UNIVERSIDAD NACIONAL AUTÓNOMA DE MÉXICO

POSGRADO EN CIENCIA E INGENIERIA DE MATERIALES
INSTITUTO DE INVESTIGACIONES EN MATERIALES

"SIMULACIÓN DE ESTRUCTURAS CRISTALINAS Y DE FORMACIÓN DE PATRONES DE DIFRACCIÓN DE ELECTRONES"

TESIS

QUE PARA OPTAR POR EL GRADO DE:
MAESTRO EN CIENCIA E INGENIERIA DE MATERIALES

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Resumen:

En esta tesis se elaboró un software que simula la estructura cristalina de los materiales y muestra el correspondiente patrón de difracción de electrones simulado (Definido por el método de la Transformada Rápida de Fourier).Una vez que el usuario define la estructura del material, se introduce en la aplicación; y a su vez esta reproduce el modelo tridimensional de la molécula, y su correspondiente patrón de difracción de electrones simulado, es posible guardar el modelo molecular en un archivo con formato PDB (Protein Data Bank).

La base para este estudio es la ley de Bragg de la difracción de electrones en un material, dando la diferencia en fase de las ondas de fotones que pasan a través del material de estudio. Se puede tener una aproximación de este patrón usando el método matemático de la Transformada Rápida de Fourier, para ver el espacio fase del material, siendo esta la representación de la estructura en el espacio recíproco. Para obtener una forma útil del espacio fase, primero necesitamos vectorizar todos los puntos de la estructura, y después graficar el resultado de la transformada de Fourier; finalmente cuando la forma en el espacio fase es la deseada se puede guardar el archivo en el formato PDB.

Una de las características de esta aplicación es que cuenta con una interfaz más accesible para el usuario, comparado con otras aplicaciones. El objetivo de esta aplicación es que el usuario al conocer el patrón de difracción de la muestra pueda refinar la estructura real de la misma, con esto podrá comparar con las micrografías de transmisión de electrones de alta resolución (High ResolutionTransmissionElectronMicroscopy).

Índice:

1. Antecedentes:

Existen dos fenómenos que se usan para el estudio y determinación de las estructuras, estos son la Difracción y la Transmisión de partículas, ya sea de fotones como en el caso de los rayos-x o de electrones como en el caso del Microscopio Electrónico de Transmisión (TEM). Esto es debido aque la longitud de onda usada en ambos casos es del mismo orden que el que existe entre losátomos de los cristales o las moléculas a estudiar; por lo tanto se generan fenómenos ópticos quepueden ser estudiados para obtener la estructura real que posee el cristal.

La difracción de Rayos – X consiste en hacer incidir un haz de rayos – x sobre la sustancia aestudiar, y debido a la simetría cristalina, éste difractará en varias direcciones, dando lugar a unpatrón de intensidades que es posible interpretar, y que nos daría información acerca de la ubicaciónfísica de los átomos en la molécula o estructura.

En el caso de la Transmisión los electrones son emitidos desde una fuente a una gran energíaCinética hacia la muestra, atravesándola y llegando a un grupo de detectores, que generan un patrónde difracción de electrones, mismo que está asociado a la forma que tiene la muestra.

El objeto de la simulación es la experimentación con un modelo de hipótesis de la estructuracristalina, por lo cual es necesario un software que sea compatible con los formatos usados en elmodelado 3D de estructuras, que genere en tiempo real patrones de difracción y difractogramas dela estructura.

El modelado formal de sistemas ha sido a través de un modelo matemático, que intenta encontrarsoluciones analíticas a problemas que permiten la predicción del comportamiento de un sistema deun conjunto de parámetros y condiciones iniciales. La simulación por computadora esfrecuentemente usada como un accesorio para, o sustitución de sistemas de modelado para los cuales las soluciones analíticas de forma cerrada simple no son posibles. Ahí se encuentran muchostipos diferentes de simulación por computadora, la característica común que todas ellas compartenes el intento por generar una muestra de escenarios representativos para un modelo en que unaenumeración completa de todos los estados posibles serían prohibitivos o imposibles.

Para crear modelos de la realidad se emplea el modelado matemático. Un modelo matemático tratade encontrar soluciones analíticas a las ecuaciones que gobiernan los procesos que se suponenresponsables del sistema que se estudia y del cual se tienen observaciones metódicas.

El objetivo es validar esas ecuaciones y posibilitar la predicción del comportamiento del sistema partiendo de un conjunto de parámetros y condiciones iniciales. Los modelos numéricos resultaron de utilizar los equipos de cómputo con el mismo propósito: resolver las ecuaciones no de forma analítica sino numérica.

Existen diversos programas para simular cristales, y entre estos también se encuentran funciones outilidades que permiten obtener la simulación de Difracción de Rayos – X; entre estos vemos que seencuentran de 2 tipos los de licencia: pública, en los que no se le requiere registro de ningún tipo, ylos que se paga cierto monto por la licencia de uso, como por ejemplo CaRIneCrystallography,CrystalMaker Software, Datasqueeze Software, HKL, Oscail, etc.

Y entre los programas libres se encuentran los que funcionan como utilidades o accesorios de

otroscomo debyer, Fullprof, Jana2006, WinGX, pero cuentan con el inconveniente de que al seraccesorios tienen que instalar programas adicionales, o son en modo consola.

Los problemas que poseen los programas de licencia restringida, es la poca compatibilidad queposeen los archivos; mientras que los de licencia libre, requieren añadir librerías o programas,cuentan con poca compatibilidad y algunos de ellos no son gráficos.También se pueden esperardificultades en la configuración de las utilidades para su conexión con los demás programas.

Haciendo estas consideraciones se observa la necesidad de un software que genera archivoscompatibles con los de modelado de estructuras (pdb), un renderizado en tiempo real (“on the fly”),e independiente de otras librerías o utilidades.

2. Planteamiento y Delimitación del problema:

Dado que no se encuentra de manera libre y de fácil acceso un software que pueda simular estructuras cristalinas a partir de datos de difracción para que sea posible determinar el tipo de estructura cristalina que los genera, es necesario desarrollar una aplicación que pueda cubrir dichos requerimientos.

3. Objetivo:

Simular estructuras cristalinas medianteun software que genera archivos compatibles con los de modelado de estructuras (pdb), un renderizado, e independiente de otras librerías o utilidades; simular patrones de difracción de electrones.

4. Hipótesis:

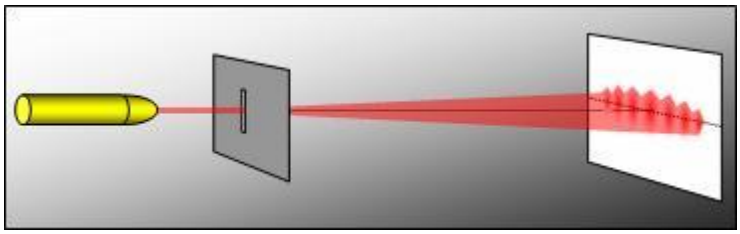
A partir del conocimiento de de una estructura cristalina y con el uso del lenguaje de programación Matlab es posible obtener simulaciones, con las cuales se podrían reproducir los resultados de difracción de electrones obtenidos porMicroscopía Electrónica de Transmisión (TEM).

5. Marco Teórico

5.1. Dispersión elástica de Rayos-X:

Difracción:

Es el fenómeno por el cual las ondas de luz son desviados de su trayectoria por medio de un objeto (en algunos casos rendija) generando un patrón de interferencia.



Fenómeno de la difracción [1]

Para el caso de los rayos – x, estos se ven desviados por el cristal siendo sus átomos y moléculas el motivo de la red cristalina, y esto genera un patrón de difracción característico. [2]

5.2. Difracción:

Debido a que la red cristalina tiene una estructura periódica en los motivos que la conforman, es posible tener un acercamiento de las densidades electrónicas que lo conforman al usar la Transformada de Fourier, dándonos un patrón de difracción que es en si la distribución de intensidades [3].

Para esto tenemos que considerar los átomos en la celda elemental del cristal como una rejilla de puntos discretos, considerando cada punto con las coordenadas tridimensionales:

$$p(x_n, y_n, z_n)$$

Siendo:

- n el índice de átomo en la red cristalina.

Para conocer las ondas resultantes de la dispersión de los puntos discretos en todas las direcciones de la estructura se usa el factor de estructura F(h,k,l):

$$F_{h,k,l} = \sum_{n=0}^{n=N} f_n e^{2\pi i\,(hx_n, ky_n, lz_n)} (1)$$

Donde:

- f_n es el factor de dispersión atómica.
- h, k, l Son los índices de Miller del cristal.
- i es el número imaginario.
- $F_{h,k,l}$ es el factor de estructura.

5.3. Factor de Estructura:

Debido a que los electrones están desviando los rayos – x se está generando una distribución de estados electrónicos donde las mayores densidades se encuentran en los puntos discretos, en este caso átomos y las menores están en los puntos intermedios a estos. Para tomar en cuenta los límites de celda que se analizan, se debe considerar los parámetros de red (a,b,c) y el volumen de celda; de forma que nuestro factor de estructura es el siguiente[3]:

$$F_{h,k,l} = \frac{V}{abc} \iiint_{000}^{abc} \rho_{x,y,z} e^{2\pi i \left[h\left(\frac{x}{a}\right)+k\left(\frac{y}{b}\right)+l\left(\frac{z}{c}\right)\right]} dx\, dy\, dz \quad (2)$$

Donde:

- V es el volumen de la celda unitaria.
- a, b, c son los parámetros de red.
- $\rho_{x,y,z}$ es la densidad electrónica en un punto x,y,z.

Para resolver esta ecuación es necesario usar la Transformada de Fourier.

5.4. Esfera de Ewald:

Si se coloca la ecuación de Bragg[4]:

$$n\lambda = 2d_{hkl} \sin\theta \quad (3)$$

Donde:

- n haces difractados.
- λ longitud de onda.
- d_{hkl} parámetro de red con los planos hkl.

- θ Angulo de difracción.

y se despeja de esta el seno del ángulo theta, tenemos que:

$$\sin\theta = \frac{\frac{1}{d_{hkl}}}{\frac{2}{\lambda}} \quad (4)$$

Llegamos a:

$$\sin\theta = \frac{\lambda}{2d_{hkl}} \quad (5)$$

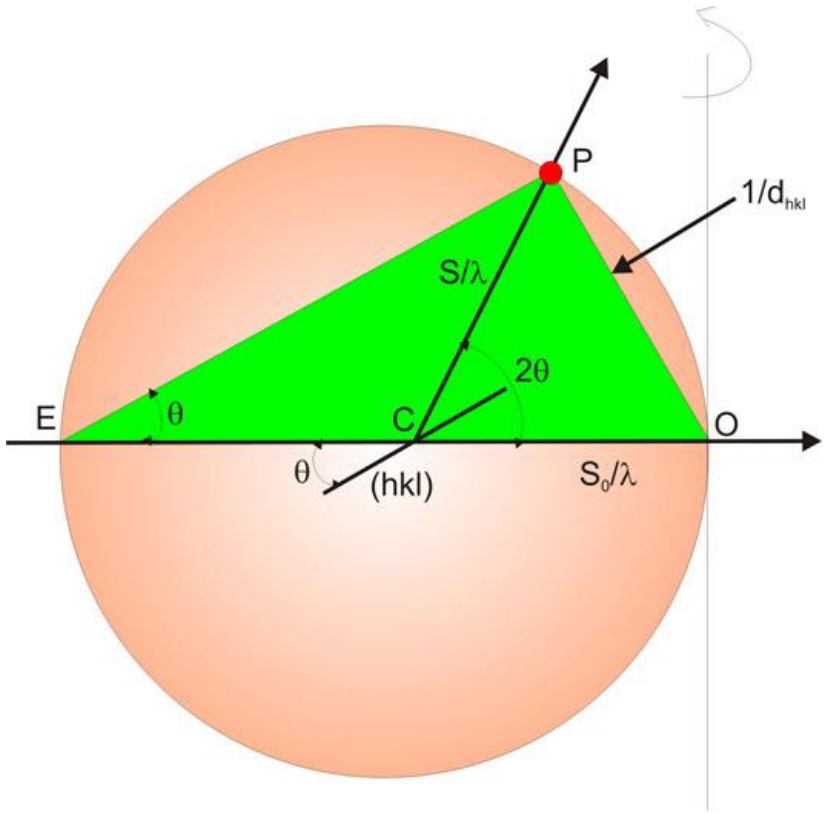


Figura 1. Representación de la Esfera de Ewald

La solución geométrica de esta ecuación es la de cualquier triángulo rectángulo, tal como el EOP de la siguiente figura:Este triángulo está inscrito en una esfera de radio 1/λ. Su diámetro coincide con la dirección de los rayos-x incidentes So. A esta esfera se le conoce como **Esfera de Ewald**.

La figura se interpreta de la siguiente forma:

- C es el cristal que se encuentra en el centro de la esfera.
- Sobre el cristal incide radiación de rayos-x indicada como So.
- El cateto OP representa al vector recíproco.
- S es el rayo difractado.
- O es el origen de nuestra construcción, donde los rayos-x abandonan la esfera de Ewald.

De esto se observa que:

Para que un plano (hkl) cualquiera difracte los rayos-x, su orientación debe ser tal que su punto recíproco representativo esté situado en la superficie de la Esfera de Ewald. Sólo en esta circunstancia se produce un rayo difractado que pasa por el punto recíproco.

5.5. Factores de Dispersión Atómica:

Es la medida de la amplitud de onda dispersada por un solo átomoaislado [5]. El factor de dispersión atómica depende de una transformada de Fourier, sobre la densidad espacial de distribución del objeto; esto es pasarlo del espacio directo al espacio reciproco. Considerando al objeto esféricamente simétrico, la densidad de distribución espacial de carga se considera como una función de radio [6]:

$$\rho = \frac{Q}{V} \quad (6)$$

Donde:

- P es la densidad de carga eléctrica.
- Q es la carga eléctrica.
- V es la unidad de Volumen en este caso de una esfera.

Se define el Factor de Dispersión Atómica como:

$$f(Q) = \int \rho(r) e^{iQr}\, d^3r \quad (7)$$

Donde:

- Q es el Vector de espacio recíproco definido como: $Q = \frac{4\pi \sin\theta}{\lambda}$
- r es el Vector de espacio real o directo.
- $\rho(r)$ es la densidad de carga eléctrica en el centro de masa, que es en $r = 0$.

Tenemos entonces el siguiente comportamiento de la función[7]:

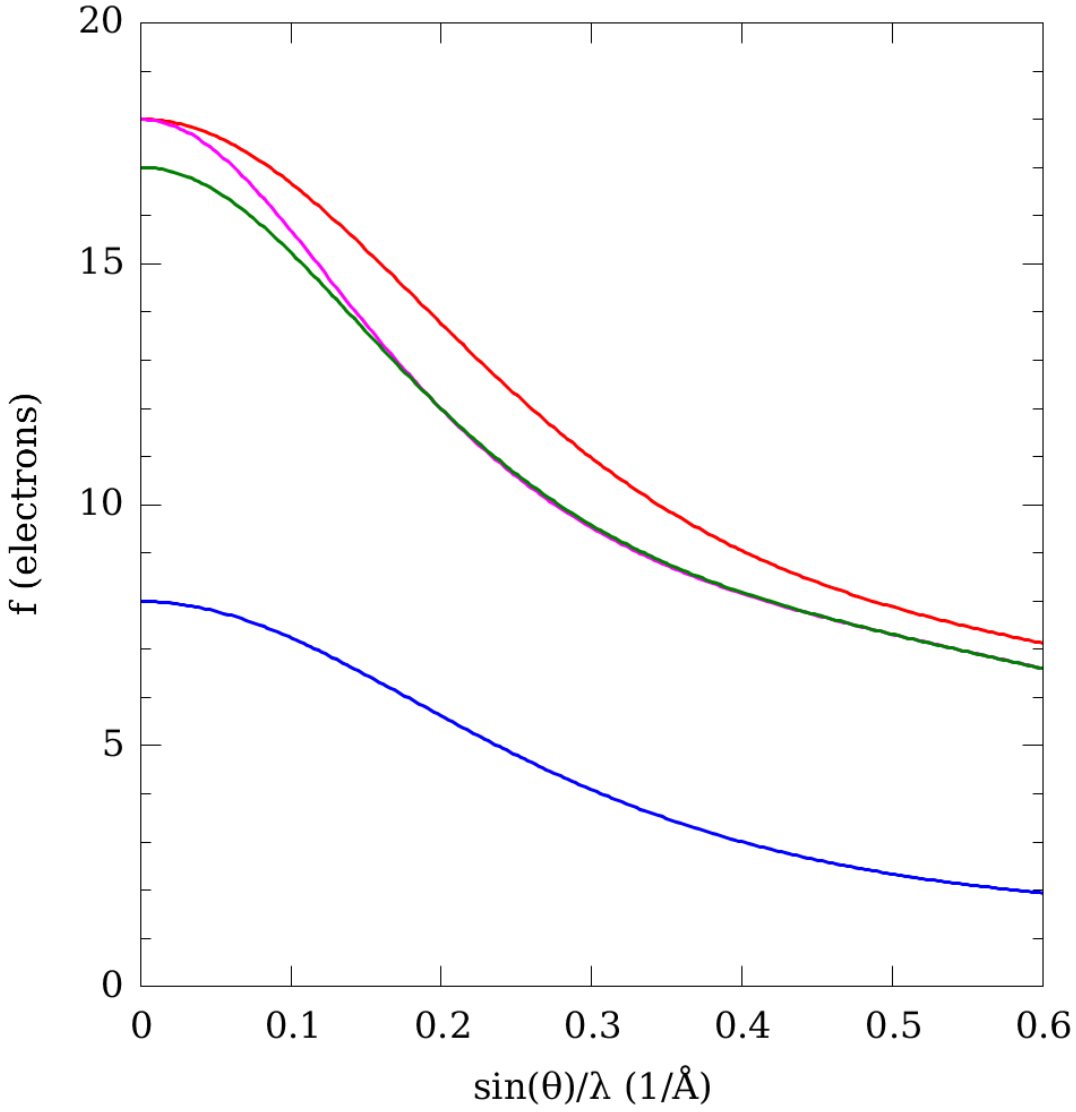


Figura 2. Comportamiento de f(Q)

5.6. Ecuación de Mott-Bethe

Esta ecuación relaciona los factores de dispersión atómica en los rayos x:

$$f_x(q)$$

Con los factores de dispersión electrónica como se muestra en la siguiente ecuación [8]:

$$f_e(q) = \frac{|e|}{16\pi^2 \varepsilon_0 |q|^2}[z - f_x(q)] \quad (8)$$

Donde:

- e es la carga del electrón.
- z es el número atómico.
- $f_x(q)$ es el factor de dispersión atómica.
- $f_e(q)$ es el factor de dispersión electrónica.
- ε_0 es la permitividad en el vacío.
- q ángulo de dispersión.

Al tener ángulos de dispersión q, pequeños en magnitud; tenemos que los factores de dispersión electrónica son más intensos que los factores de dispersión electrónica.

5.7. Transformada de Fourier:

En diversas áreas de la física se encuentran estructuras, o eventos que son de naturaleza repetitiva y están colocados a intervalos regulares entre sí; y estos se pueden presentar en una variedad de ondas de diferente tipo.[9]

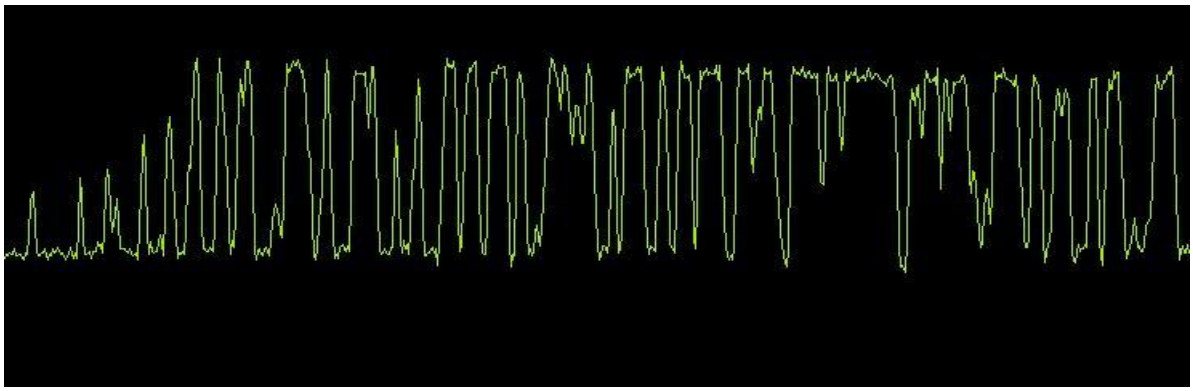


Figura 3. Espectro de una canción [10]

Estas ondas en el contexto de cristalografía de los materiales definen la estructura, se les llama ondas periódicas, siendo la densidad electrónica los puntos de red, que definen el cristal. Una función periódica la definimos como:

$$f(x) = f(x + P) \quad (9)$$

Siendo P el período entre los puntos del cristal.

Estas ondas periódicas pueden ser expresadas en términos de otras ondas sinodales, es decir en funciones de seno y funciones de coseno.Una transformada de Fourier, nombrada por el matematico Joseph Fourier, es una representación de alguna función en términos de un conjunto de ondas sinusoidales.

Este conjunto de ondas es ortogonal, es decir que ninguna de las funciones del conjunto pueden obtenerse como una combinación lineal de las otras. Se representa de forma discreta en la siguiente forma[11]:

$$A = \sum_{n=0}^{n=N} A_n \cos\left(2\pi n\left(\frac{x}{a}\right) - \alpha_n\right) \quad (10)$$

Donde:

- A es la amplitud.
- a es la distancia repetida.
- $\propto_n$ son los ángulos de fase.
- A_n son los coeficientes de Fourier.
- x es la distancia en la función periódica.

De esta ecuación se puede obtener su forma reducida en caso de que la forma de onda sea simétrica; esto es que los ángulos de fase sean 0° o 180°:

$$A = \sum_{n=0}^{n=N} A_n \cos 2\pi n\left(\frac{x}{a}\right) \quad (11)$$

Para definir su forma continúa:

$$F(\omega) = \int_{-\infty}^{\infty} f(x) e^{-2\pi i \omega x}\, dx \quad (12)$$

Donde:

- ω es su la unidad en el espacio de Fourier.

- $f(x)$es la función que se va a transformar.
- e es la función exponencial.
- i es el número imaginario.

5.8. Transformada Inversa de Fourier:

La Transformada Inversa de Fourier cuenta con las mismas propiedades que la transformada de Fourier, permite regresar el vector de puntos del espacio de frecuencias al espacio real. Se define como:

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)e^{2\pi i\omega x}\ d\omega \quad (13)$$

Donde:

- ω es su la unidad en el espacio de Fourier.
- $f(x)$es la función en el espacio real.
- e es la función exponencial.
- i es el número imaginario.
- $F(\omega)$ es la función en el espacio de Frecuencias.

Esta función se usara para reconstruir la imagen original al espacio real.

5.9. Transformada Bidimensional de Fourier:

Considerando una función $\mathbf{f(x,y)}$ definida en un plano x,y definimos a la función compleja $\boldsymbol{F(u,v)}$determinada por la formula:

$$F(u,v) = \iint_{-\infty}^{\infty} e^{2\pi(-iux-ivy)} f(x,y)\,dxdy \quad (14)$$

Donde:

- u, v son las unidades en el espacio de Fourier.
- $f(x,y)$es la función en el espacio real.

- e es la función exponencial.
- i es el número imaginario.
- $F(u,v)$ es la función en el espacio de Frecuencias.

Muchos sistemas ópticos (difracción de Fresnel, difracción de Fraunhoffer, plano focal de una lente convergente, etc.)se diseñan para reproducir la transformada bidimensional de Fourier en algún plano,[9]. Es en este punto donde se utiliza la difracción de Fresnel para Cuando un frente de onda se encuentra una lente delgada, se produce un cambio de fase de la onda iniciando su propagación tras la lente.

En el la Figura 4 se muestra el patrón de difracción del campo eléctrico definido por la integral[11]:

$$E(x,y,z) = \frac{z}{i\lambda}\iint_{-\infty}^{+\infty} E(x',y',0)\frac{e^{ikr}}{r^2}dx'dy' \quad (15)$$

Donde:

- E(x',y',0) es la apertura.
- $r = \sqrt{(x-x')^2 + (y-y')^2 + z^2}$
- $i\ es\ la\ unidad\ imaginaria.$

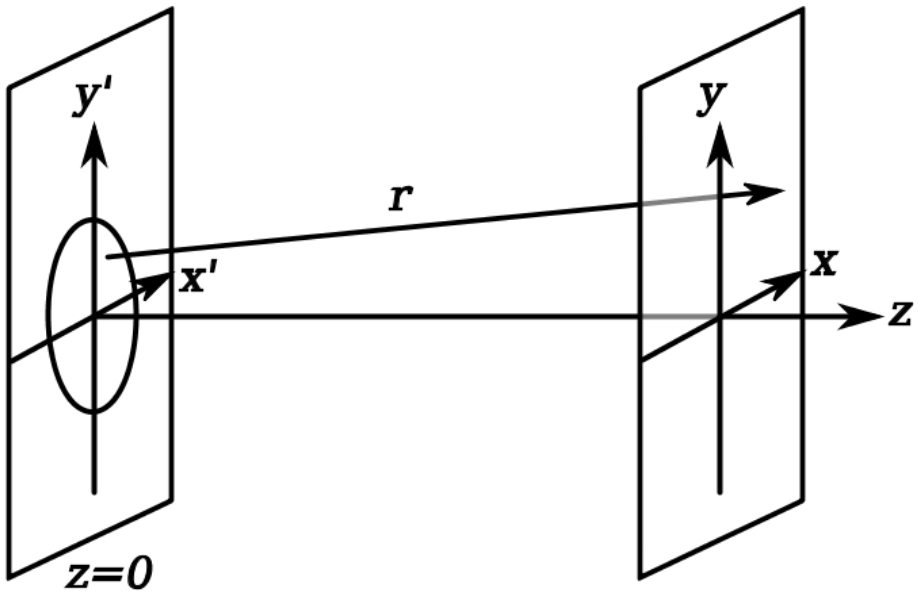


Figura 4.Patrón de difracción del campo eléctrico definido por la ecuación (15)

De esta integral es posible aproximarla numéricamente, tenemos que:

$$\rho^2 = (x - x')^2 + (y - y')^2 \quad (16)$$

Sustituyendo tenemos:

$$r = \sqrt{\rho^2 + z^2} = z\sqrt{1 + \frac{\rho^2}{z^2}} \quad (17)$$

Usando la identidad de Taylor tenemos:

$$\sqrt{1+u} = 1 + \frac{u}{2} - \frac{u^2}{8} + \cdots \quad (18)$$

Sustituyendo:

$$r = z + \frac{\rho^2}{2z} - \frac{\rho^4}{8z^3} + \cdots \quad (19)$$

Para una correcta aproximación se asume que el tercer término, es muy pequeño y se puede aproximar a cero, de forma que debe ser mucho más pequeño que el periodo de la exponencial compleja, esto es 2π:

$$k\left(\frac{\rho^4}{8z^3}\right) \ll 2\pi \; ; k = \frac{2\pi}{\lambda} \quad (20)$$

Considerando esto es posible ignorar los términos siguientes en la serie de Taylor, y solo usar el primero y el segundo término, ya que las ondas ópticas, su longitud de onda es órdenes de magnitud más pequeña que las dimensiones de la distancia a la apertura basándonos en la difracción de Fresnel:

$$F = \frac{a^2}{L\lambda} \geq 1 \quad (21)$$

Donde:

- a es el área de apertura.
- L es la distancia al punto de observación de la apertura
- λ Es la longitud de onda

Retomando:

$$r \approx z + \frac{\rho^2}{2z} = z + \frac{(x - x')^2 + (y - y')^2}{2z} \quad (22)$$

Considerando que:

$$L \gg \lambda \quad (23)$$

Tenemos que la integraldel patrón de difracción del campo eléctrico queda:

$$E(x,y,z) = \frac{e^{ikz}}{i\lambda z}\iint_{-\infty}^{+\infty} E(x',y',0)e^{\frac{ikz}{2z}[\frac{(x-x')^2+(y-y')^2}{1}]}dx'dy' \quad (24)$$

5.10. Dispersión de onda en un Sólido:

Consideramos un grupo de ondas de rayos – x atravesando un sólido, se va a ver desviado por el grupo de electrones de cada átomo, de la siguiente forma:

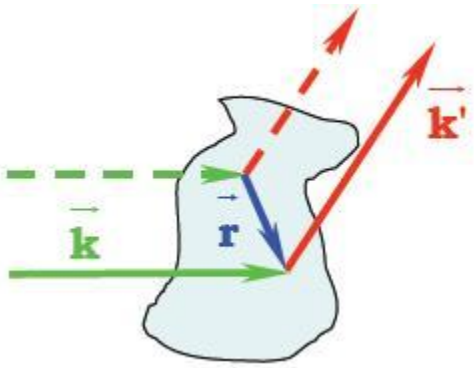


Figura 5. Dispersión de una onda por un sólido

- $\vec{K}$ es el haz incidente.
- $\overrightarrow{K'}$ es el haz refractado.
- $|\vec{K}| = |\vec{K}'| = \frac{1}{\lambda}$ es la magnitud del haz.

En este diagrama se debe de tomar un punto de origen desde el cual las ondas se empiezan a contar, en el cual las ondas son los vectores que se presentan en la gráfica.

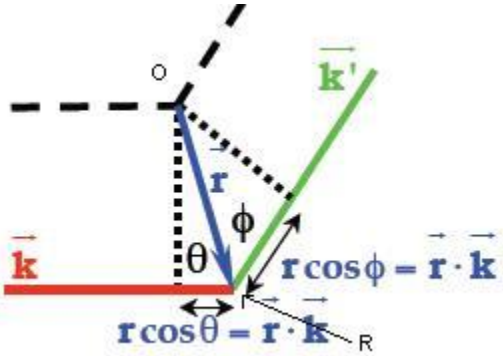


Figura 6.

- O es el origen.
- R es el siguiente haz que refracta en el cristal.

Se calcula la diferencia entre los puntos R y o:

$$R - o = \bar{r} \quad (25)$$

Con esto obtenemos un cambio de fase, según la ley de Bragg:

$$n\lambda = 2d \sin\theta \quad (26)$$

Donde:

- n es el enésimo haz de rayos-x.
- λ es la longitud de onda.
- d es el espaciado inter atómico.
- θes el ángulo de difracción.

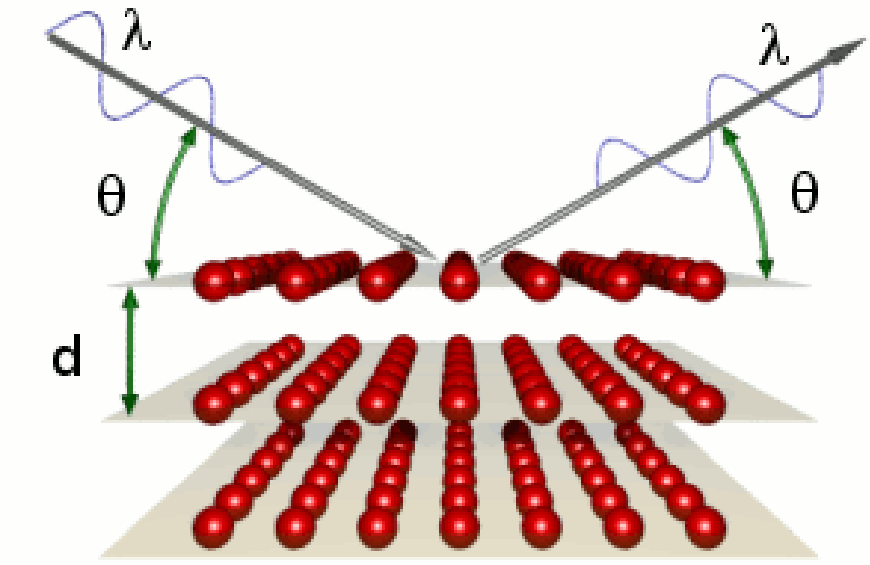


Figura 7. Representación gráfica de la Ley de Bragg[4]

Calculamos la diferencia de Trayectoria:

$$\text{Diferencia Trayectoria} = \bar{r}(\bar{k} - \overline{k'}) \quad (26)$$

De esta relación obtenemos la diferencia de fase:

$$\text{Diferencia fase} = \frac{2\pi}{\lambda}\bar{r}\left(\bar{k} - \bar{k'}\right) \quad (27)$$

De ambas ecuaciones definimos al vector:

$$\bar{s} = \left(\bar{k} - \bar{k'}\right) \quad (28)$$

Definimos la capacidad de dispersión de cada átomo con la letra p(r) tenemos la distribución de dispersión en un sólido definida por:

$$F(\bar{s}) = \int_0^V p(\bar{r}) e^{2\pi i \bar{r}\bar{s}} dr \quad (29)$$

Donde:

- $F(\bar{s})$ es la Función de Distribución de dispersión en un sólido.
- $r(x, y, z)$ es un punto tridimensional en el espacio.
- $p(r)$ es la capacidad de dispersión de cada átomo.
- V es el volumen en la celda.

5.11. Dispersión de Rutherford

La dispersión de partículas alfa de los núcleos, se puede modelar a partir de la fuerza de Coulomb y tratarla como una órbita. El proceso de dispersión puede ser tratado estadísticamente en términos de la sección transversal para la interacción, con un núcleo que se considera como una carga puntual Ze. Para un detector en un ángulo específico con respecto al haz incidente, el número de partículas por unidad de área que golpean el detector está dada por la fórmula de Rutherford[13]:

$$N(\theta) = \frac{N_i n L Z^2 k^2 e^4}{4r^2 K E^2 \sin^4\left(\frac{\theta}{2}\right)} \quad (30)$$

Donde:

- N_i número de partículas alfa incidentes.
- n átomos por unidad de volumen en el objeto.
- L Grosor del objeto.

- Z número atómico del objeto.
- e carga del electrón.
- k constante de Coulomb.
- r distancia del objeto al detector.
- KE energía cinética de las partículas alfa.
- θ ángulo de dispersión.

La variación prevista de partículas alfas detectadas con un ángulo dado, está muy de acuerdo con los datos de Geiger-Marsden. Para obtener la fracción dispersada, la fórmula anterior incluye la sección transversal de dispersión para un núcleo dado, y la naturaleza de la película de dispersión. Otra forma común para la ecuación de Rutherford en la dispersión de un núcleo determinado, es solamente la sección transversal diferencial:

$$\frac{d\sigma}{d\cos\theta} = \frac{\pi}{2} z^2 Z^2 \alpha^2 \left(\frac{\hbar c}{KE}\right)^2 \frac{1}{(1-\cos\theta)^2} \quad (31)$$

Donde:

- $\sigma = \pi r^2$ Es la sección eficaz, es decir al area efectiva para colisión.
- Z número atómico.
- α constante de estructura fina.
- c velocidad de la luz.
- KE energía cinética de las partículas alfa.
- $\hbar$ constante de Plank.

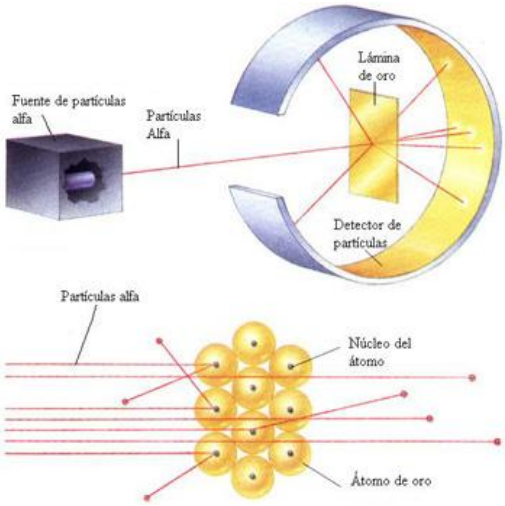


Figura 8. Dispersión de las partículas alfa por el nucleo [13].

5.12. Funcionamiento TEM (Microscopio Electrónico de Transmisión)

Es un microscopio que utiliza un haz de electrones para visualizar un objeto, debido a que la potencia amplificadora de un microscopio óptico está limitada por la longitud de onda de la luz visible. Lo característico de este microscopio es el uso de una muestra ultra fina y que la imagen se obtenga de los electrones que atraviesan la muestra.
Debido a que los electrones tienen una longitud de onda mucho menor que la de la luz visible, pueden mostrar estructuras mucho más pequeñas.

Las partes principales de un microscopio electrónico de transmisión se muestran en la figura 9.

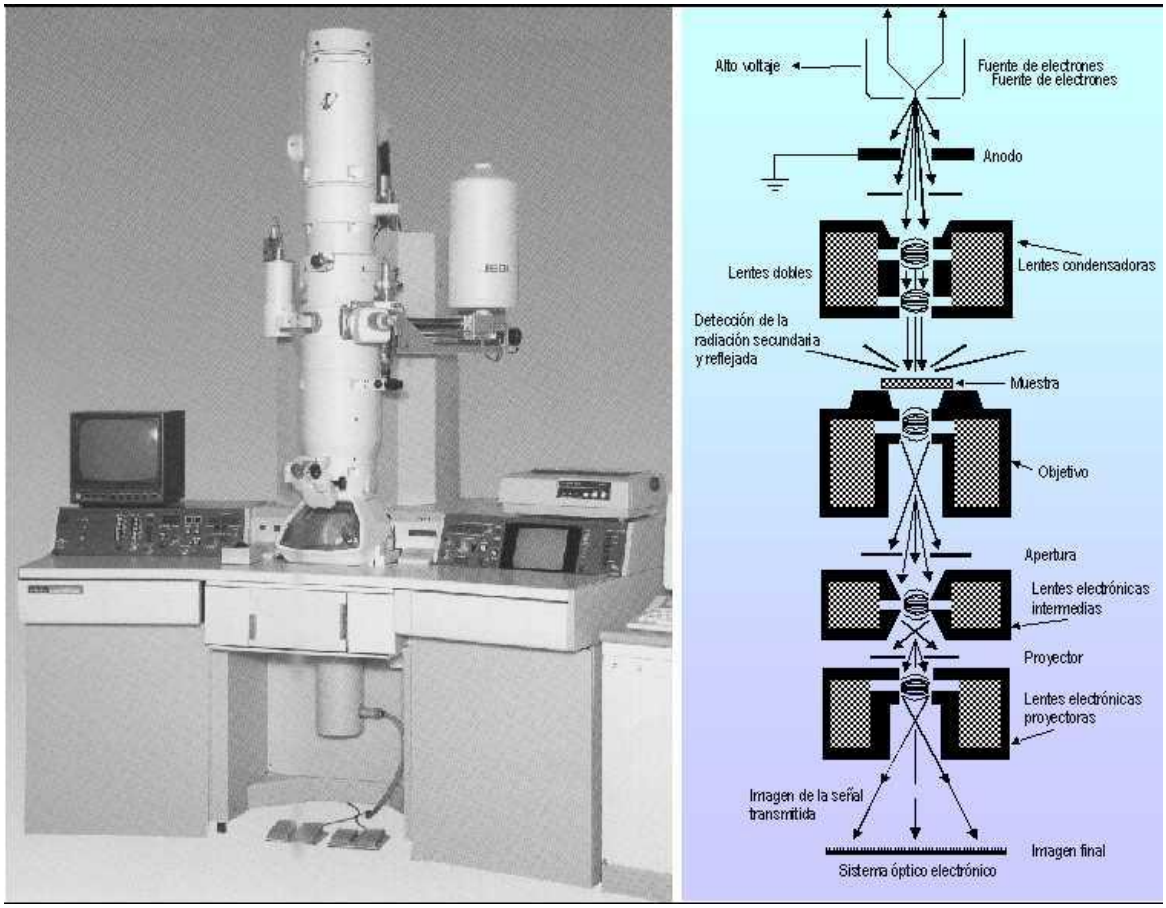


Figura 9. Esquema general del TEM (TransmissionElectronMicroscopy)[14]

- Cañón de electrones, que emite los electrones que chocan o atraviesan el espécimen (dependiendo que tipo de microscopio electrónico es), creando una imagen aumentada.
- Lentes magnéticas para crear campos que dirigen y enfocan el haz de electrones, ya que las lentes convencionales utilizadas en los microscopios ópticos no funcionan con los electrones.
- Sistema de vacío es una parte muy importante del microscopio electrónico. Debido a que los electrones pueden ser desviados por las moléculas del aire, se debe hacer un vacío casi total en el interior de un microscopio de estas características.

- Placa fotográfica o pantalla fluorescente que se coloca detrás del objeto a visualizar para registrar la imagen aumentada.
- Sistema de registro que muestra la imagen que producen los electrones, que suele ser una computadora.

El microscopio electrónico de transmisión emite un haz de electrones dirigido hacia el objeto que se desea aumentar. Una parte de los electrones rebotan o son absorbidos por el objeto y otros lo atraviesan formando una imagen aumentada de la muestra.

Para utilizar un microscopio electrónico de transmisión debe cortarse la muestra en capas finas, no mayores de un par de miles de angstroms. Los microscopios electrónicos de transmisión pueden aumentar un objeto hasta un millón de veces.
Teóricamente la resolución máxima d alcanzable con un microscopio óptico se encuentra en principio limitada por la longitud de onda λ de la luz que se utiliza para examinar la muestra, y por la apertura numérica NA del sistema.

Los físicos de principios del siglo XX teorizaron sobre posibles maneras de superar las limitaciones impuestas por la relativamente grande longitud de onda de la luz visible (de 400 a 700 nm) mediante el uso de electrones. Como toda la materia, los electrones exhiben propiedades tanto de onda como de partícula (como ya propuso Louis-Víctor de Broglie). Como consecuencia se puede hacer que un haz de electrones se comporte como un haz de radiación electromagnética. La longitud de onda del electrón se obtiene igualando la ecuación de Broglie a la energía cinética de un electrón. Debe introducirse una corrección relativista adicional, ya que los electrones en un equipo TEM alcanzan velocidades próximas a la de la luz c.

En un microscopio electrónico los electrones se producen generalmente en un filamento, normalmente de tungsteno, parecido al de una bombilla, mediante un proceso conocido como emisión termoiónica o bien mediante emisión de campo. Los electrones emitidos se aceleran entonces con ayuda de un potencial eléctrico (medido en V, o voltios) y se focalizan mediante lentes electrostáticas o electromagnéticas.

La principal función del microscopio electrónico de transmisión es estudio de los metales y minerales y el estudio de las células a nivel molecular. Siendo así un papel muy importante en la industria de la metalurgia. A su vez se utiliza en la microbiología, para observar la estructura de los virus. También es usado en Anatomía patológica, para diagnosticar partiendo de la ultra estructura celular.

5.12.1. Método Multicapa

El algoritmo multicapa es el método para la simulación de la interacción de un haz de electrones con la materia, y esto incluye los efectos de dispersión elástica. El método esta documentado en el libro de John M. Cowley[15]y es usado para la simulación de HR-TEM (High ResolutionTransmissionElectronMicroscopy).

En 1957 Cowley y Moodie[16] demostraron que usando la ecuación de Schrödinger puede ser solucionado analíticamente para evaluar las amplitudes de el haz difractado. De esta forma los efectos de difracción dinámica pueden ser calculados y la imagen simulada mostraría una buena aproximación con la imagen tomada de un microscopio electrónico.

El método multicapa es una aproximación para resolver la ecuación de onda de Schrödinger:

$$-\frac{\hbar^2}{2m}\frac{\partial\Psi(x,t)}{\partial x^2}+V(x,t)\Psi(x,t)=E\Psi(x,t) \quad (32)$$

La ecuación anterior se puede expresar también como onda incidente y onda difractada:

$$\Psi(r)=\Psi_0(r)+\int G(r,r')V(r')\Psi(r')dr' \quad (33)$$

Donde:

- $G(r,r')$ Donde G representa la amplitud de la función de onda del electrón.
- r es el punto actual del electrón.
- r' es la fuente de electrones.

Considerando la ecuación de onda incidente como:

$$\Psi(r)=e^{ikr} \quad (34)$$

La ecuación de onda de Schrödinger se representa como:

$$\Psi(r)=e^{ikr}-\frac{m}{2\pi\hbar^2}\int\frac{e^{ik|r-r'|}}{|r-r'|}V(r')\Psi(r')dr' \quad (35)$$

Se ajusta el sistema de coordenadas de forma que se impacte la muestra en (0,0,0) a lo largo del eje z.

Y consideramos a la función de onda anterior con una función de modulación $\phi(r)$ para la amplitud.

La función de modulación se define como:

$$\phi(r) = 1 - \frac{m}{2\pi\hbar^2}\int \frac{e^{ik|r-r'|-ik|r-r'|}}{|r-r'|}V(r')\phi(r')dr' \quad (36)$$

Cambiando al sistema de coordenadas al que hemos seleccionado tenemos:

$$k(r-r') = k(z-z') \quad (37)$$

$$|r-r'| \approx +\frac{(z-z') + (X-X')^2}{2(z-z')} \quad (38)$$

Con esto tenemos:

$$\phi(r) = 1 - i\frac{\pi}{E\lambda}\int\int_{z'=-\infty}^{z'=z} V(X',z')\phi(X',z')\frac{1}{i\lambda(z-z')}e^{ik\frac{(X-X')^2}{2(z-z')}}dX'dz' \quad (39)$$

Donde:

- $\lambda = \frac{2\pi}{k}$ Es la longitud de onda.
- $E = \frac{\hbar^2 k^2}{2m}$ la energía de los electrones.

En las ecuaciones anteriores se definió la mecánica de las ondas, sin embargo falta agregar la dispersión del material. Definimos la constante de interacción como:

$$\sigma = \frac{\pi}{E\lambda} \quad (40)$$

Se define la función de propagación transversal, basándonos en los términos, de la propagación de Fresnel:

$$p(X,z) = \frac{1}{iz\lambda}e^{(ik\frac{X^2}{2z})} \quad (41)$$

Considerando la simulación multicapa el grosor de cada capa es pequeño, entonces el campo de potencial se puede considerar constante en cada iteración, de la forma V(X,z') de esta forma se presenta la función de modulación como:

$$\phi(X, z_{n+1}) = \int p(X - X', z_{n+1} - z_n)\phi(X, z_n)e^{(-i\sigma \int_{z_n}^{z_{n+1}} V(X,z')dz')}dX' \quad (42)$$

La función de la modulación es la siguiente:

$$\phi_{n+1=}\phi(X, z_{n+1}) = [q_n(X)\phi_n] * p_n \quad (43)$$

Donde:

- $q(X) = e^{-i\sigma \int_{z_n}^{z_{n+1}} V(X,z)dz'}$ Define la función de transmisión de la capa.
- $p_n = p(X, z_{n+1} - z_n)$ Es la función de propagación transversal.
- $*$ símbolo de la consolación del operador.

Consideraciones Prácticas:

La premisa básica es calcular la difracción de cada capa de átomos usando Transformadas Rápidas de Fourier (FFT) y multiplicando cada una por un término de rejilla de fase. La onda se multiplica entonces por un propagador, se le aplica la Fourier transformada inversa, y se vuelve a multiplicar por un término rejilla de fase una vez más, y el proceso se repite[17].

5.12.2. Lente de Electrones

Es la parte más importante del microscopio electrónico, y sirve para emular la función de los lentes convergentes en un microscopio normal, esto es de la siguiente forma:

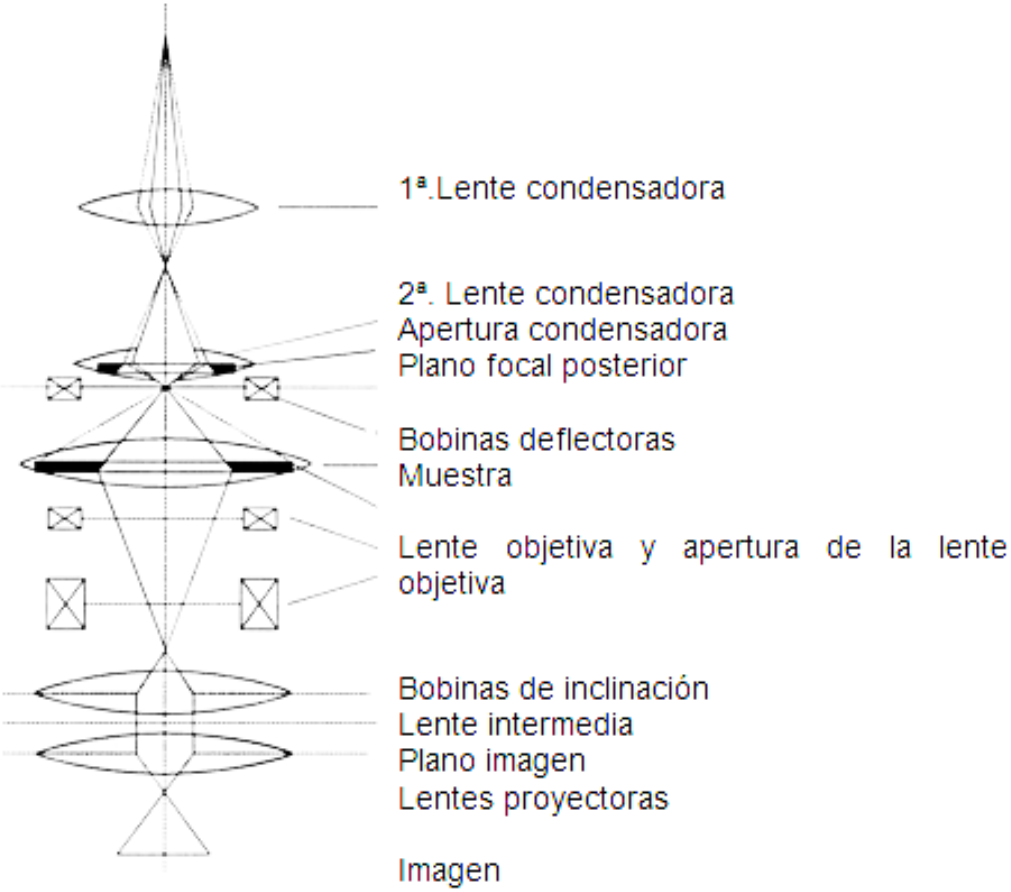
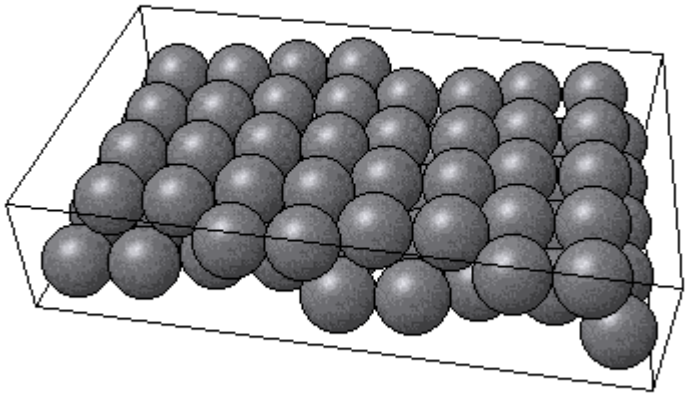
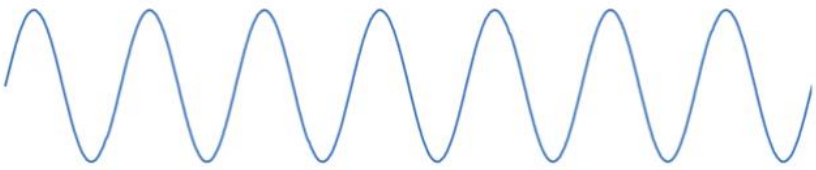
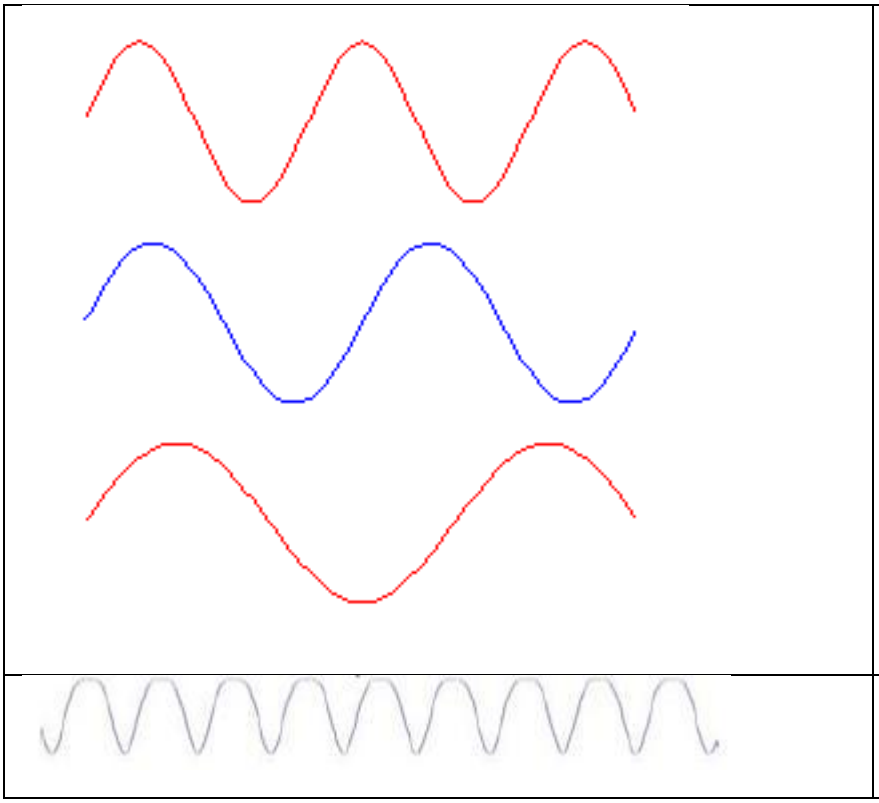


Figura 10. Lentes electromagnéticas en la microscopia electrónica.[18]

A su vez las lentes van cambiando la ecuación de onda[19]:

Diagrama	Ecuación de Onda
 Amplitud Fase	$\Psi_{incidente}\ (r) = e^{ikz}$
[20].- Muestra de material 	$V_{proj}\ (r)$
Onda de salida:  Lentes Objetivo	$\Psi_{salida}\ (r)$ $= \Psi_{\text{incidente}}\ (\text{r}) e^{i\pi\lambda V_{\text{proj}}\ (\text{r})}$



$\Psi_{aberraci\ ón}(r) = \Psi_{\text{salida}}\ (\text{r}) \otimes e^{i\chi(\text{r})}$

$I(r) = |\Psi_{ab}|^2$

Figura 11. Esquema de funcionamiento de lentes de electrones.

Donde:

- $\Psi_{incidente}\ (r)$ es la onda definida por los electrones que surgen del microscopio electrónico.
- $V_{proj}\ (r)$ Potencial proyectado por el cristal muestra.
- $\Psi_{salida}\ (\text{r})$ Onda de salida que es la unión del potencial proyectado del cristal, junto con la onda incidente.
- $e^{i\chi(\text{r})}$ es la onda generada por las aberraciones del sistema.
- $\Psi_{aberraci\ ón}(r)$ es la onda con aberraciones debido al efecto de los lentes electromagnéticos.
- $I(r)$ es la intensidad de las ondas que está definida como el cuadrado de la onda y va hacia el detector.

5.12.3. Astigmatismo:

El astigmatismo ocurre cuando los electrones son afectados por un campo magnético no uniforme en su trayectoria en espiral alrededor del eje óptico.

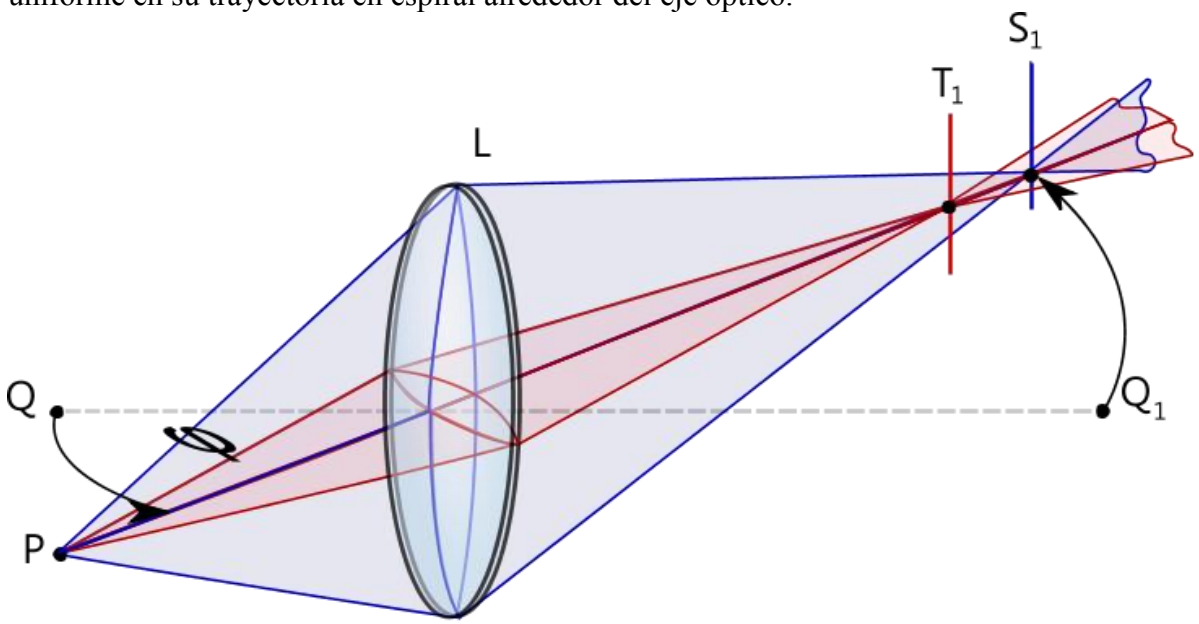


Figura 12. Esquema que muestra el astigmatismo en lente.[21]

El defecto en el TEM se origina debido a que no es posible un maquinado simétricamente cilíndrico a través del calibre de las piezas polares que son hechas de acero dulce.

Este acero dulce puede tener inhomogeneidades microestructurales las cuales causan variaciones locales en la magnitud del campo magnético. Las aperturas que tenemos en cada una de las lentes, pueden alterar el campo si estas no estan exactamente centradas alrededor del eje.

Otro efecto que produce astigmatismo es la contaminación que se produce alrededor de las aperturas, haciendo que estas partículas contaminantes (principalmente carbón) se carguen desviando el haz.

Afortunadamente el astigmatismo se corrige fácilmente usando los astigmadores, los cuales son pequeños octupolos que introducen un campo de compensación para balancear las inhomogeneidades que causan el astigmatismo[18].

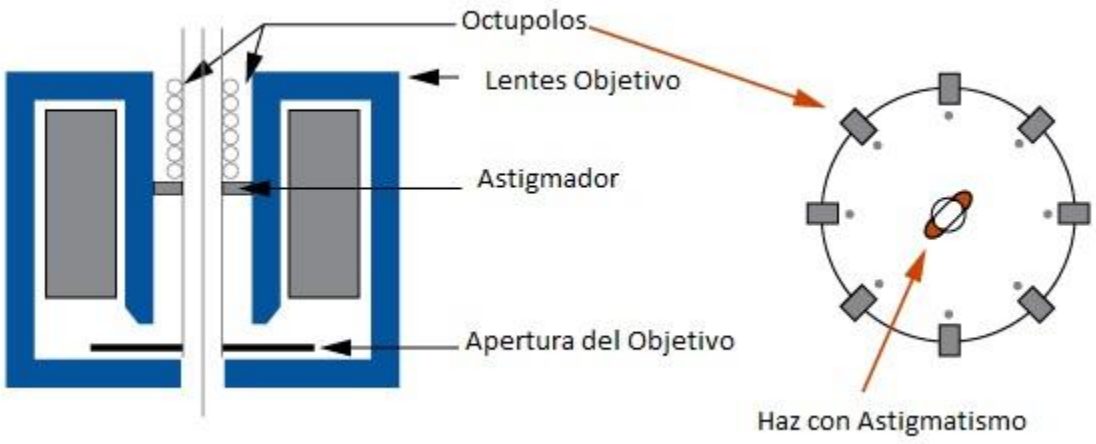


Figura 13. Octupolos en el TEM.[22]

La ecuación de astigmatismo en el TEM la definimos como:

$$X_{astigmatismo}\ (\vartheta, \varphi) = \frac{1}{2}|A_1|\vartheta^2 \cos(2[\varphi - \varphi_{22}]) \quad (44)$$

Donde:

- $\vartheta = \sin^{-1}|q|\lambda \approx |q|\,\lambda$ definida la q basada en las tablas de Dispersión Atómica.
- $\varphi = \tan^{-1}\left(\frac{q_y}{qx}\right)$ ángulo de cambio de fase.
- A_1 Amplitud del Haz.

5.12.4. Coma

Se llama así porque la forma de la imagen de un punto es similar a un cometa. Se origina por la dependencia del aumento lateral con la excentricidad del haz, esto es cuando los puntos del haz que entran a diferente altura; focalizan en distintos puntos del plano imagen. El desplazamiento es mayor cuanto más alejado del eje esta el punto origen [23].

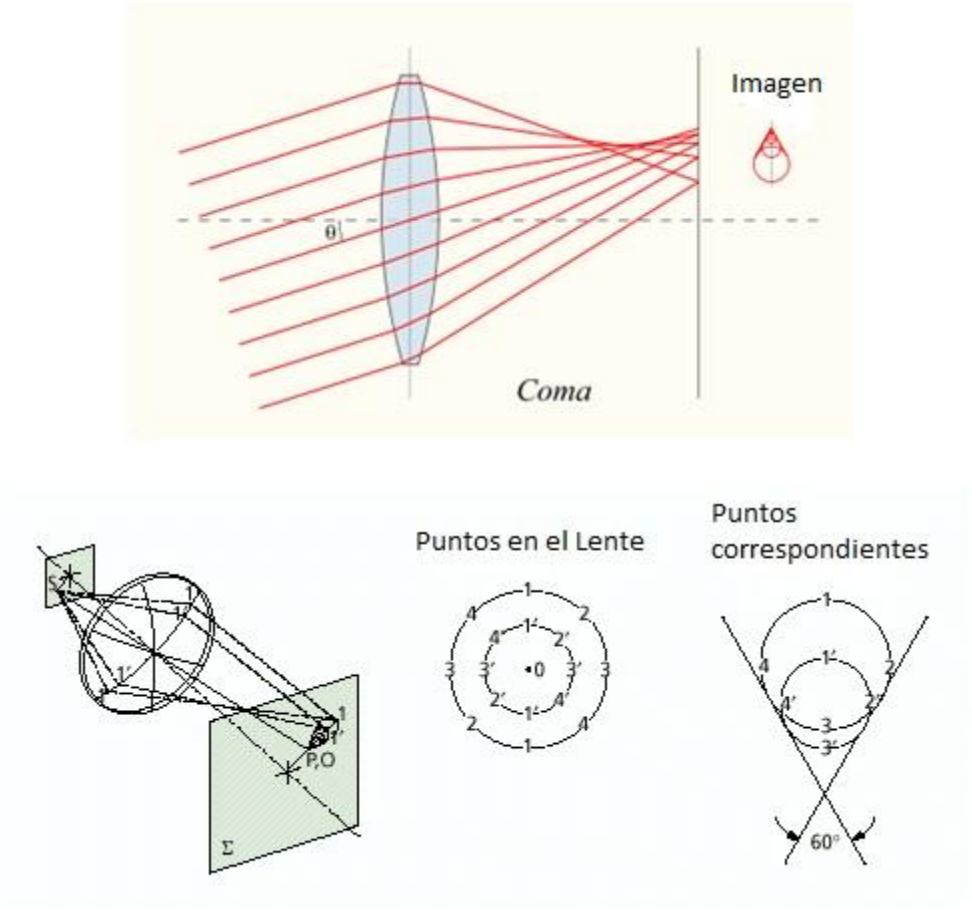


Figura 14. Esquema que muestra el efecto de la coma.[23]

Afecta en:

- Objetos descentrados.
- Objetos extensos.
- Sistemas descentrados.

Se define como:

$$X_{Coma}\,(\vartheta,\varphi) = \frac{1}{3}|B_2|\vartheta^3\cos(\varphi-\varphi_{31}) \quad (45)$$

Donde:

- $\vartheta = \sin^{-1}|q|\lambda \approx |q|\,\lambda$ definida la q basada en las tablas de Dispersión Atómica.
- $\varphi = \tan^{-1}\left(\frac{q_y}{qx}\right)$ ángulo de cambio de fase.
- B_2 Amplitud del Haz.

5.12.5. Astigmatismo de Tercer Orden

En tercer orden el astigmatismo se forma por medio de los haces; focos sagital y transversal a diferentes distancias a lo largo del eje óptico. Estos focos se llaman el enfoque sagital y el enfoque transversal, respectivamente. En la presencia de astigmatismo, un punto fuera del eje en el objeto no aparezca nítidamente por el sistema óptico. En lugar de ello, las líneas agudas están formadas en los focos sagital y transversal. La imagen en el foco transversal es una línea corta, orientada en la dirección del plano sagital; imágenes de círculos centrados en el eje óptica o líneas tangenciales a dichos círculos, será fuertes en este plano[24].

La imagen en el foco sagital es una línea corta, orientada en la dirección tangencial, las imágenes de rayos que irradian desde el centro son agudas en este enfoque. En medio de estos dos focos, se forma una imagen circular y a menudo " borrosa". Esto se denomina el enfoque medial o círculo de menor confusión.

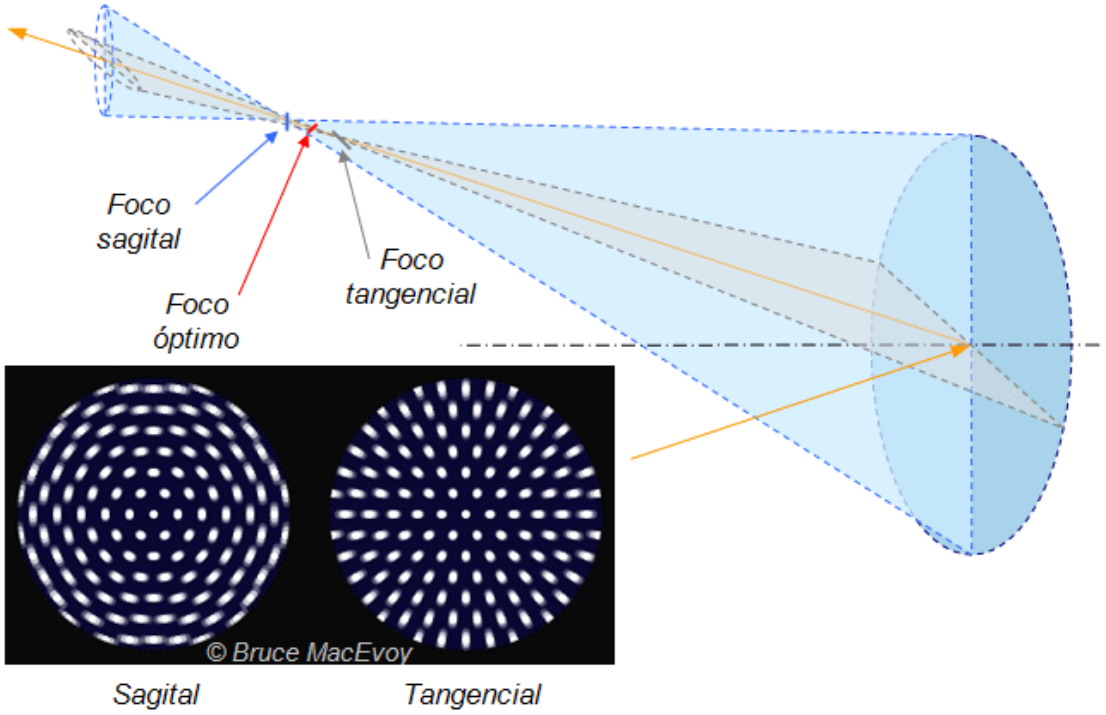


Figura 15. Astigmatismo de Tercer orden.[25].

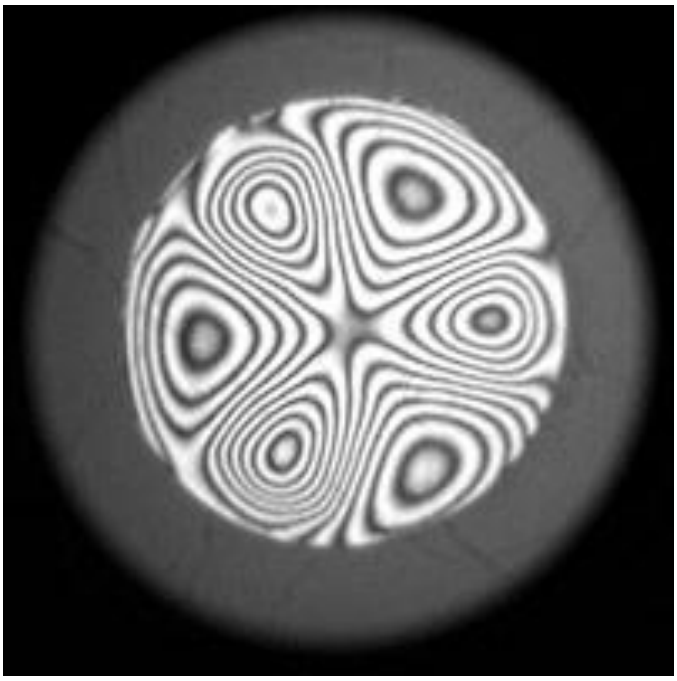


Figura 16. Efectos del Astigmatismo de Tercer Orden[26] .

La definimos como:

$$X_{astigmatismo\ \ 3}(\vartheta,\varphi) = \frac{1}{3}|A_2|\vartheta^3\cos(3[\varphi-\varphi_{33}]) \quad (46)$$

Donde:

- $\vartheta = \sin^{-1}|q|\lambda \approx |q|\,\lambda$ definida la q basada en las tablas de Dispersión Atómica.
- $\varphi = \tan^{-1}\left(\frac{q_y}{qx}\right)$ ángulo de cambio de fase.
- A_2 Amplitud del Haz.

5.12.6. Desenfoque

Es cuando la imagen se forma en una posición distinta de la correspondiente a la imagen Gaussiana. Es la traslación del foco, a lo largo del eje óptico más allá de la superficie del plano o del mejor punto focal.

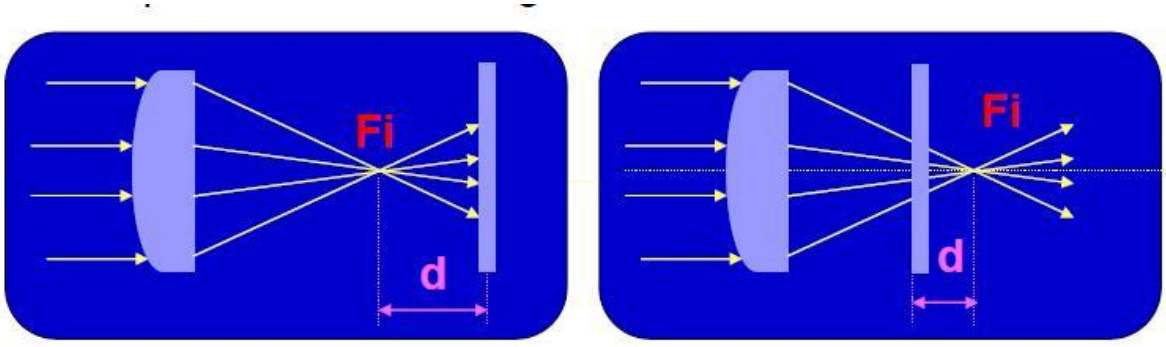


Figura 17. Desenfoque en una lente.[27]

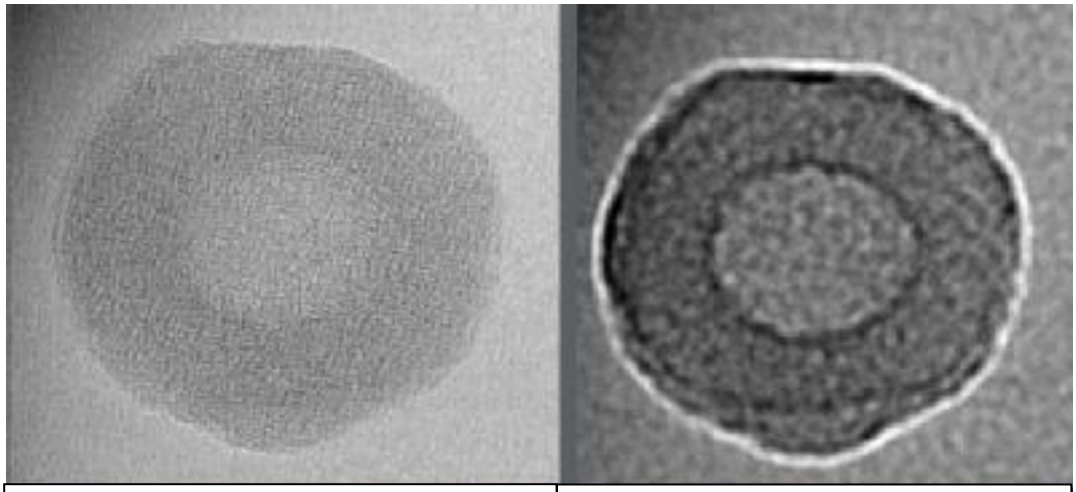


Imagen TEM de polimersoma con 0 enfoque a 200K aumentos usando JEOL 2100 TEM	Imagen TEM de polimersoma con -1000nm de desenfoque a 200K aumentos usando JEOL 2100 TEM

Figura 18. Desenfoque en una muestra de Polymersoma.[28]

El Desenfoque se define como:

$$X_{Desenfoque}\ (\vartheta) = \frac{1}{2}|C_1|\vartheta^2 \quad (47)$$

Donde:

- $\vartheta = \sin^{-1}|q|\lambda \approx |q|\,\lambda$ definida la q basada en las tablas de Dispersión Atómica.
- C_1 Coeficiente de desenfoque.

5.12.7. Función de Transferencia de Contraste (CTF)

La función de transferencia de contraste debe ser usada en las imágenes con el fin de obtener estructuras de alta resolución en microscopía electrónica tridimensional, especialmente crio-microscopía electrónica. Basándonos en la ecuación de perturbación paraxial[29]. Se define como:

$$\begin{aligned}\boldsymbol{\chi(\vartheta,\phi)} &= |\boldsymbol{A_0}|\boldsymbol{\vartheta}\,\boldsymbol{\cos(\varphi-\phi_{11})} \\ &+ \frac{\mathbf{1}}{\mathbf{2}}|\boldsymbol{A_1}|\boldsymbol{\vartheta^2}\,\boldsymbol{\cos(2[\phi-\phi_{22}])} + \frac{\mathbf{1}}{\mathbf{2}}|\boldsymbol{C_1}|\boldsymbol{\vartheta^2} \\ &+ \frac{\mathbf{1}}{\mathbf{3}}|\boldsymbol{A_2}|\boldsymbol{\vartheta^3}\,\boldsymbol{\cos(\phi-\phi_{33})} + \frac{\mathbf{1}}{\mathbf{3}}|\boldsymbol{B_2}|\boldsymbol{\vartheta^3}\,\boldsymbol{\cos(\phi-\phi_{31})} \quad \mathbf{(48)}\end{aligned}$$

Donde:

- $|A_0|\vartheta\cos(\varphi-\phi_{11})$ es el cambio de imagen.

6. Software de Simulación de Estructuras

Existen diversos software de simulación de estructuras cristalinas y difracción de rayos-x; por sus características podemos clasificarlos de las siguientes maneras:

- Por el tipo de Licencia.
- Si realizan simulación de rayos-x.
- Modo gráfico o de consola.
- Como un solo programa o en forma de utilidad.

A continuación se especifica cada categoría:

6.1. Por el tipo de Licencia

En este caso nos estamos refiriendo si el software es de licencia pública o privada, de lo siguiente definimos:

Licencia Pública:

Especifica si el software es libre de añadir nuevos módulos por el usuario, libre de modificar el programa a nivel código fuente, pero siempre y cuando actualizar los cambios en el proveedor del programa original.

Acerca de su uso tenemos que es libre el usuario de actualizar el programa y añadir características al programa para incrementar su funcionalidad.

También se encuentra el usuario en capacidad de aprovechar todas las funcionalidades de dicho programa.

Las más comunes son las siguientes:

- GNU General Public License[33]
- Licencia BSD [34]
- Mozilla Public Licence (MPL) [35]

- Creative Commons [36]

Se consideran libertades[37] a el nivel de uso que se le da al programa o código fuente en cuestión siendo las siguientes:

Libertad 0:

Es la libertad de usar el programa, con cualquier propósito.

Libertad 1:

Es la libertad de estudiar cómo funciona el programa y modificarlo, adaptándolo a las necesidades del usuario.

Libertad 2:

Libertad de distribuir copias del programa.

Libertad 3:

Libertad de mejorar el programa y hacer públicos esas mejoras a los demás usuarios.

7. Aplicaciones simuladoras de Difracción de Rayos - X:

Existen diversas aplicaciones que se utilizan para simular difracción de Rayos-X entre las que se encuentran:

- CaRIne Crystallography,
- CrystalMaker Software,
- Datasqueeze Software,
- HKL,
- Oscail,
- debyer,
- Fullprof,
- Jana2006,
- WinGX

8. Modo Gráfico o de Consola:

Modo Gráfico

Definimos a modo gráfico de un programa de simulación al que involucra el uso de ventanas y otro dispositivo como el de ratón de la siguiente forma:

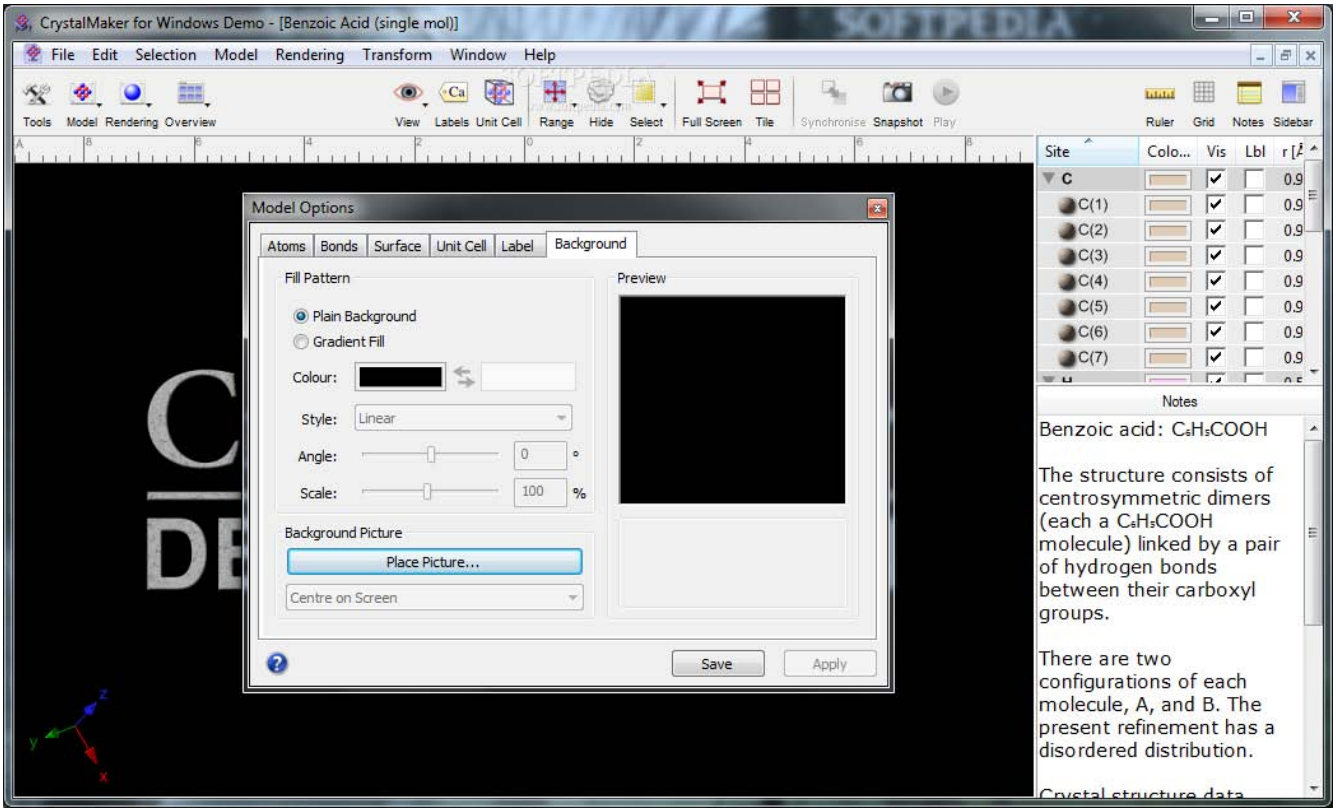


Figura 20. Modo consola de CrystalMaker.[38]

Modo Consola:

Se define al modo de consola como a aquel que los comandos son interpretados por la computadora de forma textual:

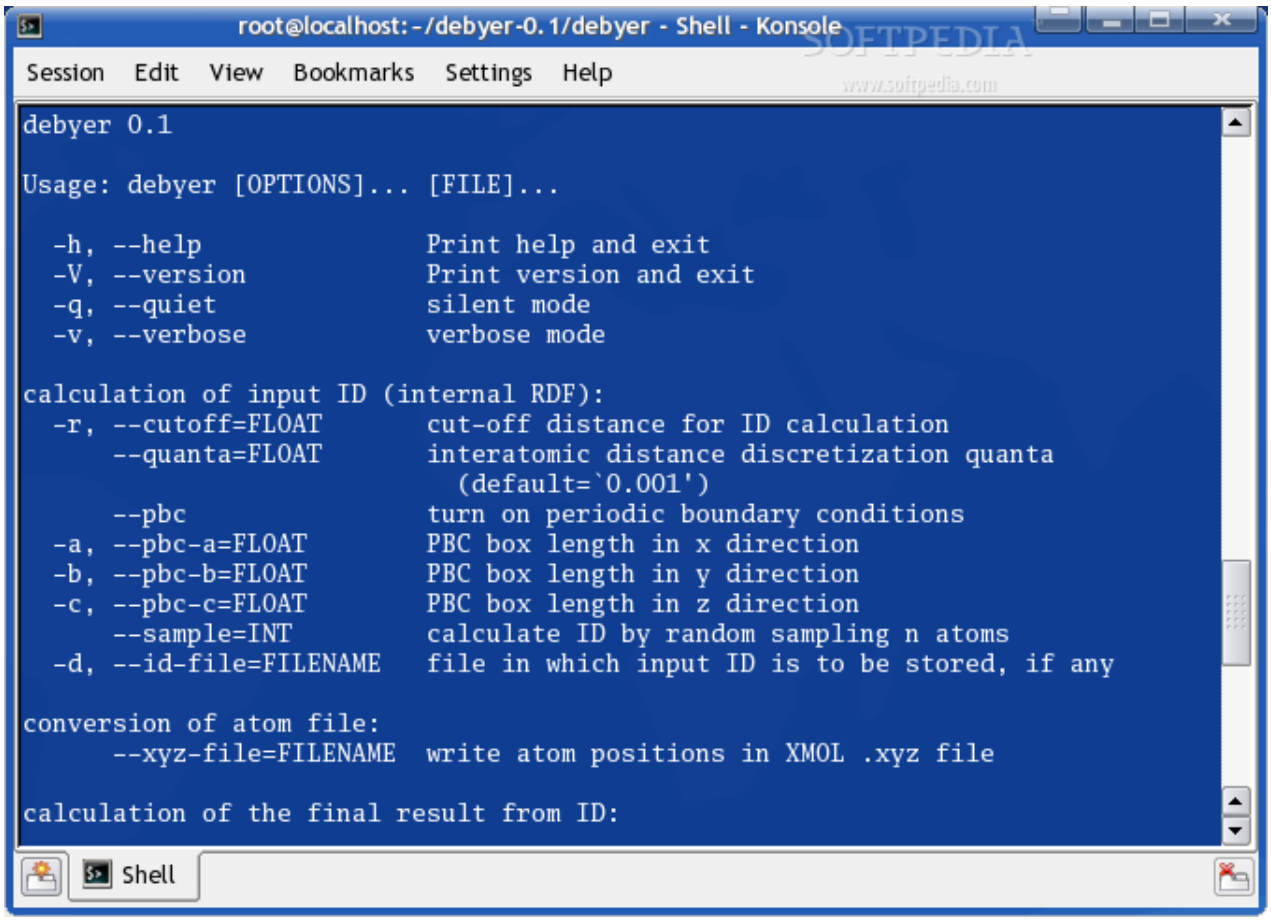


Figura 21. Modo consola de debyer.[39]

9. Aplicación o paquete de utilidades:

Aplicación

Definimos a la aplicación como al programa que posee todas las utilidades corriendo de forma dependiente de la estructura previamente definida en los comandos, y que no necesita de programas adicionales para simular la difracción de rayos-x.

Paquete de Utilidades

Es el programa que requiere la instalación y configuración de utilidades adicionales para generar una simulación de difracción de rayos-x.

10. Especificación PDB(Protein Data Bank):

El archivo PDB (Protein Data Bank) o banco de Datos de proteínas es el único repositorio mundial de información sobre las estructuras 3D de grandes moléculas biológicas, como las proteínas y los ácidos nucleicos[40].

El archivo PDB se estableció en 1971 en el Brookhaven National Laboratory y originalmente contenía 7 estructuras. En 1998, el Collaboratory Investigación Bioinformática Estructural (RCSB) se convirtió en responsable de la gestión del PDB. En 2003, el wwPDB se formó para mantener un único archivo PDB de datos macromoleculares estructurales que es libre y públicamente a disposición de la comunidad mundial. Se trata de organizaciones que actúan como depósito, proceso de datos y centros de distribución de datos PDB.

RCSB PDB personal se encuentra en Rutgers, la Universidad Estatal de Nueva Jersey y la Universidad de California, San Diego.

10.1. Obtención de la Estructura PDB

Para la obtención del formato PDB se consultó la especificación “Protein Data Bank Atomic

Coordinate Entry Format Description version 3.30” para los siguientes campos:

Columnas	**Tipo de Dato**	**Campo**	**Definición**
1 a 6	Tipo de elemento	ATOM	
7 a 11	Entero	Número de Serie	Número de Serie del átomo
13 a 16	Tipo de átomo	Símbolo en la tabla periódica	Nombre del átomo
31 a 38	Número real	X	Coordenadas ortogonales para x en Angstroms
39 a 46	Número real	Y	Coordenadas ortogonales para y en Angstroms
47 a 54	Número real	Z	Coordenadas ortogonales para z en Angstroms
55 a 60	Número real	Ocupancia	Si ocupa un átomo
61 a 66	Número real	Factor de Temperatura	Si hay un factor de temperatura
79 a 80	Número entero	Carga en el átomo	Si tiene carga el átomo

Para tener la clase contenedora de estos parámetros se generó el tipo de dato “partícula” que contiene todos los datos.

11. Desarrollo del Simulador

11.1. Pseudocódigo:

Definimos como pseudocódigo a la definición de un lenguaje intermedio entre el lenguaje de uso común y el lenguaje de programación[30]. El objetivo de este método es el de representar los pasos y acciones del algoritmo a desarrollar, de la forma más clara posible.

Siendo el siguiente pseudocódigo el siguiente:

1. Se colocan los parámetros que definen nuestra celda elemental del material de estudio.
2. Una vez definida la celda elemental se incrementa la red cristalina usando celdas previamente definidas por el usuario, usando vectores de traslación [31].
3. Se le aplica el método multicapa con el cual obtenemos patrón de difracción de rayos-x.
4. Se le aplica la Transformada Inversa de Fourier para verificar la estructura original.
5. Una ves que es aceptada la estructura como correcta, es guardado como un archivo de posiciones puntuales en formato PDB[32].

Se puede ver el diagrama de la siguiente forma:

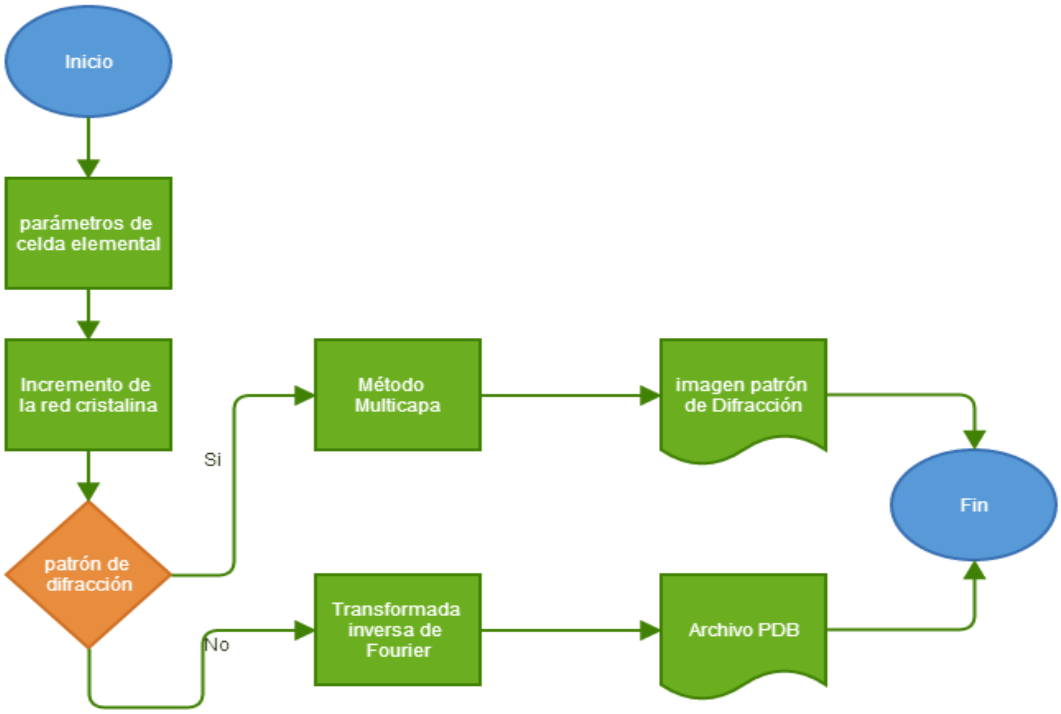
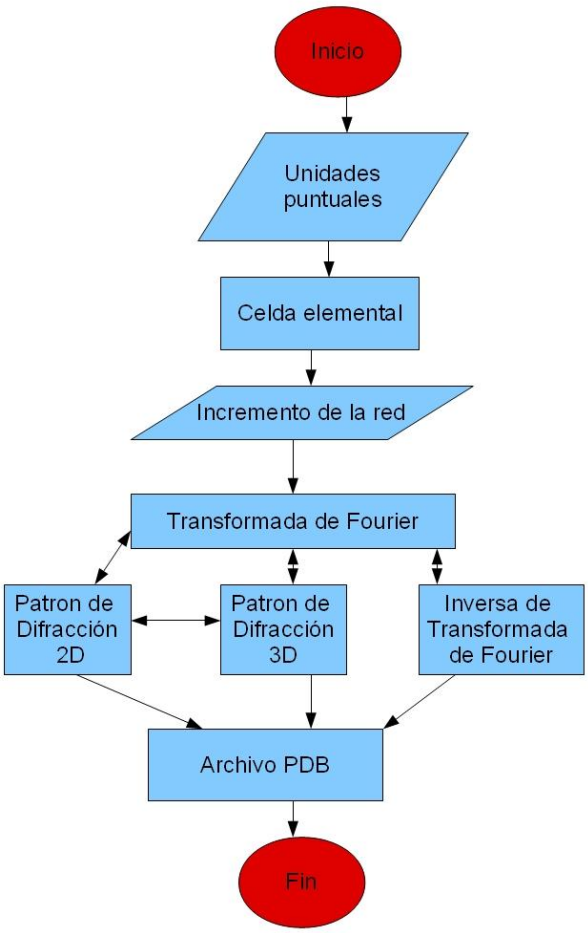


Figura 19. Diagrama de bloques que muestra los pasos y acciones del algoritmo a desarrollar.

En este diagrama de bloques explica las opciones que el usuario puede tomar ya sea si quiere solamente guardar la imagen del patrón de difracción o si desea guardar la estructura de la red cristalina en un archivo PDB.

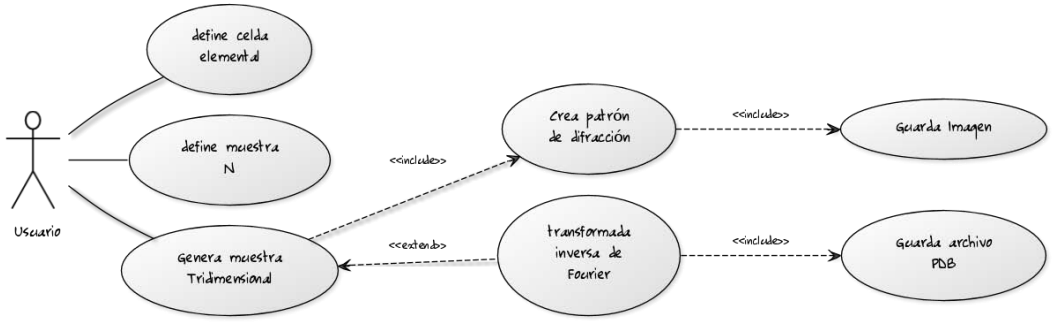
11.2. Diagrama de Flujo:



El diagrama de flujo o diagrama de actividades muestra los flujos de trabajo de un sistema, siendo en este caso el modelado de la estructura, pasando al componente de la Transformada de Fourier, y en este punto se elige entre las salidas de datos como lo es el archivo PDB o una imagen de la Transformada de Fourier de la estructura cristalina.

11.3. Diagrama de Caso de Uso:

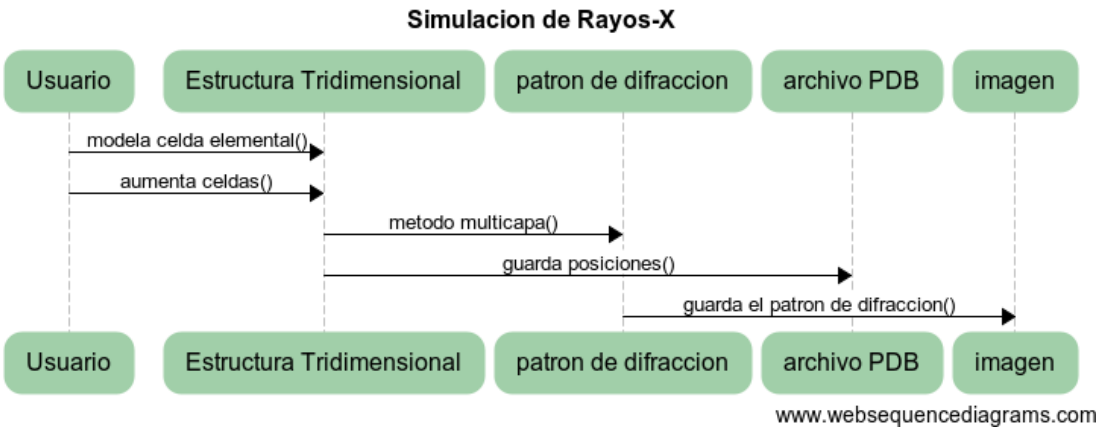
Se definen la relación entre el usuario (actor) y las metas a alcanzar (casos de uso).



En nuestro caso se definen las metas a alcanzar como las salidas del análisis de Fourier; en estos casos como archivo PDB o como imagen de la Transformada de Fourier de la estructura cristalina.

11.4. Diagrama de Secuencia [47]:

Es el diagrama que muestra la como operan entre si los procesos y en qué orden.



En nuestro caso el diagrama de secuencia nos indica en que orden entra en operación cada proceso, con esto se indica que primero se modela la estructura cristalina. Una vez definida la estructura pasamos a el método multicapa que es el que se usa para poder generar nuestra imagen de la Transformada de Fourier y finalmente obtener los datos de salida; ya sea en fomato PDB de la estructura cristalina previamente modelada o la imagen de la Transformada de Fourier de la estructura.

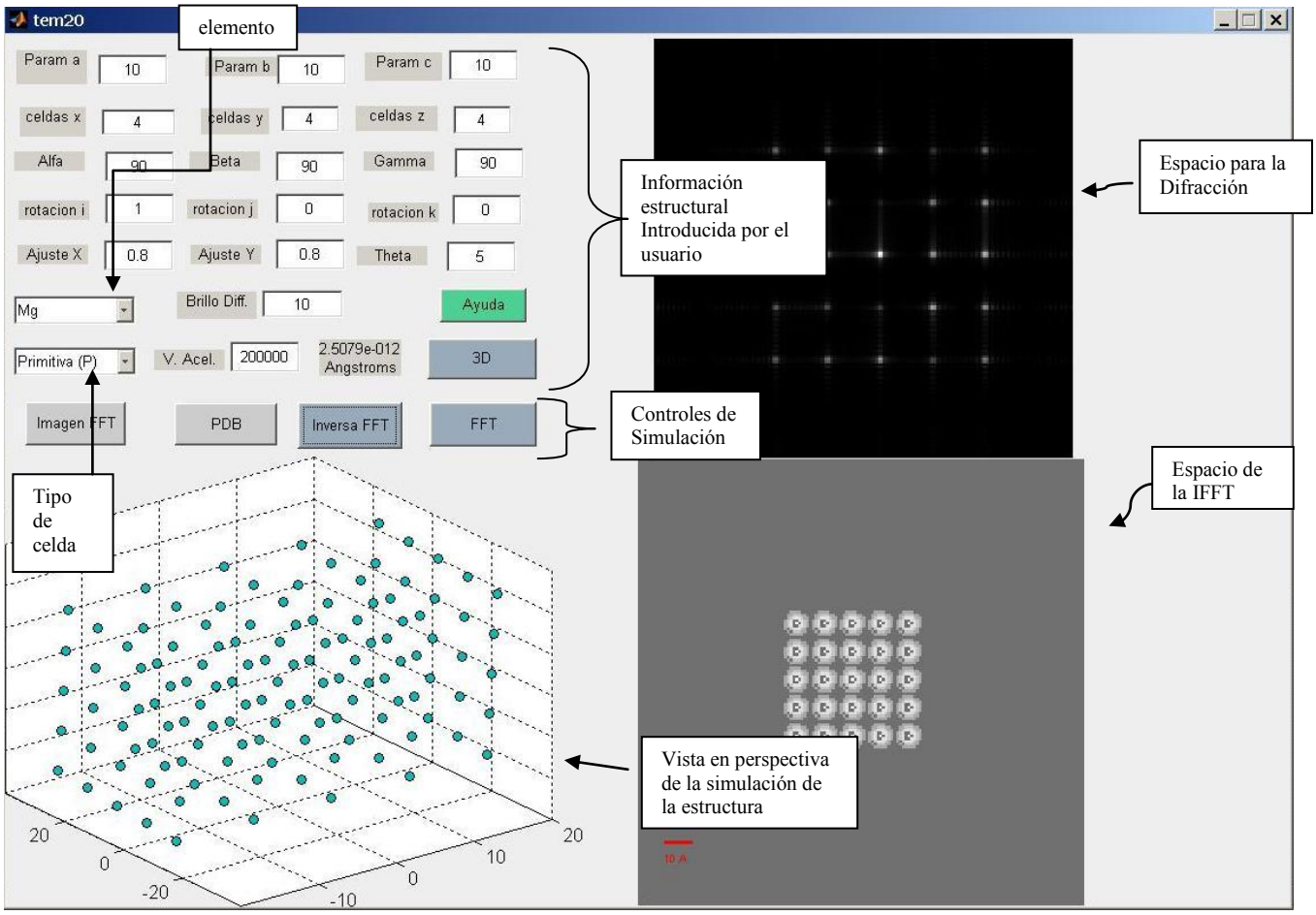
12. Resultados:

12.1 Simulación de Estructuras:

Una vez realizado el programa de simulación se obtuvieron las estructuras cristalinas, y las simulaciones de los correspondientes patrones de difracción de electrónes y los archivos pdb de dichas estructuras.

A Continuación se muestran algunos ejemplos representativos obtenidos con el software de simulación desarrollado en el presente trabajo:

Explicación de la interfaz:



Botón o campo:	Significado:
Param a	Parámetro de red a
Param b	Parámetro de red b
Param c	Parámetro de red c
Celdas x	Número de celdas a lo largo del eje x

Celdas y	Número de celdas a lo largo del eje y
Celdas z	Número de celdas a lo largo del eje z
Alfa	Ángulo alfa de la celda elemental
Beta	Ángulo beta de la celda elemental
Gamma	Ángulo gamma de la celda elemental
Rotación i	Rotación de la figura a lo largo del eje i
Rotación j	Rotación de la figura a lo largo del eje j
Rotación k	Rotación de la figura a lo largo del eje k
Theta	Ángulo de rotación de la figura
elemento	Elemento químico
Brillo Diff.	Brillo en la imagen de Diffración
Tipo de Celda	El tipo de celda de Bravais
Ajuste X	Ajuste de imagen en la Difración a lo largo de x
Ajuste Y	Ajuste de imagen en la Difración a lo largo de y
V. Acel.	Voltaje de Aceleración (en Volts)
3D	Vista en perspectiva de la simulación de la estructura
FFT	Simulación del Patrón de Difracción
IFFT	Simulación del regreso del Patrón de Difracción a espacio Real
Imagen FFT	Guarda el Patrón de Difracción como imagen
PDB	Guarda la estructura simulada en formato “PDB”

12.1.1. Estructura Cúbica Simple

En la siguiente figura veremos una estructura cúbica simple de 8 celdas por lado, 10 Angstroms en los parámetros de red a, b y c, girada 5 grados en el eje i, (en la figura se roto la vista para una mejor apreciación de los planos del cristal), a un Voltaje de aceleración de 200 KV su modelado tridimensional:

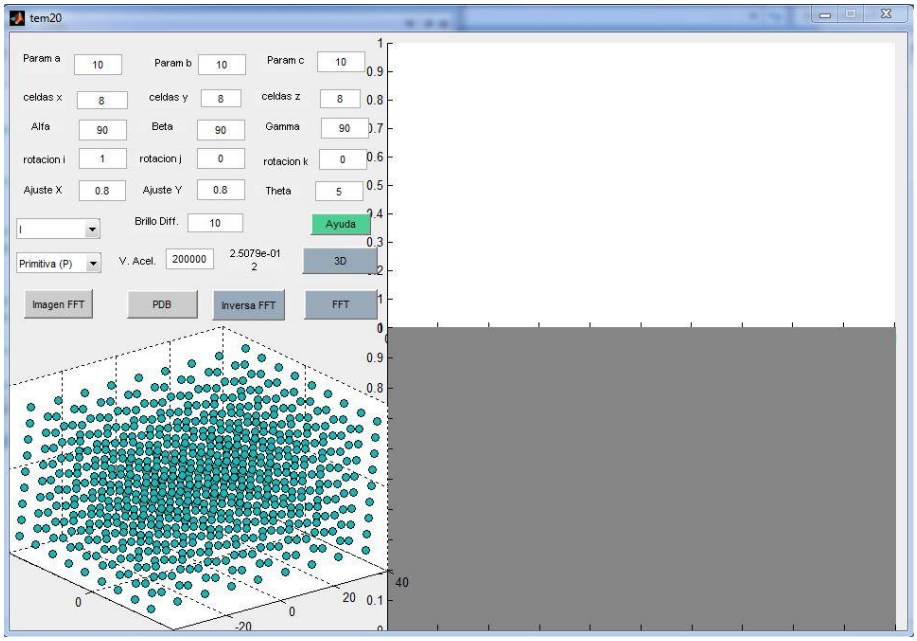


Figura 25. "Estructura Cúbica Simple 1" [44]

Y su patrón de difracción:

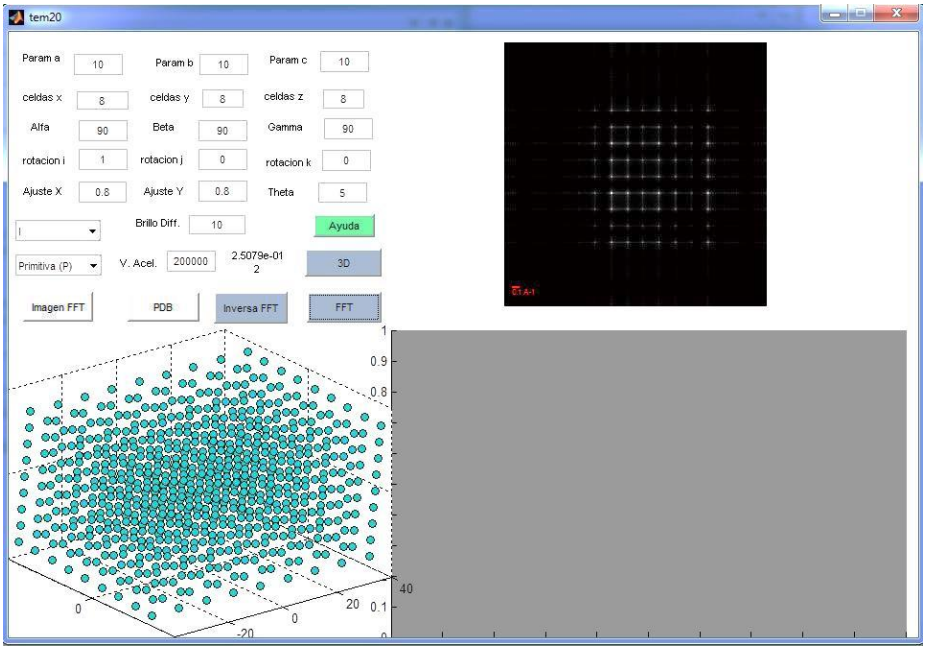


Figura 26. "Estructura Cúbica Simple 2" mostrando la simulación del patrón de difracción

de electrones (FFT) [45]

Y finalmente la transformada inversa de la estructura:

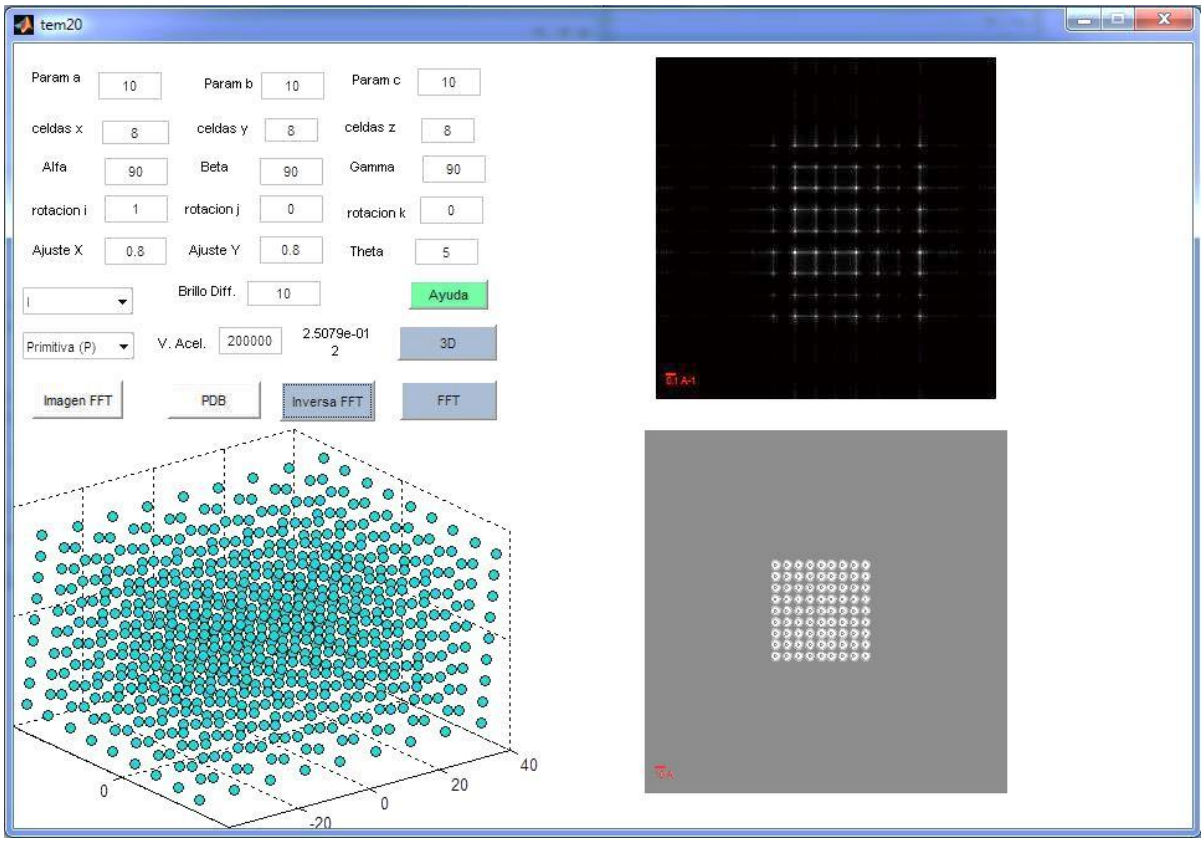


Figura 27. "Estructura Cúbica Simple 3" mostrando tanto la simulación del patrón de difracción de electrones (FFT), como la imagen reconstruida (IFFT) [46]

Una vez realizadas las simulaciones anteriores, se obtuvo el archivo PDB de la estructura también con el mismo software desarrollado en el presente trabajo (**fragmento de código**):

Campo1	**Campo2**	**Campo3**	**Campo4**	**Campo5**	**Campo6**	**Campo7**	**Campo8**	**Campo9**	**Campo 10**
Registro	serial	elemento	Numero de secuncia	Coordenadas otogonales para x	Coordenadas otogonales para y	Coordenadas otogonales para z	ocupancia	Factor de temperatura	Carga en el átomo

```
ATOM      1  I         1     -40.000 -36.362 -43.334  1.00  0.00          O
ATOM      2  I         2     -40.000 -26.400 -42.462  1.00  0.00          O
ATOM      3  I         3     -40.000 -16.438 -41.591  1.00  0.00          O
ATOM      4  I         4     -40.000  -6.476 -40.719  1.00  0.00          O
ATOM      5  I         5     -40.000   3.486 -39.848  1.00  0.00          O
ATOM      6  I         6     -40.000  13.448 -38.976  1.00  0.00          O
ATOM      7  I         7     -40.000  23.410 -38.105  1.00  0.00          O
ATOM      8  I         8     -40.000  33.372 -37.233  1.00  0.00          O
```

```
ATOM      9  I         9    -40.000  43.334 -36.362  1.00  0.00          O
ATOM     10  I        10    -30.000 -36.362 -43.334  1.00  0.00          O
ATOM     11  I        11    -30.000 -26.400 -42.462  1.00  0.00          O
ATOM     12  I        12    -30.000 -16.438 -41.591  1.00  0.00          O
ATOM     13  I        13    -30.000  -6.476 -40.719  1.00  0.00          O
ATOM     14  I        14    -30.000   3.486 -39.848  1.00  0.00          O
ATOM     15  I        15    -30.000  13.448 -38.976  1.00  0.00          O
ATOM     16  I        16    -30.000  23.410 -38.105  1.00  0.00          O
ATOM     17  I        17    -30.000  33.372 -37.233  1.00  0.00          O
ATOM     18  I        18    -30.000  43.334 -36.362  1.00  0.00          O
ATOM     19  I        19    -20.000 -36.362 -43.334  1.00  0.00          O
ATOM     20  I        20    -20.000 -26.400 -42.462  1.00  0.00          O
ATOM     21  I        21    -20.000 -16.438 -41.591  1.00  0.00          O
ATOM     22  I        22    -20.000  -6.476 -40.719  1.00  0.00          O
ATOM     23  I        23    -20.000   3.486 -39.848  1.00  0.00          O
ATOM     24  I        24    -20.000  13.448 -38.976  1.00  0.00          O
ATOM     25  I        25    -20.000  23.410 -38.105  1.00  0.00          O
ATOM     26  I        26    -20.000  33.372 -37.233  1.00  0.00          O
ATOM     27  I        27    -20.000  43.334 -36.362  1.00  0.00          O
ATOM     28  I        28    -10.000 -36.362 -43.334  1.00  0.00          O
ATOM     29  I        29    -10.000 -26.400 -42.462  1.00  0.00          O
ATOM     30  I        30    -10.000 -16.438 -41.591  1.00  0.00          O
ATOM     31  I        31    -10.000  -6.476 -40.719  1.00  0.00          O
ATOM     32  I        32    -10.000   3.486 -39.848  1.00  0.00          O
ATOM     33  I        33    -10.000  13.448 -38.976  1.00  0.00          O
ATOM     34  I        34    -10.000  23.410 -38.105  1.00  0.00          O
ATOM     35  I        35    -10.000  33.372 -37.233  1.00  0.00          O
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ATOM     37  I        37     -0.000 -36.362 -43.334  1.00  0.00          O
ATOM     38  I        38     -0.000 -26.400 -42.462  1.00  0.00          O
ATOM     39  I        39     -0.000 -16.438 -41.591  1.00  0.00          O
ATOM     40  I        40     -0.000  -6.476 -40.719  1.00  0.00          O
ATOM     41  I        41     -0.000   3.486 -39.848  1.00  0.00          O
ATOM     42  I        42     -0.000  13.448 -38.976  1.00  0.00          O
ATOM     43  I        43     -0.000  23.410 -38.105  1.00  0.00          O
ATOM     44  I        44     -0.000  33.372 -37.233  1.00  0.00          O
ATOM     45  I        45      0.000  43.334 -36.362  1.00  0.00          O
ATOM     46  I        46     10.000 -36.362 -43.334  1.00  0.00          O
ATOM     47  I        47     10.000 -26.400 -42.462  1.00  0.00          O
ATOM     48  I        48     10.000 -16.438 -41.591  1.00  0.00          O
ATOM     49  I        49     10.000  -6.476 -40.719  1.00  0.00          O
ATOM     50  I        50     10.000   3.486 -39.848  1.00  0.00          O
ATOM     51  I        51     10.000  13.448 -38.976  1.00  0.00          O
ATOM     52  I        52     10.000  23.410 -38.105  1.00  0.00          O
ATOM     53  I        53     10.000  33.372 -37.233  1.00  0.00          O
ATOM     54  I        54     10.000  43.334 -36.362  1.00  0.00          O
ATOM     55  I        55     20.000 -36.362 -43.334  1.00  0.00          O
ATOM     56  I        56     20.000 -26.400 -42.462  1.00  0.00          O
```

```
ATOM     57  I        57      20.000 -16.438 -41.591  1.00  0.00          O
ATOM     58  I        58      20.000  -6.476 -40.719  1.00  0.00          O
ATOM     59  I        59      20.000   3.486 -39.848  1.00  0.00          O
ATOM     60  I        60      20.000  13.448 -38.976  1.00  0.00          O
ATOM     61  I        61      20.000  23.410 -38.105  1.00  0.00          O
ATOM     62  I        62      20.000  33.372 -37.233  1.00  0.00          O
ATOM     63  I        63      20.000  43.334 -36.362  1.00  0.00          O
ATOM     64  I        64      30.000 -36.362 -43.334  1.00  0.00          O
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ATOM     69  I        69      30.000  13.448 -38.976  1.00  0.00          O
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ATOM     71  I        71      30.000  33.372 -37.233  1.00  0.00          O
ATOM     72  I        72      30.000  43.334 -36.362  1.00  0.00          O
ATOM     73  I        73      40.000 -36.362 -43.334  1.00  0.00          O
ATOM     74  I        74      40.000 -26.400 -42.462  1.00  0.00          O
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ATOM     78  I        78      40.000  13.448 -38.976  1.00  0.00          O
ATOM     79  I        79      40.000  23.410 -38.105  1.00  0.00          O
ATOM     80  I        80      40.000  33.372 -37.233  1.00  0.00          O
ATOM     81  I        81      40.000  43.334 -36.362  1.00  0.00          O
ATOM     82  I        82     -40.000 -37.233 -33.372  1.00  0.00          O
ATOM     83  I        83     -40.000 -27.271 -32.501  1.00  0.00          O
ATOM     84  I        84     -40.000 -17.309 -31.629  1.00  0.00          O
ATOM     85  I        85     -40.000  -7.347 -30.757  1.00  0.00          O
ATOM     86  I        86     -40.000   2.615 -29.886  1.00  0.00          O
ATOM     87  I        87     -40.000  12.577 -29.014  1.00  0.00          O
ATOM     88  I        88     -40.000  22.539 -28.143  1.00  0.00          O
ATOM     89  I        89     -40.000  32.501 -27.271  1.00  0.00          O
ATOM     90  I        90     -40.000  42.462 -26.400  1.00  0.00          O
ATOM     91  I        91     -30.000 -37.233 -33.372  1.00  0.00          O
ATOM     92  I        92     -30.000 -27.271 -32.501  1.00  0.00          O
ATOM     93  I        93     -30.000 -17.309 -31.629  1.00  0.00          O
ATOM     94  I        94     -30.000  -7.347 -30.757  1.00  0.00          O
ATOM     95  I        95     -30.000   2.615 -29.886  1.00  0.00          O
ATOM     96  I        96     -30.000  12.577 -29.014  1.00  0.00          O
ATOM     97  I        97     -30.000  22.539 -28.143  1.00  0.00          O
ATOM     98  I        98     -30.000  32.501 -27.271  1.00  0.00          O
ATOM     99  I        99     -30.000  42.462 -26.400  1.00  0.00          O
ATOM    100  I       100     -20.000 -37.233 -33.372  1.00  0.00          O
ATOM    101  I       101     -20.000 -27.271 -32.501  1.00  0.00          O
ATOM    102  I       102     -20.000 -17.309 -31.629  1.00  0.00          O
ATOM    103  I       103     -20.000  -7.347 -30.757  1.00  0.00          O
ATOM    104  I       104     -20.000   2.615 -29.886  1.00  0.00          O
```

```
ATOM    105  I        105     -20.000  12.577 -29.014  1.00  0.00          O
ATOM    106  I        106     -20.000  22.539 -28.143  1.00  0.00          O
ATOM    107  I        107     -20.000  32.501 -27.271  1.00  0.00          O
ATOM    108  I        108     -20.000  42.462 -26.400  1.00  0.00          O
ATOM    109  I        109     -10.000 -37.233 -33.372  1.00  0.00          O
ATOM    110  I        110     -10.000 -27.271 -32.501  1.00  0.00          O
ATOM    111  I        111     -10.000 -17.309 -31.629  1.00  0.00          O
ATOM    112  I        112     -10.000  -7.347 -30.757  1.00  0.00          O
ATOM    113  I        113     -10.000   2.615 -29.886  1.00  0.00          O
ATOM    114  I        114     -10.000  12.577 -29.014  1.00  0.00          O
ATOM    115  I        115     -10.000  22.539 -28.143  1.00  0.00          O
ATOM    116  I        116     -10.000  32.501 -27.271  1.00  0.00          O
ATOM    117  I        117     -10.000  42.462 -26.400  1.00  0.00          O
ATOM    118  I        118      -0.000 -37.233 -33.372  1.00  0.00          O
ATOM    119  I        119      -0.000 -27.271 -32.501  1.00  0.00          O
ATOM    120  I        120      -0.000 -17.309 -31.629  1.00  0.00          O
```

Asimismo, también se encuentra el archivo completo PDB de la estructura, en la sección 15.2.1 de los Anexos.

12.1.2. Estructura Cúbica Centrada en las Caras (FCC)

En la siguiente figura se muestra una estructura cúbica centrada en las caras de 5 celdas por lado, 8 Angstroms en los parámetros de red a, b y c, a un Voltaje de aceleración de 200 KV su modelado tridimensional:

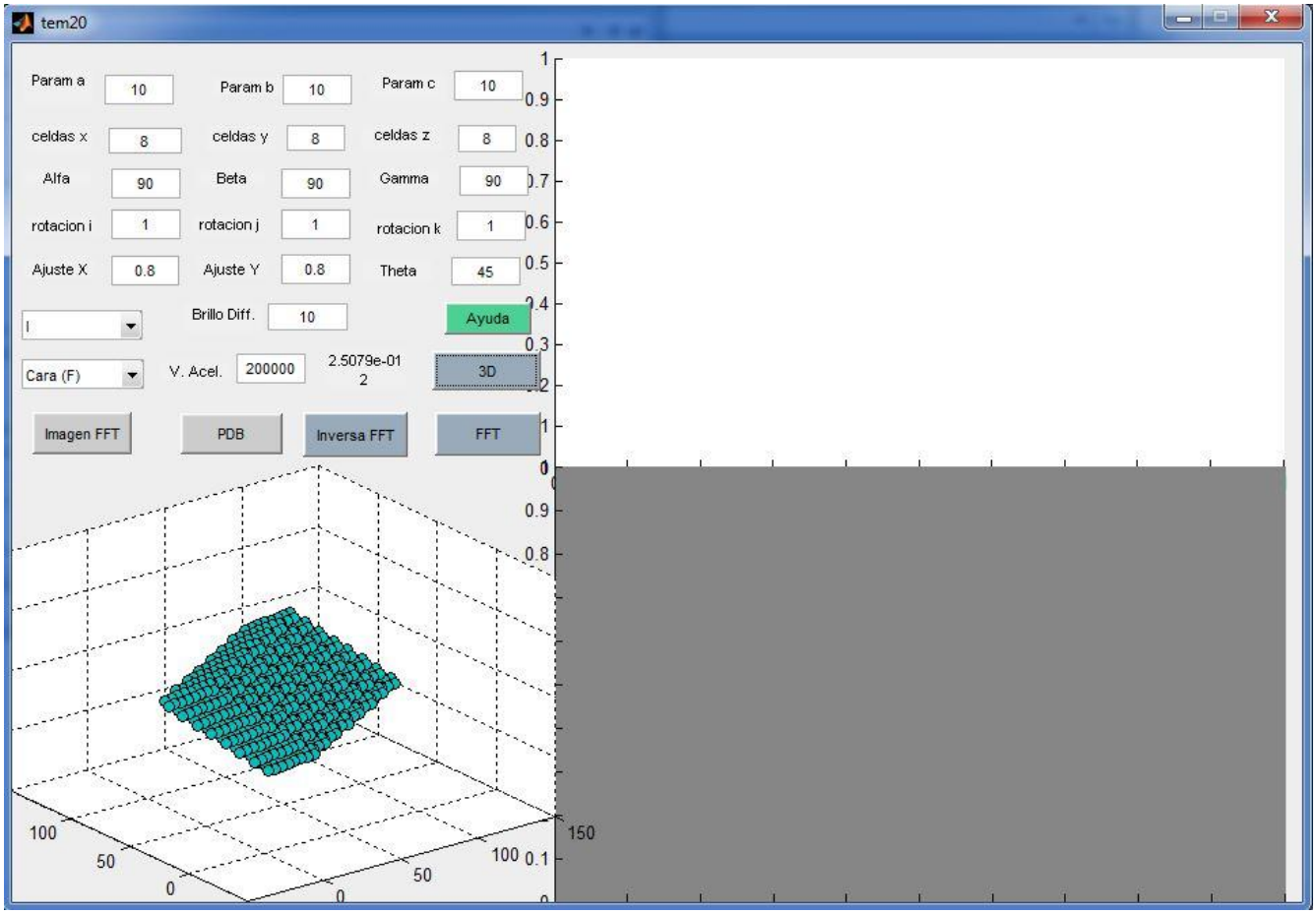

Figura 25. "Estructura Cúbica Centrada en las Caras 1" [47]

Y su patrón de difracción:

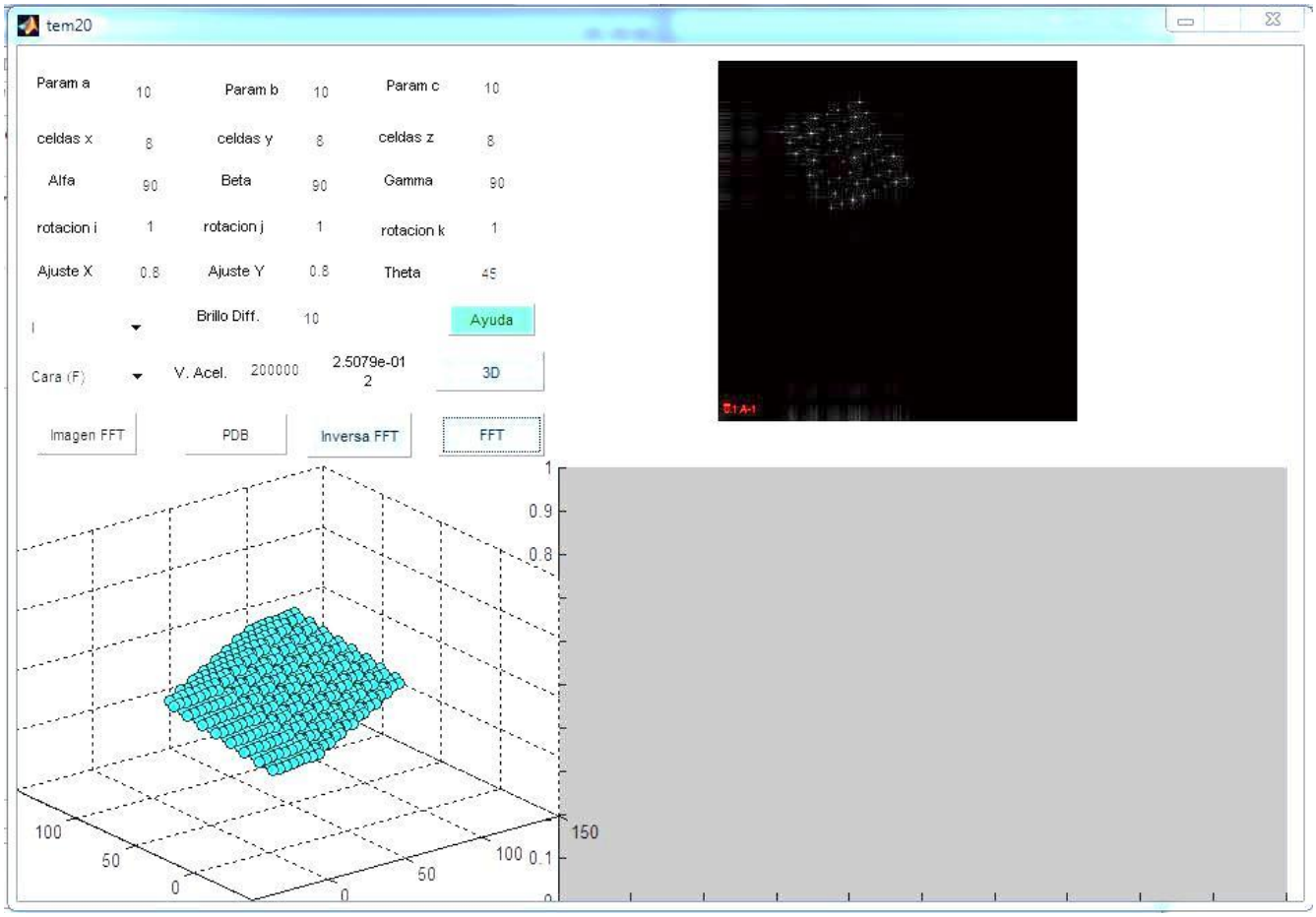

Figura 26. "Estructura Cúbica Centrada en las Caras 2" mostrando la simulación del patrón de difracción de electrones (FFT) [48]

Y finalmente la transformada inversa de la estructura:

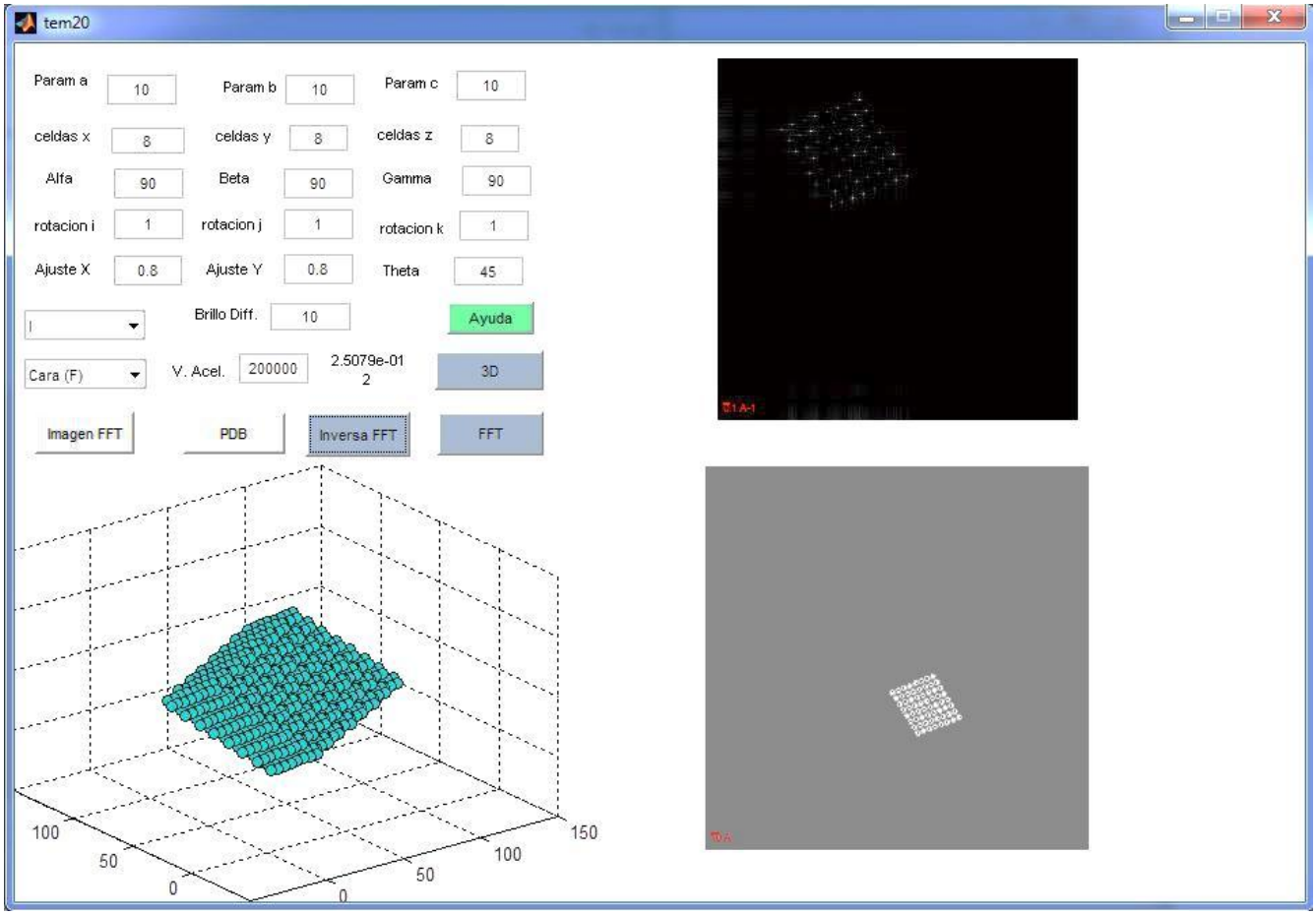

Figura 27. "Estructura Cúbica Centrada en las Caras 3" mostrando tanto la simulación del patrón de difracción de electrones (FFT), como la imagen reconstruida (IFFT) [49]

Asimismo, también se obtuvo el correspondiente archivo PDB de la estructura, el cual se encuentra en la sección 15.2.2 de los Anexos.

12.1.3. Estructura Cúbica Centrada en la Base (BCC)

En la siguiente figura veremos una estructura cúbica centrada en la Base de 8 celdas por lado, 10 Angstroms en los parámetros de red a, b, y c, a un Voltaje de aceleración de 200 KV su modelado tridimensional:

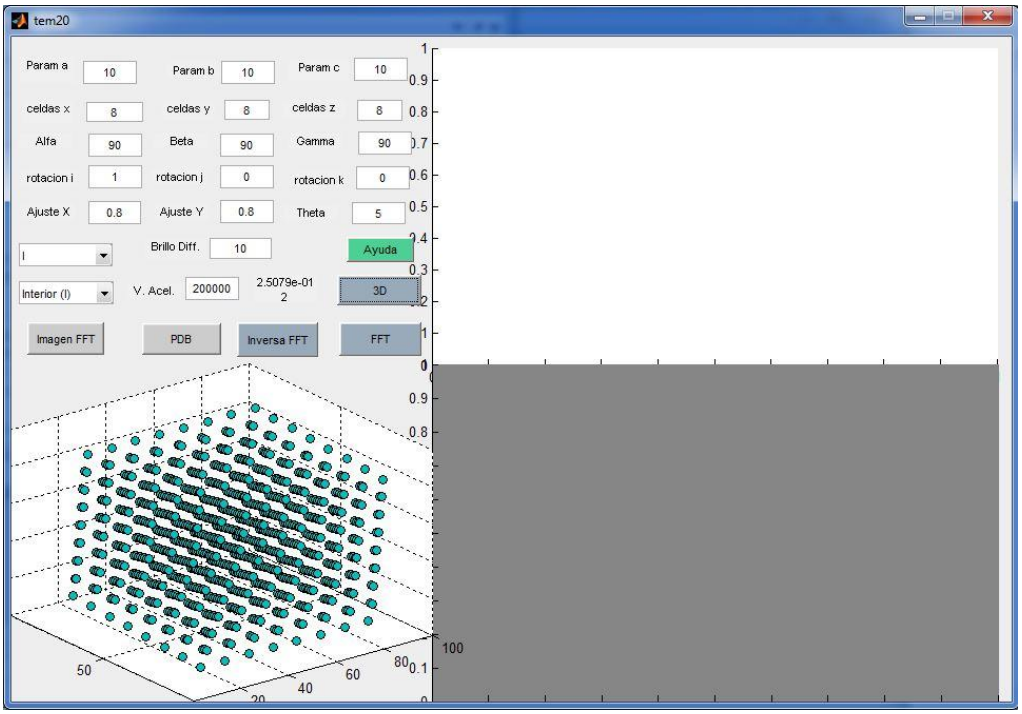

Figura 25. "Estructura Cúbica Centrada en el Cuerpo 1" [50]

Y su patrón de difracción:

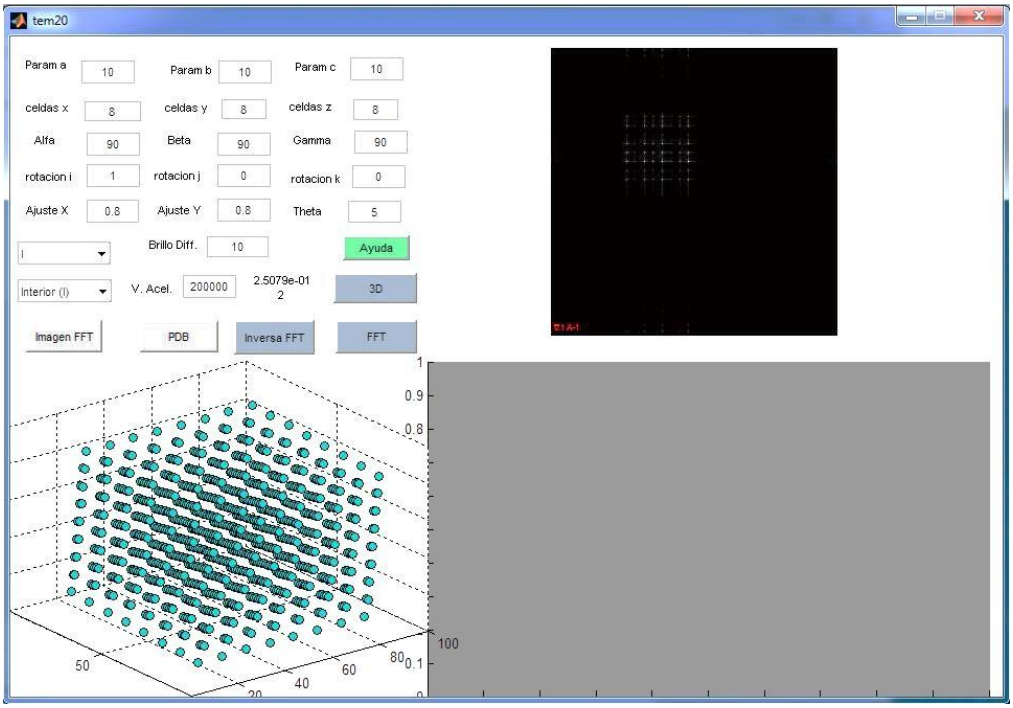

Figura 26. "Estructura Cúbica Centrada en el Cuerpo 2" mostrando la simulación del patrón de difracción de electrones (FFT) [51]

Y finalmente la transformada inversa de la estructura:

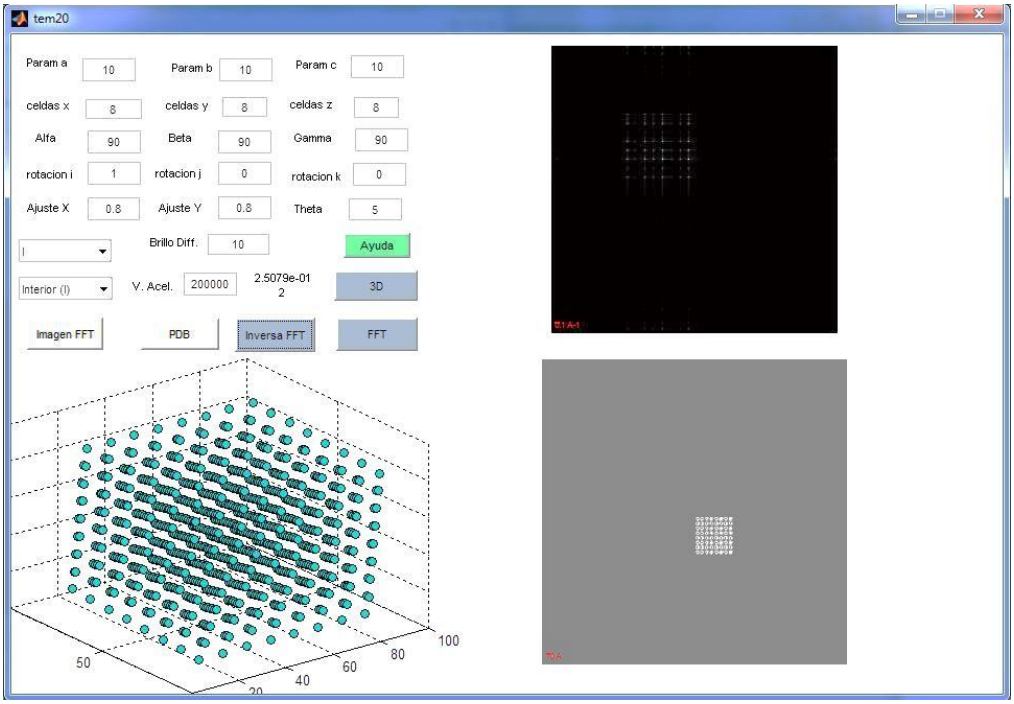

Figura 27. "Estructura Cúbica Centrada en el Cuerpo 3" mostrando tanto la simulación del patrón de difracción de electrones (FFT), como la imagen reconstruida (IFFT) [52]

Asimismo, también se obtuvo el correspondiente archivo PDB de la estructura, el cual se encuentra en la sección 15.2.3 de los Anexos.

12.1.4. Estructura Hexagonal

En la siguiente figura veremos una estructura Hexagonal de 8 celdas por lado, 10 Angstroms en los parámetros de red a y b, y 15 Angstroms en c, con ángulos alfa de 90°, beta 90° y gamma 120°; girada 5 grados en el eje i, (en la figura se roto la vista para una mejor apreciación de los planos del cristal), a un Voltaje de aceleración de 200 KV su modelado tridimensional:

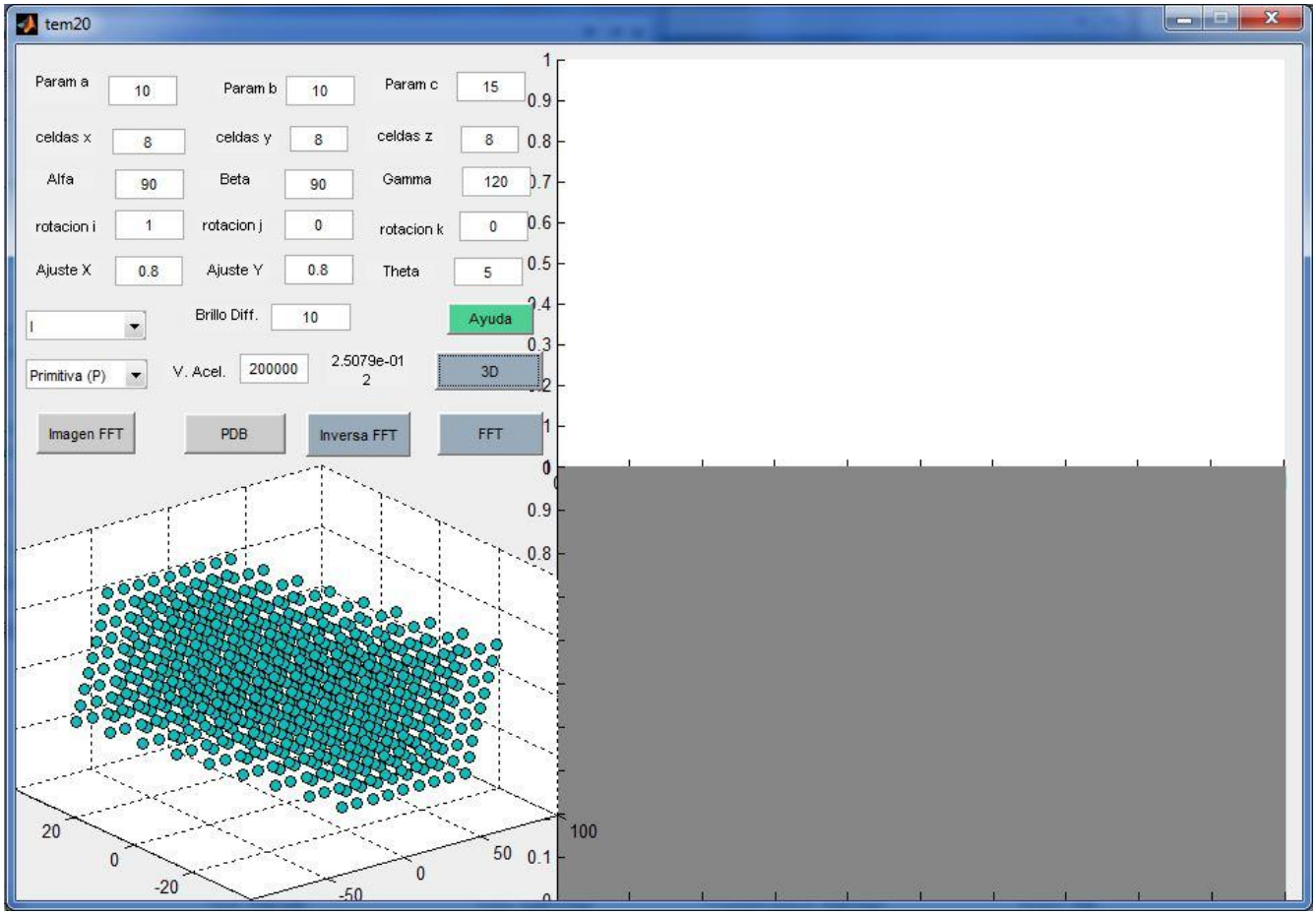

Figura 25. "Estructura Hexagonal 1" [53]

Y su patrón de difracción:

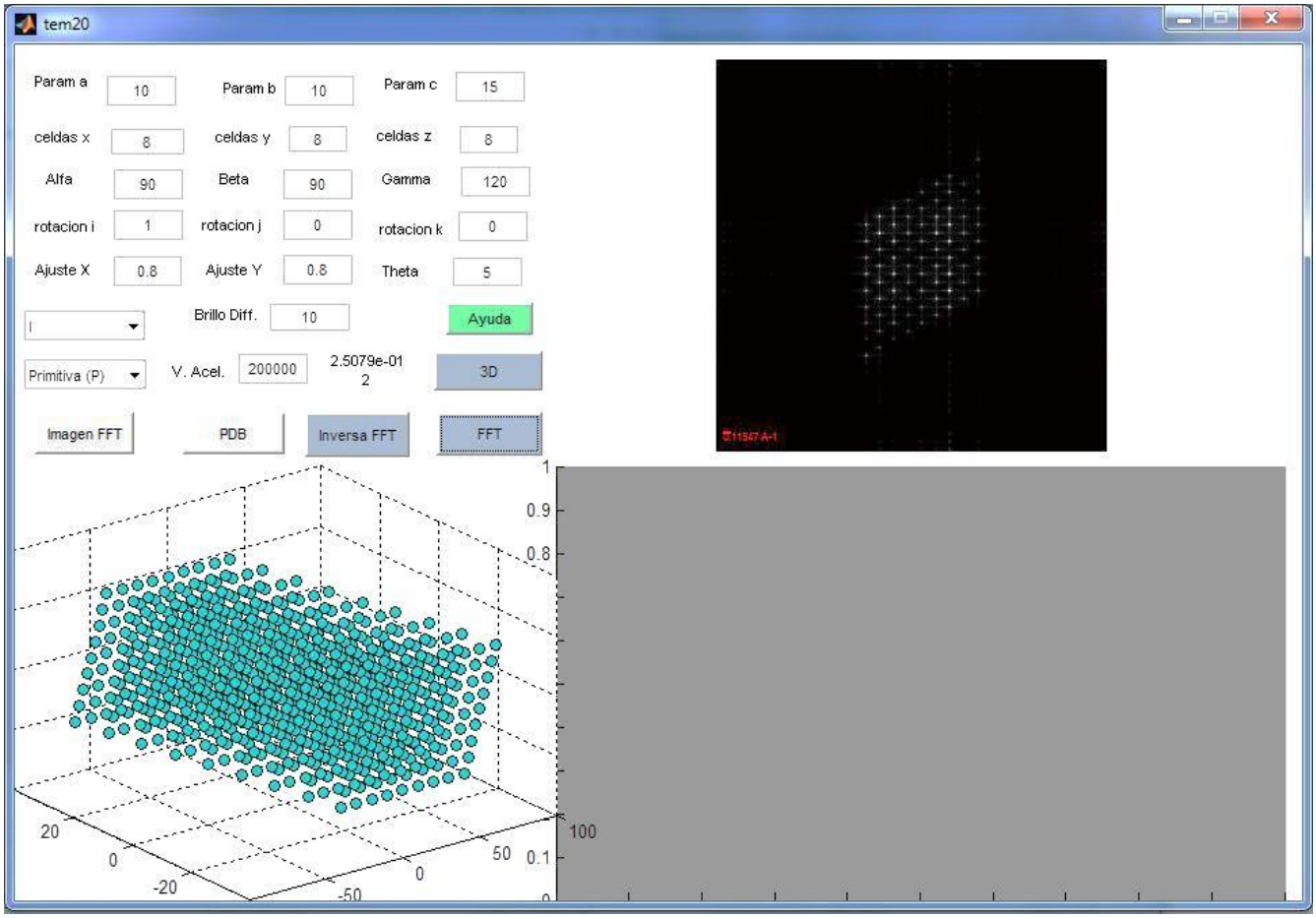

Figura 26. "Estructura Hexagonal 2" mostrando la simulación del patrón de difracción de electrones (FFT) [54]

Y finalmente la transformada inversa de la estructura:

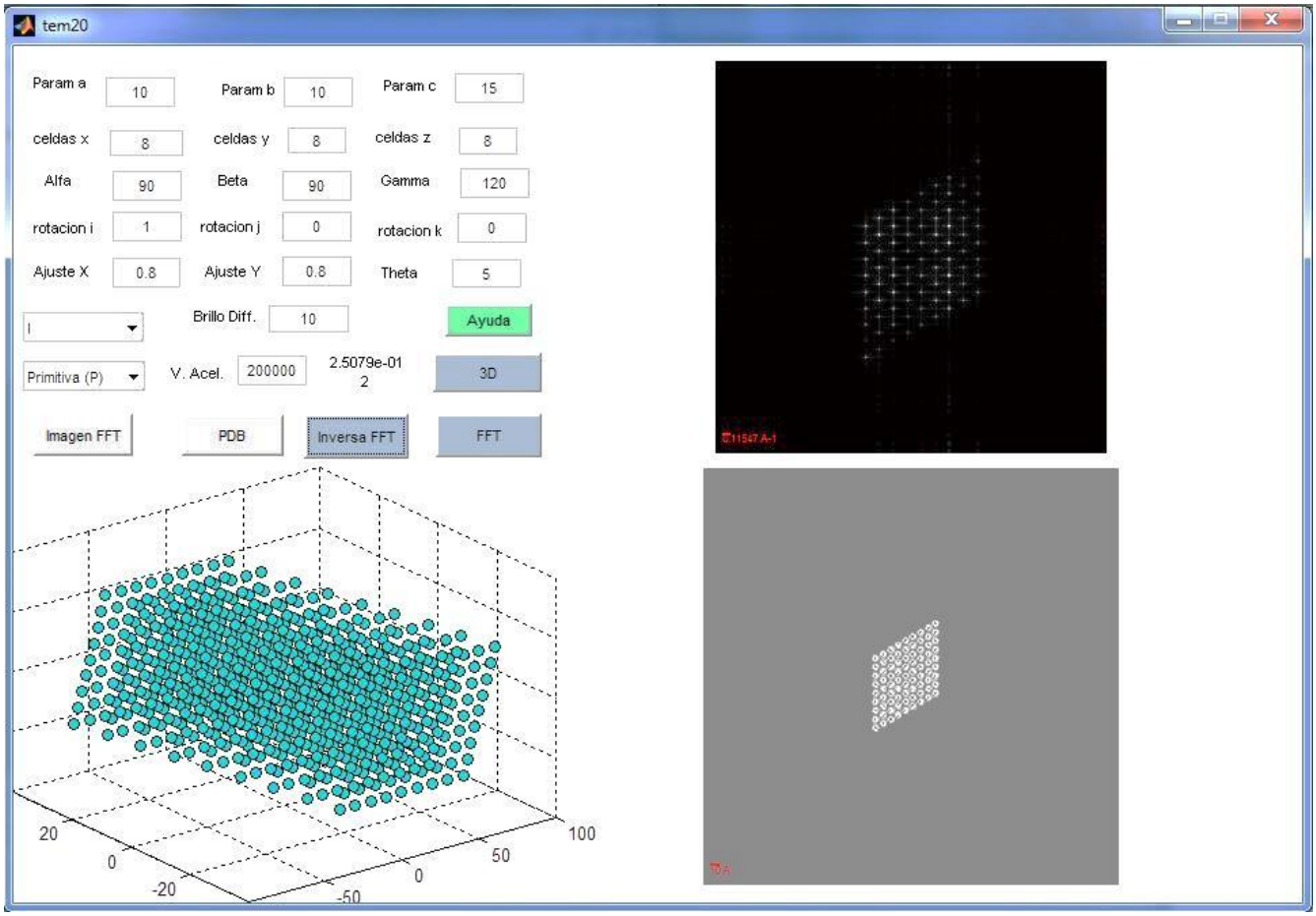

Figura 27. "Estructura Hexagonal 3" mostrando tanto la simulación del patrón de difracción de electrones (FFT), como la imagen reconstruida (IFFT) [55]

Asimismo, también se obtuvo el correspondiente archivo PDB de la estructura, el cual se encuentra en la sección 15.2.4 de los Anexos.

12.1.5. Estructura Triclínica

En la siguiente figura veremos una estructura triclínica simple de 6 celdas por lado, 10 Angstroms en el parámetro de red a, 8 Angstroms en el parámetro de red b, y 5 Angstroms en el parámetro de red c; con ángulos alfa de 80°, beta de 100°, y gamma de 120°; girada 5 grados en el eje i, (en la figura se roto la vista para una mejor apreciación de los planos del cristal), a un Voltaje de aceleración de 200 KV su modelado tridimensional:

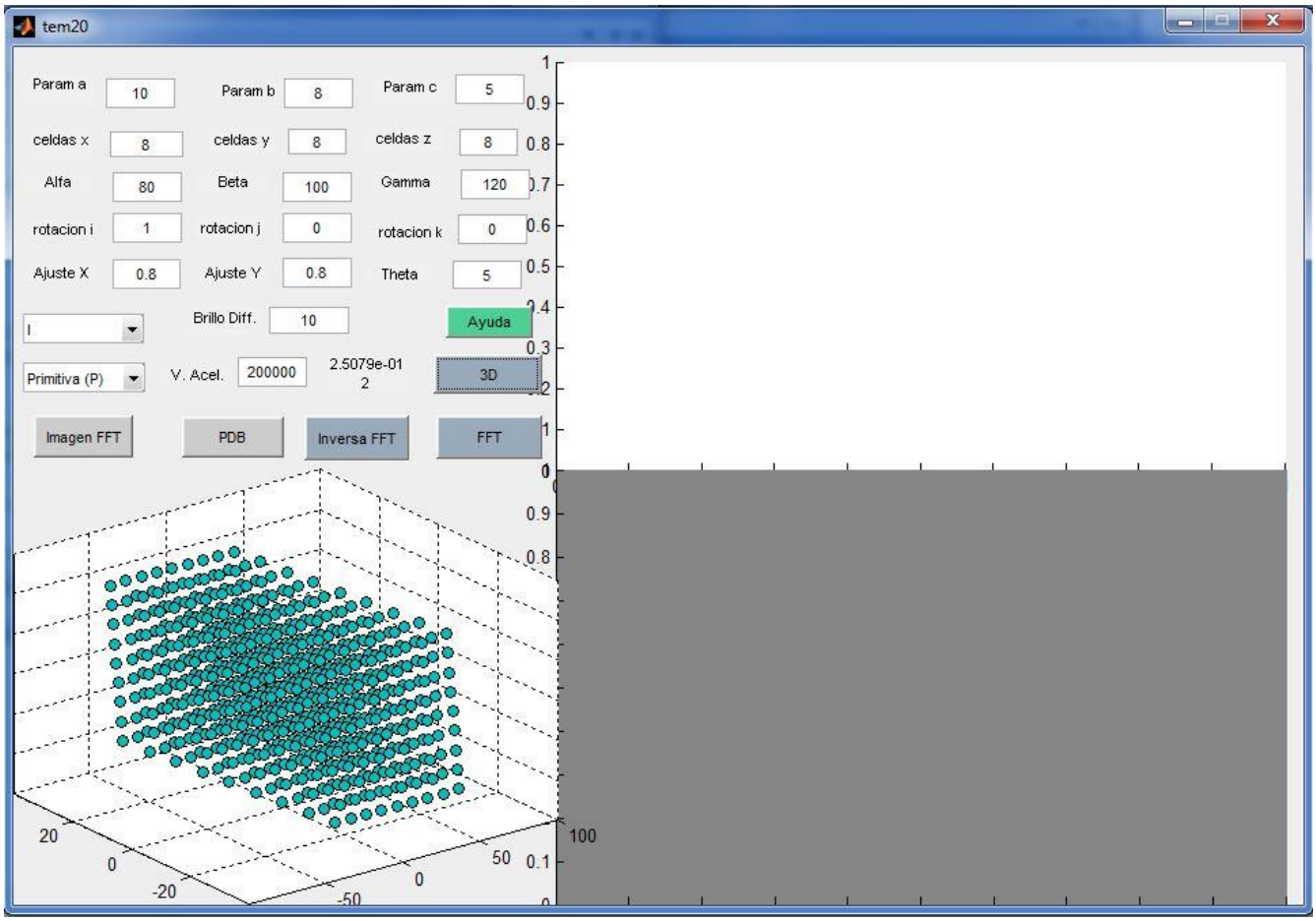

Figura 25. "Estructura Triclínica 1" [56]

Y su patrón de difracción:

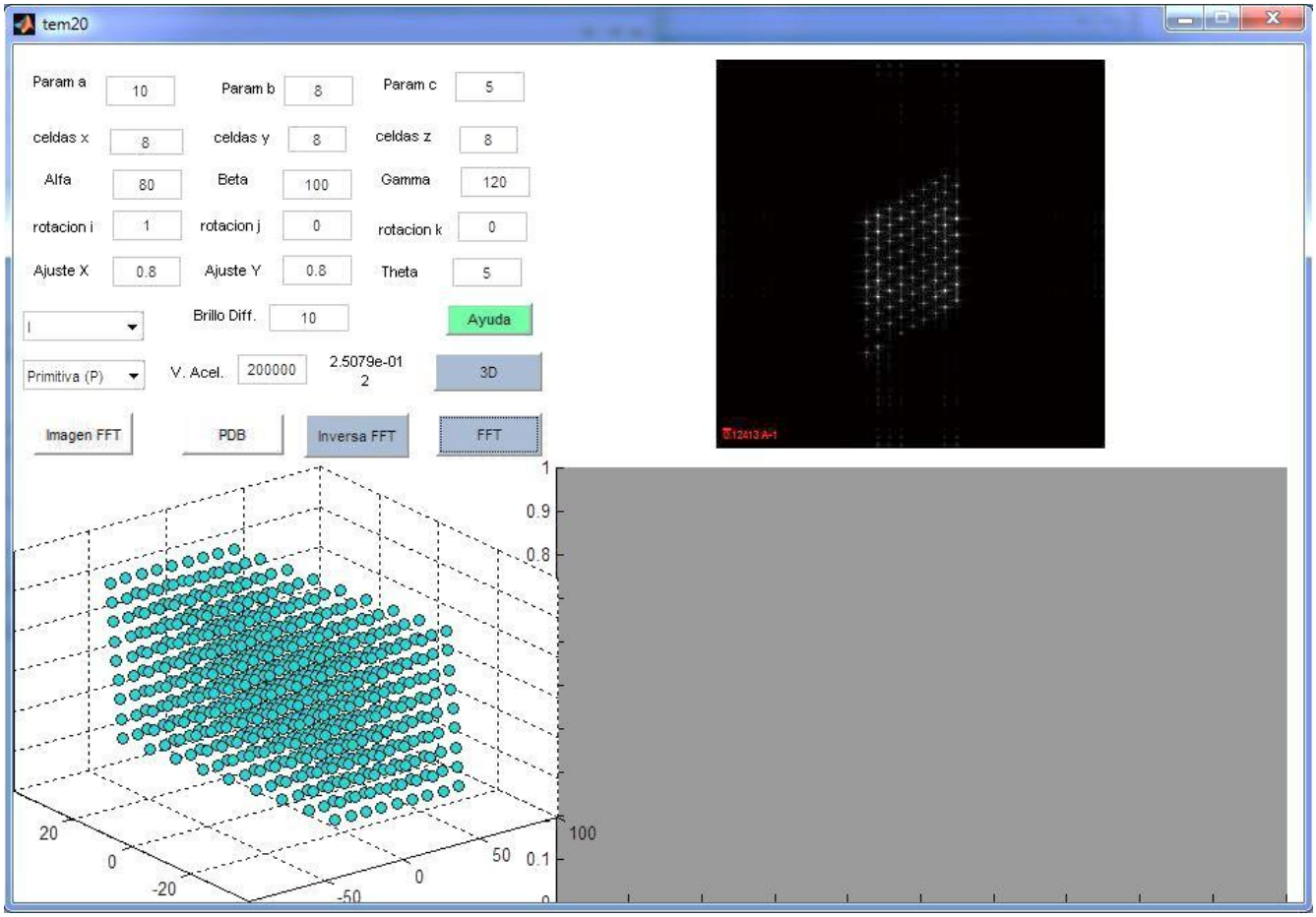

Figura 26. "Estructura Triclínica 2" mostrando la simulación del patrón de difracción de electrones (FFT) [57]

Y finalmente la transformada inversa de la estructura:

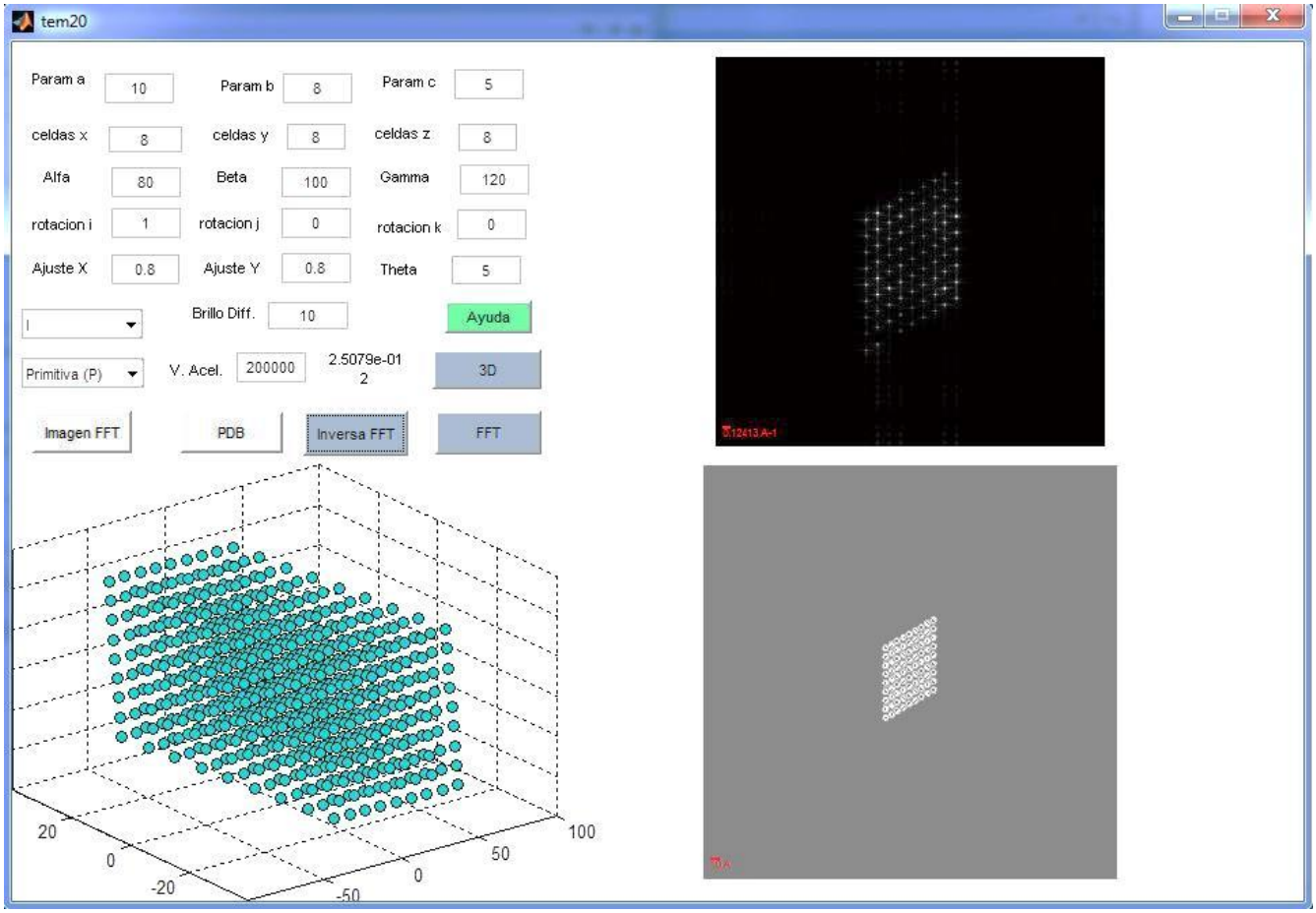

Figura 27. "Estructura Triclínica 3" mostrando tanto la simulación del patrón de difracción de electrones (FFT), como la imagen reconstruida (IFFT) [58]

Asimismo, también se obtuvo el correspondiente archivo PDB de la estructura, el cual se encuentra en la sección 15.2.5 de los Anexos.

12.1.6. Estructura Ortorrómbica

En la siguiente figura veremos una estructura ortorrómbica de 8 celdas por lado, 10 Angstroms en el parámetro de red a, 8 Angstroms en el parámetro de red b, y 5 Angstroms en el parámetro de red c, con ángulos alfa de 90°, beta de 90°y gamma de 90°; girada 5 grados en el eje i, (en la figura se roto la vista para una mejor apreciación de los planos del cristal), a un Voltaje de aceleración de 200 KV su modelado tridimensional:

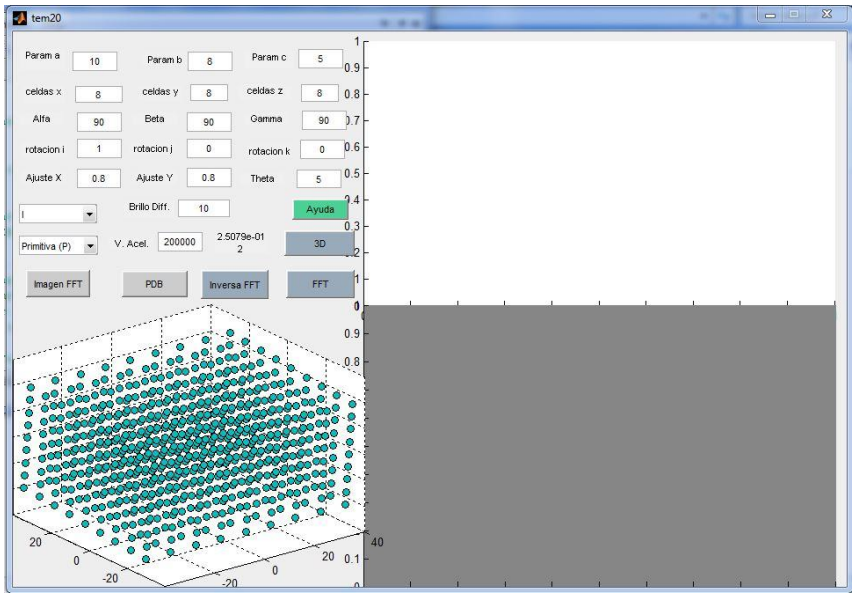

Figura 25. "Estructura Ortorrómbica 1" [59]

Y su patrón de difracción:

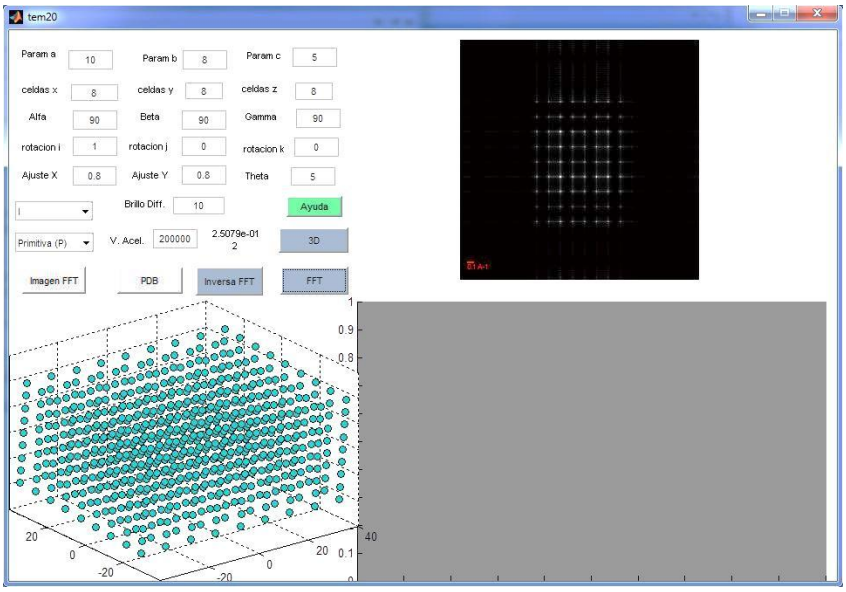

Figura 26. "Estructura Ortorrómbica 2" mostrando la simulación del patrón de difracción de electrones (FFT) [60]

Y finalmente la transformada inversa de la estructura:

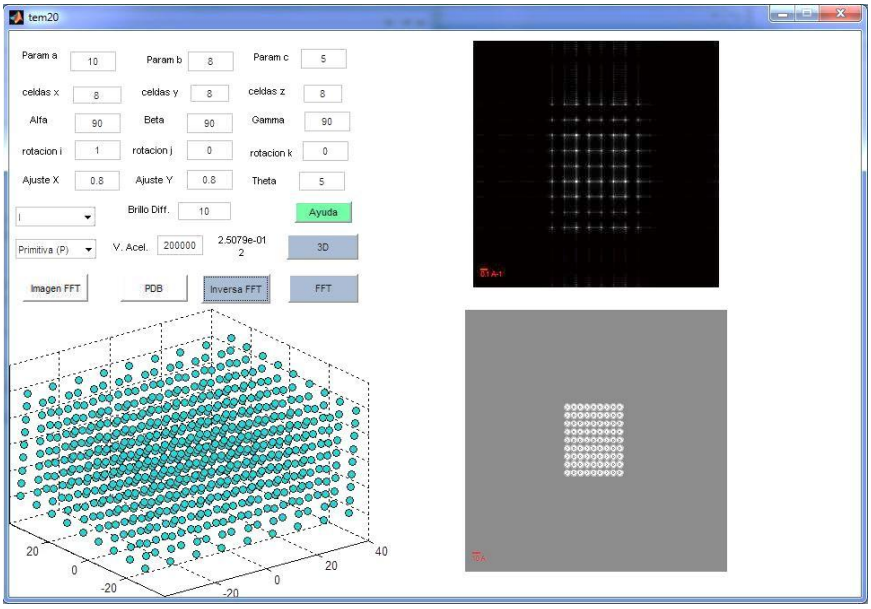

Figura 27. "Estructura Ortorrómbica 3" mostrando tanto la simulación del patrón de difracción de electrones (FFT), como la imagen reconstruida (IFFT) [61]

Asimismo, también se obtuvo el correspondiente archivo PDB de la estructura, el cual se encuentra en la sección 15.2.6 de los Anexos.

13. Conclusiones:

Se desarrolló un software como una herramienta que simula de forma precisa las estructuras cristalinas que se le colocan y es capaz de simular patrones de difracción de electrones, como los obtenidos mediante las técnicas de Microscopía Electrónica de Transmisión (TEM por sus siglas en inglés)y Microscopía Electrónica de Transmisión de Alta Resolución (HR-TEM).

Asimismo, el software desarrollado es capaz de generar archivos PDB delas estructuras simuladas, con lo cual se hace mas versátil y aporta información útil para los usuarios que estudian diferentes tipos de estructuras cristalinas. Estos archivos permiten exportar la información estructural hacia otros porgramas de visualización de estructuras.

También se pudo observar que es una herramienta auxiliar para el investigador que desee comprobar los modelos de estructuras cristalinas que analice en el microscopio electrónico con una simulación previamente programada en el software.

13.1. Perspectivas Futuras:

Además, una vez simulada la estructura de interés, es posible obtener el correspondiente archivo en formato .pdb para poder exportarlo a otras aplicaciones.

Se propone para la siguiente versión del software, un menú donde se pueda colocar el tipo de grupo espacial al que pertenece para así también incluir simulaciones con más de un tipo de átomo,así como también más opciones respecto a cómo elaborar el muestreo en el método multicapa así como más opciones para la iluminación y el corte de planos en el cristal.

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15. Anexos:

15.1. Código del programa:

```
function varargout = tem20(varargin)
% TEM20 M-file for tem20.fig
%      TEM20, by itself, creates a new TEM20 or raises the existing
%      singleton*.
%
%      H = TEM20 returns the handle to a new TEM20 or the handle to
%      the existing singleton*.
%
%      TEM20('CALLBACK',hObject,eventData,handles,...) calls the local
%      function named CALLBACK in TEM20.M with the given input arguments.
%
%      TEM20('Property','Value',...) creates a new TEM20 or raises the
%      existing singleton*.  Starting from the left, property value pairs are
%      applied to the GUI before tem20_OpeningFcn gets called.  An
%      unrecognized property name or invalid value makes property application
%      stop.  All inputs are passed to tem20_OpeningFcn via varargin.
%
%      *See GUI Options on GUIDE's Tools menu.  Choose "GUI allows only one
%      instance to run (singleton)".
%
% See also: GUIDE, GUIDATA, GUIHANDLES

% Edit the above text to modify the response to help tem20

% Last Modified by GUIDE v2.5 28-Sep-2014 21:45:33

% Begin initialization code - DO NOT EDIT
gui_Singleton = 1;
gui_State = struct('gui_Name',       mfilename, ...
                   'gui_Singleton',  gui_Singleton, ...
                   'gui_OpeningFcn', @tem20_OpeningFcn, ...
                   'gui_OutputFcn',  @tem20_OutputFcn, ...
                   'gui_LayoutFcn',  [] , ...
                   'gui_Callback',   []);
if nargin && ischar(varargin{1})
    gui_State.gui_Callback = str2func(varargin{1});
end

if nargout
    [varargout{1:nargout}] = gui_mainfcn(gui_State, varargin{:});
else
    gui_mainfcn(gui_State, varargin{:});
```

```
end
% End initialization code - DO NOT EDIT


% --- Executes just before tem20 is made visible.
function tem20_OpeningFcn(hObject, eventdata, handles, varargin)
% This function has no output args, see OutputFcn.
% hObject    handle to figure
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)
% varargin   command line arguments to tem20 (see VARARGIN)

% Choose default command line output for tem20
handles.output = hObject;

% Update handles structure
guidata(hObject, handles);

% UIWAIT makes tem20 wait for user response (see UIRESUME)
% uiwait(handles.figure1);


% --- Outputs from this function are returned to the command line.
function varargout = tem20_OutputFcn(hObject, eventdata, handles)
% varargout  cell array for returning output args (see VARARGOUT);
% hObject    handle to figure
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Get default command line output from handles structure
varargout{1} = handles.output;


% --- Executes on selection change in popupmenu1.
function popupmenu1_Callback(hObject, eventdata, handles)
% hObject    handle to popupmenu1 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: contents = cellstr(get(hObject,'String')) returns popupmenu1 contents as cell array
%        contents{get(hObject,'Value')} returns selected item from popupmenu1
elementossel=get(hObject,'String');
selecto=get(hObject,'Value');
tipoelementales=elementossel(selecto);
handles.tipoelementales=tipoelementales;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
```

```
function popupmenu1_CreateFcn(hObject, eventdata, handles)
% hObject    handle to popupmenu1 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: popupmenu controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end


% --- Executes on selection change in popupmenu2.
function popupmenu2_Callback(hObject, eventdata, handles)
% hObject    handle to popupmenu2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: contents = cellstr(get(hObject,'String')) returns popupmenu2 contents as cell array
%        contents{get(hObject,'Value')} returns selected item from popupmenu2
celgadis=cellstr(get(hObject,'String'));
tipocelda4=celgadis{get(hObject,'Value')};
handles.remplazotipo=tipocelda4;
guidata(hObject,handles);
% --- Executes during object creation, after setting all properties.
function popupmenu2_CreateFcn(hObject, eventdata, handles)
% hObject    handle to popupmenu2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: popupmenu controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end



function edit1_Callback(hObject, eventdata, handles)
% hObject    handle to edit1 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of edit1 as text
%        str2double(get(hObject,'String')) returns contents of edit1 as a double

% --- Executes during object creation, after setting all properties.
function edit1_CreateFcn(hObject, eventdata, handles)
```

```
% hObject    handle to edit1 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end



function kilovolts_Callback(hObject, eventdata, handles)
% hObject    handle to kilovolts (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of kilovolts as text
%        str2double(get(hObject,'String')) returns contents of kilovolts as a double
voltaje=str2double(get(hObject,'String'));
botonlambda1=buscalambda2(voltaje);
botonlambda2=num2str(botonlambda1);
longitud=strcat(botonlambda2,' Angstroms');
set(handles.lambda8,'String',longitud);
handles.botonlambda1=botonlambda1;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
function kilovolts_CreateFcn(hObject, eventdata, handles)
% hObject    handle to kilovolts (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end



function parama2_Callback(hObject, eventdata, handles)
% hObject    handle to parama2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of parama2 as text
%        str2double(get(hObject,'String')) returns contents of parama2 as a double
```

```
parama3=str2double(get(hObject,'String'));
handles.parama3=parama3;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
function parama2_CreateFcn(hObject, eventdata, handles)
% hObject    handle to parama2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end



function paramb2_Callback(hObject, eventdata, handles)
% hObject    handle to paramb2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of paramb2 as text
%        str2double(get(hObject,'String')) returns contents of paramb2 as a double
paramb3=str2double(get(hObject,'String'));
handles.paramb3=paramb3;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
function paramb2_CreateFcn(hObject, eventdata, handles)
% hObject    handle to paramb2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end



function paramc2_Callback(hObject, eventdata, handles)
% hObject    handle to paramc2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)
```

```
% Hints: get(hObject,'String') returns contents of paramc2 as text
%        str2double(get(hObject,'String')) returns contents of paramc2 as a double
paramc3=str2double(get(hObject,'String'));
handles.paramc3=paramc3;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
function paramc2_CreateFcn(hObject, eventdata, handles)
% hObject    handle to paramc2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end



function alfa2_Callback(hObject, eventdata, handles)
% hObject    handle to alfa2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of alfa2 as text
%        str2double(get(hObject,'String')) returns contents of alfa2 as a double
alfa3=str2double(get(hObject,'String'));
handles.alfa3=alfa3;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
function alfa2_CreateFcn(hObject, eventdata, handles)
% hObject    handle to alfa2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end



function beta2_Callback(hObject, eventdata, handles)
% hObject    handle to beta2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
```

```
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of beta2 as text
%        str2double(get(hObject,'String')) returns contents of beta2 as a double
beta3=str2double(get(hObject,'String'));
handles.beta3=beta3;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
function beta2_CreateFcn(hObject, eventdata, handles)
% hObject    handle to beta2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function gamma2_Callback(hObject, eventdata, handles)
% hObject    handle to gamma2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of gamma2 as text
%        str2double(get(hObject,'String')) returns contents of gamma2 as a double
gamma3=str2double(get(hObject,'String'));
handles.gamma3=gamma3;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
function gamma2_CreateFcn(hObject, eventdata, handles)
% hObject    handle to gamma2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function roti2_Callback(hObject, eventdata, handles)
```

```
% hObject    handle to roti2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of roti2 as text
%        str2double(get(hObject,'String')) returns contents of roti2 as a double
roti3=str2double(get(hObject,'String'));
handles.roti3=roti3;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
function roti2_CreateFcn(hObject, eventdata, handles)
% hObject    handle to roti2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end



function rotj2_Callback(hObject, eventdata, handles)
% hObject    handle to rotj2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of rotj2 as text
%        str2double(get(hObject,'String')) returns contents of rotj2 as a double
rotj3=str2double(get(hObject,'String'));
handles.rotj3=rotj3;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
function rotj2_CreateFcn(hObject, eventdata, handles)
% hObject    handle to rotj2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end
```

```
function rotk2_Callback(hObject, eventdata, handles)
% hObject    handle to rotk2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of rotk2 as text
%        str2double(get(hObject,'String')) returns contents of rotk2 as a double
rotk3=str2double(get(hObject,'String'));
handles.rotk3=rotk3;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
function rotk2_CreateFcn(hObject, eventdata, handles)
% hObject    handle to rotk2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end



function teta2_Callback(hObject, eventdata, handles)
% hObject    handle to teta2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of teta2 as text
%        str2double(get(hObject,'String')) returns contents of teta2 as a double
teta3=str2double(get(hObject,'String'));
handles.teta3=teta3;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
function teta2_CreateFcn(hObject, eventdata, handles)
% hObject    handle to teta2 (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end
```

```
function tiltx_Callback(hObject, eventdata, handles)
% hObject    handle to tiltx (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of tiltx as text
%        str2double(get(hObject,'String')) returns contents of tiltx as a double
tiltx2=str2double(get(hObject,'String'));
handles.tiltx2=tiltx2;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
function tiltx_CreateFcn(hObject, eventdata, handles)
% hObject    handle to tiltx (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end



function tilty_Callback(hObject, eventdata, handles)
% hObject    handle to tilty (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of tilty as text
%        str2double(get(hObject,'String')) returns contents of tilty as a double
tilty2=str2double(get(hObject,'String'));
handles.tilty2=tilty2;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
function tilty_CreateFcn(hObject, eventdata, handles)
% hObject    handle to tilty (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
```

```
    set(hObject,'BackgroundColor','white');
end


% --- Executes on button press in tresd.
function tresd_Callback(hObject, eventdata, handles)
% hObject    handle to tresd (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)
botonparama=handles.parama3;
botonparamb=handles.paramb3;
botonparamc=handles.paramc3;
botonalfa=handles.alfa3;
botonbeta=handles.beta3;
botongamma=handles.gamma3;
cantidadesx=handles.celdosx2;
cantidadesy=handles.celdosy2;
cantidadesz=handles.celdosz2;
botonroti=handles.roti3;
botonrotj=handles.rotj3;
botonrotk=handles.rotk3;
botonteta=handles.teta3;
seleccion=handles.remplazotipo;
if isnan(botonparama)
    errordlg('El valor debe ser numerico','ERROR');
set(handles.parama3,'String',0);
end
if isnan(botonparamb)
errordlg('El valor debe ser numerico','ERROR');
set(handles.paramb3,'String',0);
end
if isnan(botonparamc)
errordlg('El valor debe ser numerico','ERROR');
set(handles.paramc3,'String',0);
end
if isnan(botonalfa)
errordlg('El valor debe ser numerico','ERROR');
set(handles.alfa3,'String',0);
end
if isnan(botonbeta)
errordlg('El valor debe ser numerico','ERROR');
set(handles.beta3,'String',0);
end
if isnan(botongamma)
errordlg('El valor debe ser numerico','ERROR');
set(handles.gamma3,'String',0);
end
if isnan(botonroti)
```

```
errordlg('El valor debe ser numerico','ERROR');
set(handles.roti3,'String',0);
end
if isnan(botonrotj)
errordlg('El valor debe ser numerico','ERROR');
set(handles.rotj3,'String',0);
end
if isnan(botonrotk)
errordlg('El valor debe ser numerico','ERROR');
set(handles.rotk3,'String',0);
end
if isnan(botonteta)
errordlg('El valor debe ser numerico','ERROR');
set(handles.teta3,'String',0);
end
if isnan(cantidadesx)
errordlg('El valor debe ser numerico','ERROR');
set(handles.celdosx2,'String',0);
end
if isnan(cantidadesy)
errordlg('El valor debe ser numerico','ERROR');
set(handles.celdosy2,'String',0);
end
if isnan(cantidadesz)
errordlg('El valor debe ser numerico','ERROR');
   set(handles.celdosz2,'String',0);
end
precaucion=cantidadesx*cantidadesy*cantidadesz;
if precaucion>999
   warndlg('la cantidad total de celdas no debe exceder las 999 particulas','tem20');
else
   %correcto
end
sublimitex=round(cantidadesx/2);
sublimitey=round(cantidadesy/2);
sublimitez=round(cantidadesz/2);
limitex=-sublimitex:1:sublimitex;
limitey=-sublimitey:1:sublimitey;
limitez=-sublimitez:1:sublimitez;
[X1,Y1,Z1]=meshgrid(limitex,limitey,limitez);
xos=X1(:);
yos=Y1(:);
zos=Z1(:);
textop='Primitiva (P)';
textoi='Interior (I)';
textob='Base (B)';
textof='Cara (F)';
paso1=strcmp(seleccion,textop);
```

```
paso2=strcmp(seleccion,textoi);
paso3=strcmp(seleccion,textob);
paso4=strcmp(seleccion,textof);
if paso1==1

[girx,giry,girz]=lattice2(botonparama,botonparamb,botonparamc,botonalfa,botonbeta,botongamma,xos
,yos,zos);
   cortes=limitez;
elseif paso2==1

[girx,giry,girz,cortado1]=inner(botonparama,botonparamb,botonparamc,cantidadesx,cantidadesy,cantid
adesz);
   cortes=cortado1;
elseif paso3==1

[girx,giry,girz,cortado2]=base(botonparama,botonparamb,botonparamc,cantidadesx,cantidadesy,cantid
adesz);
   cortes=cortado2;
elseif paso4==1

[girx,giry,girz,cortado3]=face(botonparama,botonparamb,botonparamc,cantidadesx,cantidadesy,cantida
desz);
   cortes=cortado3;
else

[girx,giry,girz]=lattice2(botonparama,botonparamb,botonparamc,botonalfa,botonbeta,botongamma,xos
,yos,zos);
   cortes=limitez;
end
handles.limite=cortes;
guidata(hObject,handles);
[a1,b1,c1]=rotativo(girx,giry,girz,botonroti,botonrotj,botonrotk,botonteta);
handles.a1=a1;
guidata(hObject,handles);
handles.b1=b1;
guidata(hObject,handles);
handles.c1=c1;
guidata(hObject,handles);
axes(handles.axes2);
scatter3(a1,b1,c1,'MarkerEdgeColor','k','MarkerFaceColor',[0 .75 .75]);
rotate3d on;

% --- Executes on button press in diffraction.
function diffraction_Callback(hObject, eventdata, handles)
% hObject    handle to diffraction (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)
tomadosa1=handles.a1;
```

```
tomadosb1=handles.b1;
tomadosc1=handles.c1;
periodico=handles.tipoelementales;
contrastex=handles.tiltx2;
contrastey=handles.tilty2;
brilloso=handles.brillo2;
if isnan(contrastex)
   errordlg('El valor debe ser numerico','ERROR');
set(handles.tiltx2,'String',0);
end
if isnan(contrastey)
errordlg('El valor debe ser numerico','ERROR');
set(handles.tilty2,'String',0);
end
if isnan(brilloso)
errordlg('El valor debe ser numerico','ERROR');
set(handles.brillo2,'String',0);
end
grosor=length(handles.limite);
potimpar=imparidad(grosor);
rebx=tomarebanada(tomadosa1,grosor,0);
reby=tomarebanada(tomadosb1,grosor,0);
maxim1=abs(rebx);
maxim2=max(maxim1);
solotam=placa4(rebx,reby,maxim2);
[orix,oriy]=size(solotam);
dumm=zeros(orix,oriy);
salto=handles.paramc3;
lambda16=handles.botonlambda1;
ronda=0;
capa=1;
disp('grosor');
disp(grosor);
while ronda<grosor
rebanadax=tomarebanada(tomadosa1,grosor,ronda);
   rebanaday=tomarebanada(tomadosb1,grosor,ronda);
   placon=placa4(rebanadax,rebanaday,maxim2);
   [sM,sN]=size(placon);
   [propagador,dx3,dy3,x3,y3]=fresnelnu(placon,sM,sN,contrastex,contrastey,salto,lambda16);
   [f,g]=size(propagador);
   proyecciones=potencialproyectado10(potimpar,1,periodico,lambda16,f,g,brilloso);
   proyecciones2=relleno(dumm,proyecciones);
   propagador2=relleno(dumm,propagador);
   capa=capa*proyecciones2;
        roda=conv2(capa,propagador2);
   ronda=ronda+1;
end
handles.roda=roda;
```

```
guidata(hObject,handles);
imagen3=fft2(roda);
imagen4=abs(imagen3);
imagen5=mat2gray(imagen4);
axes(handles.axes1);
[altitud2,longitud2]=size(imagen5);
noleyend1=altitud2-16;
hold on;
imshow(imagen5);
[escx1,escy1,escx2,escy2,escala1]=leyenda(handles.parama3,handles.paramb3,handles.paramc3,handle
s.alfa3,handles.beta3,handles.gamma3,'fase',altitud2);
line([escx1,escx2],[escy1,escy2],'Color','r','LineWidth',2);
text(10,noleyend1,escala1,'FontSize',6,'Color','red');
hold off;
% --- Executes on button press in inversa.
function inversa_Callback(hObject, eventdata, handles)
% hObject    handle to inversa (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)
ronda2=0;
grosor2=length(handles.limite);
tomadosa2=handles.a1;
tomadosb2=handles.b1;
lambda20=handles.botonlambda1;
nuroda=handles.roda;
recxx3=tomarebanada(tomadosa2,grosor2,0);
recyy3=tomarebanada(tomadosb2,grosor2,0);
maxim3=abs(recxx3);
maxim4=max(maxim3);
while ronda2<grosor2
rebanadax2=tomarebanada(tomadosa2,grosor2,ronda2);
   rebanaday2=tomarebanada(tomadosb2,grosor2,ronda2);
   placon2=placa4(rebanadax2,rebanaday2,maxim4);
   opticot2=tretorno(placon2,1.2,lambda20,4);
   [paramix,paramiy]=size(nuroda);
   opticot3=zeros(paramix,paramiy);
   opticot4=relleno(opticot3,opticot2);
   ina2=nuroda.*opticot4;
   nunina2=abs(ina2);
   ronda2=ronda2+1;
end
[largox2,largoy2]=size(nunina2);
[datos,losx,losy]=realintensa(nunina2);
axes(handles.axes3);
imagendifuminada=difuminado(datos,losx,losy,largox2,largoy2);
[altitud,longitud]=size(imagendifuminada);
noleyend2=altitud-16;
hold on;
```

```
imshow(imagendifuminada);
[escx3,escy3,escx4,escy4,escala2]=leyenda(handles.parama3,handles.paramb3,handles.paramc3,handle
s.alfa3,handles.beta3,handles.gamma3,'real',altitud);
line([escx3,escx4],[escy3,escy4],'Color','r','LineWidth',2);
text(10,noleyend2,escala2,'FontSize',6,'Color','red');
hold off;

% --- Executes on button press in pdb.
function pdb_Callback(hObject, eventdata, handles)
% hObject    handle to pdb (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)
tomadosa3=handles.a1;
tomadosb3=handles.b1;
tomadosc3=handles.c1;
periodico4=handles.tipoelementales;
largopdb=length(tomadosa3);
indexo.outfile='estructura1.pdb';
indexo.recordName='ATOM';
indexo.X=tomadosa3;
indexo.Y=tomadosb3;
indexo.Z=tomadosc3;
preatomo=cell(1,largopdb);
preatomo(1:largopdb)=periodico4;
indexo.atomName=preatomo;
mat2PDB(indexo);

% --- Executes on button press in guardaimagen.
function guardaimagen_Callback(hObject, eventdata, handles)
% hObject    handle to guardaimagen (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)
posado=handles.roda;
imagen6=fft2(posado);
imagen7=abs(imagen6);
imagen8=mat2gray(imagen7);
guardaimagen(imagen8,'difractograma01.png','png');



function celdosx_Callback(hObject, eventdata, handles)
% hObject    handle to celdosx (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of celdosx as text
%        str2double(get(hObject,'String')) returns contents of celdosx as a double
celdosx2=str2double(get(hObject,'String'));
```

```
handles.celdosx2=celdosx2;
guidata(hObject,handles);


% --- Executes during object creation, after setting all properties.
function celdosx_CreateFcn(hObject, eventdata, handles)
% hObject    handle to celdosx (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end



function celdosy_Callback(hObject, eventdata, handles)
% hObject    handle to celdosy (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of celdosy as text
%        str2double(get(hObject,'String')) returns contents of celdosy as a double
celdosy2=str2double(get(hObject,'String'));
handles.celdosy2=celdosy2;
guidata(hObject,handles);


% --- Executes during object creation, after setting all properties.
function celdosy_CreateFcn(hObject, eventdata, handles)
% hObject    handle to celdosy (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end



function celdosz_Callback(hObject, eventdata, handles)
% hObject    handle to celdosz (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)
```

```
% Hints: get(hObject,'String') returns contents of celdosz as text
%        str2double(get(hObject,'String')) returns contents of celdosz as a double
celdosz2=str2double(get(hObject,'String'));
handles.celdosz2=celdosz2;
guidata(hObject,handles);


% --- Executes during object creation, after setting all properties.
function celdosz_CreateFcn(hObject, eventdata, handles)
% hObject    handle to celdosz (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
   set(hObject,'BackgroundColor','white');
end


% --- Executes on button press in ayuda.
function ayuda_Callback(hObject, eventdata, handles)
% hObject    handle to ayuda (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)
helpdlg({'Para no rotar  la figura colocar en i j k:',' [1 1 1] y en theta 0 ;','Valores default:','Ajuste x:
0.8','Ajuste y:0.8','Brillo Diff: 10 a 15 (mayor Z requiere mas brillo)'},'tem20');



function brillo_Callback(hObject, eventdata, handles)
% hObject    handle to brillo (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of brillo as text
%        str2double(get(hObject,'String')) returns contents of brillo as a double
brillo2=str2double(get(hObject,'String'));
handles.brillo2=brillo2;
guidata(hObject,handles);

% --- Executes during object creation, after setting all properties.
function brillo_CreateFcn(hObject, eventdata, handles)
% hObject    handle to brillo (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns called
```

```
% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'), get(0,'defaultUicontrolBackgroundColor'))
set(hObject,'BackgroundColor','white');
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function rebanada=tomarebanada(vector,placas,indice)
rebanada=[];
largotot=length(vector);
division=largotot/placas;
salto=division*indice;
        for bom=1:division
                rebanada(bom)=vector(salto+bom);
        end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function tregresas=tretorno(prebase,cs1,lambda1,defocus1)
cambio=xaberrada(cs1,lambda1,defocus1);
tregresas=prebase.*exp(-2*pi*1i*cambio);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function nux=xaberrada(cs,lambda,defocus)
u=(2*pi)/lambda;
%resolucion es dada en Angstrom
udoble=u.^2;
ucuarta=u.^4;
primero=0.5*pi*ucuarta*cs*lambda.^3;
segundo=pi*defocus*lambda*udoble;
nux=primero+segundo;
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

function apdb(nombrearchivo,elemento,xcoords,ycoords,zcoords)

fid = fopen(nombrearchivo,'w');

laroga=length(zcoords);

tipo='ATOM';

ocupancia='1.000';

miriad=1;

        while miriad<(laroga+1)

                fprintf(fid,'%s  %d   %s           %3.3f  %3.3f  %3.3f
```

```
%s\n',tipo{:},miriad,elemento{:},xcoords(miriad),ycoords(miriad),zcoords(miriad),ocupancia{:});
                miriad=miriad+1;
        end
        fclose(fid);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function apdb2(nombrearchivo,elemento,xcoords,ycoords,zcoords)
   largogen=length(xcoords);
   elementales=[];
   %atom=[];
%ocupado=[];
   for replica=1:largogen
      elementales=[elementales,elemento];
      %atom=[atom,'ATOM'];
      %ocupado=[ocupado,'1.000'];
end
   fid=fopen(nombrearchivo,'wt');
        for pro=1:largogen
                tablon={'ATOM' pro elementales(pro) xcoords(pro) ycoords(pro) zcoords(pro) '1.000'};
                formatSpec='%s  %d   %s              %3.3f  %3.3f  %3.3f    %s\n';
                fprintf(fid,formatSpec,tablon);
        end
   fclose(fid);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [cox,coy,coz,indice]=base(ba,bb,bc,l,m,n)
        N = l*m*n;
        [x,y,z] = meshgrid(1:l,1:m,1:n);
        p(1:N,1) = x(:);  p(N+1:2*N,1) = x(:)+0.5;
        p(1:N,2) = y(:);  p(N+1:2*N,2) = y(:)+0.5;
```

```
            p(1:N,3) = z(:);  p(N+1:2*N,3) = z(:);
            Xcoord = p(:,1);
            Ycoord = p(:,2);
            Zcoord = p(:,3);
            indice=unique(Zcoord);
            cox=[];
            coy=[];
            coz=[];
            for doc=1:length(indice)
voy=indice(doc);
        for interno=1:(2*N)
            if voy==Zcoord(interno)
                cox=[cox,ba*Xcoord(interno)];
                coy=[coy,bb*Ycoord(interno)];
                coz=[coz,bc*Zcoord(interno)];
            end
        end
end
end%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%
function nulambda=buscalambda2(volts)
h=6.62606957e-34;
emass=9.10938291e-31;
luz=299792458;
cdos=luz*luz;
cargaelemental=1.60217657e-19;
subter=(cargaelemental*volts)/(2*emass*cdos);
termino1=h/sqrt(2*emass*cargaelemental*volts);
termino2=1/sqrt(1+subter);
nulambda=termino1*termino2;
end
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

function regreso=difuminado(datos,posex,posey,largox,largoy)
%si se modifica a tamano variable la ventana cambiar bases por:
%bases=ones(largox,largoy);
mitadesx=round(largox/4);
mitadesy=round(largoy/4);
bases=ones(largox,largoy);
%multiplico por el gris
regreso=0.4375*bases;
%se saca porcentaje
%nos da el porcentaje
unidadcolor=(1-0.4375)/100;
%maximo total de los puntos 50 pixeles
radioreal=5;
%se elaboran los circulos
contados=1;
totaldato=length(datos);
   while contados<(totaldato+1)
      radion=radioreal;
      %colorado=0.4375-unidadcolor;
      colorado=1-unidadcolor;
      centroidex=posex(contados);
      centroidey=posey(contados);
      %se hace el centro
      regreso(centroidex,centroidey)=colorado;
      %se precolocan los circulos
      rango=colorado-0.4375;
      %exteriores
      radioext=round(radion);
      inicio=2;
      origencolor=colorado;
      tomado=(colorado-0.4375)/radioext;
      while inicio<radioext
         origencolor=origencolor-tomado;
         %se colocan los circulos
         corte=1/radioreal;
         paso=0;
         limitado=2*pi;
         while paso<limitado
            xpos=round(centroidex+(inicio*cos(paso)));
            ypos=round(centroidey+(inicio*sin(paso)));
            regreso(xpos,ypos)=origencolor;
            paso=paso+corte;
end
         inicio=inicio+1;
```

```
        end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [fox,foy,foz,indice]=face(fa,fb,fc,l,m,n)
            N = l*m*n;
            [x,y,z] = meshgrid(1:l,1:m,1:n);
            p(1:N,1) = x(:);  p(N+1:2*N,1) = x(:)+0.5;  p(2*N+1:3*N,1) = x(:)+0.5;  p(3*N+1:4*N,1) =
x(:);
            p(1:N,2) = y(:);  p(N+1:2*N,2) = y(:)+0.5;  p(2*N+1:3*N,2) = y(:);  p(3*N+1:4*N,2) =
y(:)+0.5;
            p(1:N,3) = z(:);  p(N+1:2*N,3) = z(:);  p(2*N+1:3*N,3) = z(:)+0.5;  p(3*N+1:4*N,3) = z(:)+0.5;
            Xcoord = p(:,1);
            Ycoord = p(:,2);
            Zcoord = p(:,3);
            indice=unique(Zcoord);
            fox=[];
            foy=[];
            foz=[];
            for doc=1:length(indice)
voy=indice(doc);
        for interno=1:(2*N)
if voy==Zcoord(interno)
                fox=[fox,fa*Xcoord(interno)];
                foy=[foy,fb*Ycoord(interno)];
                foz=[foz,fc*Zcoord(interno)];
            end
        end
    end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

```
function [f1,dx1,dy1,x1,y1]= fresnelnu(f0, M, N, dx0, dy0, z, lambda)
k=2*pi/lambda;
   x0=ones(N,1)*[-M/2:M/2-1]*dx0;
   y0=[-N/2:N/2-1]'*ones(1,M)*dy0;
   g=f0.*exp(j*0.5*k*(x0.^2+y0.^2)/z);
G=fftshift(fft2(g));
   du=1./(M*dx0);
dv=1./(N*dy0);
   dx1=lambda*z*du;
   dy1=lambda*z*dv;
   x1=ones(N,1)*[-M/2:M/2-1]*dx1;
   y1=[-N/2:N/2-1]'*ones(1,M)*dy1;
f1=G.*exp(i*0.5*k*(x1.^2+y1.^2)/z);
   f1=f1./(lambda*z);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function guardaimagen(matriz,nombre,formatosrec)
imwrite(matriz,nombre,formatosrec);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function correcto=imparidad(numero)
comen=mod(numero,2);
        if comen==0
                correcto=numero;
        else
                correcto=numero+1;
        end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

```
function [iox,ioy,ioz,indice]=inner(ia,ib,ic,l,m,n)
        N = l*m*n;
        [x,y,z] = meshgrid(1:l,1:m,1:n);
        p(1:N,1) = x(:);  p(N+1:2*N,1) = x(:)+0.5;
        p(1:N,2) = y(:);  p(N+1:2*N,2) = y(:)+0.5;
        p(1:N,3) = z(:);  p(N+1:2*N,3) = z(:)+0.5;
        Xcoord = p(:,1);
        Ycoord = p(:,2);
        Zcoord = p(:,3);
        indice=unique(Zcoord);
        iox=[];
        ioy=[];
        ioz=[];
        for doc=1:length(indice)
voy=indice(doc);
      for interno=1:(2*N)
if voy==Zcoord(interno)
           iox=[iox,ia*Xcoord(interno)];
           ioy=[ioy,ib*Ycoord(interno)];
           ioz=[ioz,ic*Zcoord(interno)];
        end
      end
   end
end%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%
function [bas1,bas2,bas3]=lattice2(aa,bb,cc,alfie,betie,gammie,corex,corey,corez)
alti5=deg2rad(alfie);
beti5=deg2rad(betie);
gati5=deg2rad(gammie);
doblealfa=cos(alti5).^2;
doblebeta=cos(beti5).^2;
```

```
doblegamma=cos(gati5).^2;
prevol1=aa*bb*cc;
prevol2=2*cos(alti5)*cos(beti5)*cos(gati5);
vol=prevol1*sqrt(1-doblealfa-doblebeta-doblegamma+prevol2);
a11=aa;
a12=bb*cos(gati5);
a13=cc*cos(beti5);
a21=0;
a22=bb*sin(gati5);
a23=cc*((cos(alti5)-cos(beti5)*cos(gati5))/sin(gati5));
a31=0;
a32=0;
a33=vol/(aa*bb*sin(gati5));
bas1=(corex*a11)+(corey*a12)+(corez*a13);
bas2=(corex*a21)+(corey*a22)+(corez*a23);
bas3=(corex*a31)+(corey*a32)+(corez*a33);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [leyx1,leyy1,leyx2,leyy2,leytext]=leyenda(pa,pb,pc,anga,angb,angg,tipo,alto)
    if tipo=='fase'
        anga4=degtorad(anga);
        angb4=degtorad(angb);
        angg4=degtorad(angg);
        coscuada=cos(anga4)*cos(anga4);
        coscuadb=cos(angb4)*cos(angb4);
        coscuadg=cos(angg4)*cos(angg4);
        parte1v=pa*pb*pc;
        parte2v=1-coscuada-coscuadb-coscuadg;

    parte3v=(2*cos(anga4)*cos(angb4))+(2*cos(anga4)*cos(angg4))+(2*cos(angb4)*cos(angg4));
        parte4v=parte2v+parte3v;
```

```
            parte5v=sqrt(parte4v);
            volumen=parte1v*parte5v;
            arecip=(pb*pc*sin(anga4))/volumen;
            leytext=[num2str(arecip),' A-1'];
        else
            leytext=[num2str(pa),' A'];
        end
        leyy1=alto-22;
        leyy2=alto-22;
        leyx1=10;
        leyx2=leyx1+pa;
end%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%
%% -- mat2PDB.m --
%
% this function creates a PDB from coordinate data. Represent all inputs as
% a structure field for it to be read. The output format is as given in
% online documentation (as of July 2012 when writing this program)
% http://www.wwpdb.org/documentation/format33/sect9.html#ATOM
%
% Make sure all data input is one-dimensional with the same length. If
% they are not the same length, the program ignores user input, states
% an error, and uses defaults. All string inputs should be in cell-format.
% Keep in mind the "element" and "charge" inputs are strings in
% cell-format, not numbers.
%
%
% -- required inputs (3) --
%
% input value       meaning
%
```

```
% input.X            orthagonal X coordinate data (angstroms)
% input.Y            orthagonal Y coordinate data (angstroms)
% input.Z            orthagonal Z coordinate data (angstroms)
%
% -- optional inputs (12): generates defaults when not user-specified --
%
% input value        meaning                          default value
%
% input.outfile      output file name                 "mat2PDB.pdb"
% input.recordName   output record name of atoms      "ATOM"
% input.atomNum      atom serial number               sequential number
% input.atomName     name of atoms                    "OW" (water oxygen)
% input.altLoc       alt. location indicator          " "
% input.resName      name of residue                  "SOL" (water)
%
% input.chainID      protein chain identifier         "A"
% input.resNum       residue sequence number          sequential number
% input.occupancy    occupancy factor                 "1.00"
% input.betaFactor   beta factor, temperature         "0.00"
% input.element      element symbol                   "O" (oxygen)
% input.charge       atomic charge                    " "
%
%
% -- example uses --
%
% % translates both X and Y coordinates of 3IJU.pdb by 5 angstroms
% PDBdata = pdb2mat('3IJU.pdb');
% PDBdata.X = PDBdata.X + 5;
% PDBdata.Y = PDBdata.Y + 5;
% mat2pdb(PDBdata)
%
% % make a PDB with 30 atoms in random places within a 10 angstrom box
```

```
% data.X = rand(1,20)*10;
% data.Y = rand(1,20)*10;
% data.Z = rand(1,20)*10;
% mat2pdb(data)
%
%

function mat2pdb(input)
	%% review XYZ coordinate data

	% coordinate data is required! Checking XYZ input
	if ~isfield(input, 'X') || ~isfield(input, 'Y') || ~isfield(input, 'Z')
		fprintf('we need xyz coordinate data to make a PDB!!\n\texiting...\n');
		return;
	end
	X = input.X;
	Y = input.Y;
	Z = input.Z;
	if length(X) ~= length(Y) || length(X) ~= length(Z)
		fprintf('xyz coordinate data is not of equal lengths!\n\texiting...\n');
		return;
	end

	%% review optional data inputs

	% in case optional data data not given, fill in blanks
	if ~isfield(input, 'outfile')
		input.outfile = 'mat2PDB.pdb';
	end
	if ~isfield(input, 'recordName')
		input.recordName = cell(1,length(X));
		input.recordName(1:end) = {'ATOM'};
```

```
end
if ~isfield(input, 'atomNum')
        input.atomNum = 1:length(X);
end
if ~isfield(input, 'atomName')
        input.atomName = cell(1,length(X));
        input.atomName(1:end) = {'OW'};
end
if ~isfield(input, 'altLoc')
        input.altLoc = cell(1,length(X));
        input.altLoc(1:end) = {' '};
end
if ~isfield(input, 'resName')
        input.resName = cell(1,length(X));
        input.resName(1:end) = {'   '};%iba SOL
end
if ~isfield(input, 'chainID')
        input.chainID = cell(1,length(X));
        input.chainID(1:end) = {' '};%iba A
end
if ~isfield(input, 'resNum')
        input.resNum = 1:length(X);
end
if ~isfield(input, 'occupancy')
        input.occupancy = ones(1,length(X));
end
if ~isfield(input, 'betaFactor')
        input.betaFactor = zeros(1, length(X));
end
if ~isfield(input, 'element')
        input.element = cell(1,length(X));
        input.element(1:end) = {'O'};
```

```
end
if ~isfield(input, 'charge')
        input.charge = cell(1,length(X));
        input.charge(1:end) = {' '};
end

outfile    = input.outfile;
recordName = input.recordName;
atomNum    = input.atomNum;
atomName   = input.atomName;
altLoc     = input.altLoc;
resName    = input.resName;
chainID    = input.chainID;
resNum     = input.resNum;
occupancy  = input.occupancy;
betaFactor = input.betaFactor;
element    = input.element;
charge     = input.charge;

%% remove faulty inputs

if length(recordName) ~= length(X)
        fprintf('recordName input is not the correct length!\n\tignoring user input\n');
        recordName = cell(1,length(X));
        recordName(1:end) = {'ATOM'};
end
if length(atomNum) ~= length(X)
        fprintf('atom serial number input is not the correct length!\n\tignoring user input\n');
        atomNum = 1:length(X);
end
if length(atomName) ~= length(X)
        fprintf('atom name input is not the correct length!\n\tignoring user input\n');
```

```
        atomName = cell(1,length(X));
        atomName(1:end) = {'OW'};
end
if length(altLoc) ~= length(X)
        fprintf('alternate location input is not the correct length!\n\tignoring user input\n');
        altLoc = cell(1,length(X));
        altLoc(1:end) = {' '};
end
if length(resName) ~= length(X)
        fprintf('residue name input is not the correct length!\n\tignoring user input\n');
        resName = cell(1,length(X));
        resName(1:end) = {'   '};%iba SOL
end
if length(chainID) ~= length(X)
        fprintf('chain ID input is not the correct length!\n\tignoring user input\n');
        chainID = cell(1,length(X));
        chainID(1:end) = {' '};% iba A
end
if length(resNum) ~= length(X)
        fprintf('residue number input is not the correct length!\n\tignoring user input\n');
        resNum = 1:length(X);
end
if length(occupancy) ~= length(X)
        fprintf('occupancy input is not the correct length!\n\tignoring user input\n');
        occupancy = ones(1,length(X));
end
if length(betaFactor) ~= length(X)
        fprintf('beta factor input is not the correct length!\n\tignoring user input\n');
        betaFactor = zeros(1, length(X));
end
if length(element) ~= length(X)
        fprintf('element symbol input is not the correct length!\n\tignoring user input\n');
```

```
        element = cell(1,length(X));
        element(1:end) = {'O'};
    end
    if length(charge) ~= length(X)
        fprintf('charge input is not the correct length!\n\tignoring user input\n');
        charge = cell(1,length(X));
        charge(1:end) = {' '};
    end

    % fix atomName spacing
    for n = 1:length(atomName)
        atomName(n) = {sprintf('%-3s',cell2mat(atomName(n)))};
    end


    %% create PDB

    % open file
    fprintf('outputting PDB in file %s\n', outfile);
    FILE = fopen(outfile, 'w');

    % output data
    for n = 1:length(atomNum)

        % standard PDB output line
        fprintf( FILE, '%-6s%5u%5s%1.1s%3s
%1.1s%4u%12.3f%8.3f%8.3f%6.2f%6.2f%12s%2s\n', ...
        cell2mat(recordName(n)), atomNum(n), cell2mat(atomName(n)), ...
        cell2mat(altLoc(n)), cell2mat(resName(n)), cell2mat(chainID(n)), ...
        resNum(n), X(n), Y(n), Z(n), occupancy(n), betaFactor(n), ...
        cell2mat(element(n)), cell2mat(charge(n)));
```

```
		% output progress in terminal
		if ~mod(n,400)
			fprintf('   %6.2f%%', 100*n / length(atomNum));
		if ~mod(n, 4000)
			fprintf('\n');
		end
		end

	end
	fprintf( FILE, 'END\n');

	% close file
	fprintf('   %6.2f%%\n    done! closing file...\n', 100);

	fclose(FILE);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function imagen4=placa4(xv,yv,maxima)
eltotal=round(maxima*4);
centro=floor(eltotal/2);
base=zeros(eltotal,eltotal);
redonx=round(xv);
redony=round(yv);
larg=length(yv);
	for dato=1:larg
		posx=centro+redonx(dato);
		posy=centro+redony(dato);
		base(posx,posy)=1;
	end
	imagen4=mat2gray(base);
end
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function estructura=potencialatomico(atomosdim,tipo)
[ya1,yb1,ya2,yb2,ya3,yb3,ya4,yb4,ya5,yb5]=tablascater5(tipo);
constanteplanck=6.626068e-34;
planck2=constanteplanck.^2;
masaelectron=9.10938188e-31;
cargaelemental=1.60217646e-19;
angstrom=0.1;
volt=1;
cuadradoangs=angstrom.^2;
prea1=(masaelectron*cargaelemental)/(cuadradoangs*volt);
prea2=(4*sqrt(pi)*planck2)/prea1;
preb=4*pi.^2;
%se llena el vector
muba1=prea2*yb1.^-1.5;
muba2=prea2*yb2.^-1.5;
muba3=prea2*yb3.^-1.5;
muba4=prea2*yb4.^-1.5;
muba5=prea2*yb5.^-1.5;
mubb1=preb/yb1;
mubb2=preb/yb2;
mubb3=preb/yb3;
mubb4=preb/yb4;
mubb5=preb/yb5;
mus=1;
%se llena el u2
limo=atomosdim/2;
        for k=-limo:limo
                for j=-limo:limo
                        for i=-limo:limo
                                u2=k.^2+j.^2+i.^2;
```

```
                    vas1=muba1*exp(-mubb1*u2);
                    vas2=muba2*exp(-mubb2*u2);
                    vas3=muba3*exp(-mubb3*u2);
                    vas4=muba4*exp(-mubb4*u2);
                    vas5=muba5*exp(-mubb5*u2);
                    vasil=vas1+vas2+vas3+vas4+vas5;
                    estructura(mus).x=i;
                    estructura(mus).y=j;
                    estructura(mus).z=k;
                    estructura(mus).vp=vasil;
                    mus=mus+1;
                end
            end
        end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function nuevopoti=potencialproyectado10(largoxyz,zi,tipode,lambda13,mx,ny,brillos)
%se genera estructura
estructurado=potencialatomico(largoxyz,tipode);
segundamul=rointeraccion(lambda13);
nuevopoti=zeros(mx,ny);
misx=mx/2;
misy=ny/2;
mosi=length(estructurado);
base=1;
while base<mosi
        if estructurado(base).z==zi
            dofx=estructurado(base).x;
            dofy=estructurado(base).y;
            mors=exp(-1i*segundamul*brillos*estructurado(base).vp);
suex=round(misx+dofx);
```

```
        suey=round(misy+dofy);
                nuevopoti(suex,suey)=mors;
            end
            base=base+1;
end%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%
function [vreal,xcoor,ycoor]=realintensa(matriz)
[ex,ey]=find(matriz);
vali=[];
lorga=length(ex);
%
raudo=1;
            while raudo<(lorga+1)
                nuxi=ex(raudo);
                nuyi=ey(raudo);
                valores=matriz(nuxi,nuyi);
                vali=[vali,valores];
                raudo=raudo+1;
            end
            xcoor=ex;
            ycoor=ey;
            maxi=max(vali);
            vreal=(vali*1)/maxi;
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function nuimagen=relleno(Base,inserta)
[m,n]=size(Base);
basex=floor(m/2)-floor(size(inserta,1)/2);
basey=floor(n/2)-floor(size(inserta,2)/2);
%voy aqui
```

```
nuimagen=Base;
for u=1:size(inserta,1)
        for v=1:size(inserta,2)
                nuimagen(basex+u,basey+v)=inserta(u,v);
        end
end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function interactivo=rointeraccion(lambda12)
masivo=9.10938188e-31;
planck=6.626068e-34;
planckdos=planck.^2;
interactivo=(2*pi*masivo*lambda12)/planckdos;
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [rotitax,rotitay,rotitaz]=rotativo(vectorx,vectory,vectorz,x,y,z,angulo)
rotitax=[];
rotitay=[];
rotitaz=[];
angulo2=deg2rad(angulo);
elev=(x*x)+(y*y)+(z*z);
k=1/(sqrt(elev));
x2=x*k;
y2=y*k;
z2=z*k;
cs=cos(angulo2);
sn=sin(angulo2);
cord1=cs+(x2*x2*(1-cs));
cord2=(x2*y2*(1-cs))-(z2*sn);
cord3=(x2*z2*(1-cs))+(y2*sn);
```

```
cord4=(x2*y2*(1-cs))+(z2*sn);
cord5=cs+(y2*y2*(1-cs));
cord6=(y2*z2*(1-cs))-(x2*sn);
cord7=(x2*z2*(1-cs))-(y2*sn);
cord8=(y2*z2*(1-cs))+(x2*sn);
cord9=cs+(z2*z2*(1-cs));
roto=[cord1 cord2 cord3; cord4 cord5 cord6; cord7 cord8 cord9];
largos=length(vectorx);
rotx=0;
roty=0;
rotz=0;
montado=1;
  while montado<(largos+1)
    rotx=vectorx(montado);
    roty=vectory(montado);
    rotz=vectorz(montado);
    prevos=[rotx 0 0;0 roty 0;0 0 rotz];
    rotita=roto*prevos;
    prex=rotita(1,1)+rotita(1,2)+rotita(1,3);
      prey=rotita(2,1)+rotita(2,2)+rotita(2,3);
      prez=rotita(3,1)+rotita(3,2)+rotita(3,3);
      rotitax=[rotitax,prex];
      rotitay=[rotitay,prey];
      rotitaz=[rotitaz,prez];
    montado=montado+1;
end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [ga1,gb1,ga2,gb2,ga3,gb3,ga4,gb4,ga5,gb5]=tablascater5(elemental)
tablon(1).elemento='H';
tablon(1).a1=0.1671;
```

```
tablon(1).a2=0.2563;
tablon(1).a3=0.0393;
tablon(1).a4=0.0596;
tablon(1).a5=0.0078;
tablon(1).b1=6.0583;
tablon(1).b2=20.3093;
tablon(1).b3=70.2973;
tablon(1).b4=1.3067;
tablon(1).b5=0.0102;
tablon(2).elemento='He';
tablon(2).a1=0.1227;
tablon(2).a2=0.1579;
tablon(2).a3=0.0089;
tablon(2).a4=0.0926;
tablon(2).a5=0.0358;
tablon(2).b1=14.1248;
tablon(2).b2=5.0260;
tablon(2).b3=36.9356;
tablon(2).b4=1.6644;
tablon(2).b5=0.2832;
tablon(3).elemento='Li';
tablon(3).a1=0.7762;
tablon(3).a2=0.0644;
tablon(3).a3=0.2118;
tablon(3).a4=1.0882;
tablon(3).a5=1.1218;
tablon(3).b1=16.2591;
tablon(3).b2=0.3254;
tablon(3).b3=2.5832;
tablon(3).b4=85.6315;
tablon(3).b5=80.5508;
tablon(4).elemento='Be';
```

```
tablon(4).a1=0.0197;
tablon(4).a2=1.5392;
tablon(4).a3=0.2990;
tablon(4).a4=0.1283;
tablon(4).a5=1.0548;
tablon(4).b1=0.0243;
tablon(4).b2=52.2488;
tablon(4).b3=4.1219;
tablon(4).b4=0.8202;
tablon(4).b5=15.6590;
tablon(5).elemento='B';
tablon(5).a1=0.4441;
tablon(5).a2=0.0720;
tablon(5).a3=1.1248;
tablon(5).a4=0.9794;
tablon(5).a5=0.1695;
tablon(5).b1=5.2074;
tablon(5).b2=0.2374;
tablon(5).b3=15.0436;
tablon(5).b4=44.6563;
tablon(5).b5=1.4821;
tablon(6).elemento='C';
tablon(6).a1=1.0392;
tablon(6).a2=0.5255;
tablon(6).a3=0.2246;
tablon(6).a4=0.0861;
tablon(6).a5=0.6326;
tablon(6).b1=15.4799;
tablon(6).b2=42.5178;
tablon(6).b3=1.5692;
tablon(6).b4=0.2390;
tablon(6).b5=5.5375;
```

```
tablon(7).elemento='N';
tablon(7).a1=0.9271;
tablon(7).a2=0.4702;
tablon(7).a3=0.0611;
tablon(7).a4=0.5487;
tablon(7).a5=0.2047;
tablon(7).b1=11.0027;
tablon(7).b2=32.1051;
tablon(7).b3=0.1308;
tablon(7).b4=3.8783;
tablon(7).b5=1.0445;
tablon(8).elemento='O';
tablon(8).a1=0.7118;
tablon(8).a2=0.2561;
tablon(8).a3=0.6403;
tablon(8).a4=0.2767;
tablon(8).a5=0.0983;
tablon(8).b1=11.5989;
tablon(8).b2=29.7811;
tablon(8).b3=4.4138;
tablon(8).b4=1.3555;
tablon(8).b5=0.2103;
tablon(9).elemento='F';
tablon(9).a1=0.2917;
tablon(9).a2=0.6223;
tablon(9).a3=0.6257;
tablon(9).a4=0.1632;
tablon(9).a5=0.0983;
tablon(9).b1=1.2215;
tablon(9).b2=10.6435;
tablon(9).b3=3.9383;
tablon(9).b4=27.6191;
```

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tablon(9).b5=0.1846;
tablon(10).elemento='Ne';
tablon(10).a1=0.1250;
tablon(10).a2=0.1644;
tablon(10).a3=0.4632;
tablon(10).a4=0.5452;
tablon(10).a5=0.3541;
tablon(10).b1=0.2162;
tablon(10).b2=22.1640;
tablon(10).b3=9.1228;
tablon(10).b4=3.9942;
tablon(10).b5=1.3653;
tablon(11).elemento='Na';
tablon(11).a1=1.0417;
tablon(11).a2=0.6892;
tablon(11).a3=0.1996;
tablon(11).a4=1.2693;
tablon(11).a5=1.5679;
tablon(11).b1=12.4203;
tablon(11).b2=2.1683;
tablon(11).b3=0.3158;
tablon(11).b4=131.093;
tablon(11).b5=62.9926;
tablon(12).elemento='Mg';
tablon(12).a1=0.6946;
tablon(12).a2=0.1704;
tablon(12).a3=2.0512;
tablon(12).a4=1.8009;
tablon(12).a5=0.4841;
tablon(12).b1=5.5229;
tablon(12).b2=0.2462;
tablon(12).b3=77.5613;
```

```
tablon(12).b4=24.3472;
tablon(12).b5=1.5433;
tablon(13).elemento='Al';
tablon(13).a1=0.5217;
tablon(13).a2=0.1944;
tablon(13).a3=0.7933;
tablon(13).a4=2.4057;
tablon(13).a5=1.9661;
tablon(13).b1=1.6064;
tablon(13).b2=0.2596;
tablon(13).b3=6.3070;
tablon(13).b4=24.1637;
tablon(13).b5=78.1749;
tablon(14).elemento='Si';
tablon(14).a1=1.8563;
tablon(14).a2=0.8424;
tablon(14).a3=0.4860;
tablon(14).a4=2.4408;
tablon(14).a5=0.1954;
tablon(14).b1=61.6656;
tablon(14).b2=5.6894;
tablon(14).b3=1.4450;
tablon(14).b4=19.8377;
tablon(14).b5=0.2430;
tablon(15).elemento='P';
tablon(15).a1=2.2615;
tablon(15).a2=1.8096;
tablon(15).a3=0.4399;
tablon(15).a4=0.7882;
tablon(15).a5=0.1817;
tablon(15).b1=15.0540;
tablon(15).b2=45.2182;
```

```
tablon(15).b3=1.2297;
tablon(15).b4=4.6428;
tablon(15).b5=0.2100;
tablon(16).elemento='S';
tablon(16).a1=1.0234;
tablon(16).a2=1.2139;
tablon(16).a3=0.4932;
tablon(16).a4=2.1986;
tablon(16).a5=0.2293;
tablon(16).b1=5.5511;
tablon(16).b2=41.8781;
tablon(16).b3=1.4617;
tablon(16).b4=15.4568;
tablon(16).b5=0.2477;
tablon(17).elemento='Cl';
tablon(17).a1=0.5037;
tablon(17).a2=0.2446;
tablon(17).a3=0.9581;
tablon(17).a4=1.9974;
tablon(17).a5=1.1525;
tablon(17).b1=1.4730;
tablon(17).b2=0.2489;
tablon(17).b3=36.5515;
tablon(17).b4=14.2213;
tablon(17).b5=5.4897;
tablon(18).elemento='Ar';
tablon(18).a1=0.8942;
tablon(18).a2=1.9768;
tablon(18).a3=0.1070;
tablon(18).a4=1.1841;
tablon(18).a5=0.4159;
tablon(18).b1=3.4094;
```

```
tablon(18).b2=9.8793;
tablon(18).b3=0.0763;
tablon(18).b4=27.1976;
tablon(18).b5=0.7596;
tablon(19).elemento='K';
tablon(19).a1=0.3371;
tablon(19).a2=0.8878;
tablon(19).a3=2.5273;
tablon(19).a4=2.4758;
tablon(19).a5=2.6079;
tablon(19).b1=0.3315;
tablon(19).b2=2.2665;
tablon(19).b3=9.0998;
tablon(19).b4=101.835;
tablon(19).b5=85.6052;
tablon(20).elemento='Ca';
tablon(20).a1=0.6173;
tablon(20).a2=0.2885;
tablon(20).a3=1.6416;
tablon(20).a4=2.1460;
tablon(20).a5=5.1654;
tablon(20).b1=1.6400;
tablon(20).b2=0.2468;
tablon(20).b3=5.5582;
tablon(20).b4=18.0165;
tablon(20).b5=86.4565;
tablon(21).elemento='Sc';
tablon(21).a1=1.7260;
tablon(21).a2=2.3637;
tablon(21).a3=0.2989;
tablon(21).a4=4.1911;
tablon(21).a5=0.6974;
```

```
tablon(21).b1=5.6109;
tablon(21).b2=20.8270;
tablon(21).b3=0.2446;
tablon(21).b4=83.9145;
tablon(21).b5=1.6783;
tablon(22).elemento='Ti';
tablon(22).a1=1.7508;
tablon(22).a2=2.4914;
tablon(22).a3=0.7528;
tablon(22).a4=0.3070;
tablon(22).a5=3.4557;
tablon(22).b1=5.5714;
tablon(22).b2=22.1798;
tablon(22).b3=1.6591;
tablon(22).b4=0.2448;
tablon(22).b5=82.7864;
tablon(23).elemento='V';
tablon(23).a1=0.3225;
tablon(23).a2=2.4858;
tablon(23).a3=0.8123;
tablon(23).a4=2.9576;
tablon(23).a5=1.7139;
tablon(23).b1=0.2477;
tablon(23).b2=22.3821;
tablon(23).b3=1.6916;
tablon(23).b4=80.5410;
tablon(23).b5=5.4920;
tablon(24).elemento='Cr';
tablon(24).a1=1.6778;
tablon(24).a2=0.8399;
tablon(24).a3=1.9966;
tablon(24).a4=0.3165;
```

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tablon(24).a5=2.1247;
tablon(24).b1=5.2661;
tablon(24).b2=1.6077;
tablon(24).b3=20.1030;
tablon(24).b4=0.2328;
tablon(24).b5=82.4882;
tablon(25).elemento='Mn';
tablon(25).a1=0.8970;
tablon(25).a2=2.3635;
tablon(25).a3=0.3296;
tablon(25).a4=1.6190;
tablon(25).a5=2.2893;
tablon(25).b1=1.6174;
tablon(25).b2=74.1583;
tablon(25).b3=0.2464;
tablon(25).b4=5.2368;
tablon(25).b5=21.2391;
tablon(26).elemento='Fe';
tablon(26).a1=0.9641;
tablon(26).a2=0.3397;
tablon(26).a3=2.1773;
tablon(26).a4=2.0815;
tablon(26).a5=1.5664;
tablon(26).b1=1.6217;
tablon(26).b2=0.2341;
tablon(26).b3=21.1950;
tablon(26).b4=70.7154;
tablon(26).b5=5.3081;
tablon(27).elemento='Co';
tablon(27).a1=2.0668;
tablon(27).a2=1.4921;
tablon(27).a3=0.3477;
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tablon(27).a4=0.9572;
tablon(27).a5=1.9833;
tablon(27).b1=19.7711;
tablon(27).b2=5.0028;
tablon(27).b3=0.2315;
tablon(27).b4=1.5690;
tablon(27).b5=68.3097;
tablon(28).elemento='Ni';
tablon(28).a1=1.8929;
tablon(28).a2=1.9648;
tablon(28).a3=0.9275;
tablon(28).a4=1.4477;
tablon(28).a5=0.3288;
tablon(28).b1=64.4272;
tablon(28).b2=18.2869;
tablon(28).b3=1.4276;
tablon(28).b4=4.5981;
tablon(28).b5=0.2091;
tablon(29).elemento='Cu';
tablon(29).a1=1.4292;
tablon(29).a2=0.9819;
tablon(29).a3=1.2946;
tablon(29).a4=0.3448;
tablon(29).a5=1.5426;
tablon(29).b1=4.7334;
tablon(29).b2=1.4435;
tablon(29).b3=71.8921;
tablon(29).b4=0.2258;
tablon(29).b5=18.3285;
tablon(30).elemento='Zn';
tablon(30).a1=1.5439;
tablon(30).a2=1.7832;
```

```
tablon(30).a3=1.0213;
tablon(30).a4=1.3392;
tablon(30).a5=0.3722;
tablon(30).b1=62.0393;
tablon(30).b2=18.4854;
tablon(30).b3=1.4805;
tablon(30).b4=4.7984;
tablon(30).b5=0.2250;
tablon(31).elemento='Ga';
tablon(31).a1=1.1303;
tablon(31).a2=1.3643;
tablon(31).a3=0.4097;
tablon(31).a4=2.3827;
tablon(31).a5=1.8133;
tablon(31).b1=1.5844;
tablon(31).b2=5.5819;
tablon(31).b3=0.2414;
tablon(31).b4=22.0962;
tablon(31).b5=76.1567;
tablon(32).elemento='Ge';
tablon(32).a1=2.6367;
tablon(32).a2=1.3324;
tablon(32).a3=0.4029;
tablon(32).a4=1.0846;
tablon(32).a5=1.9141;
tablon(32).b1=19.7849;
tablon(32).b2=5.2086;
tablon(32).b3=0.2298;
tablon(32).b4=1.4807;
tablon(32).b5=64.0820;
tablon(33).elemento='As';
tablon(33).a1=2.6865;
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tablon(33).a2=1.2748;
tablon(33).a3=0.3853;
tablon(33).a4=1.0297;
tablon(33).a5=1.9382;
tablon(33).b1=16.7493;
tablon(33).b2=4.7274;
tablon(33).b3=0.2125;
tablon(33).b4=1.3530;
tablon(33).b5=50.8067;
tablon(34).elemento='Se';
tablon(34).a1=1.1632;
tablon(34).a2=1.0534;
tablon(34).a3=2.7186;
tablon(34).a4=0.3958;
tablon(34).a5=1.8692;
tablon(34).b1=4.6405;
tablon(34).b2=1.3573;
tablon(34).b3=14.6754;
tablon(34).b4=0.2104;
tablon(34).b5=42.7844;
tablon(35).elemento='Br';
tablon(35).a1=2.7310;
tablon(35).a2=1.6535;
tablon(35).a3=1.2619;
tablon(35).a4=0.4015;
tablon(35).a5=1.0081;
tablon(35).b1=13.8481;
tablon(35).b2=38.1205;
tablon(35).b3=4.6020;
tablon(35).b4=0.2098;
tablon(35).b5=1.2880;
tablon(36).elemento='Kr';
```

```
tablon(36).a1=2.7163;
tablon(36).a2=1.2399;
tablon(36).a3=1.6285;
tablon(36).a4=0.3668;
tablon(36).a5=0.9433;
tablon(36).b1=12.0800;
tablon(36).b2=4.0874;
tablon(36).b3=32.8791;
tablon(36).b4=0.1977;
tablon(36).b5=1.1280;
tablon(37).elemento='Rb';
tablon(37).a1=0.4637;
tablon(37).a2=0.8657;
tablon(37).a3=5.7261;
tablon(37).a4=3.6288;
tablon(37).a5=0.9655;
tablon(37).b1=0.2420;
tablon(37).b2=1.1826;
tablon(37).b3=106.6006;
tablon(37).b4=11.2431;
tablon(37).b5=4.0022;
tablon(38).elemento='Sr';
tablon(38).a1=3.0069;
tablon(38).a2=1.7449;
tablon(38).a3=6.5739;
tablon(38).a4=1.1999;
tablon(38).a5=0.5062;
tablon(38).b1=15.5935;
tablon(38).b2=6.2286;
tablon(38).b3=92.0409;
tablon(38).b4=1.5694;
tablon(38).b5=0.2374;
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tablon(39).elemento='Y';
tablon(39).a1=2.2413;
tablon(39).a2=3.2281;
tablon(39).a3=1.0127;
tablon(39).a4=5.6088;
tablon(39).a5=0.4937;
tablon(39).b1=5.5921;
tablon(39).b2=18.4113;
tablon(39).b3=1.3346;
tablon(39).b4=83.3015;
tablon(39).b5=0.2361;
tablon(40).elemento='Zr';
tablon(40).a1=0.5090;
tablon(40).a2=3.5092;
tablon(40).a3=1.0341;
tablon(40).a4=4.5954;
tablon(40).a5=2.4670;
tablon(40).b1=0.2341;
tablon(40).b2=20.5167;
tablon(40).b3=1.3658;
tablon(40).b4=82.1291;
tablon(40).b5=5.6990;
tablon(41).elemento='Nb';
tablon(41).a1=2.5661;
tablon(41).a2=1.0335;
tablon(41).a3=3.3941;
tablon(41).a4=3.1423;
tablon(41).a5=0.5083;
tablon(41).b1=5.5531;
tablon(41).b2=1.3433;
tablon(41).b3=19.7223;
tablon(41).b4=81.3820;
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tablon(41).b5=0.2265;
tablon(42).elemento='Mo';
tablon(42).a1=2.6130;
tablon(42).a2=3.2953;
tablon(42).a3=0.5370;
tablon(42).a4=1.0379;
tablon(42).a5=2.7607;
tablon(42).b1=5.4630;
tablon(42).b2=19.1458;
tablon(42).b3=0.2343;
tablon(42).b4=1.3838;
tablon(42).b5=78.5426;
tablon(43).elemento='Tc';
tablon(43).a1=2.6630;
tablon(43).a2=3.4140;
tablon(43).a3=1.0671;
tablon(43).a4=0.5563;
tablon(43).a5=3.1287;
tablon(43).b1=5.4012;
tablon(43).b2=19.7416;
tablon(43).b3=1.4296;
tablon(43).b4=0.2352;
tablon(43).b5=73.4475;
tablon(44).elemento='Ru';
tablon(44).a1=2.2004;
tablon(44).a2=3.0256;
tablon(44).a3=1.0724;
tablon(44).a4=0.5667;
tablon(44).a5=2.6688;
tablon(44).b1=73.3132;
tablon(44).b2=18.0130;
tablon(44).b3=1.4301;
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tablon(44).b4=0.2345;
tablon(44).b5=5.2267;
tablon(45).elemento='Rh';
tablon(45).a1=2.6577;
tablon(45).a2=2.9019;
tablon(45).a3=0.5614;
tablon(45).a4=1.0653;
tablon(45).a5=2.0332;
tablon(45).b1=4.9678;
tablon(45).b2=17.0684;
tablon(45).b3=0.2387;
tablon(45).b4=1.3751;
tablon(45).b5=70.7299;
tablon(46).elemento='Pd';
tablon(46).a1=2.5413;
tablon(46).a2=2.1993;
tablon(46).a3=0.5259;
tablon(46).a4=0.9384;
tablon(46).a5=1.3647;
tablon(46).b1=11.3044;
tablon(46).b2=4.0573;
tablon(46).b3=0.2084;
tablon(46).b4=1.2112;
tablon(46).b5=37.2810;
tablon(47).elemento='Ag';
tablon(47).a1=1.8384;
tablon(47).a2=2.3312;
tablon(47).a3=2.7903;
tablon(47).a4=1.0877;
tablon(47).a5=0.6126;
tablon(47).b1=65.8402;
tablon(47).b2=16.6748;
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tablon(47).b3=4.4648;
tablon(47).b4=1.6473;
tablon(47).b5=0.2208;
tablon(48).elemento='Cd';
tablon(48).a1=2.6685;
tablon(48).a2=2.1385;
tablon(48).a3=2.6325;
tablon(48).a4=1.1951;
tablon(48).a5=0.5889;
tablon(48).b1=16.8333;
tablon(48).b2=62.4892;
tablon(48).b3=4.7990;
tablon(48).b4=1.4484;
tablon(48).b5=0.2229;
tablon(49).elemento='In';
tablon(49).a1=2.6440;
tablon(49).a2=3.1524;
tablon(49).a3=2.6224;
tablon(49).a4=0.6344;
tablon(49).a5=1.3668;
tablon(49).b1=5.1688;
tablon(49).b2=20.1585;
tablon(49).b3=74.9156;
tablon(49).b4=0.2357;
tablon(49).b5=1.6104;
tablon(50).elemento='Sn';
tablon(50).a1=2.5195;
tablon(50).a2=1.3462;
tablon(50).a3=3.4633;
tablon(50).a4=0.6255;
tablon(50).a5=2.8933;
tablon(50).b1=4.8336;
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tablon(50).b2=1.5451;
tablon(50).b3=18.9352;
tablon(50).b4=0.2287;
tablon(50).b5=65.4807;
tablon(51).elemento='Sb';
tablon(51).a1=1.3188;
tablon(51).a2=3.0205;
tablon(51).a3=2.4045;
tablon(51).a4=0.6121;
tablon(51).a5=3.6070;
tablon(51).b1=1.4835;
tablon(51).b2=54.8259;
tablon(51).b3=4.4975;
tablon(51).b4=0.2180;
tablon(51).b5=17.3120;
tablon(52).elemento='Te';
tablon(52).a1=1.3955;
tablon(52).a2=2.2768;
tablon(52).a3=3.7388;
tablon(52).a4=0.6198;
tablon(52).a5=2.9538;
tablon(52).b1=1.4883;
tablon(52).b2=4.5170;
tablon(52).b3=16.3599;
tablon(52).b4=0.2185;
tablon(52).b5=48.3219;
tablon(53).elemento='I';
tablon(53).a1=2.1533;
tablon(53).a2=3.8460;
tablon(53).a3=1.4118;
tablon(53).a4=2.8707;
tablon(53).a5=0.6161;
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tablon(53).b1=4.3665;
tablon(53).b2=15.0853;
tablon(53).b3=1.4545;
tablon(53).b4=42.9408;
tablon(53).b5=0.2133;
tablon(54).elemento='Xe';
tablon(54).a1=3.9274;
tablon(54).a2=2.0577;
tablon(54).a3=2.8684;
tablon(54).a4=0.5981;
tablon(54).a5=1.3354;
tablon(54).b1=13.5943;
tablon(54).b2=3.9880;
tablon(54).b3=37.9476;
tablon(54).b4=0.2036;
tablon(54).b5=1.3570;
tablon(55).elemento='Cs';
tablon(55).a1=-0.668;
tablon(55).a2=5.5571;
tablon(55).a3=7.4047;
tablon(55).a4=3.1363;
tablon(55).a5=0.9480;
tablon(55).b1=116.2077;
tablon(55).b2=16.1736;
tablon(55).b3=130.5351;
tablon(55).b4=3.0163;
tablon(55).b5=0.3151;
tablon(56).elemento='Ba';
tablon(56).a1=4.9425;
tablon(56).a2=1.7545;
tablon(56).a3=1.5258;
tablon(56).a4=0.6531;
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tablon(56).a5=9.2106;
tablon(56).b1=12.8126;
tablon(56).b2=4.4419;
tablon(56).b3=1.4331;
tablon(56).b4=0.2207;
tablon(56).b5=94.6924;
tablon(57).elemento='La';
tablon(57).a1=2.2875;
tablon(57).a2=4.9018;
tablon(57).a3=8.1591;
tablon(57).a4=0.6608;
tablon(57).a5=1.5861;
tablon(57).b1=4.8334;
tablon(57).b2=14.9771;
tablon(57).b3=85.6484;
tablon(57).b4=0.2146;
tablon(57).b5=1.4768;
tablon(58).elemento='Ce';
tablon(58).a1=4.7170;
tablon(58).a2=2.3595;
tablon(58).a3=0.6537;
tablon(58).a4=7.7855;
tablon(58).a5=1.6735;
tablon(58).b1=15.2154;
tablon(58).b2=4.9884;
tablon(58).b3=0.2064;
tablon(58).b4=85.0290;
tablon(58).b5=1.4784;
tablon(59).elemento='Pr';
tablon(59).a1=1.4556;
tablon(59).a2=7.9891;
tablon(59).a3=0.6898;
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tablon(59).a4=2.1328;
tablon(59).a5=4.4767;
tablon(59).b1=1.2831;
tablon(59).b2=88.5581;
tablon(59).b3=0.2415;
tablon(59).b4=4.5188;
tablon(59).b5=12.9865;
tablon(60).elemento='Nd';
tablon(60).a1=2.2056;
tablon(60).a2=1.5448;
tablon(60).a3=0.6045;
tablon(60).a4=4.2878;
tablon(60).a5=7.6905;
tablon(60).b1=4.3697;
tablon(60).b2=1.2638;
tablon(60).b3=0.1862;
tablon(60).b4=13.0088;
tablon(60).b5=85.9794;
tablon(61).elemento='Pm';
tablon(61).a1=2.2450;
tablon(61).a2=1.6102;
tablon(61).a3=0.6410;
tablon(61).a4=4.0937;
tablon(61).a5=7.4307;
tablon(61).b1=4.5693;
tablon(61).b2=1.3109;
tablon(61).b3=0.1971;
tablon(61).b4=13.2392;
tablon(61).b5=86.9048;
tablon(62).elemento='Sm';
tablon(62).a1=1.6045;
tablon(62).a2=2.2588;
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tablon(62).a3=0.6559;
tablon(62).a4=7.1214;
tablon(62).a5=4.0662;
tablon(62).b1=1.3015;
tablon(62).b2=4.4541;
tablon(62).b3=0.2003;
tablon(62).b4=87.0279;
tablon(62).b5=13.5148;
tablon(63).elemento='Eu';
tablon(63).a1=3.8096;
tablon(63).a2=2.3219;
tablon(63).a3=1.6964;
tablon(63).a4=0.6868;
tablon(63).a5=6.9420;
tablon(63).b1=13.7564;
tablon(63).b2=4.7841;
tablon(63).b3=1.3480;
tablon(63).b4=0.2086;
tablon(63).b5=87.7834;
tablon(64).elemento='Gd';
tablon(64).a1=3.8749;
tablon(64).a2=2.7972;
tablon(64).a3=0.6963;
tablon(64).a4=1.7629;
tablon(64).a5=6.0304;
tablon(64).b1=17.0522;
tablon(64).b2=5.2416;
tablon(64).b3=0.2074;
tablon(64).b4=1.3628;
tablon(64).b5=83.1903;
tablon(65).elemento='Tb';
tablon(65).a1=0.6498;
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tablon(65).a2=1.6649;
tablon(65).a3=3.5427;
tablon(65).a4=2.4129;
tablon(65).a5=6.5029;
tablon(65).b1=0.1991;
tablon(65).b2=1.2318;
tablon(65).b3=13.7926;
tablon(65).b4=4.5019;
tablon(65).b5=83.3409;
tablon(66).elemento='Dy';
tablon(66).a1=2.4738;
tablon(66).a2=6.1335;
tablon(66).a3=1.7776;
tablon(66).a4=0.6959;
tablon(66).a5=3.4270;
tablon(66).b1=4.8493;
tablon(66).b2=85.4899;
tablon(66).b3=1.3396;
tablon(66).b4=0.1969;
tablon(66).b5=14.8320;
tablon(67).elemento='Ho';
tablon(67).a1=1.8098;
tablon(67).a2=0.7445;
tablon(67).a3=3.6104;
tablon(67).a4=5.2182;
tablon(67).a5=2.9453;
tablon(67).b1=1.3701;
tablon(67).b2=0.2133;
tablon(67).b3=19.1664;
tablon(67).b4=82.8910;
tablon(67).b5=5.4014;
tablon(68).elemento='Er';
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tablon(68).a1=2.5628;
tablon(68).a2=1.7106;
tablon(68).a3=0.6949;
tablon(68).a4=3.2366;
tablon(68).a5=5.7506;
tablon(68).b1=4.6974;
tablon(68).b2=1.2429;
tablon(68).b3=0.1955;
tablon(68).b4=15.0116;
tablon(68).b5=83.5002;
tablon(69).elemento='Tm';
tablon(69).a1=1.7198;
tablon(69).a2=5.5250;
tablon(69).a3=2.6164;
tablon(69).a4=0.7377;
tablon(69).a5=3.1045;
tablon(69).b1=1.2690;
tablon(69).b2=83.9429;
tablon(69).b3=4.8412;
tablon(69).b4=0.2077;
tablon(69).b5=15.5758;
tablon(70).elemento='Yb';
tablon(70).a1=0.7372;
tablon(70).a2=3.0525;
tablon(70).a3=2.5715;
tablon(70).a4=1.7210;
tablon(70).a5=5.3674;
tablon(70).b1=0.2046;
tablon(70).b2=15.7384;
tablon(70).b3=4.7264;
tablon(70).b4=1.2520;
tablon(70).b5=83.1496;
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tablon(71).elemento='Lu';
tablon(71).a1=1.8020;
tablon(71).a2=0.7869;
tablon(71).a3=3.4122;
tablon(71).a4=2.8794;
tablon(71).a5=4.5570;
tablon(71).b1=1.3302;
tablon(71).b2=0.2139;
tablon(71).b3=20.1865;
tablon(71).b4=5.2475;
tablon(71).b5=81.9125;
tablon(72).elemento='Hf';
tablon(72).a1=3.9427;
tablon(72).a2=3.6345;
tablon(72).a3=1.8274;
tablon(72).a4=0.8219;
tablon(72).a5=2.9228;
tablon(72).b1=77.0186;
tablon(72).b2=20.8925;
tablon(72).b3=1.3673;
tablon(72).b4=0.2205;
tablon(72).b5=5.3852;
tablon(73).elemento='Ta';
tablon(73).a1=0.8327;
tablon(73).a2=3.7562;
tablon(73).a3=2.9475;
tablon(73).a4=1.8085;
tablon(73).a5=3.4870;
tablon(73).b1=0.2208;
tablon(73).b2=20.3697;
tablon(73).b3=5.3281;
tablon(73).b4=1.3533;
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tablon(73).b5=72.6270;
tablon(74).elemento='W';
tablon(74).a1=0.8296;
tablon(74).a2=3.1549;
tablon(74).a3=2.9461;
tablon(74).a4=1.7764;
tablon(74).a5=3.8167;
tablon(74).b1=0.2160;
tablon(74).b2=68.5278;
tablon(74).b3=5.1589;
tablon(74).b4=1.3249;
tablon(74).b5=19.3610;
tablon(75).elemento='Re';
tablon(75).a1=3.7785;
tablon(75).a2=2.9524;
tablon(75).a3=1.7648;
tablon(75).a4=0.8541;
tablon(75).a5=2.8968;
tablon(75).b1=18.5062;
tablon(75).b2=5.1211;
tablon(75).b3=1.3309;
tablon(75).b4=0.2202;
tablon(75).b5=64.2221;
tablon(76).elemento='Os';
tablon(76).a1=3.7057;
tablon(76).a2=2.8390;
tablon(76).a3=0.8161;
tablon(76).a4=1.6999;
tablon(76).a5=2.8998;
tablon(76).b1=16.5584;
tablon(76).b2=58.1703;
tablon(76).b3=0.2070;
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tablon(76).b4=1.2417;
tablon(76).b5=4.7727;
tablon(77).elemento='Ir';
tablon(77).a1=1.6972;
tablon(77).a2=0.8463;
tablon(77).a3=3.6636;
tablon(77).a4=2.5472;
tablon(77).a5=2.9490;
tablon(77).b1=1.2614;
tablon(77).b2=0.2126;
tablon(77).b3=16.3008;
tablon(77).b4=56.7139;
tablon(77).b5=4.7925;
tablon(78).elemento='Pt';
tablon(78).a1=3.3756;
tablon(78).a2=1.9202;
tablon(78).a3=1.6818;
tablon(78).a4=0.8701;
tablon(78).a5=2.9537;
tablon(78).b1=15.0204;
tablon(78).b2=53.3690;
tablon(78).b3=1.2708;
tablon(78).b4=0.2162;
tablon(78).b5=4.7357;
tablon(79).elemento='Au';
tablon(79).a1=0.8239;
tablon(79).a2=1.6166;
tablon(79).a3=3.3603;
tablon(79).a4=1.8342;
tablon(79).a5=2.9307;
tablon(79).b1=0.2015;
tablon(79).b2=1.1760;
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tablon(79).b3=13.8414;
tablon(79).b4=50.2016;
tablon(79).b5=4.4106;
tablon(80).elemento='Hg';
tablon(80).a1=3.3429;
tablon(80).a2=1.9700;
tablon(80).a3=1.6900;
tablon(80).a4=0.9145;
tablon(80).a5=3.0414;
tablon(80).b1=14.9551;
tablon(80).b2=51.2359;
tablon(80).b3=1.3061;
tablon(80).b4=0.2209;
tablon(80).b5=4.7166;
tablon(81).elemento='Tl';
tablon(81).a1=2.4154;
tablon(81).a2=3.7157;
tablon(81).a3=1.7410;
tablon(81).a4=3.2675;
tablon(81).a5=0.9469;
tablon(81).b1=66.8719;
tablon(81).b2=17.5708;
tablon(81).b3=1.3552;
tablon(81).b4=4.9322;
tablon(81).b5=0.2258;
tablon(82).elemento='Pb';
tablon(82).a1=1.7224;
tablon(82).a2=0.9381;
tablon(82).a3=2.7140;
tablon(82).a4=3.9155;
tablon(82).a5=3.2667;
tablon(82).b1=1.3349;
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tablon(82).b2=0.2202;
tablon(82).b3=61.8636;
tablon(82).b4=17.4937;
tablon(82).b5=4.8583;
tablon(83).elemento='Bi';
tablon(83).a1=3.1838;
tablon(83).a2=4.1659;
tablon(83).a3=0.9545;
tablon(83).a4=3.0415;
tablon(83).a5=1.7389;
tablon(83).b1=4.7027;
tablon(83).b2=16.9894;
tablon(83).b3=0.2215;
tablon(83).b4=57.5155;
tablon(83).b5=1.3394;
tablon(84).elemento='Po';
tablon(84).a1=3.0981;
tablon(84).a2=1.6868;
tablon(84).a3=0.9255;
tablon(84).a4=4.3552;
tablon(84).a5=3.2795;
tablon(84).b1=4.4110;
tablon(84).b2=1.2698;
tablon(84).b3=0.2119;
tablon(84).b4=15.9020;
tablon(84).b5=51.2527;
tablon(85).elemento='At';
tablon(85).a1=4.4662;
tablon(85).a2=3.0129;
tablon(85).a3=3.3002;
tablon(85).a4=1.7249;
tablon(85).a5=0.9516;
```

```
tablon(85).b1=15.3682;
tablon(85).b2=4.4009;
tablon(85).b3=46.5313;
tablon(85).b4=1.3060;
tablon(85).b5=0.2154;
tablon(86).elemento='Rn';
tablon(86).a1=4.6212;
tablon(86).a2=2.9312;
tablon(86).a3=1.6640;
tablon(86).a4=0.9154;
tablon(86).a5=3.3501;
tablon(86).b1=14.2812;
tablon(86).b2=4.1129;
tablon(86).b3=1.2241;
tablon(86).b4=0.2046;
tablon(86).b5=42.0807;
tablon(87).elemento='Fr';
tablon(87).a1=6.1056;
tablon(87).a2=-0.314;
tablon(87).a3=3.0127;
tablon(87).a4=8.0414;
tablon(87).a5=1.3720;
tablon(87).b1=11.2782;
tablon(87).b2=77.9414;
tablon(87).b3=2.3975;
tablon(87).b4=88.8819;
tablon(87).b5=0.3074;
tablon(88).elemento='Ra';
tablon(88).a1=2.7718;
tablon(88).a2=1.5937;
tablon(88).a3=9.1922;
tablon(88).a4=5.8530;
```

```
tablon(88).a5=0.8400;
tablon(88).b1=3.6817;
tablon(88).b2=1.0968;
tablon(88).b3=88.4473;
tablon(88).b4=13.4212;
tablon(88).b5=0.1798;
tablon(89).elemento='Ac';
tablon(89).a1=3.1041;
tablon(89).a2=1.9460;
tablon(89).a3=5.7975;
tablon(89).a4=8.4287;
tablon(89).a5=1.0283;
tablon(89).b1=4.8348;
tablon(89).b2=1.4065;
tablon(89).b3=16.1952;
tablon(89).b4=84.2792;
tablon(89).b5=0.2249;
tablon(90).elemento='Th';
tablon(90).a1=1.0606;
tablon(90).a2=6.1558;
tablon(90).a3=2.1278;
tablon(90).a4=7.2005;
tablon(90).a5=3.5299;
tablon(90).b1=0.2277;
tablon(90).b2=19.1693;
tablon(90).b3=1.5027;
tablon(90).b4=83.1842;
tablon(90).b5=5.4688;
tablon(91).elemento='Pa';
tablon(91).a1=3.3789;
tablon(91).a2=2.1098;
tablon(91).a3=7.2538;
```

```
tablon(91).a4=1.0752;
tablon(91).a5=5.6246;
tablon(91).b1=5.2199;
tablon(91).b2=1.4967;
tablon(91).b3=83.0861;
tablon(91).b4=0.2301;
tablon(91).b5=17.2570;
tablon(92).elemento='U';
tablon(92).a1=2.1845;
tablon(92).a2=1.0774;
tablon(92).a3=5.4600;
tablon(92).a4=3.5175;
tablon(92).a5=6.8170;
tablon(92).b1=1.5185;
tablon(92).b2=0.2261;
tablon(92).b3=17.5536;
tablon(92).b4=5.3832;
tablon(92).b5=83.9202;
tablon(93).elemento='Np';
tablon(93).a1=1.0605;
tablon(93).a2=5.3227;
tablon(93).a3=2.1706;
tablon(93).a4=6.4498;
tablon(93).a5=3.6607;
tablon(93).b1=0.2209;
tablon(93).b2=17.6673;
tablon(93).b3=1.4668;
tablon(93).b4=82.6385;
tablon(93).b5=5.3317;
tablon(94).elemento='Pu';
tablon(94).a1=5.0018;
tablon(94).a2=3.3635;
```

```
tablon(94).a3=1.0312;
tablon(94).a4=2.0638;
tablon(94).a5=6.5815;
tablon(94).b1=15.0396;
tablon(94).b2=4.7751;
tablon(94).b3=0.2118;
tablon(94).b4=1.3854;
tablon(94).b5=83.8012;
tablon(95).elemento='Am';
tablon(95).a1=2.1135;
tablon(95).a2=3.4848;
tablon(95).a3=1.0497;
tablon(95).a4=4.8075;
tablon(95).a5=6.2502;
tablon(95).b1=1.4178;
tablon(95).b2=4.8644;
tablon(95).b3=0.2126;
tablon(95).b4=15.4049;
tablon(95).b5=83.6486;
tablon(96).elemento='Cm';
tablon(96).a1=2.3024;
tablon(96).a2=3.8828;
tablon(96).a3=1.0947;
tablon(96).a4=5.5030;
tablon(96).a5=4.8629;
tablon(96).b1=1.5087;
tablon(96).b2=5.4420;
tablon(96).b3=0.2212;
tablon(96).b4=82.1515;
tablon(96).b5=18.6116;
tablon(97).elemento='Bk';
tablon(97).a1=3.9615;
```

```
tablon(97).a2=4.7078;
tablon(97).a3=1.1034;
tablon(97).a4=5.2136;
tablon(97).a5=2.3627;
tablon(97).b1=5.5156;
tablon(97).b2=19.1735;
tablon(97).b3=0.2330;
tablon(97).b4=82.2191;
tablon(97).b5=1.5087;
tablon(98).elemento='Cf';
tablon(98).a1=3.9176;
tablon(98).a2=5.1700;
tablon(98).a3=2.3428;
tablon(98).a4=1.0923;
tablon(98).a5=4.4169;
tablon(98).b1=5.3363;
tablon(98).b2=75.3300;
tablon(98).b3=1.4895;
tablon(98).b4=0.2161;
tablon(98).b5=18.2466;
boli=length(tablon);
        for roti=1:boli
                probando=tablon(roti).elemento;
    verel=strcmp(elemental,probando);
                if  verel==1
                        ga1=tablon(roti).a1;
                        gb1=tablon(roti).b1;
                        ga2=tablon(roti).a2;
                        gb2=tablon(roti).b2;
                        ga3=tablon(roti).a3;
                        gb3=tablon(roti).b3;
                        ga4=tablon(roti).a4;
```

```
                gb4=tablon(roti).b4;
                ga5=tablon(roti).a5;
                gb5=tablon(roti).b5;
            end
        end
end
```

15.2 Archivos PDB generados de las estructuras Simuladas

15.2.1 Archivo PDB Estructura Cúbica Simple

Archivo PDB generado correspondiente a la estructura cúbica simple de 4 celdas por lado, 10 Angstroms en los parámetros de red a, b y c:

Campo1	Campo2	Campo3	Campo4	Campo5	Campo6	Campo7	Campo8	Campo9	Campo 10
Registro	serial	elemento	Numero de secuncia	Coordenadas otogonales para x	Coordenadas otogonales para y	Coordenadas otogonales para z	ocupancia	Factor de temperatura	Carga en el átomo

```
ATOM      1  I        1     -40.000 -36.362 -43.334  1.00  0.00          O
ATOM      2  I        2     -40.000 -26.400 -42.462  1.00  0.00          O
ATOM      3  I        3     -40.000 -16.438 -41.591  1.00  0.00          O
ATOM      4  I        4     -40.000  -6.476 -40.719  1.00  0.00          O
ATOM      5  I        5     -40.000   3.486 -39.848  1.00  0.00          O
ATOM      6  I        6     -40.000  13.448 -38.976  1.00  0.00          O
ATOM      7  I        7     -40.000  23.410 -38.105  1.00  0.00          O
ATOM      8  I        8     -40.000  33.372 -37.233  1.00  0.00          O
ATOM      9  I        9     -40.000  43.334 -36.362  1.00  0.00          O
ATOM     10  I       10     -30.000 -36.362 -43.334  1.00  0.00          O
ATOM     11  I       11     -30.000 -26.400 -42.462  1.00  0.00          O
ATOM     12  I       12     -30.000 -16.438 -41.591  1.00  0.00          O
ATOM     13  I       13     -30.000  -6.476 -40.719  1.00  0.00          O
ATOM     14  I       14     -30.000   3.486 -39.848  1.00  0.00          O
ATOM     15  I       15     -30.000  13.448 -38.976  1.00  0.00          O
ATOM     16  I       16     -30.000  23.410 -38.105  1.00  0.00          O
ATOM     17  I       17     -30.000  33.372 -37.233  1.00  0.00          O
ATOM     18  I       18     -30.000  43.334 -36.362  1.00  0.00          O
ATOM     19  I       19     -20.000 -36.362 -43.334  1.00  0.00          O
ATOM     20  I       20     -20.000 -26.400 -42.462  1.00  0.00          O
ATOM     21  I       21     -20.000 -16.438 -41.591  1.00  0.00          O
ATOM     22  I       22     -20.000  -6.476 -40.719  1.00  0.00          O
ATOM     23  I       23     -20.000   3.486 -39.848  1.00  0.00          O
ATOM     24  I       24     -20.000  13.448 -38.976  1.00  0.00          O
ATOM     25  I       25     -20.000  23.410 -38.105  1.00  0.00          O
ATOM     26  I       26     -20.000  33.372 -37.233  1.00  0.00          O
ATOM     27  I       27     -20.000  43.334 -36.362  1.00  0.00          O
ATOM     28  I       28     -10.000 -36.362 -43.334  1.00  0.00          O
ATOM     29  I       29     -10.000 -26.400 -42.462  1.00  0.00          O
ATOM     30  I       30     -10.000 -16.438 -41.591  1.00  0.00          O
ATOM     31  I       31     -10.000  -6.476 -40.719  1.00  0.00          O
ATOM     32  I       32     -10.000   3.486 -39.848  1.00  0.00          O
ATOM     33  I       33     -10.000  13.448 -38.976  1.00  0.00          O
ATOM     34  I       34     -10.000  23.410 -38.105  1.00  0.00          O
ATOM     35  I       35     -10.000  33.372 -37.233  1.00  0.00          O
```

```
ATOM     36  I        36    -10.000  43.334 -36.362  1.00  0.00          O
ATOM     37  I        37     -0.000 -36.362 -43.334  1.00  0.00          O
ATOM     38  I        38     -0.000 -26.400 -42.462  1.00  0.00          O
ATOM     39  I        39     -0.000 -16.438 -41.591  1.00  0.00          O
ATOM     40  I        40     -0.000  -6.476 -40.719  1.00  0.00          O
ATOM     41  I        41     -0.000   3.486 -39.848  1.00  0.00          O
ATOM     42  I        42     -0.000  13.448 -38.976  1.00  0.00          O
ATOM     43  I        43     -0.000  23.410 -38.105  1.00  0.00          O
ATOM     44  I        44     -0.000  33.372 -37.233  1.00  0.00          O
ATOM     45  I        45      0.000  43.334 -36.362  1.00  0.00          O
ATOM     46  I        46     10.000 -36.362 -43.334  1.00  0.00          O
ATOM     47  I        47     10.000 -26.400 -42.462  1.00  0.00          O
ATOM     48  I        48     10.000 -16.438 -41.591  1.00  0.00          O
ATOM     49  I        49     10.000  -6.476 -40.719  1.00  0.00          O
ATOM     50  I        50     10.000   3.486 -39.848  1.00  0.00          O
ATOM     51  I        51     10.000  13.448 -38.976  1.00  0.00          O
ATOM     52  I        52     10.000  23.410 -38.105  1.00  0.00          O
ATOM     53  I        53     10.000  33.372 -37.233  1.00  0.00          O
ATOM     54  I        54     10.000  43.334 -36.362  1.00  0.00          O
ATOM     55  I        55     20.000 -36.362 -43.334  1.00  0.00          O
ATOM     56  I        56     20.000 -26.400 -42.462  1.00  0.00          O
ATOM     57  I        57     20.000 -16.438 -41.591  1.00  0.00          O
ATOM     58  I        58     20.000  -6.476 -40.719  1.00  0.00          O
ATOM     59  I        59     20.000   3.486 -39.848  1.00  0.00          O
ATOM     60  I        60     20.000  13.448 -38.976  1.00  0.00          O
ATOM     61  I        61     20.000  23.410 -38.105  1.00  0.00          O
ATOM     62  I        62     20.000  33.372 -37.233  1.00  0.00          O
ATOM     63  I        63     20.000  43.334 -36.362  1.00  0.00          O
ATOM     64  I        64     30.000 -36.362 -43.334  1.00  0.00          O
ATOM     65  I        65     30.000 -26.400 -42.462  1.00  0.00          O
ATOM     66  I        66     30.000 -16.438 -41.591  1.00  0.00          O
ATOM     67  I        67     30.000  -6.476 -40.719  1.00  0.00          O
ATOM     68  I        68     30.000   3.486 -39.848  1.00  0.00          O
ATOM     69  I        69     30.000  13.448 -38.976  1.00  0.00          O
ATOM     70  I        70     30.000  23.410 -38.105  1.00  0.00          O
ATOM     71  I        71     30.000  33.372 -37.233  1.00  0.00          O
ATOM     72  I        72     30.000  43.334 -36.362  1.00  0.00          O
ATOM     73  I        73     40.000 -36.362 -43.334  1.00  0.00          O
ATOM     74  I        74     40.000 -26.400 -42.462  1.00  0.00          O
ATOM     75  I        75     40.000 -16.438 -41.591  1.00  0.00          O
ATOM     76  I        76     40.000  -6.476 -40.719  1.00  0.00          O
ATOM     77  I        77     40.000   3.486 -39.848  1.00  0.00          O
ATOM     78  I        78     40.000  13.448 -38.976  1.00  0.00          O
ATOM     79  I        79     40.000  23.410 -38.105  1.00  0.00          O
ATOM     80  I        80     40.000  33.372 -37.233  1.00  0.00          O
ATOM     81  I        81     40.000  43.334 -36.362  1.00  0.00          O
ATOM     82  I        82    -40.000 -37.233 -33.372  1.00  0.00          O
ATOM     83  I        83    -40.000 -27.271 -32.501  1.00  0.00          O
```

```
ATOM     84  I       84     -40.000 -17.309 -31.629  1.00  0.00          O
ATOM     85  I       85     -40.000  -7.347 -30.757  1.00  0.00          O
ATOM     86  I       86     -40.000   2.615 -29.886  1.00  0.00          O
ATOM     87  I       87     -40.000  12.577 -29.014  1.00  0.00          O
ATOM     88  I       88     -40.000  22.539 -28.143  1.00  0.00          O
ATOM     89  I       89     -40.000  32.501 -27.271  1.00  0.00          O
ATOM     90  I       90     -40.000  42.462 -26.400  1.00  0.00          O
ATOM     91  I       91     -30.000 -37.233 -33.372  1.00  0.00          O
ATOM     92  I       92     -30.000 -27.271 -32.501  1.00  0.00          O
ATOM     93  I       93     -30.000 -17.309 -31.629  1.00  0.00          O
ATOM     94  I       94     -30.000  -7.347 -30.757  1.00  0.00          O
ATOM     95  I       95     -30.000   2.615 -29.886  1.00  0.00          O
ATOM     96  I       96     -30.000  12.577 -29.014  1.00  0.00          O
ATOM     97  I       97     -30.000  22.539 -28.143  1.00  0.00          O
ATOM     98  I       98     -30.000  32.501 -27.271  1.00  0.00          O
ATOM     99  I       99     -30.000  42.462 -26.400  1.00  0.00          O
ATOM    100  I      100     -20.000 -37.233 -33.372  1.00  0.00          O
ATOM    101  I      101     -20.000 -27.271 -32.501  1.00  0.00          O
ATOM    102  I      102     -20.000 -17.309 -31.629  1.00  0.00          O
ATOM    103  I      103     -20.000  -7.347 -30.757  1.00  0.00          O
ATOM    104  I      104     -20.000   2.615 -29.886  1.00  0.00          O
ATOM    105  I      105     -20.000  12.577 -29.014  1.00  0.00          O
ATOM    106  I      106     -20.000  22.539 -28.143  1.00  0.00          O
ATOM    107  I      107     -20.000  32.501 -27.271  1.00  0.00          O
ATOM    108  I      108     -20.000  42.462 -26.400  1.00  0.00          O
ATOM    109  I      109     -10.000 -37.233 -33.372  1.00  0.00          O
ATOM    110  I      110     -10.000 -27.271 -32.501  1.00  0.00          O
ATOM    111  I      111     -10.000 -17.309 -31.629  1.00  0.00          O
ATOM    112  I      112     -10.000  -7.347 -30.757  1.00  0.00          O
ATOM    113  I      113     -10.000   2.615 -29.886  1.00  0.00          O
ATOM    114  I      114     -10.000  12.577 -29.014  1.00  0.00          O
ATOM    115  I      115     -10.000  22.539 -28.143  1.00  0.00          O
ATOM    116  I      116     -10.000  32.501 -27.271  1.00  0.00          O
ATOM    117  I      117     -10.000  42.462 -26.400  1.00  0.00          O
ATOM    118  I      118      -0.000 -37.233 -33.372  1.00  0.00          O
ATOM    119  I      119      -0.000 -27.271 -32.501  1.00  0.00          O
ATOM    120  I      120      -0.000 -17.309 -31.629  1.00  0.00          O
ATOM    121  I      121      -0.000  -7.347 -30.757  1.00  0.00          O
ATOM    122  I      122      -0.000   2.615 -29.886  1.00  0.00          O
ATOM    123  I      123      -0.000  12.577 -29.014  1.00  0.00          O
ATOM    124  I      124      -0.000  22.539 -28.143  1.00  0.00          O
ATOM    125  I      125       0.000  32.501 -27.271  1.00  0.00          O
ATOM    126  I      126       0.000  42.462 -26.400  1.00  0.00          O
ATOM    127  I      127      10.000 -37.233 -33.372  1.00  0.00          O
ATOM    128  I      128      10.000 -27.271 -32.501  1.00  0.00          O
ATOM    129  I      129      10.000 -17.309 -31.629  1.00  0.00          O
ATOM    130  I      130      10.000  -7.347 -30.757  1.00  0.00          O
ATOM    131  I      131      10.000   2.615 -29.886  1.00  0.00          O
```

```
ATOM    132  I       132      10.000  12.577 -29.014  1.00  0.00          O
ATOM    133  I       133      10.000  22.539 -28.143  1.00  0.00          O
ATOM    134  I       134      10.000  32.501 -27.271  1.00  0.00          O
ATOM    135  I       135      10.000  42.462 -26.400  1.00  0.00          O
ATOM    136  I       136      20.000 -37.233 -33.372  1.00  0.00          O
ATOM    137  I       137      20.000 -27.271 -32.501  1.00  0.00          O
ATOM    138  I       138      20.000 -17.309 -31.629  1.00  0.00          O
ATOM    139  I       139      20.000  -7.347 -30.757  1.00  0.00          O
ATOM    140  I       140      20.000   2.615 -29.886  1.00  0.00          O
ATOM    141  I       141      20.000  12.577 -29.014  1.00  0.00          O
ATOM    142  I       142      20.000  22.539 -28.143  1.00  0.00          O
ATOM    143  I       143      20.000  32.501 -27.271  1.00  0.00          O
ATOM    144  I       144      20.000  42.462 -26.400  1.00  0.00          O
ATOM    145  I       145      30.000 -37.233 -33.372  1.00  0.00          O
ATOM    146  I       146      30.000 -27.271 -32.501  1.00  0.00          O
ATOM    147  I       147      30.000 -17.309 -31.629  1.00  0.00          O
ATOM    148  I       148      30.000  -7.347 -30.757  1.00  0.00          O
ATOM    149  I       149      30.000   2.615 -29.886  1.00  0.00          O
ATOM    150  I       150      30.000  12.577 -29.014  1.00  0.00          O
ATOM    151  I       151      30.000  22.539 -28.143  1.00  0.00          O
ATOM    152  I       152      30.000  32.501 -27.271  1.00  0.00          O
ATOM    153  I       153      30.000  42.462 -26.400  1.00  0.00          O
ATOM    154  I       154      40.000 -37.233 -33.372  1.00  0.00          O
ATOM    155  I       155      40.000 -27.271 -32.501  1.00  0.00          O
ATOM    156  I       156      40.000 -17.309 -31.629  1.00  0.00          O
ATOM    157  I       157      40.000  -7.347 -30.757  1.00  0.00          O
ATOM    158  I       158      40.000   2.615 -29.886  1.00  0.00          O
ATOM    159  I       159      40.000  12.577 -29.014  1.00  0.00          O
ATOM    160  I       160      40.000  22.539 -28.143  1.00  0.00          O
ATOM    161  I       161      40.000  32.501 -27.271  1.00  0.00          O
ATOM    162  I       162      40.000  42.462 -26.400  1.00  0.00          O
ATOM    163  I       163     -40.000 -38.105 -23.410  1.00  0.00          O
ATOM    164  I       164     -40.000 -28.143 -22.539  1.00  0.00          O
ATOM    165  I       165     -40.000 -18.181 -21.667  1.00  0.00          O
ATOM    166  I       166     -40.000  -8.219 -20.795  1.00  0.00          O
ATOM    167  I       167     -40.000   1.743 -19.924  1.00  0.00          O
ATOM    168  I       168     -40.000  11.705 -19.052  1.00  0.00          O
ATOM    169  I       169     -40.000  21.667 -18.181  1.00  0.00          O
ATOM    170  I       170     -40.000  31.629 -17.309  1.00  0.00          O
ATOM    171  I       171     -40.000  41.591 -16.438  1.00  0.00          O
ATOM    172  I       172     -30.000 -38.105 -23.410  1.00  0.00          O
ATOM    173  I       173     -30.000 -28.143 -22.539  1.00  0.00          O
ATOM    174  I       174     -30.000 -18.181 -21.667  1.00  0.00          O
ATOM    175  I       175     -30.000  -8.219 -20.795  1.00  0.00          O
ATOM    176  I       176     -30.000   1.743 -19.924  1.00  0.00          O
ATOM    177  I       177     -30.000  11.705 -19.052  1.00  0.00          O
ATOM    178  I       178     -30.000  21.667 -18.181  1.00  0.00          O
ATOM    179  I       179     -30.000  31.629 -17.309  1.00  0.00          O
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ATOM    180  I       180    -30.000  41.591 -16.438  1.00  0.00          O
ATOM    181  I       181    -20.000 -38.105 -23.410  1.00  0.00          O
ATOM    182  I       182    -20.000 -28.143 -22.539  1.00  0.00          O
ATOM    183  I       183    -20.000 -18.181 -21.667  1.00  0.00          O
ATOM    184  I       184    -20.000  -8.219 -20.795  1.00  0.00          O
ATOM    185  I       185    -20.000   1.743 -19.924  1.00  0.00          O
ATOM    186  I       186    -20.000  11.705 -19.052  1.00  0.00          O
ATOM    187  I       187    -20.000  21.667 -18.181  1.00  0.00          O
ATOM    188  I       188    -20.000  31.629 -17.309  1.00  0.00          O
ATOM    189  I       189    -20.000  41.591 -16.438  1.00  0.00          O
ATOM    190  I       190    -10.000 -38.105 -23.410  1.00  0.00          O
ATOM    191  I       191    -10.000 -28.143 -22.539  1.00  0.00          O
ATOM    192  I       192    -10.000 -18.181 -21.667  1.00  0.00          O
ATOM    193  I       193    -10.000  -8.219 -20.795  1.00  0.00          O
ATOM    194  I       194    -10.000   1.743 -19.924  1.00  0.00          O
ATOM    195  I       195    -10.000  11.705 -19.052  1.00  0.00          O
ATOM    196  I       196    -10.000  21.667 -18.181  1.00  0.00          O
ATOM    197  I       197    -10.000  31.629 -17.309  1.00  0.00          O
ATOM    198  I       198    -10.000  41.591 -16.438  1.00  0.00          O
ATOM    199  I       199     -0.000 -38.105 -23.410  1.00  0.00          O
ATOM    200  I       200     -0.000 -28.143 -22.539  1.00  0.00          O
ATOM    201  I       201     -0.000 -18.181 -21.667  1.00  0.00          O
ATOM    202  I       202     -0.000  -8.219 -20.795  1.00  0.00          O
ATOM    203  I       203     -0.000   1.743 -19.924  1.00  0.00          O
ATOM    204  I       204     -0.000  11.705 -19.052  1.00  0.00          O
ATOM    205  I       205      0.000  21.667 -18.181  1.00  0.00          O
ATOM    206  I       206      0.000  31.629 -17.309  1.00  0.00          O
ATOM    207  I       207      0.000  41.591 -16.438  1.00  0.00          O
ATOM    208  I       208     10.000 -38.105 -23.410  1.00  0.00          O
ATOM    209  I       209     10.000 -28.143 -22.539  1.00  0.00          O
ATOM    210  I       210     10.000 -18.181 -21.667  1.00  0.00          O
ATOM    211  I       211     10.000  -8.219 -20.795  1.00  0.00          O
ATOM    212  I       212     10.000   1.743 -19.924  1.00  0.00          O
ATOM    213  I       213     10.000  11.705 -19.052  1.00  0.00          O
ATOM    214  I       214     10.000  21.667 -18.181  1.00  0.00          O
ATOM    215  I       215     10.000  31.629 -17.309  1.00  0.00          O
ATOM    216  I       216     10.000  41.591 -16.438  1.00  0.00          O
ATOM    217  I       217     20.000 -38.105 -23.410  1.00  0.00          O
ATOM    218  I       218     20.000 -28.143 -22.539  1.00  0.00          O
ATOM    219  I       219     20.000 -18.181 -21.667  1.00  0.00          O
ATOM    220  I       220     20.000  -8.219 -20.795  1.00  0.00          O
ATOM    221  I       221     20.000   1.743 -19.924  1.00  0.00          O
ATOM    222  I       222     20.000  11.705 -19.052  1.00  0.00          O
ATOM    223  I       223     20.000  21.667 -18.181  1.00  0.00          O
ATOM    224  I       224     20.000  31.629 -17.309  1.00  0.00          O
ATOM    225  I       225     20.000  41.591 -16.438  1.00  0.00          O
ATOM    226  I       226     30.000 -38.105 -23.410  1.00  0.00          O
ATOM    227  I       227     30.000 -28.143 -22.539  1.00  0.00          O
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ATOM    228  I       228      30.000 -18.181 -21.667  1.00  0.00          O
ATOM    229  I       229      30.000  -8.219 -20.795  1.00  0.00          O
ATOM    230  I       230      30.000   1.743 -19.924  1.00  0.00          O
ATOM    231  I       231      30.000  11.705 -19.052  1.00  0.00          O
ATOM    232  I       232      30.000  21.667 -18.181  1.00  0.00          O
ATOM    233  I       233      30.000  31.629 -17.309  1.00  0.00          O
ATOM    234  I       234      30.000  41.591 -16.438  1.00  0.00          O
ATOM    235  I       235      40.000 -38.105 -23.410  1.00  0.00          O
ATOM    236  I       236      40.000 -28.143 -22.539  1.00  0.00          O
ATOM    237  I       237      40.000 -18.181 -21.667  1.00  0.00          O
ATOM    238  I       238      40.000  -8.219 -20.795  1.00  0.00          O
ATOM    239  I       239      40.000   1.743 -19.924  1.00  0.00          O
ATOM    240  I       240      40.000  11.705 -19.052  1.00  0.00          O
ATOM    241  I       241      40.000  21.667 -18.181  1.00  0.00          O
ATOM    242  I       242      40.000  31.629 -17.309  1.00  0.00          O
ATOM    243  I       243      40.000  41.591 -16.438  1.00  0.00          O
ATOM    244  I       244     -40.000 -38.976 -13.448  1.00  0.00          O
ATOM    245  I       245     -40.000 -29.014 -12.577  1.00  0.00          O
ATOM    246  I       246     -40.000 -19.052 -11.705  1.00  0.00          O
ATOM    247  I       247     -40.000  -9.090 -10.834  1.00  0.00          O
ATOM    248  I       248     -40.000   0.872  -9.962  1.00  0.00          O
ATOM    249  I       249     -40.000  10.834  -9.090  1.00  0.00          O
ATOM    250  I       250     -40.000  20.795  -8.219  1.00  0.00          O
ATOM    251  I       251     -40.000  30.757  -7.347  1.00  0.00          O
ATOM    252  I       252     -40.000  40.719  -6.476  1.00  0.00          O
ATOM    253  I       253     -30.000 -38.976 -13.448  1.00  0.00          O
ATOM    254  I       254     -30.000 -29.014 -12.577  1.00  0.00          O
ATOM    255  I       255     -30.000 -19.052 -11.705  1.00  0.00          O
ATOM    256  I       256     -30.000  -9.090 -10.834  1.00  0.00          O
ATOM    257  I       257     -30.000   0.872  -9.962  1.00  0.00          O
ATOM    258  I       258     -30.000  10.834  -9.090  1.00  0.00          O
ATOM    259  I       259     -30.000  20.795  -8.219  1.00  0.00          O
ATOM    260  I       260     -30.000  30.757  -7.347  1.00  0.00          O
ATOM    261  I       261     -30.000  40.719  -6.476  1.00  0.00          O
ATOM    262  I       262     -20.000 -38.976 -13.448  1.00  0.00          O
ATOM    263  I       263     -20.000 -29.014 -12.577  1.00  0.00          O
ATOM    264  I       264     -20.000 -19.052 -11.705  1.00  0.00          O
ATOM    265  I       265     -20.000  -9.090 -10.834  1.00  0.00          O
ATOM    266  I       266     -20.000   0.872  -9.962  1.00  0.00          O
ATOM    267  I       267     -20.000  10.834  -9.090  1.00  0.00          O
ATOM    268  I       268     -20.000  20.795  -8.219  1.00  0.00          O
ATOM    269  I       269     -20.000  30.757  -7.347  1.00  0.00          O
ATOM    270  I       270     -20.000  40.719  -6.476  1.00  0.00          O
ATOM    271  I       271     -10.000 -38.976 -13.448  1.00  0.00          O
ATOM    272  I       272     -10.000 -29.014 -12.577  1.00  0.00          O
ATOM    273  I       273     -10.000 -19.052 -11.705  1.00  0.00          O
ATOM    274  I       274     -10.000  -9.090 -10.834  1.00  0.00          O
ATOM    275  I       275     -10.000   0.872  -9.962  1.00  0.00          O
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ATOM 276 I 276 -10.000 10.834 -9.090 1.00 0.00 O
ATOM 277 I 277 -10.000 20.795 -8.219 1.00 0.00 O
ATOM 278 I 278 -10.000 30.757 -7.347 1.00 0.00 O
ATOM 279 I 279 -10.000 40.719 -6.476 1.00 0.00 O
ATOM 280 I 280 -0.000 -38.976 -13.448 1.00 0.00 O
ATOM 281 I 281 -0.000 -29.014 -12.577 1.00 0.00 O
ATOM 282 I 282 -0.000 -19.052 -11.705 1.00 0.00 O
ATOM 283 I 283 -0.000 -9.090 -10.834 1.00 0.00 O
ATOM 284 I 284 -0.000 0.872 -9.962 1.00 0.00 O
ATOM 285 I 285 0.000 10.834 -9.090 1.00 0.00 O
ATOM 286 I 286 0.000 20.795 -8.219 1.00 0.00 O
ATOM 287 I 287 0.000 30.757 -7.347 1.00 0.00 O
ATOM 288 I 288 0.000 40.719 -6.476 1.00 0.00 O
ATOM 289 I 289 10.000 -38.976 -13.448 1.00 0.00 O
ATOM 290 I 290 10.000 -29.014 -12.577 1.00 0.00 O
ATOM 291 I 291 10.000 -19.052 -11.705 1.00 0.00 O
ATOM 292 I 292 10.000 -9.090 -10.834 1.00 0.00 O
ATOM 293 I 293 10.000 0.872 -9.962 1.00 0.00 O
ATOM 294 I 294 10.000 10.834 -9.090 1.00 0.00 O
ATOM 295 I 295 10.000 20.795 -8.219 1.00 0.00 O
ATOM 296 I 296 10.000 30.757 -7.347 1.00 0.00 O
ATOM 297 I 297 10.000 40.719 -6.476 1.00 0.00 O
ATOM 298 I 298 20.000 -38.976 -13.448 1.00 0.00 O
ATOM 299 I 299 20.000 -29.014 -12.577 1.00 0.00 O
ATOM 300 I 300 20.000 -19.052 -11.705 1.00 0.00 O
ATOM 301 I 301 20.000 -9.090 -10.834 1.00 0.00 O
ATOM 302 I 302 20.000 0.872 -9.962 1.00 0.00 O
ATOM 303 I 303 20.000 10.834 -9.090 1.00 0.00 O
ATOM 304 I 304 20.000 20.795 -8.219 1.00 0.00 O
ATOM 305 I 305 20.000 30.757 -7.347 1.00 0.00 O
ATOM 306 I 306 20.000 40.719 -6.476 1.00 0.00 O
ATOM 307 I 307 30.000 -38.976 -13.448 1.00 0.00 O
ATOM 308 I 308 30.000 -29.014 -12.577 1.00 0.00 O
ATOM 309 I 309 30.000 -19.052 -11.705 1.00 0.00 O
ATOM 310 I 310 30.000 -9.090 -10.834 1.00 0.00 O
ATOM 311 I 311 30.000 0.872 -9.962 1.00 0.00 O
ATOM 312 I 312 30.000 10.834 -9.090 1.00 0.00 O
ATOM 313 I 313 30.000 20.795 -8.219 1.00 0.00 O
ATOM 314 I 314 30.000 30.757 -7.347 1.00 0.00 O
ATOM 315 I 315 30.000 40.719 -6.476 1.00 0.00 O
ATOM 316 I 316 40.000 -38.976 -13.448 1.00 0.00 O
ATOM 317 I 317 40.000 -29.014 -12.577 1.00 0.00 O
ATOM 318 I 318 40.000 -19.052 -11.705 1.00 0.00 O
ATOM 319 I 319 40.000 -9.090 -10.834 1.00 0.00 O
ATOM 320 I 320 40.000 0.872 -9.962 1.00 0.00 O
ATOM 321 I 321 40.000 10.834 -9.090 1.00 0.00 O
ATOM 322 I 322 40.000 20.795 -8.219 1.00 0.00 O
ATOM 323 I 323 40.000 30.757 -7.347 1.00 0.00 O

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ATOM    324  I       324      40.000  40.719  -6.476  1.00  0.00          O
ATOM    325  I       325     -40.000 -39.848  -3.486  1.00  0.00          O
ATOM    326  I       326     -40.000 -29.886  -2.615  1.00  0.00          O
ATOM    327  I       327     -40.000 -19.924  -1.743  1.00  0.00          O
ATOM    328  I       328     -40.000  -9.962  -0.872  1.00  0.00          O
ATOM    329  I       329     -40.000   0.000   0.000  1.00  0.00          O
ATOM    330  I       330     -40.000   9.962   0.872  1.00  0.00          O
ATOM    331  I       331     -40.000  19.924   1.743  1.00  0.00          O
ATOM    332  I       332     -40.000  29.886   2.615  1.00  0.00          O
ATOM    333  I       333     -40.000  39.848   3.486  1.00  0.00          O
ATOM    334  I       334     -30.000 -39.848  -3.486  1.00  0.00          O
ATOM    335  I       335     -30.000 -29.886  -2.615  1.00  0.00          O
ATOM    336  I       336     -30.000 -19.924  -1.743  1.00  0.00          O
ATOM    337  I       337     -30.000  -9.962  -0.872  1.00  0.00          O
ATOM    338  I       338     -30.000   0.000   0.000  1.00  0.00          O
ATOM    339  I       339     -30.000   9.962   0.872  1.00  0.00          O
ATOM    340  I       340     -30.000  19.924   1.743  1.00  0.00          O
ATOM    341  I       341     -30.000  29.886   2.615  1.00  0.00          O
ATOM    342  I       342     -30.000  39.848   3.486  1.00  0.00          O
ATOM    343  I       343     -20.000 -39.848  -3.486  1.00  0.00          O
ATOM    344  I       344     -20.000 -29.886  -2.615  1.00  0.00          O
ATOM    345  I       345     -20.000 -19.924  -1.743  1.00  0.00          O
ATOM    346  I       346     -20.000  -9.962  -0.872  1.00  0.00          O
ATOM    347  I       347     -20.000   0.000   0.000  1.00  0.00          O
ATOM    348  I       348     -20.000   9.962   0.872  1.00  0.00          O
ATOM    349  I       349     -20.000  19.924   1.743  1.00  0.00          O
ATOM    350  I       350     -20.000  29.886   2.615  1.00  0.00          O
ATOM    351  I       351     -20.000  39.848   3.486  1.00  0.00          O
ATOM    352  I       352     -10.000 -39.848  -3.486  1.00  0.00          O
ATOM    353  I       353     -10.000 -29.886  -2.615  1.00  0.00          O
ATOM    354  I       354     -10.000 -19.924  -1.743  1.00  0.00          O
ATOM    355  I       355     -10.000  -9.962  -0.872  1.00  0.00          O
ATOM    356  I       356     -10.000   0.000   0.000  1.00  0.00          O
ATOM    357  I       357     -10.000   9.962   0.872  1.00  0.00          O
ATOM    358  I       358     -10.000  19.924   1.743  1.00  0.00          O
ATOM    359  I       359     -10.000  29.886   2.615  1.00  0.00          O
ATOM    360  I       360     -10.000  39.848   3.486  1.00  0.00          O
ATOM    361  I       361      -0.000 -39.848  -3.486  1.00  0.00          O
ATOM    362  I       362      -0.000 -29.886  -2.615  1.00  0.00          O
ATOM    363  I       363      -0.000 -19.924  -1.743  1.00  0.00          O
ATOM    364  I       364      -0.000  -9.962  -0.872  1.00  0.00          O
ATOM    365  I       365       0.000   0.000   0.000  1.00  0.00          O
ATOM    366  I       366       0.000   9.962   0.872  1.00  0.00          O
ATOM    367  I       367       0.000  19.924   1.743  1.00  0.00          O
ATOM    368  I       368       0.000  29.886   2.615  1.00  0.00          O
ATOM    369  I       369       0.000  39.848   3.486  1.00  0.00          O
ATOM    370  I       370      10.000 -39.848  -3.486  1.00  0.00          O
ATOM    371  I       371      10.000 -29.886  -2.615  1.00  0.00          O
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ATOM 372 I 372 10.000 -19.924 -1.743 1.00 0.00 O
ATOM 373 I 373 10.000 -9.962 -0.872 1.00 0.00 O
ATOM 374 I 374 10.000 0.000 0.000 1.00 0.00 O
ATOM 375 I 375 10.000 9.962 0.872 1.00 0.00 O
ATOM 376 I 376 10.000 19.924 1.743 1.00 0.00 O
ATOM 377 I 377 10.000 29.886 2.615 1.00 0.00 O
ATOM 378 I 378 10.000 39.848 3.486 1.00 0.00 O
ATOM 379 I 379 20.000 -39.848 -3.486 1.00 0.00 O
ATOM 380 I 380 20.000 -29.886 -2.615 1.00 0.00 O
ATOM 381 I 381 20.000 -19.924 -1.743 1.00 0.00 O
ATOM 382 I 382 20.000 -9.962 -0.872 1.00 0.00 O
ATOM 383 I 383 20.000 0.000 0.000 1.00 0.00 O
ATOM 384 I 384 20.000 9.962 0.872 1.00 0.00 O
ATOM 385 I 385 20.000 19.924 1.743 1.00 0.00 O
ATOM 386 I 386 20.000 29.886 2.615 1.00 0.00 O
ATOM 387 I 387 20.000 39.848 3.486 1.00 0.00 O
ATOM 388 I 388 30.000 -39.848 -3.486 1.00 0.00 O
ATOM 389 I 389 30.000 -29.886 -2.615 1.00 0.00 O
ATOM 390 I 390 30.000 -19.924 -1.743 1.00 0.00 O
ATOM 391 I 391 30.000 -9.962 -0.872 1.00 0.00 O
ATOM 392 I 392 30.000 0.000 0.000 1.00 0.00 O
ATOM 393 I 393 30.000 9.962 0.872 1.00 0.00 O
ATOM 394 I 394 30.000 19.924 1.743 1.00 0.00 O
ATOM 395 I 395 30.000 29.886 2.615 1.00 0.00 O
ATOM 396 I 396 30.000 39.848 3.486 1.00 0.00 O
ATOM 397 I 397 40.000 -39.848 -3.486 1.00 0.00 O
ATOM 398 I 398 40.000 -29.886 -2.615 1.00 0.00 O
ATOM 399 I 399 40.000 -19.924 -1.743 1.00 0.00 O
ATOM 400 I 400 40.000 -9.962 -0.872 1.00 0.00 O
ATOM 401 I 401 40.000 0.000 0.000 1.00 0.00 O
ATOM 402 I 402 40.000 9.962 0.872 1.00 0.00 O
ATOM 403 I 403 40.000 19.924 1.743 1.00 0.00 O
ATOM 404 I 404 40.000 29.886 2.615 1.00 0.00 O
ATOM 405 I 405 40.000 39.848 3.486 1.00 0.00 O
ATOM 406 I 406 -40.000 -40.719 6.476 1.00 0.00 O
ATOM 407 I 407 -40.000 -30.757 7.347 1.00 0.00 O
ATOM 408 I 408 -40.000 -20.795 8.219 1.00 0.00 O
ATOM 409 I 409 -40.000 -10.834 9.090 1.00 0.00 O
ATOM 410 I 410 -40.000 -0.872 9.962 1.00 0.00 O
ATOM 411 I 411 -40.000 9.090 10.834 1.00 0.00 O
ATOM 412 I 412 -40.000 19.052 11.705 1.00 0.00 O
ATOM 413 I 413 -40.000 29.014 12.577 1.00 0.00 O
ATOM 414 I 414 -40.000 38.976 13.448 1.00 0.00 O
ATOM 415 I 415 -30.000 -40.719 6.476 1.00 0.00 O
ATOM 416 I 416 -30.000 -30.757 7.347 1.00 0.00 O
ATOM 417 I 417 -30.000 -20.795 8.219 1.00 0.00 O
ATOM 418 I 418 -30.000 -10.834 9.090 1.00 0.00 O
ATOM 419 I 419 -30.000 -0.872 9.962 1.00 0.00 O

```
ATOM    420  I       420     -30.000   9.090  10.834  1.00  0.00          O
ATOM    421  I       421     -30.000  19.052  11.705  1.00  0.00          O
ATOM    422  I       422     -30.000  29.014  12.577  1.00  0.00          O
ATOM    423  I       423     -30.000  38.976  13.448  1.00  0.00          O
ATOM    424  I       424     -20.000 -40.719   6.476  1.00  0.00          O
ATOM    425  I       425     -20.000 -30.757   7.347  1.00  0.00          O
ATOM    426  I       426     -20.000 -20.795   8.219  1.00  0.00          O
ATOM    427  I       427     -20.000 -10.834   9.090  1.00  0.00          O
ATOM    428  I       428     -20.000  -0.872   9.962  1.00  0.00          O
ATOM    429  I       429     -20.000   9.090  10.834  1.00  0.00          O
ATOM    430  I       430     -20.000  19.052  11.705  1.00  0.00          O
ATOM    431  I       431     -20.000  29.014  12.577  1.00  0.00          O
ATOM    432  I       432     -20.000  38.976  13.448  1.00  0.00          O
ATOM    433  I       433     -10.000 -40.719   6.476  1.00  0.00          O
ATOM    434  I       434     -10.000 -30.757   7.347  1.00  0.00          O
ATOM    435  I       435     -10.000 -20.795   8.219  1.00  0.00          O
ATOM    436  I       436     -10.000 -10.834   9.090  1.00  0.00          O
ATOM    437  I       437     -10.000  -0.872   9.962  1.00  0.00          O
ATOM    438  I       438     -10.000   9.090  10.834  1.00  0.00          O
ATOM    439  I       439     -10.000  19.052  11.705  1.00  0.00          O
ATOM    440  I       440     -10.000  29.014  12.577  1.00  0.00          O
ATOM    441  I       441     -10.000  38.976  13.448  1.00  0.00          O
ATOM    442  I       442      -0.000 -40.719   6.476  1.00  0.00          O
ATOM    443  I       443      -0.000 -30.757   7.347  1.00  0.00          O
ATOM    444  I       444      -0.000 -20.795   8.219  1.00  0.00          O
ATOM    445  I       445       0.000 -10.834   9.090  1.00  0.00          O
ATOM    446  I       446       0.000  -0.872   9.962  1.00  0.00          O
ATOM    447  I       447       0.000   9.090  10.834  1.00  0.00          O
ATOM    448  I       448       0.000  19.052  11.705  1.00  0.00          O
ATOM    449  I       449       0.000  29.014  12.577  1.00  0.00          O
ATOM    450  I       450       0.000  38.976  13.448  1.00  0.00          O
ATOM    451  I       451      10.000 -40.719   6.476  1.00  0.00          O
ATOM    452  I       452      10.000 -30.757   7.347  1.00  0.00          O
ATOM    453  I       453      10.000 -20.795   8.219  1.00  0.00          O
ATOM    454  I       454      10.000 -10.834   9.090  1.00  0.00          O
ATOM    455  I       455      10.000  -0.872   9.962  1.00  0.00          O
ATOM    456  I       456      10.000   9.090  10.834  1.00  0.00          O
ATOM    457  I       457      10.000  19.052  11.705  1.00  0.00          O
ATOM    458  I       458      10.000  29.014  12.577  1.00  0.00          O
ATOM    459  I       459      10.000  38.976  13.448  1.00  0.00          O
ATOM    460  I       460      20.000 -40.719   6.476  1.00  0.00          O
ATOM    461  I       461      20.000 -30.757   7.347  1.00  0.00          O
ATOM    462  I       462      20.000 -20.795   8.219  1.00  0.00          O
ATOM    463  I       463      20.000 -10.834   9.090  1.00  0.00          O
ATOM    464  I       464      20.000  -0.872   9.962  1.00  0.00          O
ATOM    465  I       465      20.000   9.090  10.834  1.00  0.00          O
ATOM    466  I       466      20.000  19.052  11.705  1.00  0.00          O
ATOM    467  I       467      20.000  29.014  12.577  1.00  0.00          O
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ATOM 468 I 468 20.000 38.976 13.448 1.00 0.00 O
ATOM 469 I 469 30.000 -40.719 6.476 1.00 0.00 O
ATOM 470 I 470 30.000 -30.757 7.347 1.00 0.00 O
ATOM 471 I 471 30.000 -20.795 8.219 1.00 0.00 O
ATOM 472 I 472 30.000 -10.834 9.090 1.00 0.00 O
ATOM 473 I 473 30.000 -0.872 9.962 1.00 0.00 O
ATOM 474 I 474 30.000 9.090 10.834 1.00 0.00 O
ATOM 475 I 475 30.000 19.052 11.705 1.00 0.00 O
ATOM 476 I 476 30.000 29.014 12.577 1.00 0.00 O
ATOM 477 I 477 30.000 38.976 13.448 1.00 0.00 O
ATOM 478 I 478 40.000 -40.719 6.476 1.00 0.00 O
ATOM 479 I 479 40.000 -30.757 7.347 1.00 0.00 O
ATOM 480 I 480 40.000 -20.795 8.219 1.00 0.00 O
ATOM 481 I 481 40.000 -10.834 9.090 1.00 0.00 O
ATOM 482 I 482 40.000 -0.872 9.962 1.00 0.00 O
ATOM 483 I 483 40.000 9.090 10.834 1.00 0.00 O
ATOM 484 I 484 40.000 19.052 11.705 1.00 0.00 O
ATOM 485 I 485 40.000 29.014 12.577 1.00 0.00 O
ATOM 486 I 486 40.000 38.976 13.448 1.00 0.00 O
ATOM 487 I 487 -40.000 -41.591 16.438 1.00 0.00 O
ATOM 488 I 488 -40.000 -31.629 17.309 1.00 0.00 O
ATOM 489 I 489 -40.000 -21.667 18.181 1.00 0.00 O
ATOM 490 I 490 -40.000 -11.705 19.052 1.00 0.00 O
ATOM 491 I 491 -40.000 -1.743 19.924 1.00 0.00 O
ATOM 492 I 492 -40.000 8.219 20.795 1.00 0.00 O
ATOM 493 I 493 -40.000 18.181 21.667 1.00 0.00 O
ATOM 494 I 494 -40.000 28.143 22.539 1.00 0.00 O
ATOM 495 I 495 -40.000 38.105 23.410 1.00 0.00 O
ATOM 496 I 496 -30.000 -41.591 16.438 1.00 0.00 O
ATOM 497 I 497 -30.000 -31.629 17.309 1.00 0.00 O
ATOM 498 I 498 -30.000 -21.667 18.181 1.00 0.00 O
ATOM 499 I 499 -30.000 -11.705 19.052 1.00 0.00 O
ATOM 500 I 500 -30.000 -1.743 19.924 1.00 0.00 O
ATOM 501 I 501 -30.000 8.219 20.795 1.00 0.00 O
ATOM 502 I 502 -30.000 18.181 21.667 1.00 0.00 O
ATOM 503 I 503 -30.000 28.143 22.539 1.00 0.00 O
ATOM 504 I 504 -30.000 38.105 23.410 1.00 0.00 O
ATOM 505 I 505 -20.000 -41.591 16.438 1.00 0.00 O
ATOM 506 I 506 -20.000 -31.629 17.309 1.00 0.00 O
ATOM 507 I 507 -20.000 -21.667 18.181 1.00 0.00 O
ATOM 508 I 508 -20.000 -11.705 19.052 1.00 0.00 O
ATOM 509 I 509 -20.000 -1.743 19.924 1.00 0.00 O
ATOM 510 I 510 -20.000 8.219 20.795 1.00 0.00 O
ATOM 511 I 511 -20.000 18.181 21.667 1.00 0.00 O
ATOM 512 I 512 -20.000 28.143 22.539 1.00 0.00 O
ATOM 513 I 513 -20.000 38.105 23.410 1.00 0.00 O
ATOM 514 I 514 -10.000 -41.591 16.438 1.00 0.00 O
ATOM 515 I 515 -10.000 -31.629 17.309 1.00 0.00 O

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ATOM    516  I       516    -10.000 -21.667  18.181  1.00  0.00          O
ATOM    517  I       517    -10.000 -11.705  19.052  1.00  0.00          O
ATOM    518  I       518    -10.000  -1.743  19.924  1.00  0.00          O
ATOM    519  I       519    -10.000   8.219  20.795  1.00  0.00          O
ATOM    520  I       520    -10.000  18.181  21.667  1.00  0.00          O
ATOM    521  I       521    -10.000  28.143  22.539  1.00  0.00          O
ATOM    522  I       522    -10.000  38.105  23.410  1.00  0.00          O
ATOM    523  I       523     -0.000 -41.591  16.438  1.00  0.00          O
ATOM    524  I       524     -0.000 -31.629  17.309  1.00  0.00          O
ATOM    525  I       525      0.000 -21.667  18.181  1.00  0.00          O
ATOM    526  I       526      0.000 -11.705  19.052  1.00  0.00          O
ATOM    527  I       527      0.000  -1.743  19.924  1.00  0.00          O
ATOM    528  I       528      0.000   8.219  20.795  1.00  0.00          O
ATOM    529  I       529      0.000  18.181  21.667  1.00  0.00          O
ATOM    530  I       530      0.000  28.143  22.539  1.00  0.00          O
ATOM    531  I       531      0.000  38.105  23.410  1.00  0.00          O
ATOM    532  I       532     10.000 -41.591  16.438  1.00  0.00          O
ATOM    533  I       533     10.000 -31.629  17.309  1.00  0.00          O
ATOM    534  I       534     10.000 -21.667  18.181  1.00  0.00          O
ATOM    535  I       535     10.000 -11.705  19.052  1.00  0.00          O
ATOM    536  I       536     10.000  -1.743  19.924  1.00  0.00          O
ATOM    537  I       537     10.000   8.219  20.795  1.00  0.00          O
ATOM    538  I       538     10.000  18.181  21.667  1.00  0.00          O
ATOM    539  I       539     10.000  28.143  22.539  1.00  0.00          O
ATOM    540  I       540     10.000  38.105  23.410  1.00  0.00          O
ATOM    541  I       541     20.000 -41.591  16.438  1.00  0.00          O
ATOM    542  I       542     20.000 -31.629  17.309  1.00  0.00          O
ATOM    543  I       543     20.000 -21.667  18.181  1.00  0.00          O
ATOM    544  I       544     20.000 -11.705  19.052  1.00  0.00          O
ATOM    545  I       545     20.000  -1.743  19.924  1.00  0.00          O
ATOM    546  I       546     20.000   8.219  20.795  1.00  0.00          O
ATOM    547  I       547     20.000  18.181  21.667  1.00  0.00          O
ATOM    548  I       548     20.000  28.143  22.539  1.00  0.00          O
ATOM    549  I       549     20.000  38.105  23.410  1.00  0.00          O
ATOM    550  I       550     30.000 -41.591  16.438  1.00  0.00          O
ATOM    551  I       551     30.000 -31.629  17.309  1.00  0.00          O
ATOM    552  I       552     30.000 -21.667  18.181  1.00  0.00          O
ATOM    553  I       553     30.000 -11.705  19.052  1.00  0.00          O
ATOM    554  I       554     30.000  -1.743  19.924  1.00  0.00          O
ATOM    555  I       555     30.000   8.219  20.795  1.00  0.00          O
ATOM    556  I       556     30.000  18.181  21.667  1.00  0.00          O
ATOM    557  I       557     30.000  28.143  22.539  1.00  0.00          O
ATOM    558  I       558     30.000  38.105  23.410  1.00  0.00          O
ATOM    559  I       559     40.000 -41.591  16.438  1.00  0.00          O
ATOM    560  I       560     40.000 -31.629  17.309  1.00  0.00          O
ATOM    561  I       561     40.000 -21.667  18.181  1.00  0.00          O
ATOM    562  I       562     40.000 -11.705  19.052  1.00  0.00          O
ATOM    563  I       563     40.000  -1.743  19.924  1.00  0.00          O
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ATOM 564 I 564 40.000 8.219 20.795 1.00 0.00 O
ATOM 565 I 565 40.000 18.181 21.667 1.00 0.00 O
ATOM 566 I 566 40.000 28.143 22.539 1.00 0.00 O
ATOM 567 I 567 40.000 38.105 23.410 1.00 0.00 O
ATOM 568 I 568 -40.000 -42.462 26.400 1.00 0.00 O
ATOM 569 I 569 -40.000 -32.501 27.271 1.00 0.00 O
ATOM 570 I 570 -40.000 -22.539 28.143 1.00 0.00 O
ATOM 571 I 571 -40.000 -12.577 29.014 1.00 0.00 O
ATOM 572 I 572 -40.000 -2.615 29.886 1.00 0.00 O
ATOM 573 I 573 -40.000 7.347 30.757 1.00 0.00 O
ATOM 574 I 574 -40.000 17.309 31.629 1.00 0.00 O
ATOM 575 I 575 -40.000 27.271 32.501 1.00 0.00 O
ATOM 576 I 576 -40.000 37.233 33.372 1.00 0.00 O
ATOM 577 I 577 -30.000 -42.462 26.400 1.00 0.00 O
ATOM 578 I 578 -30.000 -32.501 27.271 1.00 0.00 O
ATOM 579 I 579 -30.000 -22.539 28.143 1.00 0.00 O
ATOM 580 I 580 -30.000 -12.577 29.014 1.00 0.00 O
ATOM 581 I 581 -30.000 -2.615 29.886 1.00 0.00 O
ATOM 582 I 582 -30.000 7.347 30.757 1.00 0.00 O
ATOM 583 I 583 -30.000 17.309 31.629 1.00 0.00 O
ATOM 584 I 584 -30.000 27.271 32.501 1.00 0.00 O
ATOM 585 I 585 -30.000 37.233 33.372 1.00 0.00 O
ATOM 586 I 586 -20.000 -42.462 26.400 1.00 0.00 O
ATOM 587 I 587 -20.000 -32.501 27.271 1.00 0.00 O
ATOM 588 I 588 -20.000 -22.539 28.143 1.00 0.00 O
ATOM 589 I 589 -20.000 -12.577 29.014 1.00 0.00 O
ATOM 590 I 590 -20.000 -2.615 29.886 1.00 0.00 O
ATOM 591 I 591 -20.000 7.347 30.757 1.00 0.00 O
ATOM 592 I 592 -20.000 17.309 31.629 1.00 0.00 O
ATOM 593 I 593 -20.000 27.271 32.501 1.00 0.00 O
ATOM 594 I 594 -20.000 37.233 33.372 1.00 0.00 O
ATOM 595 I 595 -10.000 -42.462 26.400 1.00 0.00 O
ATOM 596 I 596 -10.000 -32.501 27.271 1.00 0.00 O
ATOM 597 I 597 -10.000 -22.539 28.143 1.00 0.00 O
ATOM 598 I 598 -10.000 -12.577 29.014 1.00 0.00 O
ATOM 599 I 599 -10.000 -2.615 29.886 1.00 0.00 O
ATOM 600 I 600 -10.000 7.347 30.757 1.00 0.00 O
ATOM 601 I 601 -10.000 17.309 31.629 1.00 0.00 O
ATOM 602 I 602 -10.000 27.271 32.501 1.00 0.00 O
ATOM 603 I 603 -10.000 37.233 33.372 1.00 0.00 O
ATOM 604 I 604 -0.000 -42.462 26.400 1.00 0.00 O
ATOM 605 I 605 0.000 -32.501 27.271 1.00 0.00 O
ATOM 606 I 606 0.000 -22.539 28.143 1.00 0.00 O
ATOM 607 I 607 0.000 -12.577 29.014 1.00 0.00 O
ATOM 608 I 608 0.000 -2.615 29.886 1.00 0.00 O
ATOM 609 I 609 0.000 7.347 30.757 1.00 0.00 O
ATOM 610 I 610 0.000 17.309 31.629 1.00 0.00 O
ATOM 611 I 611 0.000 27.271 32.501 1.00 0.00 O

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ATOM    612  I       612       0.000  37.233  33.372  1.00  0.00          O
ATOM    613  I       613      10.000 -42.462  26.400  1.00  0.00          O
ATOM    614  I       614      10.000 -32.501  27.271  1.00  0.00          O
ATOM    615  I       615      10.000 -22.539  28.143  1.00  0.00          O
ATOM    616  I       616      10.000 -12.577  29.014  1.00  0.00          O
ATOM    617  I       617      10.000  -2.615  29.886  1.00  0.00          O
ATOM    618  I       618      10.000   7.347  30.757  1.00  0.00          O
ATOM    619  I       619      10.000  17.309  31.629  1.00  0.00          O
ATOM    620  I       620      10.000  27.271  32.501  1.00  0.00          O
ATOM    621  I       621      10.000  37.233  33.372  1.00  0.00          O
ATOM    622  I       622      20.000 -42.462  26.400  1.00  0.00          O
ATOM    623  I       623      20.000 -32.501  27.271  1.00  0.00          O
ATOM    624  I       624      20.000 -22.539  28.143  1.00  0.00          O
ATOM    625  I       625      20.000 -12.577  29.014  1.00  0.00          O
ATOM    626  I       626      20.000  -2.615  29.886  1.00  0.00          O
ATOM    627  I       627      20.000   7.347  30.757  1.00  0.00          O
ATOM    628  I       628      20.000  17.309  31.629  1.00  0.00          O
ATOM    629  I       629      20.000  27.271  32.501  1.00  0.00          O
ATOM    630  I       630      20.000  37.233  33.372  1.00  0.00          O
ATOM    631  I       631      30.000 -42.462  26.400  1.00  0.00          O
ATOM    632  I       632      30.000 -32.501  27.271  1.00  0.00          O
ATOM    633  I       633      30.000 -22.539  28.143  1.00  0.00          O
ATOM    634  I       634      30.000 -12.577  29.014  1.00  0.00          O
ATOM    635  I       635      30.000  -2.615  29.886  1.00  0.00          O
ATOM    636  I       636      30.000   7.347  30.757  1.00  0.00          O
ATOM    637  I       637      30.000  17.309  31.629  1.00  0.00          O
ATOM    638  I       638      30.000  27.271  32.501  1.00  0.00          O
ATOM    639  I       639      30.000  37.233  33.372  1.00  0.00          O
ATOM    640  I       640      40.000 -42.462  26.400  1.00  0.00          O
ATOM    641  I       641      40.000 -32.501  27.271  1.00  0.00          O
ATOM    642  I       642      40.000 -22.539  28.143  1.00  0.00          O
ATOM    643  I       643      40.000 -12.577  29.014  1.00  0.00          O
ATOM    644  I       644      40.000  -2.615  29.886  1.00  0.00          O
ATOM    645  I       645      40.000   7.347  30.757  1.00  0.00          O
ATOM    646  I       646      40.000  17.309  31.629  1.00  0.00          O
ATOM    647  I       647      40.000  27.271  32.501  1.00  0.00          O
ATOM    648  I       648      40.000  37.233  33.372  1.00  0.00          O
ATOM    649  I       649     -40.000 -43.334  36.362  1.00  0.00          O
ATOM    650  I       650     -40.000 -33.372  37.233  1.00  0.00          O
ATOM    651  I       651     -40.000 -23.410  38.105  1.00  0.00          O
ATOM    652  I       652     -40.000 -13.448  38.976  1.00  0.00          O
ATOM    653  I       653     -40.000  -3.486  39.848  1.00  0.00          O
ATOM    654  I       654     -40.000   6.476  40.719  1.00  0.00          O
ATOM    655  I       655     -40.000  16.438  41.591  1.00  0.00          O
ATOM    656  I       656     -40.000  26.400  42.462  1.00  0.00          O
ATOM    657  I       657     -40.000  36.362  43.334  1.00  0.00          O
ATOM    658  I       658     -30.000 -43.334  36.362  1.00  0.00          O
ATOM    659  I       659     -30.000 -33.372  37.233  1.00  0.00          O
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ATOM    660  I       660     -30.000 -23.410  38.105  1.00  0.00          O
ATOM    661  I       661     -30.000 -13.448  38.976  1.00  0.00          O
ATOM    662  I       662     -30.000  -3.486  39.848  1.00  0.00          O
ATOM    663  I       663     -30.000   6.476  40.719  1.00  0.00          O
ATOM    664  I       664     -30.000  16.438  41.591  1.00  0.00          O
ATOM    665  I       665     -30.000  26.400  42.462  1.00  0.00          O
ATOM    666  I       666     -30.000  36.362  43.334  1.00  0.00          O
ATOM    667  I       667     -20.000 -43.334  36.362  1.00  0.00          O
ATOM    668  I       668     -20.000 -33.372  37.233  1.00  0.00          O
ATOM    669  I       669     -20.000 -23.410  38.105  1.00  0.00          O
ATOM    670  I       670     -20.000 -13.448  38.976  1.00  0.00          O
ATOM    671  I       671     -20.000  -3.486  39.848  1.00  0.00          O
ATOM    672  I       672     -20.000   6.476  40.719  1.00  0.00          O
ATOM    673  I       673     -20.000  16.438  41.591  1.00  0.00          O
ATOM    674  I       674     -20.000  26.400  42.462  1.00  0.00          O
ATOM    675  I       675     -20.000  36.362  43.334  1.00  0.00          O
ATOM    676  I       676     -10.000 -43.334  36.362  1.00  0.00          O
ATOM    677  I       677     -10.000 -33.372  37.233  1.00  0.00          O
ATOM    678  I       678     -10.000 -23.410  38.105  1.00  0.00          O
ATOM    679  I       679     -10.000 -13.448  38.976  1.00  0.00          O
ATOM    680  I       680     -10.000  -3.486  39.848  1.00  0.00          O
ATOM    681  I       681     -10.000   6.476  40.719  1.00  0.00          O
ATOM    682  I       682     -10.000  16.438  41.591  1.00  0.00          O
ATOM    683  I       683     -10.000  26.400  42.462  1.00  0.00          O
ATOM    684  I       684     -10.000  36.362  43.334  1.00  0.00          O
ATOM    685  I       685       0.000 -43.334  36.362  1.00  0.00          O
ATOM    686  I       686       0.000 -33.372  37.233  1.00  0.00          O
ATOM    687  I       687       0.000 -23.410  38.105  1.00  0.00          O
ATOM    688  I       688       0.000 -13.448  38.976  1.00  0.00          O
ATOM    689  I       689       0.000  -3.486  39.848  1.00  0.00          O
ATOM    690  I       690       0.000   6.476  40.719  1.00  0.00          O
ATOM    691  I       691       0.000  16.438  41.591  1.00  0.00          O
ATOM    692  I       692       0.000  26.400  42.462  1.00  0.00          O
ATOM    693  I       693       0.000  36.362  43.334  1.00  0.00          O
ATOM    694  I       694      10.000 -43.334  36.362  1.00  0.00          O
ATOM    695  I       695      10.000 -33.372  37.233  1.00  0.00          O
ATOM    696  I       696      10.000 -23.410  38.105  1.00  0.00          O
ATOM    697  I       697      10.000 -13.448  38.976  1.00  0.00          O
ATOM    698  I       698      10.000  -3.486  39.848  1.00  0.00          O
ATOM    699  I       699      10.000   6.476  40.719  1.00  0.00          O
ATOM    700  I       700      10.000  16.438  41.591  1.00  0.00          O
ATOM    701  I       701      10.000  26.400  42.462  1.00  0.00          O
ATOM    702  I       702      10.000  36.362  43.334  1.00  0.00          O
ATOM    703  I       703      20.000 -43.334  36.362  1.00  0.00          O
ATOM    704  I       704      20.000 -33.372  37.233  1.00  0.00          O
ATOM    705  I       705      20.000 -23.410  38.105  1.00  0.00          O
ATOM    706  I       706      20.000 -13.448  38.976  1.00  0.00          O
ATOM    707  I       707      20.000  -3.486  39.848  1.00  0.00          O
```

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ATOM    708  I       708      20.000   6.476  40.719  1.00  0.00          O
ATOM    709  I       709      20.000  16.438  41.591  1.00  0.00          O
ATOM    710  I       710      20.000  26.400  42.462  1.00  0.00          O
ATOM    711  I       711      20.000  36.362  43.334  1.00  0.00          O
ATOM    712  I       712      30.000 -43.334  36.362  1.00  0.00          O
ATOM    713  I       713      30.000 -33.372  37.233  1.00  0.00          O
ATOM    714  I       714      30.000 -23.410  38.105  1.00  0.00          O
ATOM    715  I       715      30.000 -13.448  38.976  1.00  0.00          O
ATOM    716  I       716      30.000  -3.486  39.848  1.00  0.00          O
ATOM    717  I       717      30.000   6.476  40.719  1.00  0.00          O
ATOM    718  I       718      30.000  16.438  41.591  1.00  0.00          O
ATOM    719  I       719      30.000  26.400  42.462  1.00  0.00          O
ATOM    720  I       720      30.000  36.362  43.334  1.00  0.00          O
ATOM    721  I       721      40.000 -43.334  36.362  1.00  0.00          O
ATOM    722  I       722      40.000 -33.372  37.233  1.00  0.00          O
ATOM    723  I       723      40.000 -23.410  38.105  1.00  0.00          O
ATOM    724  I       724      40.000 -13.448  38.976  1.00  0.00          O
ATOM    725  I       725      40.000  -3.486  39.848  1.00  0.00          O
ATOM    726  I       726      40.000   6.476  40.719  1.00  0.00          O
ATOM    727  I       727      40.000  16.438  41.591  1.00  0.00          O
ATOM    728  I       728      40.000  26.400  42.462  1.00  0.00          O
ATOM    729  I       729      40.000  36.362  43.334  1.00  0.00          O
END
```

15.2.2 Archivo PDB Estructura Cúbica Centrada en las Caras (FCC)

Archivo PDB generado correspondiente a la estructura cúbica centrada en las caras de 4 celdas por lado, 10 Angstroms en los parámetros de red a, b y c:

Campo1	Campo2	Campo3	Campo4	Campo5	Campo6	Campo7	Campo8	Campo9	Campo 10
Registro	serial	elemento	Numero de secuncia	Coordenadas otogonales para x	Coordenadas otogonales para y	Coordenadas otogonales para z	ocupancia	Factor de temperatura	Carga en el átomo

```
ATOM      1  I         1      10.000  10.000  10.000  1.00  0.00          O
ATOM      2  I         2       6.894  18.047  15.059  1.00  0.00          O
ATOM      3  I         3       3.788  26.095  20.118  1.00  0.00          O
ATOM      4  I         4       0.681  34.142  25.176  1.00  0.00          O
ATOM      5  I         5      -2.425  42.190  30.235  1.00  0.00          O
ATOM      6  I         6      -5.531  50.237  35.294  1.00  0.00          O
ATOM      7  I         7      -8.637  58.284  40.353  1.00  0.00          O
ATOM      8  I         8     -11.743  66.332  45.412  1.00  0.00          O
ATOM      9  I         9      18.047  15.059   6.894  1.00  0.00          O
ATOM     10  I        10      14.941  23.106  11.953  1.00  0.00          O
ATOM     11  I        11      11.835  31.154  17.011  1.00  0.00          O
ATOM     12  I        12       8.729  39.201  22.070  1.00  0.00          O
ATOM     13  I        13       5.623  47.248  27.129  1.00  0.00          O
ATOM     14  I        14       2.517  55.296  32.188  1.00  0.00          O
ATOM     15  I        15      -0.590  63.343  37.247  1.00  0.00          O
ATOM     16  I        16      -3.696  71.390  42.305  1.00  0.00          O
ATOM     17  I        17      26.095  20.118   3.788  1.00  0.00          O
ATOM     18  I        18      22.989  28.165   8.846  1.00  0.00          O
ATOM     19  I        19      19.882  36.212  13.905  1.00  0.00          O
ATOM     20  I        20      16.776  44.260  18.964  1.00  0.00          O
ATOM     21  I        21      13.670  52.307  24.023  1.00  0.00          O
ATOM     22  I        22      10.564  60.354  29.082  1.00  0.00          O
ATOM     23  I        23       7.458  68.402  34.140  1.00  0.00          O
ATOM     24  I        24       4.352  76.449  39.199  1.00  0.00          O
ATOM     25  I        25      34.142  25.176   0.681  1.00  0.00          O
ATOM     26  I        26      31.036  33.224   5.740  1.00  0.00          O
ATOM     27  I        27      27.930  41.271  10.799  1.00  0.00          O
ATOM     28  I        28      24.824  49.319  15.858  1.00  0.00          O
ATOM     29  I        29      21.717  57.366  20.917  1.00  0.00          O
ATOM     30  I        30      18.611  65.413  25.975  1.00  0.00          O
ATOM     31  I        31      15.505  73.461  31.034  1.00  0.00          O
ATOM     32  I        32      12.399  81.508  36.093  1.00  0.00          O
ATOM     33  I        33      42.190  30.235  -2.425  1.00  0.00          O
ATOM     34  I        34      39.083  38.283   2.634  1.00  0.00          O
ATOM     35  I        35      35.977  46.330   7.693  1.00  0.00          O
ATOM     36  I        36      32.871  54.377  12.752  1.00  0.00          O
ATOM     37  I        37      29.765  62.425  17.810  1.00  0.00          O
```

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ATOM     38  I        38      26.659  70.472  22.869  1.00  0.00           O
ATOM     39  I        39      23.552  78.519  27.928  1.00  0.00           O
ATOM     40  I        40      20.446  86.567  32.987  1.00  0.00           O
ATOM     41  I        41      50.237  35.294  -5.531  1.00  0.00           O
ATOM     42  I        42      47.131  43.341  -0.472  1.00  0.00           O
ATOM     43  I        43      44.025  51.389   4.587  1.00  0.00           O
ATOM     44  I        44      40.918  59.436   9.646  1.00  0.00           O
ATOM     45  I        45      37.812  67.483  14.704  1.00  0.00           O
ATOM     46  I        46      34.706  75.531  19.763  1.00  0.00           O
ATOM     47  I        47      31.600  83.578  24.822  1.00  0.00           O
ATOM     48  I        48      28.494  91.626  29.881  1.00  0.00           O
ATOM     49  I        49      58.284  40.353  -8.637  1.00  0.00           O
ATOM     50  I        50      55.178  48.400  -3.578  1.00  0.00           O
ATOM     51  I        51      52.072  56.448   1.481  1.00  0.00           O
ATOM     52  I        52      48.966  64.495   6.539  1.00  0.00           O
ATOM     53  I        53      45.860  72.542  11.598  1.00  0.00           O
ATOM     54  I        54      42.753  80.590  16.657  1.00  0.00           O
ATOM     55  I        55      39.647  88.637  21.716  1.00  0.00           O
ATOM     56  I        56      36.541  96.684  26.775  1.00  0.00           O
ATOM     57  I        57      66.332  45.412 -11.743  1.00  0.00           O
ATOM     58  I        58      63.225  53.459  -6.684  1.00  0.00           O
ATOM     59  I        59      60.119  61.506  -1.626  1.00  0.00           O
ATOM     60  I        60      57.013  69.554   3.433  1.00  0.00           O
ATOM     61  I        61      53.907  77.601   8.492  1.00  0.00           O
ATOM     62  I        62      50.801  85.648  13.551  1.00  0.00           O
ATOM     63  I        63      47.695  93.696  18.610  1.00  0.00           O
ATOM     64  I        64      44.588 101.743  23.668  1.00  0.00           O
ATOM     65  I        65      12.471  16.553  10.976  1.00  0.00           O
ATOM     66  I        66       9.364  24.600  16.035  1.00  0.00           O
ATOM     67  I        67       6.258  32.648  21.094  1.00  0.00           O
ATOM     68  I        68       3.152  40.695  26.153  1.00  0.00           O
ATOM     69  I        69       0.046  48.743  31.211  1.00  0.00           O
ATOM     70  I        70      -3.060  56.790  36.270  1.00  0.00           O
ATOM     71  I        71      -6.166  64.837  41.329  1.00  0.00           O
ATOM     72  I        72      -9.273  72.885  46.388  1.00  0.00           O
ATOM     73  I        73      20.518  21.612   7.870  1.00  0.00           O
ATOM     74  I        74      17.412  29.659  12.929  1.00  0.00           O
ATOM     75  I        75      14.306  37.707  17.988  1.00  0.00           O
ATOM     76  I        76      11.199  45.754  23.047  1.00  0.00           O
ATOM     77  I        77       8.093  53.801  28.105  1.00  0.00           O
ATOM     78  I        78       4.987  61.849  33.164  1.00  0.00           O
ATOM     79  I        79       1.881  69.896  38.223  1.00  0.00           O
ATOM     80  I        80      -1.225  77.944  43.282  1.00  0.00           O
ATOM     81  I        81      28.565  26.671   4.764  1.00  0.00           O
ATOM     82  I        82      25.459  34.718   9.823  1.00  0.00           O
ATOM     83  I        83      22.353  42.765  14.882  1.00  0.00           O
ATOM     84  I        84      19.247  50.813  19.940  1.00  0.00           O
ATOM     85  I        85      16.141  58.860  24.999  1.00  0.00           O
```

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ATOM     86  I       86     13.034  66.908  30.058  1.00  0.00          O
ATOM     87  I       87      9.928  74.955  35.117  1.00  0.00          O
ATOM     88  I       88      6.822  83.002  40.176  1.00  0.00          O
ATOM     89  I       89     36.613  31.729   1.658  1.00  0.00          O
ATOM     90  I       90     33.507  39.777   6.717  1.00  0.00          O
ATOM     91  I       91     30.400  47.824  11.775  1.00  0.00          O
ATOM     92  I       92     27.294  55.872  16.834  1.00  0.00          O
ATOM     93  I       93     24.188  63.919  21.893  1.00  0.00          O
ATOM     94  I       94     21.082  71.966  26.952  1.00  0.00          O
ATOM     95  I       95     17.976  80.014  32.011  1.00  0.00          O
ATOM     96  I       96     14.870  88.061  37.069  1.00  0.00          O
ATOM     97  I       97     44.660  36.788  -1.448  1.00  0.00          O
ATOM     98  I       98     41.554  44.836   3.610  1.00  0.00          O
ATOM     99  I       99     38.448  52.883   8.669  1.00  0.00          O
ATOM    100  I      100     35.342  60.930  13.728  1.00  0.00          O
ATOM    101  I      101     32.235  68.978  18.787  1.00  0.00          O
ATOM    102  I      102     29.129  77.025  23.846  1.00  0.00          O
ATOM    103  I      103     26.023  85.073  28.904  1.00  0.00          O
ATOM    104  I      104     22.917  93.120  33.963  1.00  0.00          O
ATOM    105  I      105     52.707  41.847  -4.555  1.00  0.00          O
ATOM    106  I      106     49.601  49.894   0.504  1.00  0.00          O
ATOM    107  I      107     46.495  57.942   5.563  1.00  0.00          O
ATOM    108  I      108     43.389  65.989  10.622  1.00  0.00          O
ATOM    109  I      109     40.283  74.037  15.681  1.00  0.00          O
ATOM    110  I      110     37.177  82.084  20.739  1.00  0.00          O
ATOM    111  I      111     34.070  90.131  25.798  1.00  0.00          O
ATOM    112  I      112     30.964  98.179  30.857  1.00  0.00          O
ATOM    113  I      113     60.755  46.906  -7.661  1.00  0.00          O
ATOM    114  I      114     57.649  54.953  -2.602  1.00  0.00          O
ATOM    115  I      115     54.543  63.001   2.457  1.00  0.00          O
ATOM    116  I      116     51.436  71.048   7.516  1.00  0.00          O
ATOM    117  I      117     48.330  79.095  12.574  1.00  0.00          O
ATOM    118  I      118     45.224  87.143  17.633  1.00  0.00          O
ATOM    119  I      119     42.118  95.190  22.692  1.00  0.00          O
ATOM    120  I      120     39.012 103.237  27.751  1.00  0.00          O
ATOM    121  I      121     68.802  51.965 -10.767  1.00  0.00          O
ATOM    122  I      122     65.696  60.012  -5.708  1.00  0.00          O
ATOM    123  I      123     62.590  68.059  -0.649  1.00  0.00          O
ATOM    124  I      124     59.484  76.107   4.409  1.00  0.00          O
ATOM    125  I      125     56.378  84.154   9.468  1.00  0.00          O
ATOM    126  I      126     53.271  92.202  14.527  1.00  0.00          O
ATOM    127  I      127     50.165 100.249  19.586  1.00  0.00          O
ATOM    128  I      128     47.059 108.296  24.645  1.00  0.00          O
ATOM    129  I      129     15.059   6.894  18.047  1.00  0.00          O
ATOM    130  I      130     11.953  14.941  23.106  1.00  0.00          O
ATOM    131  I      131      8.846  22.989  28.165  1.00  0.00          O
ATOM    132  I      132      5.740  31.036  33.224  1.00  0.00          O
ATOM    133  I      133      2.634  39.083  38.283  1.00  0.00          O
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ATOM    134  I        134      -0.472  47.131  43.341  1.00  0.00          O
ATOM    135  I        135      -3.578  55.178  48.400  1.00  0.00          O
ATOM    136  I        136      -6.684  63.225  53.459  1.00  0.00          O
ATOM    137  I        137      23.106  11.953  14.941  1.00  0.00          O
ATOM    138  I        138      20.000  20.000  20.000  1.00  0.00          O
ATOM    139  I        139      16.894  28.047  25.059  1.00  0.00          O
ATOM    140  I        140      13.788  36.095  30.118  1.00  0.00          O
ATOM    141  I        141      10.681  44.142  35.176  1.00  0.00          O
ATOM    142  I        142       7.575  52.190  40.235  1.00  0.00          O
ATOM    143  I        143       4.469  60.237  45.294  1.00  0.00          O
ATOM    144  I        144       1.363  68.284  50.353  1.00  0.00          O
ATOM    145  I        145      31.154  17.011  11.835  1.00  0.00          O
ATOM    146  I        146      28.047  25.059  16.894  1.00  0.00          O
ATOM    147  I        147      24.941  33.106  21.953  1.00  0.00          O
ATOM    148  I        148      21.835  41.154  27.011  1.00  0.00          O
ATOM    149  I        149      18.729  49.201  32.070  1.00  0.00          O
ATOM    150  I        150      15.623  57.248  37.129  1.00  0.00          O
ATOM    151  I        151      12.517  65.296  42.188  1.00  0.00          O
ATOM    152  I        152       9.410  73.343  47.247  1.00  0.00          O
ATOM    153  I        153      39.201  22.070   8.729  1.00  0.00          O
ATOM    154  I        154      36.095  30.118  13.788  1.00  0.00          O
ATOM    155  I        155      32.989  38.165  18.846  1.00  0.00          O
ATOM    156  I        156      29.882  46.212  23.905  1.00  0.00          O
ATOM    157  I        157      26.776  54.260  28.964  1.00  0.00          O
ATOM    158  I        158      23.670  62.307  34.023  1.00  0.00          O
ATOM    159  I        159      20.564  70.354  39.082  1.00  0.00          O
ATOM    160  I        160      17.458  78.402  44.140  1.00  0.00          O
ATOM    161  I        161      47.248  27.129   5.623  1.00  0.00          O
ATOM    162  I        162      44.142  35.176  10.681  1.00  0.00          O
ATOM    163  I        163      41.036  43.224  15.740  1.00  0.00          O
ATOM    164  I        164      37.930  51.271  20.799  1.00  0.00          O
ATOM    165  I        165      34.824  59.319  25.858  1.00  0.00          O
ATOM    166  I        166      31.717  67.366  30.917  1.00  0.00          O
ATOM    167  I        167      28.611  75.413  35.975  1.00  0.00          O
ATOM    168  I        168      25.505  83.461  41.034  1.00  0.00          O
ATOM    169  I        169      55.296  32.188   2.517  1.00  0.00          O
ATOM    170  I        170      52.190  40.235   7.575  1.00  0.00          O
ATOM    171  I        171      49.083  48.283  12.634  1.00  0.00          O
ATOM    172  I        172      45.977  56.330  17.693  1.00  0.00          O
ATOM    173  I        173      42.871  64.377  22.752  1.00  0.00          O
ATOM    174  I        174      39.765  72.425  27.810  1.00  0.00          O
ATOM    175  I        175      36.659  80.472  32.869  1.00  0.00          O
ATOM    176  I        176      33.552  88.519  37.928  1.00  0.00          O
ATOM    177  I        177      63.343  37.247  -0.590  1.00  0.00          O
ATOM    178  I        178      60.237  45.294   4.469  1.00  0.00          O
ATOM    179  I        179      57.131  53.341   9.528  1.00  0.00          O
ATOM    180  I        180      54.025  61.389  14.587  1.00  0.00          O
ATOM    181  I        181      50.918  69.436  19.646  1.00  0.00          O
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ATOM    182  I       182      47.812  77.483  24.704  1.00  0.00          O
ATOM    183  I       183      44.706  85.531  29.763  1.00  0.00          O
ATOM    184  I       184      41.600  93.578  34.822  1.00  0.00          O
ATOM    185  I       185      71.390  42.305  -3.696  1.00  0.00          O
ATOM    186  I       186      68.284  50.353   1.363  1.00  0.00          O
ATOM    187  I       187      65.178  58.400   6.422  1.00  0.00          O
ATOM    188  I       188      62.072  66.448  11.481  1.00  0.00          O
ATOM    189  I       189      58.966  74.495  16.539  1.00  0.00          O
ATOM    190  I       190      55.860  82.542  21.598  1.00  0.00          O
ATOM    191  I       191      52.753  90.590  26.657  1.00  0.00          O
ATOM    192  I       192      49.647  98.637  31.716  1.00  0.00          O
ATOM    193  I       193      17.529  13.447  19.024  1.00  0.00          O
ATOM    194  I       194      14.423  21.494  24.082  1.00  0.00          O
ATOM    195  I       195      11.317  29.542  29.141  1.00  0.00          O
ATOM    196  I       196       8.211  37.589  34.200  1.00  0.00          O
ATOM    197  I       197       5.105  45.636  39.259  1.00  0.00          O
ATOM    198  I       198       1.999  53.684  44.318  1.00  0.00          O
ATOM    199  I       199      -1.108  61.731  49.376  1.00  0.00          O
ATOM    200  I       200      -4.214  69.779  54.435  1.00  0.00          O
ATOM    201  I       201      25.577  18.506  15.918  1.00  0.00          O
ATOM    202  I       202      22.471  26.553  20.976  1.00  0.00          O
ATOM    203  I       203      19.364  34.600  26.035  1.00  0.00          O
ATOM    204  I       204      16.258  42.648  31.094  1.00  0.00          O
ATOM    205  I       205      13.152  50.695  36.153  1.00  0.00          O
ATOM    206  I       206      10.046  58.743  41.211  1.00  0.00          O
ATOM    207  I       207       6.940  66.790  46.270  1.00  0.00          O
ATOM    208  I       208       3.834  74.837  51.329  1.00  0.00          O
ATOM    209  I       209      33.624  23.565  12.811  1.00  0.00          O
ATOM    210  I       210      30.518  31.612  17.870  1.00  0.00          O
ATOM    211  I       211      27.412  39.659  22.929  1.00  0.00          O
ATOM    212  I       212      24.306  47.707  27.988  1.00  0.00          O
ATOM    213  I       213      21.199  55.754  33.047  1.00  0.00          O
ATOM    214  I       214      18.093  63.801  38.105  1.00  0.00          O
ATOM    215  I       215      14.987  71.849  43.164  1.00  0.00          O
ATOM    216  I       216      11.881  79.896  48.223  1.00  0.00          O
ATOM    217  I       217      41.672  28.623   9.705  1.00  0.00          O
ATOM    218  I       218      38.565  36.671  14.764  1.00  0.00          O
ATOM    219  I       219      35.459  44.718  19.823  1.00  0.00          O
ATOM    220  I       220      32.353  52.765  24.882  1.00  0.00          O
ATOM    221  I       221      29.247  60.813  29.940  1.00  0.00          O
ATOM    222  I       222      26.141  68.860  34.999  1.00  0.00          O
ATOM    223  I       223      23.034  76.908  40.058  1.00  0.00          O
ATOM    224  I       224      19.928  84.955  45.117  1.00  0.00          O
ATOM    225  I       225      49.719  33.682   6.599  1.00  0.00          O
ATOM    226  I       226      46.613  41.729  11.658  1.00  0.00          O
ATOM    227  I       227      43.507  49.777  16.717  1.00  0.00          O
ATOM    228  I       228      40.400  57.824  21.775  1.00  0.00          O
ATOM    229  I       229      37.294  65.872  26.834  1.00  0.00          O
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ATOM    230  I       230      34.188  73.919  31.893  1.00  0.00          O
ATOM    231  I       231      31.082  81.966  36.952  1.00  0.00          O
ATOM    232  I       232      27.976  90.014  42.011  1.00  0.00          O
ATOM    233  I       233      57.766  38.741   3.493  1.00  0.00          O
ATOM    234  I       234      54.660  46.788   8.552  1.00  0.00          O
ATOM    235  I       235      51.554  54.836  13.610  1.00  0.00          O
ATOM    236  I       236      48.448  62.883  18.669  1.00  0.00          O
ATOM    237  I       237      45.342  70.930  23.728  1.00  0.00          O
ATOM    238  I       238      42.235  78.978  28.787  1.00  0.00          O
ATOM    239  I       239      39.129  87.025  33.846  1.00  0.00          O
ATOM    240  I       240      36.023  95.073  38.904  1.00  0.00          O
ATOM    241  I       241      65.814  43.800   0.387  1.00  0.00          O
ATOM    242  I       242      62.707  51.847   5.445  1.00  0.00          O
ATOM    243  I       243      59.601  59.894  10.504  1.00  0.00          O
ATOM    244  I       244      56.495  67.942  15.563  1.00  0.00          O
ATOM    245  I       245      53.389  75.989  20.622  1.00  0.00          O
ATOM    246  I       246      50.283  84.037  25.681  1.00  0.00          O
ATOM    247  I       247      47.177  92.084  30.739  1.00  0.00          O
ATOM    248  I       248      44.070 100.131  35.798  1.00  0.00          O
ATOM    249  I       249      73.861  48.858  -2.720  1.00  0.00          O
ATOM    250  I       250      70.755  56.906   2.339  1.00  0.00          O
ATOM    251  I       251      67.649  64.953   7.398  1.00  0.00          O
ATOM    252  I       252      64.543  73.001  12.457  1.00  0.00          O
ATOM    253  I       253      61.436  81.048  17.516  1.00  0.00          O
ATOM    254  I       254      58.330  89.095  22.574  1.00  0.00          O
ATOM    255  I       255      55.224  97.143  27.633  1.00  0.00          O
ATOM    256  I       256      52.118 105.190  32.692  1.00  0.00          O
ATOM    257  I       257      20.118   3.788  26.095  1.00  0.00          O
ATOM    258  I       258      17.011  11.835  31.154  1.00  0.00          O
ATOM    259  I       259      13.905  19.882  36.212  1.00  0.00          O
ATOM    260  I       260      10.799  27.930  41.271  1.00  0.00          O
ATOM    261  I       261       7.693  35.977  46.330  1.00  0.00          O
ATOM    262  I       262       4.587  44.025  51.389  1.00  0.00          O
ATOM    263  I       263       1.481  52.072  56.448  1.00  0.00          O
ATOM    264  I       264      -1.626  60.119  61.506  1.00  0.00          O
ATOM    265  I       265      28.165   8.846  22.989  1.00  0.00          O
ATOM    266  I       266      25.059  16.894  28.047  1.00  0.00          O
ATOM    267  I       267      21.953  24.941  33.106  1.00  0.00          O
ATOM    268  I       268      18.846  32.989  38.165  1.00  0.00          O
ATOM    269  I       269      15.740  41.036  43.224  1.00  0.00          O
ATOM    270  I       270      12.634  49.083  48.283  1.00  0.00          O
ATOM    271  I       271       9.528  57.131  53.341  1.00  0.00          O
ATOM    272  I       272       6.422  65.178  58.400  1.00  0.00          O
ATOM    273  I       273      36.212  13.905  19.882  1.00  0.00          O
ATOM    274  I       274      33.106  21.953  24.941  1.00  0.00          O
ATOM    275  I       275      30.000  30.000  30.000  1.00  0.00          O
ATOM    276  I       276      26.894  38.047  35.059  1.00  0.00          O
ATOM    277  I       277      23.788  46.095  40.118  1.00  0.00          O
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ATOM    278  I       278      20.681  54.142  45.176  1.00  0.00          O
ATOM    279  I       279      17.575  62.190  50.235  1.00  0.00          O
ATOM    280  I       280      14.469  70.237  55.294  1.00  0.00          O
ATOM    281  I       281      44.260  18.964  16.776  1.00  0.00          O
ATOM    282  I       282      41.154  27.011  21.835  1.00  0.00          O
ATOM    283  I       283      38.047  35.059  26.894  1.00  0.00          O
ATOM    284  I       284      34.941  43.106  31.953  1.00  0.00          O
ATOM    285  I       285      31.835  51.154  37.011  1.00  0.00          O
ATOM    286  I       286      28.729  59.201  42.070  1.00  0.00          O
ATOM    287  I       287      25.623  67.248  47.129  1.00  0.00          O
ATOM    288  I       288      22.517  75.296  52.188  1.00  0.00          O
ATOM    289  I       289      52.307  24.023  13.670  1.00  0.00          O
ATOM    290  I       290      49.201  32.070  18.729  1.00  0.00          O
ATOM    291  I       291      46.095  40.118  23.788  1.00  0.00          O
ATOM    292  I       292      42.989  48.165  28.846  1.00  0.00          O
ATOM    293  I       293      39.882  56.212  33.905  1.00  0.00          O
ATOM    294  I       294      36.776  64.260  38.964  1.00  0.00          O
ATOM    295  I       295      33.670  72.307  44.023  1.00  0.00          O
ATOM    296  I       296      30.564  80.354  49.082  1.00  0.00          O
ATOM    297  I       297      60.354  29.082  10.564  1.00  0.00          O
ATOM    298  I       298      57.248  37.129  15.623  1.00  0.00          O
ATOM    299  I       299      54.142  45.176  20.681  1.00  0.00          O
ATOM    300  I       300      51.036  53.224  25.740  1.00  0.00          O
ATOM    301  I       301      47.930  61.271  30.799  1.00  0.00          O
ATOM    302  I       302      44.824  69.319  35.858  1.00  0.00          O
ATOM    303  I       303      41.717  77.366  40.917  1.00  0.00          O
ATOM    304  I       304      38.611  85.413  45.975  1.00  0.00          O
ATOM    305  I       305      68.402  34.140   7.458  1.00  0.00          O
ATOM    306  I       306      65.296  42.188  12.517  1.00  0.00          O
ATOM    307  I       307      62.190  50.235  17.575  1.00  0.00          O
ATOM    308  I       308      59.083  58.283  22.634  1.00  0.00          O
ATOM    309  I       309      55.977  66.330  27.693  1.00  0.00          O
ATOM    310  I       310      52.871  74.377  32.752  1.00  0.00          O
ATOM    311  I       311      49.765  82.425  37.810  1.00  0.00          O
ATOM    312  I       312      46.659  90.472  42.869  1.00  0.00          O
ATOM    313  I       313      76.449  39.199   4.352  1.00  0.00          O
ATOM    314  I       314      73.343  47.247   9.410  1.00  0.00          O
ATOM    315  I       315      70.237  55.294  14.469  1.00  0.00          O
ATOM    316  I       316      67.131  63.341  19.528  1.00  0.00          O
ATOM    317  I       317      64.025  71.389  24.587  1.00  0.00          O
ATOM    318  I       318      60.918  79.436  29.646  1.00  0.00          O
ATOM    319  I       319      57.812  87.483  34.704  1.00  0.00          O
ATOM    320  I       320      54.706  95.531  39.763  1.00  0.00          O
ATOM    321  I       321      22.588  10.341  27.071  1.00  0.00          O
ATOM    322  I       322      19.482  18.388  32.130  1.00  0.00          O
ATOM    323  I       323      16.376  26.435  37.189  1.00  0.00          O
ATOM    324  I       324      13.270  34.483  42.247  1.00  0.00          O
ATOM    325  I       325      10.164  42.530  47.306  1.00  0.00          O
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ATOM    326  I       326       7.057  50.578  52.365  1.00  0.00          O
ATOM    327  I       327       3.951  58.625  57.424  1.00  0.00          O
ATOM    328  I       328       0.845  66.672  62.483  1.00  0.00          O
ATOM    329  I       329      30.636  15.400  23.965  1.00  0.00          O
ATOM    330  I       330      27.529  23.447  29.024  1.00  0.00          O
ATOM    331  I       331      24.423  31.494  34.082  1.00  0.00          O
ATOM    332  I       332      21.317  39.542  39.141  1.00  0.00          O
ATOM    333  I       333      18.211  47.589  44.200  1.00  0.00          O
ATOM    334  I       334      15.105  55.636  49.259  1.00  0.00          O
ATOM    335  I       335      11.999  63.684  54.318  1.00  0.00          O
ATOM    336  I       336       8.892  71.731  59.376  1.00  0.00          O
ATOM    337  I       337      38.683  20.458  20.859  1.00  0.00          O
ATOM    338  I       338      35.577  28.506  25.918  1.00  0.00          O
ATOM    339  I       339      32.471  36.553  30.976  1.00  0.00          O
ATOM    340  I       340      29.364  44.600  36.035  1.00  0.00          O
ATOM    341  I       341      26.258  52.648  41.094  1.00  0.00          O
ATOM    342  I       342      23.152  60.695  46.153  1.00  0.00          O
ATOM    343  I       343      20.046  68.743  51.211  1.00  0.00          O
ATOM    344  I       344      16.940  76.790  56.270  1.00  0.00          O
ATOM    345  I       345      46.730  25.517  17.753  1.00  0.00          O
ATOM    346  I       346      43.624  33.565  22.811  1.00  0.00          O
ATOM    347  I       347      40.518  41.612  27.870  1.00  0.00          O
ATOM    348  I       348      37.412  49.659  32.929  1.00  0.00          O
ATOM    349  I       349      34.306  57.707  37.988  1.00  0.00          O
ATOM    350  I       350      31.199  65.754  43.047  1.00  0.00          O
ATOM    351  I       351      28.093  73.801  48.105  1.00  0.00          O
ATOM    352  I       352      24.987  81.849  53.164  1.00  0.00          O
ATOM    353  I       353      54.778  30.576  14.646  1.00  0.00          O
ATOM    354  I       354      51.672  38.623  19.705  1.00  0.00          O
ATOM    355  I       355      48.565  46.671  24.764  1.00  0.00          O
ATOM    356  I       356      45.459  54.718  29.823  1.00  0.00          O
ATOM    357  I       357      42.353  62.765  34.882  1.00  0.00          O
ATOM    358  I       358      39.247  70.813  39.940  1.00  0.00          O
ATOM    359  I       359      36.141  78.860  44.999  1.00  0.00          O
ATOM    360  I       360      33.034  86.908  50.058  1.00  0.00          O
ATOM    361  I       361      62.825  35.635  11.540  1.00  0.00          O
ATOM    362  I       362      59.719  43.682  16.599  1.00  0.00          O
ATOM    363  I       363      56.613  51.729  21.658  1.00  0.00          O
ATOM    364  I       364      53.507  59.777  26.717  1.00  0.00          O
ATOM    365  I       365      50.400  67.824  31.775  1.00  0.00          O
ATOM    366  I       366      47.294  75.872  36.834  1.00  0.00          O
ATOM    367  I       367      44.188  83.919  41.893  1.00  0.00          O
ATOM    368  I       368      41.082  91.966  46.952  1.00  0.00          O
ATOM    369  I       369      70.872  40.694   8.434  1.00  0.00          O
ATOM    370  I       370      67.766  48.741  13.493  1.00  0.00          O
ATOM    371  I       371      64.660  56.788  18.552  1.00  0.00          O
ATOM    372  I       372      61.554  64.836  23.610  1.00  0.00          O
ATOM    373  I       373      58.448  72.883  28.669  1.00  0.00          O
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ATOM    374  I       374      55.342  80.930  33.728  1.00  0.00          O
ATOM    375  I       375      52.235  88.978  38.787  1.00  0.00          O
ATOM    376  I       376      49.129  97.025  43.846  1.00  0.00          O
ATOM    377  I       377      78.920  45.752   5.328  1.00  0.00          O
ATOM    378  I       378      75.814  53.800  10.387  1.00  0.00          O
ATOM    379  I       379      72.707  61.847  15.445  1.00  0.00          O
ATOM    380  I       380      69.601  69.894  20.504  1.00  0.00          O
ATOM    381  I       381      66.495  77.942  25.563  1.00  0.00          O
ATOM    382  I       382      63.389  85.989  30.622  1.00  0.00          O
ATOM    383  I       383      60.283  94.037  35.681  1.00  0.00          O
ATOM    384  I       384      57.177 102.084  40.739  1.00  0.00          O
ATOM    385  I       385      25.176   0.681  34.142  1.00  0.00          O
ATOM    386  I       386      22.070   8.729  39.201  1.00  0.00          O
ATOM    387  I       387      18.964  16.776  44.260  1.00  0.00          O
ATOM    388  I       388      15.858  24.824  49.319  1.00  0.00          O
ATOM    389  I       389      12.752  32.871  54.377  1.00  0.00          O
ATOM    390  I       390       9.646  40.918  59.436  1.00  0.00          O
ATOM    391  I       391       6.539  48.966  64.495  1.00  0.00          O
ATOM    392  I       392       3.433  57.013  69.554  1.00  0.00          O
ATOM    393  I       393      33.224   5.740  31.036  1.00  0.00          O
ATOM    394  I       394      30.118  13.788  36.095  1.00  0.00          O
ATOM    395  I       395      27.011  21.835  41.154  1.00  0.00          O
ATOM    396  I       396      23.905  29.882  46.212  1.00  0.00          O
ATOM    397  I       397      20.799  37.930  51.271  1.00  0.00          O
ATOM    398  I       398      17.693  45.977  56.330  1.00  0.00          O
ATOM    399  I       399      14.587  54.025  61.389  1.00  0.00          O
ATOM    400  I       400      11.481  62.072  66.448  1.00  0.00          O
ATOM    401  I       401      41.271  10.799  27.930  1.00  0.00          O
ATOM    402  I       402      38.165  18.846  32.989  1.00  0.00          O
ATOM    403  I       403      35.059  26.894  38.047  1.00  0.00          O
ATOM    404  I       404      31.953  34.941  43.106  1.00  0.00          O
ATOM    405  I       405      28.846  42.989  48.165  1.00  0.00          O
ATOM    406  I       406      25.740  51.036  53.224  1.00  0.00          O
ATOM    407  I       407      22.634  59.083  58.283  1.00  0.00          O
ATOM    408  I       408      19.528  67.131  63.341  1.00  0.00          O
ATOM    409  I       409      49.319  15.858  24.824  1.00  0.00          O
ATOM    410  I       410      46.212  23.905  29.882  1.00  0.00          O
ATOM    411  I       411      43.106  31.953  34.941  1.00  0.00          O
ATOM    412  I       412      40.000  40.000  40.000  1.00  0.00          O
ATOM    413  I       413      36.894  48.047  45.059  1.00  0.00          O
ATOM    414  I       414      33.788  56.095  50.118  1.00  0.00          O
ATOM    415  I       415      30.681  64.142  55.176  1.00  0.00          O
ATOM    416  I       416      27.575  72.190  60.235  1.00  0.00          O
ATOM    417  I       417      57.366  20.917  21.717  1.00  0.00          O
ATOM    418  I       418      54.260  28.964  26.776  1.00  0.00          O
ATOM    419  I       419      51.154  37.011  31.835  1.00  0.00          O
ATOM    420  I       420      48.047  45.059  36.894  1.00  0.00          O
ATOM    421  I       421      44.941  53.106  41.953  1.00  0.00          O
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ATOM 422 I 422 41.835 61.154 47.011 1.00 0.00 O
ATOM 423 I 423 38.729 69.201 52.070 1.00 0.00 O
ATOM 424 I 424 35.623 77.248 57.129 1.00 0.00 O
ATOM 425 I 425 65.413 25.975 18.611 1.00 0.00 O
ATOM 426 I 426 62.307 34.023 23.670 1.00 0.00 O
ATOM 427 I 427 59.201 42.070 28.729 1.00 0.00 O
ATOM 428 I 428 56.095 50.118 33.788 1.00 0.00 O
ATOM 429 I 429 52.989 58.165 38.846 1.00 0.00 O
ATOM 430 I 430 49.882 66.212 43.905 1.00 0.00 O
ATOM 431 I 431 46.776 74.260 48.964 1.00 0.00 O
ATOM 432 I 432 43.670 82.307 54.023 1.00 0.00 O
ATOM 433 I 433 73.461 31.034 15.505 1.00 0.00 O
ATOM 434 I 434 70.354 39.082 20.564 1.00 0.00 O
ATOM 435 I 435 67.248 47.129 25.623 1.00 0.00 O
ATOM 436 I 436 64.142 55.176 30.681 1.00 0.00 O
ATOM 437 I 437 61.036 63.224 35.740 1.00 0.00 O
ATOM 438 I 438 57.930 71.271 40.799 1.00 0.00 O
ATOM 439 I 439 54.824 79.319 45.858 1.00 0.00 O
ATOM 440 I 440 51.717 87.366 50.917 1.00 0.00 O
ATOM 441 I 441 81.508 36.093 12.399 1.00 0.00 O
ATOM 442 I 442 78.402 44.140 17.458 1.00 0.00 O
ATOM 443 I 443 75.296 52.188 22.517 1.00 0.00 O
ATOM 444 I 444 72.190 60.235 27.575 1.00 0.00 O
ATOM 445 I 445 69.083 68.283 32.634 1.00 0.00 O
ATOM 446 I 446 65.977 76.330 37.693 1.00 0.00 O
ATOM 447 I 447 62.871 84.377 42.752 1.00 0.00 O
ATOM 448 I 448 59.765 92.425 47.810 1.00 0.00 O
ATOM 449 I 449 27.647 7.235 35.118 1.00 0.00 O
ATOM 450 I 450 24.541 15.282 40.177 1.00 0.00 O
ATOM 451 I 451 21.435 23.329 45.236 1.00 0.00 O
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ATOM 454 I 454 12.116 47.471 60.412 1.00 0.00 O
ATOM 455 I 455 9.010 55.519 65.471 1.00 0.00 O
ATOM 456 I 456 5.904 63.566 70.530 1.00 0.00 O
ATOM 457 I 457 35.694 12.293 32.012 1.00 0.00 O
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ATOM 633 I 633 89.037 39.540 21.423 1.00 0.00 O
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ATOM 646 I 646 19.763 34.706 75.531 1.00 0.00 O
ATOM 647 I 647 16.657 42.753 80.590 1.00 0.00 O
ATOM 648 I 648 13.551 50.801 85.648 1.00 0.00 O
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ATOM 650 I 650 40.235 7.575 52.190 1.00 0.00 O
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ATOM 658 I 658 48.283 12.634 49.083 1.00 0.00 O
ATOM 659 I 659 45.176 20.681 54.142 1.00 0.00 O
ATOM 660 I 660 42.070 28.729 59.201 1.00 0.00 O
ATOM 661 I 661 38.964 36.776 64.260 1.00 0.00 O

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ATOM    662  I        662      35.858  44.824  69.319  1.00  0.00          O
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ATOM    680  I        680      45.740  71.036  73.224  1.00  0.00          O
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ATOM    682  I        682      72.425  27.810  39.765  1.00  0.00          O
ATOM    683  I        683      69.319  35.858  44.824  1.00  0.00          O
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ATOM    685  I        685      63.106  51.953  54.941  1.00  0.00          O
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ATOM    687  I        687      56.894  68.047  65.059  1.00  0.00          O
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ATOM    692  I        692      74.260  48.964  46.776  1.00  0.00          O
ATOM    693  I        693      71.154  57.011  51.835  1.00  0.00          O
ATOM    694  I        694      68.047  65.059  56.894  1.00  0.00          O
ATOM    695  I        695      64.941  73.106  61.953  1.00  0.00          O
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ATOM    703  I        703      72.989  78.165  58.846  1.00  0.00          O
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ATOM    708  I        708      28.446  25.164  66.390  1.00  0.00          O
ATOM    709  I        709      25.340  33.212  71.448  1.00  0.00          O
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ATOM 710 I 710 22.234 41.259 76.507 1.00 0.00 O
ATOM 711 I 711 19.128 49.306 81.566 1.00 0.00 O
ATOM 712 I 712 16.021 57.354 86.625 1.00 0.00 O
ATOM 713 I 713 45.812 6.081 48.107 1.00 0.00 O
ATOM 714 I 714 42.706 14.128 53.166 1.00 0.00 O
ATOM 715 I 715 39.600 22.176 58.225 1.00 0.00 O
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ATOM 737 I 737 69.954 21.257 38.789 1.00 0.00 O
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ATOM 750 I 750 62.471 66.553 60.976 1.00 0.00 O
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ATOM 756 I 756 76.730 55.517 47.753 1.00 0.00 O
ATOM 757 I 757 73.624 63.565 52.811 1.00 0.00 O

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ATOM    758  I       758      70.518  71.612  57.870  1.00  0.00          O
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ATOM    764  I       764      84.778  60.576  44.646  1.00  0.00          O
ATOM    765  I       765      81.672  68.623  49.705  1.00  0.00          O
ATOM    766  I       766      78.565  76.671  54.764  1.00  0.00          O
ATOM    767  I       767      75.459  84.718  59.823  1.00  0.00          O
ATOM    768  I       768      72.353  92.765  64.882  1.00  0.00          O
ATOM    769  I       769      40.353  -8.637  58.284  1.00  0.00          O
ATOM    770  I       770      37.247  -0.590  63.343  1.00  0.00          O
ATOM    771  I       771      34.140   7.458  68.402  1.00  0.00          O
ATOM    772  I       772      31.034  15.505  73.461  1.00  0.00          O
ATOM    773  I       773      27.928  23.552  78.519  1.00  0.00          O
ATOM    774  I       774      24.822  31.600  83.578  1.00  0.00          O
ATOM    775  I       775      21.716  39.647  88.637  1.00  0.00          O
ATOM    776  I       776      18.610  47.695  93.696  1.00  0.00          O
ATOM    777  I       777      48.400  -3.578  55.178  1.00  0.00          O
ATOM    778  I       778      45.294   4.469  60.237  1.00  0.00          O
ATOM    779  I       779      42.188  12.517  65.296  1.00  0.00          O
ATOM    780  I       780      39.082  20.564  70.354  1.00  0.00          O
ATOM    781  I       781      35.975  28.611  75.413  1.00  0.00          O
ATOM    782  I       782      32.869  36.659  80.472  1.00  0.00          O
ATOM    783  I       783      29.763  44.706  85.531  1.00  0.00          O
ATOM    784  I       784      26.657  52.753  90.590  1.00  0.00          O
ATOM    785  I       785      56.448   1.481  52.072  1.00  0.00          O
ATOM    786  I       786      53.341   9.528  57.131  1.00  0.00          O
ATOM    787  I       787      50.235  17.575  62.190  1.00  0.00          O
ATOM    788  I       788      47.129  25.623  67.248  1.00  0.00          O
ATOM    789  I       789      44.023  33.670  72.307  1.00  0.00          O
ATOM    790  I       790      40.917  41.717  77.366  1.00  0.00          O
ATOM    791  I       791      37.810  49.765  82.425  1.00  0.00          O
ATOM    792  I       792      34.704  57.812  87.483  1.00  0.00          O
ATOM    793  I       793      64.495   6.539  48.966  1.00  0.00          O
ATOM    794  I       794      61.389  14.587  54.025  1.00  0.00          O
ATOM    795  I       795      58.283  22.634  59.083  1.00  0.00          O
ATOM    796  I       796      55.176  30.681  64.142  1.00  0.00          O
ATOM    797  I       797      52.070  38.729  69.201  1.00  0.00          O
ATOM    798  I       798      48.964  46.776  74.260  1.00  0.00          O
ATOM    799  I       799      45.858  54.824  79.319  1.00  0.00          O
ATOM    800  I       800      42.752  62.871  84.377  1.00  0.00          O
ATOM    801  I       801      72.542  11.598  45.860  1.00  0.00          O
ATOM    802  I       802      69.436  19.646  50.918  1.00  0.00          O
ATOM    803  I       803      66.330  27.693  55.977  1.00  0.00          O
ATOM    804  I       804      63.224  35.740  61.036  1.00  0.00          O
ATOM    805  I       805      60.118  43.788  66.095  1.00  0.00          O
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ATOM    806  I       806      57.011  51.835  71.154  1.00  0.00          O
ATOM    807  I       807      53.905  59.882  76.212  1.00  0.00          O
ATOM    808  I       808      50.799  67.930  81.271  1.00  0.00          O
ATOM    809  I       809      80.590  16.657  42.753  1.00  0.00          O
ATOM    810  I       810      77.483  24.704  47.812  1.00  0.00          O
ATOM    811  I       811      74.377  32.752  52.871  1.00  0.00          O
ATOM    812  I       812      71.271  40.799  57.930  1.00  0.00          O
ATOM    813  I       813      68.165  48.846  62.989  1.00  0.00          O
ATOM    814  I       814      65.059  56.894  68.047  1.00  0.00          O
ATOM    815  I       815      61.953  64.941  73.106  1.00  0.00          O
ATOM    816  I       816      58.846  72.989  78.165  1.00  0.00          O
ATOM    817  I       817      88.637  21.716  39.647  1.00  0.00          O
ATOM    818  I       818      85.531  29.763  44.706  1.00  0.00          O
ATOM    819  I       819      82.425  37.810  49.765  1.00  0.00          O
ATOM    820  I       820      79.319  45.858  54.824  1.00  0.00          O
ATOM    821  I       821      76.212  53.905  59.882  1.00  0.00          O
ATOM    822  I       822      73.106  61.953  64.941  1.00  0.00          O
ATOM    823  I       823      70.000  70.000  70.000  1.00  0.00          O
ATOM    824  I       824      66.894  78.047  75.059  1.00  0.00          O
ATOM    825  I       825      96.684  26.775  36.541  1.00  0.00          O
ATOM    826  I       826      93.578  34.822  41.600  1.00  0.00          O
ATOM    827  I       827      90.472  42.869  46.659  1.00  0.00          O
ATOM    828  I       828      87.366  50.917  51.717  1.00  0.00          O
ATOM    829  I       829      84.260  58.964  56.776  1.00  0.00          O
ATOM    830  I       830      81.154  67.011  61.835  1.00  0.00          O
ATOM    831  I       831      78.047  75.059  66.894  1.00  0.00          O
ATOM    832  I       832      74.941  83.106  71.953  1.00  0.00          O
ATOM    833  I       833      42.823  -2.084  59.261  1.00  0.00          O
ATOM    834  I       834      39.717   5.963  64.319  1.00  0.00          O
ATOM    835  I       835      36.611  14.011  69.378  1.00  0.00          O
ATOM    836  I       836      33.505  22.058  74.437  1.00  0.00          O
ATOM    837  I       837      30.399  30.106  79.496  1.00  0.00          O
ATOM    838  I       838      27.293  38.153  84.555  1.00  0.00          O
ATOM    839  I       839      24.186  46.200  89.613  1.00  0.00          O
ATOM    840  I       840      21.080  54.248  94.672  1.00  0.00          O
ATOM    841  I       841      50.871   2.975  56.154  1.00  0.00          O
ATOM    842  I       842      47.765  11.022  61.213  1.00  0.00          O
ATOM    843  I       843      44.658  19.070  66.272  1.00  0.00          O
ATOM    844  I       844      41.552  27.117  71.331  1.00  0.00          O
ATOM    845  I       845      38.446  35.164  76.390  1.00  0.00          O
ATOM    846  I       846      35.340  43.212  81.448  1.00  0.00          O
ATOM    847  I       847      32.234  51.259  86.507  1.00  0.00          O
ATOM    848  I       848      29.128  59.306  91.566  1.00  0.00          O
ATOM    849  I       849      58.918   8.034  53.048  1.00  0.00          O
ATOM    850  I       850      55.812  16.081  58.107  1.00  0.00          O
ATOM    851  I       851      52.706  24.128  63.166  1.00  0.00          O
ATOM    852  I       852      49.600  32.176  68.225  1.00  0.00          O
ATOM    853  I       853      46.493  40.223  73.283  1.00  0.00          O
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ATOM    854  I       854      43.387  48.271  78.342  1.00  0.00          O
ATOM    855  I       855      40.281  56.318  83.401  1.00  0.00          O
ATOM    856  I       856      37.175  64.365  88.460  1.00  0.00          O
ATOM    857  I       857      66.966  13.092  49.942  1.00  0.00          O
ATOM    858  I       858      63.859  21.140  55.001  1.00  0.00          O
ATOM    859  I       859      60.753  29.187  60.060  1.00  0.00          O
ATOM    860  I       860      57.647  37.235  65.118  1.00  0.00          O
ATOM    861  I       861      54.541  45.282  70.177  1.00  0.00          O
ATOM    862  I       862      51.435  53.329  75.236  1.00  0.00          O
ATOM    863  I       863      48.328  61.377  80.295  1.00  0.00          O
ATOM    864  I       864      45.222  69.424  85.354  1.00  0.00          O
ATOM    865  I       865      75.013  18.151  46.836  1.00  0.00          O
ATOM    866  I       866      71.907  26.199  51.895  1.00  0.00          O
ATOM    867  I       867      68.801  34.246  56.953  1.00  0.00          O
ATOM    868  I       868      65.694  42.293  62.012  1.00  0.00          O
ATOM    869  I       869      62.588  50.341  67.071  1.00  0.00          O
ATOM    870  I       870      59.482  58.388  72.130  1.00  0.00          O
ATOM    871  I       871      56.376  66.435  77.189  1.00  0.00          O
ATOM    872  I       872      53.270  74.483  82.247  1.00  0.00          O
ATOM    873  I       873      83.060  23.210  43.730  1.00  0.00          O
ATOM    874  I       874      79.954  31.257  48.789  1.00  0.00          O
ATOM    875  I       875      76.848  39.305  53.847  1.00  0.00          O
ATOM    876  I       876      73.742  47.352  58.906  1.00  0.00          O
ATOM    877  I       877      70.636  55.400  63.965  1.00  0.00          O
ATOM    878  I       878      67.529  63.447  69.024  1.00  0.00          O
ATOM    879  I       879      64.423  71.494  74.082  1.00  0.00          O
ATOM    880  I       880      61.317  79.542  79.141  1.00  0.00          O
ATOM    881  I       881      91.108  28.269  40.624  1.00  0.00          O
ATOM    882  I       882      88.001  36.316  45.682  1.00  0.00          O
ATOM    883  I       883      84.895  44.364  50.741  1.00  0.00          O
ATOM    884  I       884      81.789  52.411  55.800  1.00  0.00          O
ATOM    885  I       885      78.683  60.458  60.859  1.00  0.00          O
ATOM    886  I       886      75.577  68.506  65.918  1.00  0.00          O
ATOM    887  I       887      72.471  76.553  70.976  1.00  0.00          O
ATOM    888  I       888      69.364  84.600  76.035  1.00  0.00          O
ATOM    889  I       889      99.155  33.328  37.517  1.00  0.00          O
ATOM    890  I       890      96.049  41.375  42.576  1.00  0.00          O
ATOM    891  I       891      92.943  49.422  47.635  1.00  0.00          O
ATOM    892  I       892      89.836  57.470  52.694  1.00  0.00          O
ATOM    893  I       893      86.730  65.517  57.753  1.00  0.00          O
ATOM    894  I       894      83.624  73.565  62.811  1.00  0.00          O
ATOM    895  I       895      80.518  81.612  67.870  1.00  0.00          O
ATOM    896  I       896      77.412  89.659  72.929  1.00  0.00          O
ATOM    897  I       897      45.412 -11.743  66.332  1.00  0.00          O
ATOM    898  I       898      42.305  -3.696  71.390  1.00  0.00          O
ATOM    899  I       899      39.199   4.352  76.449  1.00  0.00          O
ATOM    900  I       900      36.093  12.399  81.508  1.00  0.00          O
ATOM    901  I       901      32.987  20.446  86.567  1.00  0.00          O
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ATOM 902 I 902 29.881 28.494 91.626 1.00 0.00 O
ATOM 903 I 903 26.775 36.541 96.684 1.00 0.00 O
ATOM 904 I 904 23.668 44.588 101.743 1.00 0.00 O
ATOM 905 I 905 53.459 -6.684 63.225 1.00 0.00 O
ATOM 906 I 906 50.353 1.363 68.284 1.00 0.00 O
ATOM 907 I 907 47.247 9.410 73.343 1.00 0.00 O
ATOM 908 I 908 44.140 17.458 78.402 1.00 0.00 O
ATOM 909 I 909 41.034 25.505 83.461 1.00 0.00 O
ATOM 910 I 910 37.928 33.552 88.519 1.00 0.00 O
ATOM 911 I 911 34.822 41.600 93.578 1.00 0.00 O
ATOM 912 I 912 31.716 49.647 98.637 1.00 0.00 O
ATOM 913 I 913 61.506 -1.626 60.119 1.00 0.00 O
ATOM 914 I 914 58.400 6.422 65.178 1.00 0.00 O
ATOM 915 I 915 55.294 14.469 70.237 1.00 0.00 O
ATOM 916 I 916 52.188 22.517 75.296 1.00 0.00 O
ATOM 917 I 917 49.082 30.564 80.354 1.00 0.00 O
ATOM 918 I 918 45.975 38.611 85.413 1.00 0.00 O
ATOM 919 I 919 42.869 46.659 90.472 1.00 0.00 O
ATOM 920 I 920 39.763 54.706 95.531 1.00 0.00 O
ATOM 921 I 921 69.554 3.433 57.013 1.00 0.00 O
ATOM 922 I 922 66.448 11.481 62.072 1.00 0.00 O
ATOM 923 I 923 63.341 19.528 67.131 1.00 0.00 O
ATOM 924 I 924 60.235 27.575 72.190 1.00 0.00 O
ATOM 925 I 925 57.129 35.623 77.248 1.00 0.00 O
ATOM 926 I 926 54.023 43.670 82.307 1.00 0.00 O
ATOM 927 I 927 50.917 51.717 87.366 1.00 0.00 O
ATOM 928 I 928 47.810 59.765 92.425 1.00 0.00 O
ATOM 929 I 929 77.601 8.492 53.907 1.00 0.00 O
ATOM 930 I 930 74.495 16.539 58.966 1.00 0.00 O
ATOM 931 I 931 71.389 24.587 64.025 1.00 0.00 O
ATOM 932 I 932 68.283 32.634 69.083 1.00 0.00 O
ATOM 933 I 933 65.176 40.681 74.142 1.00 0.00 O
ATOM 934 I 934 62.070 48.729 79.201 1.00 0.00 O
ATOM 935 I 935 58.964 56.776 84.260 1.00 0.00 O
ATOM 936 I 936 55.858 64.824 89.319 1.00 0.00 O
ATOM 937 I 937 85.648 13.551 50.801 1.00 0.00 O
ATOM 938 I 938 82.542 21.598 55.860 1.00 0.00 O
ATOM 939 I 939 79.436 29.646 60.918 1.00 0.00 O
ATOM 940 I 940 76.330 37.693 65.977 1.00 0.00 O
ATOM 941 I 941 73.224 45.740 71.036 1.00 0.00 O
ATOM 942 I 942 70.118 53.788 76.095 1.00 0.00 O
ATOM 943 I 943 67.011 61.835 81.154 1.00 0.00 O
ATOM 944 I 944 63.905 69.882 86.212 1.00 0.00 O
ATOM 945 I 945 93.696 18.610 47.695 1.00 0.00 O
ATOM 946 I 946 90.590 26.657 52.753 1.00 0.00 O
ATOM 947 I 947 87.483 34.704 57.812 1.00 0.00 O
ATOM 948 I 948 84.377 42.752 62.871 1.00 0.00 O
ATOM 949 I 949 81.271 50.799 67.930 1.00 0.00 O

ATOM 950 I 950 78.165 58.846 72.989 1.00 0.00 O
ATOM 951 I 951 75.059 66.894 78.047 1.00 0.00 O
ATOM 952 I 952 71.953 74.941 83.106 1.00 0.00 O
ATOM 953 I 953 101.743 23.668 44.588 1.00 0.00 O
ATOM 954 I 954 98.637 31.716 49.647 1.00 0.00 O
ATOM 955 I 955 95.531 39.763 54.706 1.00 0.00 O
ATOM 956 I 956 92.425 47.810 59.765 1.00 0.00 O
ATOM 957 I 957 89.319 55.858 64.824 1.00 0.00 O
ATOM 958 I 958 86.212 63.905 69.882 1.00 0.00 O
ATOM 959 I 959 83.106 71.953 74.941 1.00 0.00 O
ATOM 960 I 960 80.000 80.000 80.000 1.00 0.00 O
ATOM 961 I 961 47.882 -5.190 67.308 1.00 0.00 O
ATOM 962 I 962 44.776 2.857 72.367 1.00 0.00 O
ATOM 963 I 963 41.670 10.905 77.426 1.00 0.00 O
ATOM 964 I 964 38.564 18.952 82.484 1.00 0.00 O
ATOM 965 I 965 35.457 26.999 87.543 1.00 0.00 O
ATOM 966 I 966 32.351 35.047 92.602 1.00 0.00 O
ATOM 967 I 967 29.245 43.094 97.661 1.00 0.00 O
ATOM 968 I 968 26.139 51.142 102.720 1.00 0.00 O
ATOM 969 I 969 55.930 -0.131 64.202 1.00 0.00 O
ATOM 970 I 970 52.823 7.916 69.261 1.00 0.00 O
ATOM 971 I 971 49.717 15.963 74.319 1.00 0.00 O
ATOM 972 I 972 46.611 24.011 79.378 1.00 0.00 O
ATOM 973 I 973 43.505 32.058 84.437 1.00 0.00 O
ATOM 974 I 974 40.399 40.106 89.496 1.00 0.00 O
ATOM 975 I 975 37.293 48.153 94.555 1.00 0.00 O
ATOM 976 I 976 34.186 56.200 99.613 1.00 0.00 O
ATOM 977 I 977 63.977 4.927 61.096 1.00 0.00 O
ATOM 978 I 978 60.871 12.975 66.154 1.00 0.00 O
ATOM 979 I 979 57.765 21.022 71.213 1.00 0.00 O
ATOM 980 I 980 54.658 29.070 76.272 1.00 0.00 O
ATOM 981 I 981 51.552 37.117 81.331 1.00 0.00 O
ATOM 982 I 982 48.446 45.164 86.390 1.00 0.00 O
ATOM 983 I 983 45.340 53.212 91.448 1.00 0.00 O
ATOM 984 I 984 42.234 61.259 96.507 1.00 0.00 O
ATOM 985 I 985 72.024 9.986 57.989 1.00 0.00 O
ATOM 986 I 986 68.918 18.034 63.048 1.00 0.00 O
ATOM 987 I 987 65.812 26.081 68.107 1.00 0.00 O
ATOM 988 I 988 62.706 34.128 73.166 1.00 0.00 O
ATOM 989 I 989 59.600 42.176 78.225 1.00 0.00 O
ATOM 990 I 990 56.493 50.223 83.283 1.00 0.00 O
ATOM 991 I 991 53.387 58.271 88.342 1.00 0.00 O
ATOM 992 I 992 50.281 66.318 93.401 1.00 0.00 O
ATOM 993 I 993 80.072 15.045 54.883 1.00 0.00 O
ATOM 994 I 994 76.966 23.092 59.942 1.00 0.00 O
ATOM 995 I 995 73.859 31.140 65.001 1.00 0.00 O
ATOM 996 I 996 70.753 39.187 70.060 1.00 0.00 O
ATOM 997 I 997 67.647 47.235 75.118 1.00 0.00 O

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ATOM    998  I       998      64.541  55.282  80.177  1.00  0.00          O
ATOM    999  I       999      61.435  63.329  85.236  1.00  0.00          O
ATOM   1000  I      1000      58.328  71.377  90.295  1.00  0.00          O
ATOM   1001  I      1001      88.119  20.104  51.777  1.00  0.00          O
ATOM   1002  I      1002      85.013  28.151  56.836  1.00  0.00          O
ATOM   1003  I      1003      81.907  36.199  61.895  1.00  0.00          O
ATOM   1004  I      1004      78.801  44.246  66.953  1.00  0.00          O
ATOM   1005  I      1005      75.694  52.293  72.012  1.00  0.00          O
ATOM   1006  I      1006      72.588  60.341  77.071  1.00  0.00          O
ATOM   1007  I      1007      69.482  68.388  82.130  1.00  0.00          O
ATOM   1008  I      1008      66.376  76.435  87.189  1.00  0.00          O
ATOM   1009  I      1009      96.166  25.163  48.671  1.00  0.00          O
ATOM   1010  I      1010      93.060  33.210  53.730  1.00  0.00          O
ATOM   1011  I      1011      89.954  41.257  58.789  1.00  0.00          O
ATOM   1012  I      1012      86.848  49.305  63.847  1.00  0.00          O
ATOM   1013  I      1013      83.742  57.352  68.906  1.00  0.00          O
ATOM   1014  I      1014      80.636  65.400  73.965  1.00  0.00          O
ATOM   1015  I      1015      77.529  73.447  79.024  1.00  0.00          O
ATOM   1016  I      1016      74.423  81.494  84.082  1.00  0.00          O
ATOM   1017  I      1017     104.214  30.221  45.565  1.00  0.00          O
ATOM   1018  I      1018     101.108  38.269  50.624  1.00  0.00          O
ATOM   1019  I      1019      98.001  46.316  55.682  1.00  0.00          O
ATOM   1020  I      1020      94.895  54.364  60.741  1.00  0.00          O
ATOM   1021  I      1021      91.789  62.411  65.800  1.00  0.00          O
ATOM   1022  I      1022      88.683  70.458  70.859  1.00  0.00          O
ATOM   1023  I      1023      85.577  78.506  75.918  1.00  0.00          O
ATOM   1024  I      1024      82.471  86.553  80.976  1.00  0.00          O
END
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15.2.3 Archivo PDB Estructura Cúbica Centrada en el Cuerpo (BCC)

Archivo PDB generado correspondiente a la estructura cúbica centrada en el Cuerpo de 4 celdas por lado, 10 Angstroms en los parámetros de red a, b y c:

Campo1	Campo2	Campo3	Campo4	Campo5	Campo6	Campo7	Campo8	Campo9	Campo 10
Registro	serial	elemento	Numero de secuncia	Coordenadas otogonales para x	Coordenadas otogonales para y	Coordenadas otogonales para z	ocupancia	Factor de temperatura	Carga en el átomo

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ATOM      1  I         1      10.000   9.090  10.834  1.00  0.00          O
ATOM      2  I         2      10.000  19.052  11.705  1.00  0.00          O
ATOM      3  I         3      10.000  29.014  12.577  1.00  0.00          O
ATOM      4  I         4      10.000  38.976  13.448  1.00  0.00          O
ATOM      5  I         5      10.000  48.938  14.320  1.00  0.00          O
ATOM      6  I         6      10.000  58.900  15.191  1.00  0.00          O
ATOM      7  I         7      10.000  68.862  16.063  1.00  0.00          O
ATOM      8  I         8      10.000  78.824  16.934  1.00  0.00          O
ATOM      9  I         9      20.000   9.090  10.834  1.00  0.00          O
ATOM     10  I        10      20.000  19.052  11.705  1.00  0.00          O
ATOM     11  I        11      20.000  29.014  12.577  1.00  0.00          O
ATOM     12  I        12      20.000  38.976  13.448  1.00  0.00          O
ATOM     13  I        13      20.000  48.938  14.320  1.00  0.00          O
ATOM     14  I        14      20.000  58.900  15.191  1.00  0.00          O
ATOM     15  I        15      20.000  68.862  16.063  1.00  0.00          O
ATOM     16  I        16      20.000  78.824  16.934  1.00  0.00          O
ATOM     17  I        17      30.000   9.090  10.834  1.00  0.00          O
ATOM     18  I        18      30.000  19.052  11.705  1.00  0.00          O
ATOM     19  I        19      30.000  29.014  12.577  1.00  0.00          O
ATOM     20  I        20      30.000  38.976  13.448  1.00  0.00          O
ATOM     21  I        21      30.000  48.938  14.320  1.00  0.00          O
ATOM     22  I        22      30.000  58.900  15.191  1.00  0.00          O
ATOM     23  I        23      30.000  68.862  16.063  1.00  0.00          O
ATOM     24  I        24      30.000  78.824  16.934  1.00  0.00          O
ATOM     25  I        25      40.000   9.090  10.834  1.00  0.00          O
ATOM     26  I        26      40.000  19.052  11.705  1.00  0.00          O
ATOM     27  I        27      40.000  29.014  12.577  1.00  0.00          O
ATOM     28  I        28      40.000  38.976  13.448  1.00  0.00          O
ATOM     29  I        29      40.000  48.938  14.320  1.00  0.00          O
ATOM     30  I        30      40.000  58.900  15.191  1.00  0.00          O
ATOM     31  I        31      40.000  68.862  16.063  1.00  0.00          O
ATOM     32  I        32      40.000  78.824  16.934  1.00  0.00          O
ATOM     33  I        33      50.000   9.090  10.834  1.00  0.00          O
ATOM     34  I        34      50.000  19.052  11.705  1.00  0.00          O
ATOM     35  I        35      50.000  29.014  12.577  1.00  0.00          O
ATOM     36  I        36      50.000  38.976  13.448  1.00  0.00          O
```

ATOM 37 I 37 50.000 48.938 14.320 1.00 0.00 O
ATOM 38 I 38 50.000 58.900 15.191 1.00 0.00 O
ATOM 39 I 39 50.000 68.862 16.063 1.00 0.00 O
ATOM 40 I 40 50.000 78.824 16.934 1.00 0.00 O
ATOM 41 I 41 60.000 9.090 10.834 1.00 0.00 O
ATOM 42 I 42 60.000 19.052 11.705 1.00 0.00 O
ATOM 43 I 43 60.000 29.014 12.577 1.00 0.00 O
ATOM 44 I 44 60.000 38.976 13.448 1.00 0.00 O
ATOM 45 I 45 60.000 48.938 14.320 1.00 0.00 O
ATOM 46 I 46 60.000 58.900 15.191 1.00 0.00 O
ATOM 47 I 47 60.000 68.862 16.063 1.00 0.00 O
ATOM 48 I 48 60.000 78.824 16.934 1.00 0.00 O
ATOM 49 I 49 70.000 9.090 10.834 1.00 0.00 O
ATOM 50 I 50 70.000 19.052 11.705 1.00 0.00 O
ATOM 51 I 51 70.000 29.014 12.577 1.00 0.00 O
ATOM 52 I 52 70.000 38.976 13.448 1.00 0.00 O
ATOM 53 I 53 70.000 48.938 14.320 1.00 0.00 O
ATOM 54 I 54 70.000 58.900 15.191 1.00 0.00 O
ATOM 55 I 55 70.000 68.862 16.063 1.00 0.00 O
ATOM 56 I 56 70.000 78.824 16.934 1.00 0.00 O
ATOM 57 I 57 80.000 9.090 10.834 1.00 0.00 O
ATOM 58 I 58 80.000 19.052 11.705 1.00 0.00 O
ATOM 59 I 59 80.000 29.014 12.577 1.00 0.00 O
ATOM 60 I 60 80.000 38.976 13.448 1.00 0.00 O
ATOM 61 I 61 80.000 48.938 14.320 1.00 0.00 O
ATOM 62 I 62 80.000 58.900 15.191 1.00 0.00 O
ATOM 63 I 63 80.000 68.862 16.063 1.00 0.00 O
ATOM 64 I 64 80.000 78.824 16.934 1.00 0.00 O
ATOM 65 I 65 15.000 13.636 16.250 1.00 0.00 O
ATOM 66 I 66 15.000 23.598 17.122 1.00 0.00 O
ATOM 67 I 67 15.000 33.559 17.993 1.00 0.00 O
ATOM 68 I 68 15.000 43.521 18.865 1.00 0.00 O
ATOM 69 I 69 15.000 53.483 19.736 1.00 0.00 O
ATOM 70 I 70 15.000 63.445 20.608 1.00 0.00 O
ATOM 71 I 71 15.000 73.407 21.480 1.00 0.00 O
ATOM 72 I 72 15.000 83.369 22.351 1.00 0.00 O
ATOM 73 I 73 25.000 13.636 16.250 1.00 0.00 O
ATOM 74 I 74 25.000 23.598 17.122 1.00 0.00 O
ATOM 75 I 75 25.000 33.559 17.993 1.00 0.00 O
ATOM 76 I 76 25.000 43.521 18.865 1.00 0.00 O
ATOM 77 I 77 25.000 53.483 19.736 1.00 0.00 O
ATOM 78 I 78 25.000 63.445 20.608 1.00 0.00 O
ATOM 79 I 79 25.000 73.407 21.480 1.00 0.00 O
ATOM 80 I 80 25.000 83.369 22.351 1.00 0.00 O
ATOM 81 I 81 35.000 13.636 16.250 1.00 0.00 O
ATOM 82 I 82 35.000 23.598 17.122 1.00 0.00 O
ATOM 83 I 83 35.000 33.559 17.993 1.00 0.00 O
ATOM 84 I 84 35.000 43.521 18.865 1.00 0.00 O

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ATOM    85  I       85     35.000  53.483  19.736  1.00  0.00          O
ATOM    86  I       86     35.000  63.445  20.608  1.00  0.00          O
ATOM    87  I       87     35.000  73.407  21.480  1.00  0.00          O
ATOM    88  I       88     35.000  83.369  22.351  1.00  0.00          O
ATOM    89  I       89     45.000  13.636  16.250  1.00  0.00          O
ATOM    90  I       90     45.000  23.598  17.122  1.00  0.00          O
ATOM    91  I       91     45.000  33.559  17.993  1.00  0.00          O
ATOM    92  I       92     45.000  43.521  18.865  1.00  0.00          O
ATOM    93  I       93     45.000  53.483  19.736  1.00  0.00          O
ATOM    94  I       94     45.000  63.445  20.608  1.00  0.00          O
ATOM    95  I       95     45.000  73.407  21.480  1.00  0.00          O
ATOM    96  I       96     45.000  83.369  22.351  1.00  0.00          O
ATOM    97  I       97     55.000  13.636  16.250  1.00  0.00          O
ATOM    98  I       98     55.000  23.598  17.122  1.00  0.00          O
ATOM    99  I       99     55.000  33.559  17.993  1.00  0.00          O
ATOM   100  I      100     55.000  43.521  18.865  1.00  0.00          O
ATOM   101  I      101     55.000  53.483  19.736  1.00  0.00          O
ATOM   102  I      102     55.000  63.445  20.608  1.00  0.00          O
ATOM   103  I      103     55.000  73.407  21.480  1.00  0.00          O
ATOM   104  I      104     55.000  83.369  22.351  1.00  0.00          O
ATOM   105  I      105     65.000  13.636  16.250  1.00  0.00          O
ATOM   106  I      106     65.000  23.598  17.122  1.00  0.00          O
ATOM   107  I      107     65.000  33.559  17.993  1.00  0.00          O
ATOM   108  I      108     65.000  43.521  18.865  1.00  0.00          O
ATOM   109  I      109     65.000  53.483  19.736  1.00  0.00          O
ATOM   110  I      110     65.000  63.445  20.608  1.00  0.00          O
ATOM   111  I      111     65.000  73.407  21.480  1.00  0.00          O
ATOM   112  I      112     65.000  83.369  22.351  1.00  0.00          O
ATOM   113  I      113     75.000  13.636  16.250  1.00  0.00          O
ATOM   114  I      114     75.000  23.598  17.122  1.00  0.00          O
ATOM   115  I      115     75.000  33.559  17.993  1.00  0.00          O
ATOM   116  I      116     75.000  43.521  18.865  1.00  0.00          O
ATOM   117  I      117     75.000  53.483  19.736  1.00  0.00          O
ATOM   118  I      118     75.000  63.445  20.608  1.00  0.00          O
ATOM   119  I      119     75.000  73.407  21.480  1.00  0.00          O
ATOM   120  I      120     75.000  83.369  22.351  1.00  0.00          O
ATOM   121  I      121     85.000  13.636  16.250  1.00  0.00          O
ATOM   122  I      122     85.000  23.598  17.122  1.00  0.00          O
ATOM   123  I      123     85.000  33.559  17.993  1.00  0.00          O
ATOM   124  I      124     85.000  43.521  18.865  1.00  0.00          O
ATOM   125  I      125     85.000  53.483  19.736  1.00  0.00          O
ATOM   126  I      126     85.000  63.445  20.608  1.00  0.00          O
ATOM   127  I      127     85.000  73.407  21.480  1.00  0.00          O
ATOM   128  I      128     85.000  83.369  22.351  1.00  0.00          O
ATOM   129  I      129     10.000   8.219  20.795  1.00  0.00          O
ATOM   130  I      130     10.000  18.181  21.667  1.00  0.00          O
ATOM   131  I      131     10.000  28.143  22.539  1.00  0.00          O
ATOM   132  I      132     10.000  38.105  23.410  1.00  0.00          O
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ATOM    133  I       133      10.000  48.067  24.282  1.00  0.00          O
ATOM    134  I       134      10.000  58.029  25.153  1.00  0.00          O
ATOM    135  I       135      10.000  67.991  26.025  1.00  0.00          O
ATOM    136  I       136      10.000  77.952  26.896  1.00  0.00          O
ATOM    137  I       137      20.000   8.219  20.795  1.00  0.00          O
ATOM    138  I       138      20.000  18.181  21.667  1.00  0.00          O
ATOM    139  I       139      20.000  28.143  22.539  1.00  0.00          O
ATOM    140  I       140      20.000  38.105  23.410  1.00  0.00          O
ATOM    141  I       141      20.000  48.067  24.282  1.00  0.00          O
ATOM    142  I       142      20.000  58.029  25.153  1.00  0.00          O
ATOM    143  I       143      20.000  67.991  26.025  1.00  0.00          O
ATOM    144  I       144      20.000  77.952  26.896  1.00  0.00          O
ATOM    145  I       145      30.000   8.219  20.795  1.00  0.00          O
ATOM    146  I       146      30.000  18.181  21.667  1.00  0.00          O
ATOM    147  I       147      30.000  28.143  22.539  1.00  0.00          O
ATOM    148  I       148      30.000  38.105  23.410  1.00  0.00          O
ATOM    149  I       149      30.000  48.067  24.282  1.00  0.00          O
ATOM    150  I       150      30.000  58.029  25.153  1.00  0.00          O
ATOM    151  I       151      30.000  67.991  26.025  1.00  0.00          O
ATOM    152  I       152      30.000  77.952  26.896  1.00  0.00          O
ATOM    153  I       153      40.000   8.219  20.795  1.00  0.00          O
ATOM    154  I       154      40.000  18.181  21.667  1.00  0.00          O
ATOM    155  I       155      40.000  28.143  22.539  1.00  0.00          O
ATOM    156  I       156      40.000  38.105  23.410  1.00  0.00          O
ATOM    157  I       157      40.000  48.067  24.282  1.00  0.00          O
ATOM    158  I       158      40.000  58.029  25.153  1.00  0.00          O
ATOM    159  I       159      40.000  67.991  26.025  1.00  0.00          O
ATOM    160  I       160      40.000  77.952  26.896  1.00  0.00          O
ATOM    161  I       161      50.000   8.219  20.795  1.00  0.00          O
ATOM    162  I       162      50.000  18.181  21.667  1.00  0.00          O
ATOM    163  I       163      50.000  28.143  22.539  1.00  0.00          O
ATOM    164  I       164      50.000  38.105  23.410  1.00  0.00          O
ATOM    165  I       165      50.000  48.067  24.282  1.00  0.00          O
ATOM    166  I       166      50.000  58.029  25.153  1.00  0.00          O
ATOM    167  I       167      50.000  67.991  26.025  1.00  0.00          O
ATOM    168  I       168      50.000  77.952  26.896  1.00  0.00          O
ATOM    169  I       169      60.000   8.219  20.795  1.00  0.00          O
ATOM    170  I       170      60.000  18.181  21.667  1.00  0.00          O
ATOM    171  I       171      60.000  28.143  22.539  1.00  0.00          O
ATOM    172  I       172      60.000  38.105  23.410  1.00  0.00          O
ATOM    173  I       173      60.000  48.067  24.282  1.00  0.00          O
ATOM    174  I       174      60.000  58.029  25.153  1.00  0.00          O
ATOM    175  I       175      60.000  67.991  26.025  1.00  0.00          O
ATOM    176  I       176      60.000  77.952  26.896  1.00  0.00          O
ATOM    177  I       177      70.000   8.219  20.795  1.00  0.00          O
ATOM    178  I       178      70.000  18.181  21.667  1.00  0.00          O
ATOM    179  I       179      70.000  28.143  22.539  1.00  0.00          O
ATOM    180  I       180      70.000  38.105  23.410  1.00  0.00          O
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ATOM 181 I 181 70.000 48.067 24.282 1.00 0.00 O
ATOM 182 I 182 70.000 58.029 25.153 1.00 0.00 O
ATOM 183 I 183 70.000 67.991 26.025 1.00 0.00 O
ATOM 184 I 184 70.000 77.952 26.896 1.00 0.00 O
ATOM 185 I 185 80.000 8.219 20.795 1.00 0.00 O
ATOM 186 I 186 80.000 18.181 21.667 1.00 0.00 O
ATOM 187 I 187 80.000 28.143 22.539 1.00 0.00 O
ATOM 188 I 188 80.000 38.105 23.410 1.00 0.00 O
ATOM 189 I 189 80.000 48.067 24.282 1.00 0.00 O
ATOM 190 I 190 80.000 58.029 25.153 1.00 0.00 O
ATOM 191 I 191 80.000 67.991 26.025 1.00 0.00 O
ATOM 192 I 192 80.000 77.952 26.896 1.00 0.00 O
ATOM 193 I 193 15.000 12.764 26.212 1.00 0.00 O
ATOM 194 I 194 15.000 22.726 27.084 1.00 0.00 O
ATOM 195 I 195 15.000 32.688 27.955 1.00 0.00 O
ATOM 196 I 196 15.000 42.650 28.827 1.00 0.00 O
ATOM 197 I 197 15.000 52.612 29.698 1.00 0.00 O
ATOM 198 I 198 15.000 62.574 30.570 1.00 0.00 O
ATOM 199 I 199 15.000 72.536 31.442 1.00 0.00 O
ATOM 200 I 200 15.000 82.498 32.313 1.00 0.00 O
ATOM 201 I 201 25.000 12.764 26.212 1.00 0.00 O
ATOM 202 I 202 25.000 22.726 27.084 1.00 0.00 O
ATOM 203 I 203 25.000 32.688 27.955 1.00 0.00 O
ATOM 204 I 204 25.000 42.650 28.827 1.00 0.00 O
ATOM 205 I 205 25.000 52.612 29.698 1.00 0.00 O
ATOM 206 I 206 25.000 62.574 30.570 1.00 0.00 O
ATOM 207 I 207 25.000 72.536 31.442 1.00 0.00 O
ATOM 208 I 208 25.000 82.498 32.313 1.00 0.00 O
ATOM 209 I 209 35.000 12.764 26.212 1.00 0.00 O
ATOM 210 I 210 35.000 22.726 27.084 1.00 0.00 O
ATOM 211 I 211 35.000 32.688 27.955 1.00 0.00 O
ATOM 212 I 212 35.000 42.650 28.827 1.00 0.00 O
ATOM 213 I 213 35.000 52.612 29.698 1.00 0.00 O
ATOM 214 I 214 35.000 62.574 30.570 1.00 0.00 O
ATOM 215 I 215 35.000 72.536 31.442 1.00 0.00 O
ATOM 216 I 216 35.000 82.498 32.313 1.00 0.00 O
ATOM 217 I 217 45.000 12.764 26.212 1.00 0.00 O
ATOM 218 I 218 45.000 22.726 27.084 1.00 0.00 O
ATOM 219 I 219 45.000 32.688 27.955 1.00 0.00 O
ATOM 220 I 220 45.000 42.650 28.827 1.00 0.00 O
ATOM 221 I 221 45.000 52.612 29.698 1.00 0.00 O
ATOM 222 I 222 45.000 62.574 30.570 1.00 0.00 O
ATOM 223 I 223 45.000 72.536 31.442 1.00 0.00 O
ATOM 224 I 224 45.000 82.498 32.313 1.00 0.00 O
ATOM 225 I 225 55.000 12.764 26.212 1.00 0.00 O
ATOM 226 I 226 55.000 22.726 27.084 1.00 0.00 O
ATOM 227 I 227 55.000 32.688 27.955 1.00 0.00 O
ATOM 228 I 228 55.000 42.650 28.827 1.00 0.00 O

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ATOM    229  I     229      55.000  52.612  29.698  1.00  0.00          O
ATOM    230  I     230      55.000  62.574  30.570  1.00  0.00          O
ATOM    231  I     231      55.000  72.536  31.442  1.00  0.00          O
ATOM    232  I     232      55.000  82.498  32.313  1.00  0.00          O
ATOM    233  I     233      65.000  12.764  26.212  1.00  0.00          O
ATOM    234  I     234      65.000  22.726  27.084  1.00  0.00          O
ATOM    235  I     235      65.000  32.688  27.955  1.00  0.00          O
ATOM    236  I     236      65.000  42.650  28.827  1.00  0.00          O
ATOM    237  I     237      65.000  52.612  29.698  1.00  0.00          O
ATOM    238  I     238      65.000  62.574  30.570  1.00  0.00          O
ATOM    239  I     239      65.000  72.536  31.442  1.00  0.00          O
ATOM    240  I     240      65.000  82.498  32.313  1.00  0.00          O
ATOM    241  I     241      75.000  12.764  26.212  1.00  0.00          O
ATOM    242  I     242      75.000  22.726  27.084  1.00  0.00          O
ATOM    243  I     243      75.000  32.688  27.955  1.00  0.00          O
ATOM    244  I     244      75.000  42.650  28.827  1.00  0.00          O
ATOM    245  I     245      75.000  52.612  29.698  1.00  0.00          O
ATOM    246  I     246      75.000  62.574  30.570  1.00  0.00          O
ATOM    247  I     247      75.000  72.536  31.442  1.00  0.00          O
ATOM    248  I     248      75.000  82.498  32.313  1.00  0.00          O
ATOM    249  I     249      85.000  12.764  26.212  1.00  0.00          O
ATOM    250  I     250      85.000  22.726  27.084  1.00  0.00          O
ATOM    251  I     251      85.000  32.688  27.955  1.00  0.00          O
ATOM    252  I     252      85.000  42.650  28.827  1.00  0.00          O
ATOM    253  I     253      85.000  52.612  29.698  1.00  0.00          O
ATOM    254  I     254      85.000  62.574  30.570  1.00  0.00          O
ATOM    255  I     255      85.000  72.536  31.442  1.00  0.00          O
ATOM    256  I     256      85.000  82.498  32.313  1.00  0.00          O
ATOM    257  I     257      10.000   7.347  30.757  1.00  0.00          O
ATOM    258  I     258      10.000  17.309  31.629  1.00  0.00          O
ATOM    259  I     259      10.000  27.271  32.501  1.00  0.00          O
ATOM    260  I     260      10.000  37.233  33.372  1.00  0.00          O
ATOM    261  I     261      10.000  47.195  34.244  1.00  0.00          O
ATOM    262  I     262      10.000  57.157  35.115  1.00  0.00          O
ATOM    263  I     263      10.000  67.119  35.987  1.00  0.00          O
ATOM    264  I     264      10.000  77.081  36.858  1.00  0.00          O
ATOM    265  I     265      20.000   7.347  30.757  1.00  0.00          O
ATOM    266  I     266      20.000  17.309  31.629  1.00  0.00          O
ATOM    267  I     267      20.000  27.271  32.501  1.00  0.00          O
ATOM    268  I     268      20.000  37.233  33.372  1.00  0.00          O
ATOM    269  I     269      20.000  47.195  34.244  1.00  0.00          O
ATOM    270  I     270      20.000  57.157  35.115  1.00  0.00          O
ATOM    271  I     271      20.000  67.119  35.987  1.00  0.00          O
ATOM    272  I     272      20.000  77.081  36.858  1.00  0.00          O
ATOM    273  I     273      30.000   7.347  30.757  1.00  0.00          O
ATOM    274  I     274      30.000  17.309  31.629  1.00  0.00          O
ATOM    275  I     275      30.000  27.271  32.501  1.00  0.00          O
ATOM    276  I     276      30.000  37.233  33.372  1.00  0.00          O
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ATOM 277 I 277 30.000 47.195 34.244 1.00 0.00 O
ATOM 278 I 278 30.000 57.157 35.115 1.00 0.00 O
ATOM 279 I 279 30.000 67.119 35.987 1.00 0.00 O
ATOM 280 I 280 30.000 77.081 36.858 1.00 0.00 O
ATOM 281 I 281 40.000 7.347 30.757 1.00 0.00 O
ATOM 282 I 282 40.000 17.309 31.629 1.00 0.00 O
ATOM 283 I 283 40.000 27.271 32.501 1.00 0.00 O
ATOM 284 I 284 40.000 37.233 33.372 1.00 0.00 O
ATOM 285 I 285 40.000 47.195 34.244 1.00 0.00 O
ATOM 286 I 286 40.000 57.157 35.115 1.00 0.00 O
ATOM 287 I 287 40.000 67.119 35.987 1.00 0.00 O
ATOM 288 I 288 40.000 77.081 36.858 1.00 0.00 O
ATOM 289 I 289 50.000 7.347 30.757 1.00 0.00 O
ATOM 290 I 290 50.000 17.309 31.629 1.00 0.00 O
ATOM 291 I 291 50.000 27.271 32.501 1.00 0.00 O
ATOM 292 I 292 50.000 37.233 33.372 1.00 0.00 O
ATOM 293 I 293 50.000 47.195 34.244 1.00 0.00 O
ATOM 294 I 294 50.000 57.157 35.115 1.00 0.00 O
ATOM 295 I 295 50.000 67.119 35.987 1.00 0.00 O
ATOM 296 I 296 50.000 77.081 36.858 1.00 0.00 O
ATOM 297 I 297 60.000 7.347 30.757 1.00 0.00 O
ATOM 298 I 298 60.000 17.309 31.629 1.00 0.00 O
ATOM 299 I 299 60.000 27.271 32.501 1.00 0.00 O
ATOM 300 I 300 60.000 37.233 33.372 1.00 0.00 O
ATOM 301 I 301 60.000 47.195 34.244 1.00 0.00 O
ATOM 302 I 302 60.000 57.157 35.115 1.00 0.00 O
ATOM 303 I 303 60.000 67.119 35.987 1.00 0.00 O
ATOM 304 I 304 60.000 77.081 36.858 1.00 0.00 O
ATOM 305 I 305 70.000 7.347 30.757 1.00 0.00 O
ATOM 306 I 306 70.000 17.309 31.629 1.00 0.00 O
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ATOM 308 I 308 70.000 37.233 33.372 1.00 0.00 O
ATOM 309 I 309 70.000 47.195 34.244 1.00 0.00 O
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ATOM 313 I 313 80.000 7.347 30.757 1.00 0.00 O
ATOM 314 I 314 80.000 17.309 31.629 1.00 0.00 O
ATOM 315 I 315 80.000 27.271 32.501 1.00 0.00 O
ATOM 316 I 316 80.000 37.233 33.372 1.00 0.00 O
ATOM 317 I 317 80.000 47.195 34.244 1.00 0.00 O
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ATOM 319 I 319 80.000 67.119 35.987 1.00 0.00 O
ATOM 320 I 320 80.000 77.081 36.858 1.00 0.00 O
ATOM 321 I 321 15.000 11.892 36.174 1.00 0.00 O
ATOM 322 I 322 15.000 21.854 37.046 1.00 0.00 O
ATOM 323 I 323 15.000 31.816 37.917 1.00 0.00 O
ATOM 324 I 324 15.000 41.778 38.789 1.00 0.00 O

ATOM 325 I 325 15.000 51.740 39.660 1.00 0.00 O
ATOM 326 I 326 15.000 61.702 40.532 1.00 0.00 O
ATOM 327 I 327 15.000 71.664 41.403 1.00 0.00 O
ATOM 328 I 328 15.000 81.626 42.275 1.00 0.00 O
ATOM 329 I 329 25.000 11.892 36.174 1.00 0.00 O
ATOM 330 I 330 25.000 21.854 37.046 1.00 0.00 O
ATOM 331 I 331 25.000 31.816 37.917 1.00 0.00 O
ATOM 332 I 332 25.000 41.778 38.789 1.00 0.00 O
ATOM 333 I 333 25.000 51.740 39.660 1.00 0.00 O
ATOM 334 I 334 25.000 61.702 40.532 1.00 0.00 O
ATOM 335 I 335 25.000 71.664 41.403 1.00 0.00 O
ATOM 336 I 336 25.000 81.626 42.275 1.00 0.00 O
ATOM 337 I 337 35.000 11.892 36.174 1.00 0.00 O
ATOM 338 I 338 35.000 21.854 37.046 1.00 0.00 O
ATOM 339 I 339 35.000 31.816 37.917 1.00 0.00 O
ATOM 340 I 340 35.000 41.778 38.789 1.00 0.00 O
ATOM 341 I 341 35.000 51.740 39.660 1.00 0.00 O
ATOM 342 I 342 35.000 61.702 40.532 1.00 0.00 O
ATOM 343 I 343 35.000 71.664 41.403 1.00 0.00 O
ATOM 344 I 344 35.000 81.626 42.275 1.00 0.00 O
ATOM 345 I 345 45.000 11.892 36.174 1.00 0.00 O
ATOM 346 I 346 45.000 21.854 37.046 1.00 0.00 O
ATOM 347 I 347 45.000 31.816 37.917 1.00 0.00 O
ATOM 348 I 348 45.000 41.778 38.789 1.00 0.00 O
ATOM 349 I 349 45.000 51.740 39.660 1.00 0.00 O
ATOM 350 I 350 45.000 61.702 40.532 1.00 0.00 O
ATOM 351 I 351 45.000 71.664 41.403 1.00 0.00 O
ATOM 352 I 352 45.000 81.626 42.275 1.00 0.00 O
ATOM 353 I 353 55.000 11.892 36.174 1.00 0.00 O
ATOM 354 I 354 55.000 21.854 37.046 1.00 0.00 O
ATOM 355 I 355 55.000 31.816 37.917 1.00 0.00 O
ATOM 356 I 356 55.000 41.778 38.789 1.00 0.00 O
ATOM 357 I 357 55.000 51.740 39.660 1.00 0.00 O
ATOM 358 I 358 55.000 61.702 40.532 1.00 0.00 O
ATOM 359 I 359 55.000 71.664 41.403 1.00 0.00 O
ATOM 360 I 360 55.000 81.626 42.275 1.00 0.00 O
ATOM 361 I 361 65.000 11.892 36.174 1.00 0.00 O
ATOM 362 I 362 65.000 21.854 37.046 1.00 0.00 O
ATOM 363 I 363 65.000 31.816 37.917 1.00 0.00 O
ATOM 364 I 364 65.000 41.778 38.789 1.00 0.00 O
ATOM 365 I 365 65.000 51.740 39.660 1.00 0.00 O
ATOM 366 I 366 65.000 61.702 40.532 1.00 0.00 O
ATOM 367 I 367 65.000 71.664 41.403 1.00 0.00 O
ATOM 368 I 368 65.000 81.626 42.275 1.00 0.00 O
ATOM 369 I 369 75.000 11.892 36.174 1.00 0.00 O
ATOM 370 I 370 75.000 21.854 37.046 1.00 0.00 O
ATOM 371 I 371 75.000 31.816 37.917 1.00 0.00 O
ATOM 372 I 372 75.000 41.778 38.789 1.00 0.00 O

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ATOM    373  I       373      75.000  51.740  39.660  1.00  0.00          O
ATOM    374  I       374      75.000  61.702  40.532  1.00  0.00          O
ATOM    375  I       375      75.000  71.664  41.403  1.00  0.00          O
ATOM    376  I       376      75.000  81.626  42.275  1.00  0.00          O
ATOM    377  I       377      85.000  11.892  36.174  1.00  0.00          O
ATOM    378  I       378      85.000  21.854  37.046  1.00  0.00          O
ATOM    379  I       379      85.000  31.816  37.917  1.00  0.00          O
ATOM    380  I       380      85.000  41.778  38.789  1.00  0.00          O
ATOM    381  I       381      85.000  51.740  39.660  1.00  0.00          O
ATOM    382  I       382      85.000  61.702  40.532  1.00  0.00          O
ATOM    383  I       383      85.000  71.664  41.403  1.00  0.00          O
ATOM    384  I       384      85.000  81.626  42.275  1.00  0.00          O
ATOM    385  I       385      10.000   6.476  40.719  1.00  0.00          O
ATOM    386  I       386      10.000  16.438  41.591  1.00  0.00          O
ATOM    387  I       387      10.000  26.400  42.462  1.00  0.00          O
ATOM    388  I       388      10.000  36.362  43.334  1.00  0.00          O
ATOM    389  I       389      10.000  46.324  44.206  1.00  0.00          O
ATOM    390  I       390      10.000  56.285  45.077  1.00  0.00          O
ATOM    391  I       391      10.000  66.247  45.949  1.00  0.00          O
ATOM    392  I       392      10.000  76.209  46.820  1.00  0.00          O
ATOM    393  I       393      20.000   6.476  40.719  1.00  0.00          O
ATOM    394  I       394      20.000  16.438  41.591  1.00  0.00          O
ATOM    395  I       395      20.000  26.400  42.462  1.00  0.00          O
ATOM    396  I       396      20.000  36.362  43.334  1.00  0.00          O
ATOM    397  I       397      20.000  46.324  44.206  1.00  0.00          O
ATOM    398  I       398      20.000  56.285  45.077  1.00  0.00          O
ATOM    399  I       399      20.000  66.247  45.949  1.00  0.00          O
ATOM    400  I       400      20.000  76.209  46.820  1.00  0.00          O
ATOM    401  I       401      30.000   6.476  40.719  1.00  0.00          O
ATOM    402  I       402      30.000  16.438  41.591  1.00  0.00          O
ATOM    403  I       403      30.000  26.400  42.462  1.00  0.00          O
ATOM    404  I       404      30.000  36.362  43.334  1.00  0.00          O
ATOM    405  I       405      30.000  46.324  44.206  1.00  0.00          O
ATOM    406  I       406      30.000  56.285  45.077  1.00  0.00          O
ATOM    407  I       407      30.000  66.247  45.949  1.00  0.00          O
ATOM    408  I       408      30.000  76.209  46.820  1.00  0.00          O
ATOM    409  I       409      40.000   6.476  40.719  1.00  0.00          O
ATOM    410  I       410      40.000  16.438  41.591  1.00  0.00          O
ATOM    411  I       411      40.000  26.400  42.462  1.00  0.00          O
ATOM    412  I       412      40.000  36.362  43.334  1.00  0.00          O
ATOM    413  I       413      40.000  46.324  44.206  1.00  0.00          O
ATOM    414  I       414      40.000  56.285  45.077  1.00  0.00          O
ATOM    415  I       415      40.000  66.247  45.949  1.00  0.00          O
ATOM    416  I       416      40.000  76.209  46.820  1.00  0.00          O
ATOM    417  I       417      50.000   6.476  40.719  1.00  0.00          O
ATOM    418  I       418      50.000  16.438  41.591  1.00  0.00          O
ATOM    419  I       419      50.000  26.400  42.462  1.00  0.00          O
ATOM    420  I       420      50.000  36.362  43.334  1.00  0.00          O
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ATOM 421 I 421 50.000 46.324 44.206 1.00 0.00 O
ATOM 422 I 422 50.000 56.285 45.077 1.00 0.00 O
ATOM 423 I 423 50.000 66.247 45.949 1.00 0.00 O
ATOM 424 I 424 50.000 76.209 46.820 1.00 0.00 O
ATOM 425 I 425 60.000 6.476 40.719 1.00 0.00 O
ATOM 426 I 426 60.000 16.438 41.591 1.00 0.00 O
ATOM 427 I 427 60.000 26.400 42.462 1.00 0.00 O
ATOM 428 I 428 60.000 36.362 43.334 1.00 0.00 O
ATOM 429 I 429 60.000 46.324 44.206 1.00 0.00 O
ATOM 430 I 430 60.000 56.285 45.077 1.00 0.00 O
ATOM 431 I 431 60.000 66.247 45.949 1.00 0.00 O
ATOM 432 I 432 60.000 76.209 46.820 1.00 0.00 O
ATOM 433 I 433 70.000 6.476 40.719 1.00 0.00 O
ATOM 434 I 434 70.000 16.438 41.591 1.00 0.00 O
ATOM 435 I 435 70.000 26.400 42.462 1.00 0.00 O
ATOM 436 I 436 70.000 36.362 43.334 1.00 0.00 O
ATOM 437 I 437 70.000 46.324 44.206 1.00 0.00 O
ATOM 438 I 438 70.000 56.285 45.077 1.00 0.00 O
ATOM 439 I 439 70.000 66.247 45.949 1.00 0.00 O
ATOM 440 I 440 70.000 76.209 46.820 1.00 0.00 O
ATOM 441 I 441 80.000 6.476 40.719 1.00 0.00 O
ATOM 442 I 442 80.000 16.438 41.591 1.00 0.00 O
ATOM 443 I 443 80.000 26.400 42.462 1.00 0.00 O
ATOM 444 I 444 80.000 36.362 43.334 1.00 0.00 O
ATOM 445 I 445 80.000 46.324 44.206 1.00 0.00 O
ATOM 446 I 446 80.000 56.285 45.077 1.00 0.00 O
ATOM 447 I 447 80.000 66.247 45.949 1.00 0.00 O
ATOM 448 I 448 80.000 76.209 46.820 1.00 0.00 O
ATOM 449 I 449 15.000 11.021 46.136 1.00 0.00 O
ATOM 450 I 450 15.000 20.983 47.008 1.00 0.00 O
ATOM 451 I 451 15.000 30.945 47.879 1.00 0.00 O
ATOM 452 I 452 15.000 40.907 48.751 1.00 0.00 O
ATOM 453 I 453 15.000 50.869 49.622 1.00 0.00 O
ATOM 454 I 454 15.000 60.831 50.494 1.00 0.00 O
ATOM 455 I 455 15.000 70.793 51.365 1.00 0.00 O
ATOM 456 I 456 15.000 80.755 52.237 1.00 0.00 O
ATOM 457 I 457 25.000 11.021 46.136 1.00 0.00 O
ATOM 458 I 458 25.000 20.983 47.008 1.00 0.00 O
ATOM 459 I 459 25.000 30.945 47.879 1.00 0.00 O
ATOM 460 I 460 25.000 40.907 48.751 1.00 0.00 O
ATOM 461 I 461 25.000 50.869 49.622 1.00 0.00 O
ATOM 462 I 462 25.000 60.831 50.494 1.00 0.00 O
ATOM 463 I 463 25.000 70.793 51.365 1.00 0.00 O
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ATOM 472 I 472 35.000 80.755 52.237 1.00 0.00 O
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ATOM 474 I 474 45.000 20.983 47.008 1.00 0.00 O
ATOM 475 I 475 45.000 30.945 47.879 1.00 0.00 O
ATOM 476 I 476 45.000 40.907 48.751 1.00 0.00 O
ATOM 477 I 477 45.000 50.869 49.622 1.00 0.00 O
ATOM 478 I 478 45.000 60.831 50.494 1.00 0.00 O
ATOM 479 I 479 45.000 70.793 51.365 1.00 0.00 O
ATOM 480 I 480 45.000 80.755 52.237 1.00 0.00 O
ATOM 481 I 481 55.000 11.021 46.136 1.00 0.00 O
ATOM 482 I 482 55.000 20.983 47.008 1.00 0.00 O
ATOM 483 I 483 55.000 30.945 47.879 1.00 0.00 O
ATOM 484 I 484 55.000 40.907 48.751 1.00 0.00 O
ATOM 485 I 485 55.000 50.869 49.622 1.00 0.00 O
ATOM 486 I 486 55.000 60.831 50.494 1.00 0.00 O
ATOM 487 I 487 55.000 70.793 51.365 1.00 0.00 O
ATOM 488 I 488 55.000 80.755 52.237 1.00 0.00 O
ATOM 489 I 489 65.000 11.021 46.136 1.00 0.00 O
ATOM 490 I 490 65.000 20.983 47.008 1.00 0.00 O
ATOM 491 I 491 65.000 30.945 47.879 1.00 0.00 O
ATOM 492 I 492 65.000 40.907 48.751 1.00 0.00 O
ATOM 493 I 493 65.000 50.869 49.622 1.00 0.00 O
ATOM 494 I 494 65.000 60.831 50.494 1.00 0.00 O
ATOM 495 I 495 65.000 70.793 51.365 1.00 0.00 O
ATOM 496 I 496 65.000 80.755 52.237 1.00 0.00 O
ATOM 497 I 497 75.000 11.021 46.136 1.00 0.00 O
ATOM 498 I 498 75.000 20.983 47.008 1.00 0.00 O
ATOM 499 I 499 75.000 30.945 47.879 1.00 0.00 O
ATOM 500 I 500 75.000 40.907 48.751 1.00 0.00 O
ATOM 501 I 501 75.000 50.869 49.622 1.00 0.00 O
ATOM 502 I 502 75.000 60.831 50.494 1.00 0.00 O
ATOM 503 I 503 75.000 70.793 51.365 1.00 0.00 O
ATOM 504 I 504 75.000 80.755 52.237 1.00 0.00 O
ATOM 505 I 505 85.000 11.021 46.136 1.00 0.00 O
ATOM 506 I 506 85.000 20.983 47.008 1.00 0.00 O
ATOM 507 I 507 85.000 30.945 47.879 1.00 0.00 O
ATOM 508 I 508 85.000 40.907 48.751 1.00 0.00 O
ATOM 509 I 509 85.000 50.869 49.622 1.00 0.00 O
ATOM 510 I 510 85.000 60.831 50.494 1.00 0.00 O
ATOM 511 I 511 85.000 70.793 51.365 1.00 0.00 O
ATOM 512 I 512 85.000 80.755 52.237 1.00 0.00 O
ATOM 513 I 513 10.000 5.604 50.681 1.00 0.00 O
ATOM 514 I 514 10.000 15.566 51.553 1.00 0.00 O
ATOM 515 I 515 10.000 25.528 52.424 1.00 0.00 O
ATOM 516 I 516 10.000 35.490 53.296 1.00 0.00 O

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ATOM    517  I       517      10.000  45.452  54.168  1.00  0.00          O
ATOM    518  I       518      10.000  55.414  55.039  1.00  0.00          O
ATOM    519  I       519      10.000  65.376  55.911  1.00  0.00          O
ATOM    520  I       520      10.000  75.338  56.782  1.00  0.00          O
ATOM    521  I       521      20.000   5.604  50.681  1.00  0.00          O
ATOM    522  I       522      20.000  15.566  51.553  1.00  0.00          O
ATOM    523  I       523      20.000  25.528  52.424  1.00  0.00          O
ATOM    524  I       524      20.000  35.490  53.296  1.00  0.00          O
ATOM    525  I       525      20.000  45.452  54.168  1.00  0.00          O
ATOM    526  I       526      20.000  55.414  55.039  1.00  0.00          O
ATOM    527  I       527      20.000  65.376  55.911  1.00  0.00          O
ATOM    528  I       528      20.000  75.338  56.782  1.00  0.00          O
ATOM    529  I       529      30.000   5.604  50.681  1.00  0.00          O
ATOM    530  I       530      30.000  15.566  51.553  1.00  0.00          O
ATOM    531  I       531      30.000  25.528  52.424  1.00  0.00          O
ATOM    532  I       532      30.000  35.490  53.296  1.00  0.00          O
ATOM    533  I       533      30.000  45.452  54.168  1.00  0.00          O
ATOM    534  I       534      30.000  55.414  55.039  1.00  0.00          O
ATOM    535  I       535      30.000  65.376  55.911  1.00  0.00          O
ATOM    536  I       536      30.000  75.338  56.782  1.00  0.00          O
ATOM    537  I       537      40.000   5.604  50.681  1.00  0.00          O
ATOM    538  I       538      40.000  15.566  51.553  1.00  0.00          O
ATOM    539  I       539      40.000  25.528  52.424  1.00  0.00          O
ATOM    540  I       540      40.000  35.490  53.296  1.00  0.00          O
ATOM    541  I       541      40.000  45.452  54.168  1.00  0.00          O
ATOM    542  I       542      40.000  55.414  55.039  1.00  0.00          O
ATOM    543  I       543      40.000  65.376  55.911  1.00  0.00          O
ATOM    544  I       544      40.000  75.338  56.782  1.00  0.00          O
ATOM    545  I       545      50.000   5.604  50.681  1.00  0.00          O
ATOM    546  I       546      50.000  15.566  51.553  1.00  0.00          O
ATOM    547  I       547      50.000  25.528  52.424  1.00  0.00          O
ATOM    548  I       548      50.000  35.490  53.296  1.00  0.00          O
ATOM    549  I       549      50.000  45.452  54.168  1.00  0.00          O
ATOM    550  I       550      50.000  55.414  55.039  1.00  0.00          O
ATOM    551  I       551      50.000  65.376  55.911  1.00  0.00          O
ATOM    552  I       552      50.000  75.338  56.782  1.00  0.00          O
ATOM    553  I       553      60.000   5.604  50.681  1.00  0.00          O
ATOM    554  I       554      60.000  15.566  51.553  1.00  0.00          O
ATOM    555  I       555      60.000  25.528  52.424  1.00  0.00          O
ATOM    556  I       556      60.000  35.490  53.296  1.00  0.00          O
ATOM    557  I       557      60.000  45.452  54.168  1.00  0.00          O
ATOM    558  I       558      60.000  55.414  55.039  1.00  0.00          O
ATOM    559  I       559      60.000  65.376  55.911  1.00  0.00          O
ATOM    560  I       560      60.000  75.338  56.782  1.00  0.00          O
ATOM    561  I       561      70.000   5.604  50.681  1.00  0.00          O
ATOM    562  I       562      70.000  15.566  51.553  1.00  0.00          O
ATOM    563  I       563      70.000  25.528  52.424  1.00  0.00          O
ATOM    564  I       564      70.000  35.490  53.296  1.00  0.00          O
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ATOM    565  I       565      70.000  45.452  54.168  1.00  0.00          O
ATOM    566  I       566      70.000  55.414  55.039  1.00  0.00          O
ATOM    567  I       567      70.000  65.376  55.911  1.00  0.00          O
ATOM    568  I       568      70.000  75.338  56.782  1.00  0.00          O
ATOM    569  I       569      80.000   5.604  50.681  1.00  0.00          O
ATOM    570  I       570      80.000  15.566  51.553  1.00  0.00          O
ATOM    571  I       571      80.000  25.528  52.424  1.00  0.00          O
ATOM    572  I       572      80.000  35.490  53.296  1.00  0.00          O
ATOM    573  I       573      80.000  45.452  54.168  1.00  0.00          O
ATOM    574  I       574      80.000  55.414  55.039  1.00  0.00          O
ATOM    575  I       575      80.000  65.376  55.911  1.00  0.00          O
ATOM    576  I       576      80.000  75.338  56.782  1.00  0.00          O
ATOM    577  I       577      15.000  10.149  56.098  1.00  0.00          O
ATOM    578  I       578      15.000  20.111  56.970  1.00  0.00          O
ATOM    579  I       579      15.000  30.073  57.841  1.00  0.00          O
ATOM    580  I       580      15.000  40.035  58.713  1.00  0.00          O
ATOM    581  I       581      15.000  49.997  59.584  1.00  0.00          O
ATOM    582  I       582      15.000  59.959  60.456  1.00  0.00          O
ATOM    583  I       583      15.000  69.921  61.327  1.00  0.00          O
ATOM    584  I       584      15.000  79.883  62.199  1.00  0.00          O
ATOM    585  I       585      25.000  10.149  56.098  1.00  0.00          O
ATOM    586  I       586      25.000  20.111  56.970  1.00  0.00          O
ATOM    587  I       587      25.000  30.073  57.841  1.00  0.00          O
ATOM    588  I       588      25.000  40.035  58.713  1.00  0.00          O
ATOM    589  I       589      25.000  49.997  59.584  1.00  0.00          O
ATOM    590  I       590      25.000  59.959  60.456  1.00  0.00          O
ATOM    591  I       591      25.000  69.921  61.327  1.00  0.00          O
ATOM    592  I       592      25.000  79.883  62.199  1.00  0.00          O
ATOM    593  I       593      35.000  10.149  56.098  1.00  0.00          O
ATOM    594  I       594      35.000  20.111  56.970  1.00  0.00          O
ATOM    595  I       595      35.000  30.073  57.841  1.00  0.00          O
ATOM    596  I       596      35.000  40.035  58.713  1.00  0.00          O
ATOM    597  I       597      35.000  49.997  59.584  1.00  0.00          O
ATOM    598  I       598      35.000  59.959  60.456  1.00  0.00          O
ATOM    599  I       599      35.000  69.921  61.327  1.00  0.00          O
ATOM    600  I       600      35.000  79.883  62.199  1.00  0.00          O
ATOM    601  I       601      45.000  10.149  56.098  1.00  0.00          O
ATOM    602  I       602      45.000  20.111  56.970  1.00  0.00          O
ATOM    603  I       603      45.000  30.073  57.841  1.00  0.00          O
ATOM    604  I       604      45.000  40.035  58.713  1.00  0.00          O
ATOM    605  I       605      45.000  49.997  59.584  1.00  0.00          O
ATOM    606  I       606      45.000  59.959  60.456  1.00  0.00          O
ATOM    607  I       607      45.000  69.921  61.327  1.00  0.00          O
ATOM    608  I       608      45.000  79.883  62.199  1.00  0.00          O
ATOM    609  I       609      55.000  10.149  56.098  1.00  0.00          O
ATOM    610  I       610      55.000  20.111  56.970  1.00  0.00          O
ATOM    611  I       611      55.000  30.073  57.841  1.00  0.00          O
ATOM    612  I       612      55.000  40.035  58.713  1.00  0.00          O
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ATOM 613 I 613 55.000 49.997 59.584 1.00 0.00 O
ATOM 614 I 614 55.000 59.959 60.456 1.00 0.00 O
ATOM 615 I 615 55.000 69.921 61.327 1.00 0.00 O
ATOM 616 I 616 55.000 79.883 62.199 1.00 0.00 O
ATOM 617 I 617 65.000 10.149 56.098 1.00 0.00 O
ATOM 618 I 618 65.000 20.111 56.970 1.00 0.00 O
ATOM 619 I 619 65.000 30.073 57.841 1.00 0.00 O
ATOM 620 I 620 65.000 40.035 58.713 1.00 0.00 O
ATOM 621 I 621 65.000 49.997 59.584 1.00 0.00 O
ATOM 622 I 622 65.000 59.959 60.456 1.00 0.00 O
ATOM 623 I 623 65.000 69.921 61.327 1.00 0.00 O
ATOM 624 I 624 65.000 79.883 62.199 1.00 0.00 O
ATOM 625 I 625 75.000 10.149 56.098 1.00 0.00 O
ATOM 626 I 626 75.000 20.111 56.970 1.00 0.00 O
ATOM 627 I 627 75.000 30.073 57.841 1.00 0.00 O
ATOM 628 I 628 75.000 40.035 58.713 1.00 0.00 O
ATOM 629 I 629 75.000 49.997 59.584 1.00 0.00 O
ATOM 630 I 630 75.000 59.959 60.456 1.00 0.00 O
ATOM 631 I 631 75.000 69.921 61.327 1.00 0.00 O
ATOM 632 I 632 75.000 79.883 62.199 1.00 0.00 O
ATOM 633 I 633 85.000 10.149 56.098 1.00 0.00 O
ATOM 634 I 634 85.000 20.111 56.970 1.00 0.00 O
ATOM 635 I 635 85.000 30.073 57.841 1.00 0.00 O
ATOM 636 I 636 85.000 40.035 58.713 1.00 0.00 O
ATOM 637 I 637 85.000 49.997 59.584 1.00 0.00 O
ATOM 638 I 638 85.000 59.959 60.456 1.00 0.00 O
ATOM 639 I 639 85.000 69.921 61.327 1.00 0.00 O
ATOM 640 I 640 85.000 79.883 62.199 1.00 0.00 O
ATOM 641 I 641 10.000 4.733 60.643 1.00 0.00 O
ATOM 642 I 642 10.000 14.695 61.515 1.00 0.00 O
ATOM 643 I 643 10.000 24.656 62.386 1.00 0.00 O
ATOM 644 I 644 10.000 34.618 63.258 1.00 0.00 O
ATOM 645 I 645 10.000 44.580 64.129 1.00 0.00 O
ATOM 646 I 646 10.000 54.542 65.001 1.00 0.00 O
ATOM 647 I 647 10.000 64.504 65.873 1.00 0.00 O
ATOM 648 I 648 10.000 74.466 66.744 1.00 0.00 O
ATOM 649 I 649 20.000 4.733 60.643 1.00 0.00 O
ATOM 650 I 650 20.000 14.695 61.515 1.00 0.00 O
ATOM 651 I 651 20.000 24.656 62.386 1.00 0.00 O
ATOM 652 I 652 20.000 34.618 63.258 1.00 0.00 O
ATOM 653 I 653 20.000 44.580 64.129 1.00 0.00 O
ATOM 654 I 654 20.000 54.542 65.001 1.00 0.00 O
ATOM 655 I 655 20.000 64.504 65.873 1.00 0.00 O
ATOM 656 I 656 20.000 74.466 66.744 1.00 0.00 O
ATOM 657 I 657 30.000 4.733 60.643 1.00 0.00 O
ATOM 658 I 658 30.000 14.695 61.515 1.00 0.00 O
ATOM 659 I 659 30.000 24.656 62.386 1.00 0.00 O
ATOM 660 I 660 30.000 34.618 63.258 1.00 0.00 O

ATOM 661 I 661 30.000 44.580 64.129 1.00 0.00 O
ATOM 662 I 662 30.000 54.542 65.001 1.00 0.00 O
ATOM 663 I 663 30.000 64.504 65.873 1.00 0.00 O
ATOM 664 I 664 30.000 74.466 66.744 1.00 0.00 O
ATOM 665 I 665 40.000 4.733 60.643 1.00 0.00 O
ATOM 666 I 666 40.000 14.695 61.515 1.00 0.00 O
ATOM 667 I 667 40.000 24.656 62.386 1.00 0.00 O
ATOM 668 I 668 40.000 34.618 63.258 1.00 0.00 O
ATOM 669 I 669 40.000 44.580 64.129 1.00 0.00 O
ATOM 670 I 670 40.000 54.542 65.001 1.00 0.00 O
ATOM 671 I 671 40.000 64.504 65.873 1.00 0.00 O
ATOM 672 I 672 40.000 74.466 66.744 1.00 0.00 O
ATOM 673 I 673 50.000 4.733 60.643 1.00 0.00 O
ATOM 674 I 674 50.000 14.695 61.515 1.00 0.00 O
ATOM 675 I 675 50.000 24.656 62.386 1.00 0.00 O
ATOM 676 I 676 50.000 34.618 63.258 1.00 0.00 O
ATOM 677 I 677 50.000 44.580 64.129 1.00 0.00 O
ATOM 678 I 678 50.000 54.542 65.001 1.00 0.00 O
ATOM 679 I 679 50.000 64.504 65.873 1.00 0.00 O
ATOM 680 I 680 50.000 74.466 66.744 1.00 0.00 O
ATOM 681 I 681 60.000 4.733 60.643 1.00 0.00 O
ATOM 682 I 682 60.000 14.695 61.515 1.00 0.00 O
ATOM 683 I 683 60.000 24.656 62.386 1.00 0.00 O
ATOM 684 I 684 60.000 34.618 63.258 1.00 0.00 O
ATOM 685 I 685 60.000 44.580 64.129 1.00 0.00 O
ATOM 686 I 686 60.000 54.542 65.001 1.00 0.00 O
ATOM 687 I 687 60.000 64.504 65.873 1.00 0.00 O
ATOM 688 I 688 60.000 74.466 66.744 1.00 0.00 O
ATOM 689 I 689 70.000 4.733 60.643 1.00 0.00 O
ATOM 690 I 690 70.000 14.695 61.515 1.00 0.00 O
ATOM 691 I 691 70.000 24.656 62.386 1.00 0.00 O
ATOM 692 I 692 70.000 34.618 63.258 1.00 0.00 O
ATOM 693 I 693 70.000 44.580 64.129 1.00 0.00 O
ATOM 694 I 694 70.000 54.542 65.001 1.00 0.00 O
ATOM 695 I 695 70.000 64.504 65.873 1.00 0.00 O
ATOM 696 I 696 70.000 74.466 66.744 1.00 0.00 O
ATOM 697 I 697 80.000 4.733 60.643 1.00 0.00 O
ATOM 698 I 698 80.000 14.695 61.515 1.00 0.00 O
ATOM 699 I 699 80.000 24.656 62.386 1.00 0.00 O
ATOM 700 I 700 80.000 34.618 63.258 1.00 0.00 O
ATOM 701 I 701 80.000 44.580 64.129 1.00 0.00 O
ATOM 702 I 702 80.000 54.542 65.001 1.00 0.00 O
ATOM 703 I 703 80.000 64.504 65.873 1.00 0.00 O
ATOM 704 I 704 80.000 74.466 66.744 1.00 0.00 O
ATOM 705 I 705 15.000 9.278 66.060 1.00 0.00 O
ATOM 706 I 706 15.000 19.240 66.932 1.00 0.00 O
ATOM 707 I 707 15.000 29.202 67.803 1.00 0.00 O
ATOM 708 I 708 15.000 39.164 68.675 1.00 0.00 O

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ATOM    709  I       709      15.000  49.126  69.546  1.00  0.00          O
ATOM    710  I       710      15.000  59.088  70.418  1.00  0.00          O
ATOM    711  I       711      15.000  69.049  71.289  1.00  0.00          O
ATOM    712  I       712      15.000  79.011  72.161  1.00  0.00          O
ATOM    713  I       713      25.000   9.278  66.060  1.00  0.00          O
ATOM    714  I       714      25.000  19.240  66.932  1.00  0.00          O
ATOM    715  I       715      25.000  29.202  67.803  1.00  0.00          O
ATOM    716  I       716      25.000  39.164  68.675  1.00  0.00          O
ATOM    717  I       717      25.000  49.126  69.546  1.00  0.00          O
ATOM    718  I       718      25.000  59.088  70.418  1.00  0.00          O
ATOM    719  I       719      25.000  69.049  71.289  1.00  0.00          O
ATOM    720  I       720      25.000  79.011  72.161  1.00  0.00          O
ATOM    721  I       721      35.000   9.278  66.060  1.00  0.00          O
ATOM    722  I       722      35.000  19.240  66.932  1.00  0.00          O
ATOM    723  I       723      35.000  29.202  67.803  1.00  0.00          O
ATOM    724  I       724      35.000  39.164  68.675  1.00  0.00          O
ATOM    725  I       725      35.000  49.126  69.546  1.00  0.00          O
ATOM    726  I       726      35.000  59.088  70.418  1.00  0.00          O
ATOM    727  I       727      35.000  69.049  71.289  1.00  0.00          O
ATOM    728  I       728      35.000  79.011  72.161  1.00  0.00          O
ATOM    729  I       729      45.000   9.278  66.060  1.00  0.00          O
ATOM    730  I       730      45.000  19.240  66.932  1.00  0.00          O
ATOM    731  I       731      45.000  29.202  67.803  1.00  0.00          O
ATOM    732  I       732      45.000  39.164  68.675  1.00  0.00          O
ATOM    733  I       733      45.000  49.126  69.546  1.00  0.00          O
ATOM    734  I       734      45.000  59.088  70.418  1.00  0.00          O
ATOM    735  I       735      45.000  69.049  71.289  1.00  0.00          O
ATOM    736  I       736      45.000  79.011  72.161  1.00  0.00          O
ATOM    737  I       737      55.000   9.278  66.060  1.00  0.00          O
ATOM    738  I       738      55.000  19.240  66.932  1.00  0.00          O
ATOM    739  I       739      55.000  29.202  67.803  1.00  0.00          O
ATOM    740  I       740      55.000  39.164  68.675  1.00  0.00          O
ATOM    741  I       741      55.000  49.126  69.546  1.00  0.00          O
ATOM    742  I       742      55.000  59.088  70.418  1.00  0.00          O
ATOM    743  I       743      55.000  69.049  71.289  1.00  0.00          O
ATOM    744  I       744      55.000  79.011  72.161  1.00  0.00          O
ATOM    745  I       745      65.000   9.278  66.060  1.00  0.00          O
ATOM    746  I       746      65.000  19.240  66.932  1.00  0.00          O
ATOM    747  I       747      65.000  29.202  67.803  1.00  0.00          O
ATOM    748  I       748      65.000  39.164  68.675  1.00  0.00          O
ATOM    749  I       749      65.000  49.126  69.546  1.00  0.00          O
ATOM    750  I       750      65.000  59.088  70.418  1.00  0.00          O
ATOM    751  I       751      65.000  69.049  71.289  1.00  0.00          O
ATOM    752  I       752      65.000  79.011  72.161  1.00  0.00          O
ATOM    753  I       753      75.000   9.278  66.060  1.00  0.00          O
ATOM    754  I       754      75.000  19.240  66.932  1.00  0.00          O
ATOM    755  I       755      75.000  29.202  67.803  1.00  0.00          O
ATOM    756  I       756      75.000  39.164  68.675  1.00  0.00          O
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ATOM    757  I       757      75.000  49.126  69.546  1.00  0.00          O
ATOM    758  I       758      75.000  59.088  70.418  1.00  0.00          O
ATOM    759  I       759      75.000  69.049  71.289  1.00  0.00          O
ATOM    760  I       760      75.000  79.011  72.161  1.00  0.00          O
ATOM    761  I       761      85.000   9.278  66.060  1.00  0.00          O
ATOM    762  I       762      85.000  19.240  66.932  1.00  0.00          O
ATOM    763  I       763      85.000  29.202  67.803  1.00  0.00          O
ATOM    764  I       764      85.000  39.164  68.675  1.00  0.00          O
ATOM    765  I       765      85.000  49.126  69.546  1.00  0.00          O
ATOM    766  I       766      85.000  59.088  70.418  1.00  0.00          O
ATOM    767  I       767      85.000  69.049  71.289  1.00  0.00          O
ATOM    768  I       768      85.000  79.011  72.161  1.00  0.00          O
ATOM    769  I       769      10.000   3.861  70.605  1.00  0.00          O
ATOM    770  I       770      10.000  13.823  71.477  1.00  0.00          O
ATOM    771  I       771      10.000  23.785  72.348  1.00  0.00          O
ATOM    772  I       772      10.000  33.747  73.220  1.00  0.00          O
ATOM    773  I       773      10.000  43.709  74.091  1.00  0.00          O
ATOM    774  I       774      10.000  53.671  74.963  1.00  0.00          O
ATOM    775  I       775      10.000  63.633  75.835  1.00  0.00          O
ATOM    776  I       776      10.000  73.595  76.706  1.00  0.00          O
ATOM    777  I       777      20.000   3.861  70.605  1.00  0.00          O
ATOM    778  I       778      20.000  13.823  71.477  1.00  0.00          O
ATOM    779  I       779      20.000  23.785  72.348  1.00  0.00          O
ATOM    780  I       780      20.000  33.747  73.220  1.00  0.00          O
ATOM    781  I       781      20.000  43.709  74.091  1.00  0.00          O
ATOM    782  I       782      20.000  53.671  74.963  1.00  0.00          O
ATOM    783  I       783      20.000  63.633  75.835  1.00  0.00          O
ATOM    784  I       784      20.000  73.595  76.706  1.00  0.00          O
ATOM    785  I       785      30.000   3.861  70.605  1.00  0.00          O
ATOM    786  I       786      30.000  13.823  71.477  1.00  0.00          O
ATOM    787  I       787      30.000  23.785  72.348  1.00  0.00          O
ATOM    788  I       788      30.000  33.747  73.220  1.00  0.00          O
ATOM    789  I       789      30.000  43.709  74.091  1.00  0.00          O
ATOM    790  I       790      30.000  53.671  74.963  1.00  0.00          O
ATOM    791  I       791      30.000  63.633  75.835  1.00  0.00          O
ATOM    792  I       792      30.000  73.595  76.706  1.00  0.00          O
ATOM    793  I       793      40.000   3.861  70.605  1.00  0.00          O
ATOM    794  I       794      40.000  13.823  71.477  1.00  0.00          O
ATOM    795  I       795      40.000  23.785  72.348  1.00  0.00          O
ATOM    796  I       796      40.000  33.747  73.220  1.00  0.00          O
ATOM    797  I       797      40.000  43.709  74.091  1.00  0.00          O
ATOM    798  I       798      40.000  53.671  74.963  1.00  0.00          O
ATOM    799  I       799      40.000  63.633  75.835  1.00  0.00          O
ATOM    800  I       800      40.000  73.595  76.706  1.00  0.00          O
ATOM    801  I       801      50.000   3.861  70.605  1.00  0.00          O
ATOM    802  I       802      50.000  13.823  71.477  1.00  0.00          O
ATOM    803  I       803      50.000  23.785  72.348  1.00  0.00          O
ATOM    804  I       804      50.000  33.747  73.220  1.00  0.00          O
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ATOM    805  I       805      50.000  43.709  74.091  1.00  0.00          O
ATOM    806  I       806      50.000  53.671  74.963  1.00  0.00          O
ATOM    807  I       807      50.000  63.633  75.835  1.00  0.00          O
ATOM    808  I       808      50.000  73.595  76.706  1.00  0.00          O
ATOM    809  I       809      60.000   3.861  70.605  1.00  0.00          O
ATOM    810  I       810      60.000  13.823  71.477  1.00  0.00          O
ATOM    811  I       811      60.000  23.785  72.348  1.00  0.00          O
ATOM    812  I       812      60.000  33.747  73.220  1.00  0.00          O
ATOM    813  I       813      60.000  43.709  74.091  1.00  0.00          O
ATOM    814  I       814      60.000  53.671  74.963  1.00  0.00          O
ATOM    815  I       815      60.000  63.633  75.835  1.00  0.00          O
ATOM    816  I       816      60.000  73.595  76.706  1.00  0.00          O
ATOM    817  I       817      70.000   3.861  70.605  1.00  0.00          O
ATOM    818  I       818      70.000  13.823  71.477  1.00  0.00          O
ATOM    819  I       819      70.000  23.785  72.348  1.00  0.00          O
ATOM    820  I       820      70.000  33.747  73.220  1.00  0.00          O
ATOM    821  I       821      70.000  43.709  74.091  1.00  0.00          O
ATOM    822  I       822      70.000  53.671  74.963  1.00  0.00          O
ATOM    823  I       823      70.000  63.633  75.835  1.00  0.00          O
ATOM    824  I       824      70.000  73.595  76.706  1.00  0.00          O
ATOM    825  I       825      80.000   3.861  70.605  1.00  0.00          O
ATOM    826  I       826      80.000  13.823  71.477  1.00  0.00          O
ATOM    827  I       827      80.000  23.785  72.348  1.00  0.00          O
ATOM    828  I       828      80.000  33.747  73.220  1.00  0.00          O
ATOM    829  I       829      80.000  43.709  74.091  1.00  0.00          O
ATOM    830  I       830      80.000  53.671  74.963  1.00  0.00          O
ATOM    831  I       831      80.000  63.633  75.835  1.00  0.00          O
ATOM    832  I       832      80.000  73.595  76.706  1.00  0.00          O
ATOM    833  I       833      15.000   8.406  76.022  1.00  0.00          O
ATOM    834  I       834      15.000  18.368  76.893  1.00  0.00          O
ATOM    835  I       835      15.000  28.330  77.765  1.00  0.00          O
ATOM    836  I       836      15.000  38.292  78.637  1.00  0.00          O
ATOM    837  I       837      15.000  48.254  79.508  1.00  0.00          O
ATOM    838  I       838      15.000  58.216  80.380  1.00  0.00          O
ATOM    839  I       839      15.000  68.178  81.251  1.00  0.00          O
ATOM    840  I       840      15.000  78.140  82.123  1.00  0.00          O
ATOM    841  I       841      25.000   8.406  76.022  1.00  0.00          O
ATOM    842  I       842      25.000  18.368  76.893  1.00  0.00          O
ATOM    843  I       843      25.000  28.330  77.765  1.00  0.00          O
ATOM    844  I       844      25.000  38.292  78.637  1.00  0.00          O
ATOM    845  I       845      25.000  48.254  79.508  1.00  0.00          O
ATOM    846  I       846      25.000  58.216  80.380  1.00  0.00          O
ATOM    847  I       847      25.000  68.178  81.251  1.00  0.00          O
ATOM    848  I       848      25.000  78.140  82.123  1.00  0.00          O
ATOM    849  I       849      35.000   8.406  76.022  1.00  0.00          O
ATOM    850  I       850      35.000  18.368  76.893  1.00  0.00          O
ATOM    851  I       851      35.000  28.330  77.765  1.00  0.00          O
ATOM    852  I       852      35.000  38.292  78.637  1.00  0.00          O
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ATOM    853  I       853      35.000  48.254  79.508  1.00  0.00          O
ATOM    854  I       854      35.000  58.216  80.380  1.00  0.00          O
ATOM    855  I       855      35.000  68.178  81.251  1.00  0.00          O
ATOM    856  I       856      35.000  78.140  82.123  1.00  0.00          O
ATOM    857  I       857      45.000   8.406  76.022  1.00  0.00          O
ATOM    858  I       858      45.000  18.368  76.893  1.00  0.00          O
ATOM    859  I       859      45.000  28.330  77.765  1.00  0.00          O
ATOM    860  I       860      45.000  38.292  78.637  1.00  0.00          O
ATOM    861  I       861      45.000  48.254  79.508  1.00  0.00          O
ATOM    862  I       862      45.000  58.216  80.380  1.00  0.00          O
ATOM    863  I       863      45.000  68.178  81.251  1.00  0.00          O
ATOM    864  I       864      45.000  78.140  82.123  1.00  0.00          O
ATOM    865  I       865      55.000   8.406  76.022  1.00  0.00          O
ATOM    866  I       866      55.000  18.368  76.893  1.00  0.00          O
ATOM    867  I       867      55.000  28.330  77.765  1.00  0.00          O
ATOM    868  I       868      55.000  38.292  78.637  1.00  0.00          O
ATOM    869  I       869      55.000  48.254  79.508  1.00  0.00          O
ATOM    870  I       870      55.000  58.216  80.380  1.00  0.00          O
ATOM    871  I       871      55.000  68.178  81.251  1.00  0.00          O
ATOM    872  I       872      55.000  78.140  82.123  1.00  0.00          O
ATOM    873  I       873      65.000   8.406  76.022  1.00  0.00          O
ATOM    874  I       874      65.000  18.368  76.893  1.00  0.00          O
ATOM    875  I       875      65.000  28.330  77.765  1.00  0.00          O
ATOM    876  I       876      65.000  38.292  78.637  1.00  0.00          O
ATOM    877  I       877      65.000  48.254  79.508  1.00  0.00          O
ATOM    878  I       878      65.000  58.216  80.380  1.00  0.00          O
ATOM    879  I       879      65.000  68.178  81.251  1.00  0.00          O
ATOM    880  I       880      65.000  78.140  82.123  1.00  0.00          O
ATOM    881  I       881      75.000   8.406  76.022  1.00  0.00          O
ATOM    882  I       882      75.000  18.368  76.893  1.00  0.00          O
ATOM    883  I       883      75.000  28.330  77.765  1.00  0.00          O
ATOM    884  I       884      75.000  38.292  78.637  1.00  0.00          O
ATOM    885  I       885      75.000  48.254  79.508  1.00  0.00          O
ATOM    886  I       886      75.000  58.216  80.380  1.00  0.00          O
ATOM    887  I       887      75.000  68.178  81.251  1.00  0.00          O
ATOM    888  I       888      75.000  78.140  82.123  1.00  0.00          O
ATOM    889  I       889      85.000   8.406  76.022  1.00  0.00          O
ATOM    890  I       890      85.000  18.368  76.893  1.00  0.00          O
ATOM    891  I       891      85.000  28.330  77.765  1.00  0.00          O
ATOM    892  I       892      85.000  38.292  78.637  1.00  0.00          O
ATOM    893  I       893      85.000  48.254  79.508  1.00  0.00          O
ATOM    894  I       894      85.000  58.216  80.380  1.00  0.00          O
ATOM    895  I       895      85.000  68.178  81.251  1.00  0.00          O
ATOM    896  I       896      85.000  78.140  82.123  1.00  0.00          O
ATOM    897  I       897      10.000   2.989  80.567  1.00  0.00          O
ATOM    898  I       898      10.000  12.951  81.439  1.00  0.00          O
ATOM    899  I       899      10.000  22.913  82.310  1.00  0.00          O
ATOM    900  I       900      10.000  32.875  83.182  1.00  0.00          O
```

ATOM 901 I 901 10.000 42.837 84.053 1.00 0.00 O
ATOM 902 I 902 10.000 52.799 84.925 1.00 0.00 O
ATOM 903 I 903 10.000 62.761 85.796 1.00 0.00 O
ATOM 904 I 904 10.000 72.723 86.668 1.00 0.00 O
ATOM 905 I 905 20.000 2.989 80.567 1.00 0.00 O
ATOM 906 I 906 20.000 12.951 81.439 1.00 0.00 O
ATOM 907 I 907 20.000 22.913 82.310 1.00 0.00 O
ATOM 908 I 908 20.000 32.875 83.182 1.00 0.00 O
ATOM 909 I 909 20.000 42.837 84.053 1.00 0.00 O
ATOM 910 I 910 20.000 52.799 84.925 1.00 0.00 O
ATOM 911 I 911 20.000 62.761 85.796 1.00 0.00 O
ATOM 912 I 912 20.000 72.723 86.668 1.00 0.00 O
ATOM 913 I 913 30.000 2.989 80.567 1.00 0.00 O
ATOM 914 I 914 30.000 12.951 81.439 1.00 0.00 O
ATOM 915 I 915 30.000 22.913 82.310 1.00 0.00 O
ATOM 916 I 916 30.000 32.875 83.182 1.00 0.00 O
ATOM 917 I 917 30.000 42.837 84.053 1.00 0.00 O
ATOM 918 I 918 30.000 52.799 84.925 1.00 0.00 O
ATOM 919 I 919 30.000 62.761 85.796 1.00 0.00 O
ATOM 920 I 920 30.000 72.723 86.668 1.00 0.00 O
ATOM 921 I 921 40.000 2.989 80.567 1.00 0.00 O
ATOM 922 I 922 40.000 12.951 81.439 1.00 0.00 O
ATOM 923 I 923 40.000 22.913 82.310 1.00 0.00 O
ATOM 924 I 924 40.000 32.875 83.182 1.00 0.00 O
ATOM 925 I 925 40.000 42.837 84.053 1.00 0.00 O
ATOM 926 I 926 40.000 52.799 84.925 1.00 0.00 O
ATOM 927 I 927 40.000 62.761 85.796 1.00 0.00 O
ATOM 928 I 928 40.000 72.723 86.668 1.00 0.00 O
ATOM 929 I 929 50.000 2.989 80.567 1.00 0.00 O
ATOM 930 I 930 50.000 12.951 81.439 1.00 0.00 O
ATOM 931 I 931 50.000 22.913 82.310 1.00 0.00 O
ATOM 932 I 932 50.000 32.875 83.182 1.00 0.00 O
ATOM 933 I 933 50.000 42.837 84.053 1.00 0.00 O
ATOM 934 I 934 50.000 52.799 84.925 1.00 0.00 O
ATOM 935 I 935 50.000 62.761 85.796 1.00 0.00 O
ATOM 936 I 936 50.000 72.723 86.668 1.00 0.00 O
ATOM 937 I 937 60.000 2.989 80.567 1.00 0.00 O
ATOM 938 I 938 60.000 12.951 81.439 1.00 0.00 O
ATOM 939 I 939 60.000 22.913 82.310 1.00 0.00 O
ATOM 940 I 940 60.000 32.875 83.182 1.00 0.00 O
ATOM 941 I 941 60.000 42.837 84.053 1.00 0.00 O
ATOM 942 I 942 60.000 52.799 84.925 1.00 0.00 O
ATOM 943 I 943 60.000 62.761 85.796 1.00 0.00 O
ATOM 944 I 944 60.000 72.723 86.668 1.00 0.00 O
ATOM 945 I 945 70.000 2.989 80.567 1.00 0.00 O
ATOM 946 I 946 70.000 12.951 81.439 1.00 0.00 O
ATOM 947 I 947 70.000 22.913 82.310 1.00 0.00 O
ATOM 948 I 948 70.000 32.875 83.182 1.00 0.00 O

ATOM 949 I 949 70.000 42.837 84.053 1.00 0.00 O
ATOM 950 I 950 70.000 52.799 84.925 1.00 0.00 O
ATOM 951 I 951 70.000 62.761 85.796 1.00 0.00 O
ATOM 952 I 952 70.000 72.723 86.668 1.00 0.00 O
ATOM 953 I 953 80.000 2.989 80.567 1.00 0.00 O
ATOM 954 I 954 80.000 12.951 81.439 1.00 0.00 O
ATOM 955 I 955 80.000 22.913 82.310 1.00 0.00 O
ATOM 956 I 956 80.000 32.875 83.182 1.00 0.00 O
ATOM 957 I 957 80.000 42.837 84.053 1.00 0.00 O
ATOM 958 I 958 80.000 52.799 84.925 1.00 0.00 O
ATOM 959 I 959 80.000 62.761 85.796 1.00 0.00 O
ATOM 960 I 960 80.000 72.723 86.668 1.00 0.00 O
ATOM 961 I 961 15.000 7.535 85.984 1.00 0.00 O
ATOM 962 I 962 15.000 17.497 86.855 1.00 0.00 O
ATOM 963 I 963 15.000 27.459 87.727 1.00 0.00 O
ATOM 964 I 964 15.000 37.421 88.599 1.00 0.00 O
ATOM 965 I 965 15.000 47.382 89.470 1.00 0.00 O
ATOM 966 I 966 15.000 57.344 90.342 1.00 0.00 O
ATOM 967 I 967 15.000 67.306 91.213 1.00 0.00 O
ATOM 968 I 968 15.000 77.268 92.085 1.00 0.00 O
ATOM 969 I 969 25.000 7.535 85.984 1.00 0.00 O
ATOM 970 I 970 25.000 17.497 86.855 1.00 0.00 O
ATOM 971 I 971 25.000 27.459 87.727 1.00 0.00 O
ATOM 972 I 972 25.000 37.421 88.599 1.00 0.00 O
ATOM 973 I 973 25.000 47.382 89.470 1.00 0.00 O
ATOM 974 I 974 25.000 57.344 90.342 1.00 0.00 O
ATOM 975 I 975 25.000 67.306 91.213 1.00 0.00 O
ATOM 976 I 976 25.000 77.268 92.085 1.00 0.00 O
ATOM 977 I 977 35.000 7.535 85.984 1.00 0.00 O
ATOM 978 I 978 35.000 17.497 86.855 1.00 0.00 O
ATOM 979 I 979 35.000 27.459 87.727 1.00 0.00 O
ATOM 980 I 980 35.000 37.421 88.599 1.00 0.00 O
ATOM 981 I 981 35.000 47.382 89.470 1.00 0.00 O
ATOM 982 I 982 35.000 57.344 90.342 1.00 0.00 O
ATOM 983 I 983 35.000 67.306 91.213 1.00 0.00 O
ATOM 984 I 984 35.000 77.268 92.085 1.00 0.00 O
ATOM 985 I 985 45.000 7.535 85.984 1.00 0.00 O
ATOM 986 I 986 45.000 17.497 86.855 1.00 0.00 O
ATOM 987 I 987 45.000 27.459 87.727 1.00 0.00 O
ATOM 988 I 988 45.000 37.421 88.599 1.00 0.00 O
ATOM 989 I 989 45.000 47.382 89.470 1.00 0.00 O
ATOM 990 I 990 45.000 57.344 90.342 1.00 0.00 O
ATOM 991 I 991 45.000 67.306 91.213 1.00 0.00 O
ATOM 992 I 992 45.000 77.268 92.085 1.00 0.00 O
ATOM 993 I 993 55.000 7.535 85.984 1.00 0.00 O
ATOM 994 I 994 55.000 17.497 86.855 1.00 0.00 O
ATOM 995 I 995 55.000 27.459 87.727 1.00 0.00 O
ATOM 996 I 996 55.000 37.421 88.599 1.00 0.00 O

```
ATOM    997  I       997     55.000  47.382  89.470  1.00  0.00          O
ATOM    998  I       998     55.000  57.344  90.342  1.00  0.00          O
ATOM    999  I       999     55.000  67.306  91.213  1.00  0.00          O
ATOM   1000  I      1000     55.000  77.268  92.085  1.00  0.00          O
ATOM   1001  I      1001     65.000   7.535  85.984  1.00  0.00          O
ATOM   1002  I      1002     65.000  17.497  86.855  1.00  0.00          O
ATOM   1003  I      1003     65.000  27.459  87.727  1.00  0.00          O
ATOM   1004  I      1004     65.000  37.421  88.599  1.00  0.00          O
ATOM   1005  I      1005     65.000  47.382  89.470  1.00  0.00          O
ATOM   1006  I      1006     65.000  57.344  90.342  1.00  0.00          O
ATOM   1007  I      1007     65.000  67.306  91.213  1.00  0.00          O
ATOM   1008  I      1008     65.000  77.268  92.085  1.00  0.00          O
ATOM   1009  I      1009     75.000   7.535  85.984  1.00  0.00          O
ATOM   1010  I      1010     75.000  17.497  86.855  1.00  0.00          O
ATOM   1011  I      1011     75.000  27.459  87.727  1.00  0.00          O
ATOM   1012  I      1012     75.000  37.421  88.599  1.00  0.00          O
ATOM   1013  I      1013     75.000  47.382  89.470  1.00  0.00          O
ATOM   1014  I      1014     75.000  57.344  90.342  1.00  0.00          O
ATOM   1015  I      1015     75.000  67.306  91.213  1.00  0.00          O
ATOM   1016  I      1016     75.000  77.268  92.085  1.00  0.00          O
ATOM   1017  I      1017     85.000   7.535  85.984  1.00  0.00          O
ATOM   1018  I      1018     85.000  17.497  86.855  1.00  0.00          O
ATOM   1019  I      1019     85.000  27.459  87.727  1.00  0.00          O
ATOM   1020  I      1020     85.000  37.421  88.599  1.00  0.00          O
ATOM   1021  I      1021     85.000  47.382  89.470  1.00  0.00          O
ATOM   1022  I      1022     85.000  57.344  90.342  1.00  0.00          O
ATOM   1023  I      1023     85.000  67.306  91.213  1.00  0.00          O
ATOM   1024  I      1024     85.000  77.268  92.085  1.00  0.00          O
END
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15.2.4 Archivo PDB Estructura Hexagonal

Archivo PDB generado correspondiente a la estructura Hexagonal de 4 celdas por lado, 10 Angstroms en los parámetros de red a, b y 15 Angstroms en el parámetroc con 90º en alfa y beta y 120º en gamma:

Campo1	Campo2	Campo3	Campo4	Campo5	Campo6	Campo7	Campo8	Campo9	Campo 10
Registro	serial	elemento	Numero de secuncia	Coordenadas otogonales para x	Coordenadas otogonales para y	Coordenadas otogonales para z	ocupancia	Factor de temperatura	Carga en el átomo

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ATOM      1  I         1     -20.000 -29.280 -62.791  1.00  0.00          O
ATOM      2  I         2     -25.000 -20.653 -62.036  1.00  0.00          O
ATOM      3  I         3     -30.000 -12.025 -61.281  1.00  0.00          O
ATOM      4  I         4     -35.000  -3.398 -60.526  1.00  0.00          O
ATOM      5  I         5     -40.000   5.229 -59.772  1.00  0.00          O
ATOM      6  I         6     -45.000  13.857 -59.017  1.00  0.00          O
ATOM      7  I         7     -50.000  22.484 -58.262  1.00  0.00          O
ATOM      8  I         8     -55.000  31.111 -57.507  1.00  0.00          O
ATOM      9  I         9     -60.000  39.739 -56.753  1.00  0.00          O
ATOM     10  I        10      -10.000 -29.280 -62.791  1.00  0.00          O
ATOM     11  I        11      -15.000 -20.653 -62.036  1.00  0.00          O
ATOM     12  I        12      -20.000 -12.025 -61.281  1.00  0.00          O
ATOM     13  I        13      -25.000  -3.398 -60.526  1.00  0.00          O
ATOM     14  I        14      -30.000   5.229 -59.772  1.00  0.00          O
ATOM     15  I        15      -35.000  13.857 -59.017  1.00  0.00          O
ATOM     16  I        16      -40.000  22.484 -58.262  1.00  0.00          O
ATOM     17  I        17      -45.000  31.111 -57.507  1.00  0.00          O
ATOM     18  I        18      -50.000  39.739 -56.753  1.00  0.00          O
ATOM     19  I        19       -0.000 -29.280 -62.791  1.00  0.00          O
ATOM     20  I        20       -5.000 -20.653 -62.036  1.00  0.00          O
ATOM     21  I        21      -10.000 -12.025 -61.281  1.00  0.00          O
ATOM     22  I        22      -15.000  -3.398 -60.526  1.00  0.00          O
ATOM     23  I        23      -20.000   5.229 -59.772  1.00  0.00          O
ATOM     24  I        24      -25.000  13.857 -59.017  1.00  0.00          O
ATOM     25  I        25      -30.000  22.484 -58.262  1.00  0.00          O
ATOM     26  I        26      -35.000  31.111 -57.507  1.00  0.00          O
ATOM     27  I        27      -40.000  39.739 -56.753  1.00  0.00          O
ATOM     28  I        28       10.000 -29.280 -62.791  1.00  0.00          O
ATOM     29  I        29        5.000 -20.653 -62.036  1.00  0.00          O
ATOM     30  I        30       -0.000 -12.025 -61.281  1.00  0.00          O
ATOM     31  I        31       -5.000  -3.398 -60.526  1.00  0.00          O
ATOM     32  I        32      -10.000   5.229 -59.772  1.00  0.00          O
ATOM     33  I        33      -15.000  13.857 -59.017  1.00  0.00          O
ATOM     34  I        34      -20.000  22.484 -58.262  1.00  0.00          O
ATOM     35  I        35      -25.000  31.111 -57.507  1.00  0.00          O
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ATOM     36  I        36    -30.000  39.739 -56.753  1.00  0.00          O
ATOM     37  I        37     20.000 -29.280 -62.791  1.00  0.00          O
ATOM     38  I        38     15.000 -20.653 -62.036  1.00  0.00          O
ATOM     39  I        39     10.000 -12.025 -61.281  1.00  0.00          O
ATOM     40  I        40      5.000  -3.398 -60.526  1.00  0.00          O
ATOM     41  I        41     -0.000   5.229 -59.772  1.00  0.00          O
ATOM     42  I        42     -5.000  13.857 -59.017  1.00  0.00          O
ATOM     43  I        43    -10.000  22.484 -58.262  1.00  0.00          O
ATOM     44  I        44    -15.000  31.111 -57.507  1.00  0.00          O
ATOM     45  I        45    -20.000  39.739 -56.753  1.00  0.00          O
ATOM     46  I        46     30.000 -29.280 -62.791  1.00  0.00          O
ATOM     47  I        47     25.000 -20.653 -62.036  1.00  0.00          O
ATOM     48  I        48     20.000 -12.025 -61.281  1.00  0.00          O
ATOM     49  I        49     15.000  -3.398 -60.526  1.00  0.00          O
ATOM     50  I        50     10.000   5.229 -59.772  1.00  0.00          O
ATOM     51  I        51      5.000  13.857 -59.017  1.00  0.00          O
ATOM     52  I        52     -0.000  22.484 -58.262  1.00  0.00          O
ATOM     53  I        53     -5.000  31.111 -57.507  1.00  0.00          O
ATOM     54  I        54    -10.000  39.739 -56.753  1.00  0.00          O
ATOM     55  I        55     40.000 -29.280 -62.791  1.00  0.00          O
ATOM     56  I        56     35.000 -20.653 -62.036  1.00  0.00          O
ATOM     57  I        57     30.000 -12.025 -61.281  1.00  0.00          O
ATOM     58  I        58     25.000  -3.398 -60.526  1.00  0.00          O
ATOM     59  I        59     20.000   5.229 -59.772  1.00  0.00          O
ATOM     60  I        60     15.000  13.857 -59.017  1.00  0.00          O
ATOM     61  I        61     10.000  22.484 -58.262  1.00  0.00          O
ATOM     62  I        62      5.000  31.111 -57.507  1.00  0.00          O
ATOM     63  I        63      0.000  39.739 -56.753  1.00  0.00          O
ATOM     64  I        64     50.000 -29.280 -62.791  1.00  0.00          O
ATOM     65  I        65     45.000 -20.653 -62.036  1.00  0.00          O
ATOM     66  I        66     40.000 -12.025 -61.281  1.00  0.00          O
ATOM     67  I        67     35.000  -3.398 -60.526  1.00  0.00          O
ATOM     68  I        68     30.000   5.229 -59.772  1.00  0.00          O
ATOM     69  I        69     25.000  13.857 -59.017  1.00  0.00          O
ATOM     70  I        70     20.000  22.484 -58.262  1.00  0.00          O
ATOM     71  I        71     15.000  31.111 -57.507  1.00  0.00          O
ATOM     72  I        72     10.000  39.739 -56.753  1.00  0.00          O
ATOM     73  I        73     60.000 -29.280 -62.791  1.00  0.00          O
ATOM     74  I        74     55.000 -20.653 -62.036  1.00  0.00          O
ATOM     75  I        75     50.000 -12.025 -61.281  1.00  0.00          O
ATOM     76  I        76     45.000  -3.398 -60.526  1.00  0.00          O
ATOM     77  I        77     40.000   5.229 -59.772  1.00  0.00          O
ATOM     78  I        78     35.000  13.857 -59.017  1.00  0.00          O
ATOM     79  I        79     30.000  22.484 -58.262  1.00  0.00          O
ATOM     80  I        80     25.000  31.111 -57.507  1.00  0.00          O
ATOM     81  I        81     20.000  39.739 -56.753  1.00  0.00          O
ATOM     82  I        82    -20.000 -30.587 -47.848  1.00  0.00          O
ATOM     83  I        83    -25.000 -21.960 -47.093  1.00  0.00          O
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ATOM     84  I       84    -30.000 -13.333 -46.338  1.00  0.00          O
ATOM     85  I       85    -35.000  -4.705 -45.584  1.00  0.00          O
ATOM     86  I       86    -40.000   3.922 -44.829  1.00  0.00          O
ATOM     87  I       87    -45.000  12.549 -44.074  1.00  0.00          O
ATOM     88  I       88    -50.000  21.177 -43.319  1.00  0.00          O
ATOM     89  I       89    -55.000  29.804 -42.564  1.00  0.00          O
ATOM     90  I       90    -60.000  38.431 -41.810  1.00  0.00          O
ATOM     91  I       91    -10.000 -30.587 -47.848  1.00  0.00          O
ATOM     92  I       92    -15.000 -21.960 -47.093  1.00  0.00          O
ATOM     93  I       93    -20.000 -13.333 -46.338  1.00  0.00          O
ATOM     94  I       94    -25.000  -4.705 -45.584  1.00  0.00          O
ATOM     95  I       95    -30.000   3.922 -44.829  1.00  0.00          O
ATOM     96  I       96    -35.000  12.549 -44.074  1.00  0.00          O
ATOM     97  I       97    -40.000  21.177 -43.319  1.00  0.00          O
ATOM     98  I       98    -45.000  29.804 -42.564  1.00  0.00          O
ATOM     99  I       99    -50.000  38.431 -41.810  1.00  0.00          O
ATOM    100  I      100     -0.000 -30.587 -47.848  1.00  0.00          O
ATOM    101  I      101     -5.000 -21.960 -47.093  1.00  0.00          O
ATOM    102  I      102    -10.000 -13.333 -46.338  1.00  0.00          O
ATOM    103  I      103    -15.000  -4.705 -45.584  1.00  0.00          O
ATOM    104  I      104    -20.000   3.922 -44.829  1.00  0.00          O
ATOM    105  I      105    -25.000  12.549 -44.074  1.00  0.00          O
ATOM    106  I      106    -30.000  21.177 -43.319  1.00  0.00          O
ATOM    107  I      107    -35.000  29.804 -42.564  1.00  0.00          O
ATOM    108  I      108    -40.000  38.431 -41.810  1.00  0.00          O
ATOM    109  I      109     10.000 -30.587 -47.848  1.00  0.00          O
ATOM    110  I      110      5.000 -21.960 -47.093  1.00  0.00          O
ATOM    111  I      111     -0.000 -13.333 -46.338  1.00  0.00          O
ATOM    112  I      112     -5.000  -4.705 -45.584  1.00  0.00          O
ATOM    113  I      113    -10.000   3.922 -44.829  1.00  0.00          O
ATOM    114  I      114    -15.000  12.549 -44.074  1.00  0.00          O
ATOM    115  I      115    -20.000  21.177 -43.319  1.00  0.00          O
ATOM    116  I      116    -25.000  29.804 -42.564  1.00  0.00          O
ATOM    117  I      117    -30.000  38.431 -41.810  1.00  0.00          O
ATOM    118  I      118     20.000 -30.587 -47.848  1.00  0.00          O
ATOM    119  I      119     15.000 -21.960 -47.093  1.00  0.00          O
ATOM    120  I      120     10.000 -13.333 -46.338  1.00  0.00          O
ATOM    121  I      121      5.000  -4.705 -45.584  1.00  0.00          O
ATOM    122  I      122     -0.000   3.922 -44.829  1.00  0.00          O
ATOM    123  I      123     -5.000  12.549 -44.074  1.00  0.00          O
ATOM    124  I      124    -10.000  21.177 -43.319  1.00  0.00          O
ATOM    125  I      125    -15.000  29.804 -42.564  1.00  0.00          O
ATOM    126  I      126    -20.000  38.431 -41.810  1.00  0.00          O
ATOM    127  I      127     30.000 -30.587 -47.848  1.00  0.00          O
ATOM    128  I      128     25.000 -21.960 -47.093  1.00  0.00          O
ATOM    129  I      129     20.000 -13.333 -46.338  1.00  0.00          O
ATOM    130  I      130     15.000  -4.705 -45.584  1.00  0.00          O
ATOM    131  I      131     10.000   3.922 -44.829  1.00  0.00          O
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ATOM    132  I       132       5.000  12.549 -44.074  1.00  0.00          O
ATOM    133  I       133       0.000  21.177 -43.319  1.00  0.00          O
ATOM    134  I       134      -5.000  29.804 -42.564  1.00  0.00          O
ATOM    135  I       135     -10.000  38.431 -41.810  1.00  0.00          O
ATOM    136  I       136      40.000 -30.587 -47.848  1.00  0.00          O
ATOM    137  I       137      35.000 -21.960 -47.093  1.00  0.00          O
ATOM    138  I       138      30.000 -13.333 -46.338  1.00  0.00          O
ATOM    139  I       139      25.000  -4.705 -45.584  1.00  0.00          O
ATOM    140  I       140      20.000   3.922 -44.829  1.00  0.00          O
ATOM    141  I       141      15.000  12.549 -44.074  1.00  0.00          O
ATOM    142  I       142      10.000  21.177 -43.319  1.00  0.00          O
ATOM    143  I       143       5.000  29.804 -42.564  1.00  0.00          O
ATOM    144  I       144       0.000  38.431 -41.810  1.00  0.00          O
ATOM    145  I       145      50.000 -30.587 -47.848  1.00  0.00          O
ATOM    146  I       146      45.000 -21.960 -47.093  1.00  0.00          O
ATOM    147  I       147      40.000 -13.333 -46.338  1.00  0.00          O
ATOM    148  I       148      35.000  -4.705 -45.584  1.00  0.00          O
ATOM    149  I       149      30.000   3.922 -44.829  1.00  0.00          O
ATOM    150  I       150      25.000  12.549 -44.074  1.00  0.00          O
ATOM    151  I       151      20.000  21.177 -43.319  1.00  0.00          O
ATOM    152  I       152      15.000  29.804 -42.564  1.00  0.00          O
ATOM    153  I       153      10.000  38.431 -41.810  1.00  0.00          O
ATOM    154  I       154      60.000 -30.587 -47.848  1.00  0.00          O
ATOM    155  I       155      55.000 -21.960 -47.093  1.00  0.00          O
ATOM    156  I       156      50.000 -13.333 -46.338  1.00  0.00          O
ATOM    157  I       157      45.000  -4.705 -45.584  1.00  0.00          O
ATOM    158  I       158      40.000   3.922 -44.829  1.00  0.00          O
ATOM    159  I       159      35.000  12.549 -44.074  1.00  0.00          O
ATOM    160  I       160      30.000  21.177 -43.319  1.00  0.00          O
ATOM    161  I       161      25.000  29.804 -42.564  1.00  0.00          O
ATOM    162  I       162      20.000  38.431 -41.810  1.00  0.00          O
ATOM    163  I       163     -20.000 -31.895 -32.905  1.00  0.00          O
ATOM    164  I       164     -25.000 -23.267 -32.150  1.00  0.00          O
ATOM    165  I       165     -30.000 -14.640 -31.395  1.00  0.00          O
ATOM    166  I       166     -35.000  -6.013 -30.641  1.00  0.00          O
ATOM    167  I       167     -40.000   2.615 -29.886  1.00  0.00          O
ATOM    168  I       168     -45.000  11.242 -29.131  1.00  0.00          O
ATOM    169  I       169     -50.000  19.869 -28.376  1.00  0.00          O
ATOM    170  I       170     -55.000  28.497 -27.621  1.00  0.00          O
ATOM    171  I       171     -60.000  37.124 -26.867  1.00  0.00          O
ATOM    172  I       172     -10.000 -31.895 -32.905  1.00  0.00          O
ATOM    173  I       173     -15.000 -23.267 -32.150  1.00  0.00          O
ATOM    174  I       174     -20.000 -14.640 -31.395  1.00  0.00          O
ATOM    175  I       175     -25.000  -6.013 -30.641  1.00  0.00          O
ATOM    176  I       176     -30.000   2.615 -29.886  1.00  0.00          O
ATOM    177  I       177     -35.000  11.242 -29.131  1.00  0.00          O
ATOM    178  I       178     -40.000  19.869 -28.376  1.00  0.00          O
ATOM    179  I       179     -45.000  28.497 -27.621  1.00  0.00          O
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ATOM    180  I       180     -50.000  37.124 -26.867  1.00  0.00          O
ATOM    181  I       181      -0.000 -31.895 -32.905  1.00  0.00          O
ATOM    182  I       182      -5.000 -23.267 -32.150  1.00  0.00          O
ATOM    183  I       183     -10.000 -14.640 -31.395  1.00  0.00          O
ATOM    184  I       184     -15.000  -6.013 -30.641  1.00  0.00          O
ATOM    185  I       185     -20.000   2.615 -29.886  1.00  0.00          O
ATOM    186  I       186     -25.000  11.242 -29.131  1.00  0.00          O
ATOM    187  I       187     -30.000  19.869 -28.376  1.00  0.00          O
ATOM    188  I       188     -35.000  28.497 -27.621  1.00  0.00          O
ATOM    189  I       189     -40.000  37.124 -26.867  1.00  0.00          O
ATOM    190  I       190      10.000 -31.895 -32.905  1.00  0.00          O
ATOM    191  I       191       5.000 -23.267 -32.150  1.00  0.00          O
ATOM    192  I       192      -0.000 -14.640 -31.395  1.00  0.00          O
ATOM    193  I       193      -5.000  -6.013 -30.641  1.00  0.00          O
ATOM    194  I       194     -10.000   2.615 -29.886  1.00  0.00          O
ATOM    195  I       195     -15.000  11.242 -29.131  1.00  0.00          O
ATOM    196  I       196     -20.000  19.869 -28.376  1.00  0.00          O
ATOM    197  I       197     -25.000  28.497 -27.621  1.00  0.00          O
ATOM    198  I       198     -30.000  37.124 -26.867  1.00  0.00          O
ATOM    199  I       199      20.000 -31.895 -32.905  1.00  0.00          O
ATOM    200  I       200      15.000 -23.267 -32.150  1.00  0.00          O
ATOM    201  I       201      10.000 -14.640 -31.395  1.00  0.00          O
ATOM    202  I       202       5.000  -6.013 -30.641  1.00  0.00          O
ATOM    203  I       203      -0.000   2.615 -29.886  1.00  0.00          O
ATOM    204  I       204      -5.000  11.242 -29.131  1.00  0.00          O
ATOM    205  I       205     -10.000  19.869 -28.376  1.00  0.00          O
ATOM    206  I       206     -15.000  28.497 -27.621  1.00  0.00          O
ATOM    207  I       207     -20.000  37.124 -26.867  1.00  0.00          O
ATOM    208  I       208      30.000 -31.895 -32.905  1.00  0.00          O
ATOM    209  I       209      25.000 -23.267 -32.150  1.00  0.00          O
ATOM    210  I       210      20.000 -14.640 -31.395  1.00  0.00          O
ATOM    211  I       211      15.000  -6.013 -30.641  1.00  0.00          O
ATOM    212  I       212      10.000   2.615 -29.886  1.00  0.00          O
ATOM    213  I       213       5.000  11.242 -29.131  1.00  0.00          O
ATOM    214  I       214       0.000  19.869 -28.376  1.00  0.00          O
ATOM    215  I       215      -5.000  28.497 -27.621  1.00  0.00          O
ATOM    216  I       216     -10.000  37.124 -26.867  1.00  0.00          O
ATOM    217  I       217      40.000 -31.895 -32.905  1.00  0.00          O
ATOM    218  I       218      35.000 -23.267 -32.150  1.00  0.00          O
ATOM    219  I       219      30.000 -14.640 -31.395  1.00  0.00          O
ATOM    220  I       220      25.000  -6.013 -30.641  1.00  0.00          O
ATOM    221  I       221      20.000   2.615 -29.886  1.00  0.00          O
ATOM    222  I       222      15.000  11.242 -29.131  1.00  0.00          O
ATOM    223  I       223      10.000  19.869 -28.376  1.00  0.00          O
ATOM    224  I       224       5.000  28.497 -27.621  1.00  0.00          O
ATOM    225  I       225       0.000  37.124 -26.867  1.00  0.00          O
ATOM    226  I       226      50.000 -31.895 -32.905  1.00  0.00          O
ATOM    227  I       227      45.000 -23.267 -32.150  1.00  0.00          O
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ATOM 228 I 228 40.000 -14.640 -31.395 1.00 0.00 O
ATOM 229 I 229 35.000 -6.013 -30.641 1.00 0.00 O
ATOM 230 I 230 30.000 2.615 -29.886 1.00 0.00 O
ATOM 231 I 231 25.000 11.242 -29.131 1.00 0.00 O
ATOM 232 I 232 20.000 19.869 -28.376 1.00 0.00 O
ATOM 233 I 233 15.000 28.497 -27.621 1.00 0.00 O
ATOM 234 I 234 10.000 37.124 -26.867 1.00 0.00 O
ATOM 235 I 235 60.000 -31.895 -32.905 1.00 0.00 O
ATOM 236 I 236 55.000 -23.267 -32.150 1.00 0.00 O
ATOM 237 I 237 50.000 -14.640 -31.395 1.00 0.00 O
ATOM 238 I 238 45.000 -6.013 -30.641 1.00 0.00 O
ATOM 239 I 239 40.000 2.615 -29.886 1.00 0.00 O
ATOM 240 I 240 35.000 11.242 -29.131 1.00 0.00 O
ATOM 241 I 241 30.000 19.869 -28.376 1.00 0.00 O
ATOM 242 I 242 25.000 28.497 -27.621 1.00 0.00 O
ATOM 243 I 243 20.000 37.124 -26.867 1.00 0.00 O
ATOM 244 I 244 -20.000 -33.202 -17.962 1.00 0.00 O
ATOM 245 I 245 -25.000 -24.575 -17.207 1.00 0.00 O
ATOM 246 I 246 -30.000 -15.947 -16.453 1.00 0.00 O
ATOM 247 I 247 -35.000 -7.320 -15.698 1.00 0.00 O
ATOM 248 I 248 -40.000 1.307 -14.943 1.00 0.00 O
ATOM 249 I 249 -45.000 9.935 -14.188 1.00 0.00 O
ATOM 250 I 250 -50.000 18.562 -13.433 1.00 0.00 O
ATOM 251 I 251 -55.000 27.189 -12.679 1.00 0.00 O
ATOM 252 I 252 -60.000 35.817 -11.924 1.00 0.00 O
ATOM 253 I 253 -10.000 -33.202 -17.962 1.00 0.00 O
ATOM 254 I 254 -15.000 -24.575 -17.207 1.00 0.00 O
ATOM 255 I 255 -20.000 -15.947 -16.453 1.00 0.00 O
ATOM 256 I 256 -25.000 -7.320 -15.698 1.00 0.00 O
ATOM 257 I 257 -30.000 1.307 -14.943 1.00 0.00 O
ATOM 258 I 258 -35.000 9.935 -14.188 1.00 0.00 O
ATOM 259 I 259 -40.000 18.562 -13.433 1.00 0.00 O
ATOM 260 I 260 -45.000 27.189 -12.679 1.00 0.00 O
ATOM 261 I 261 -50.000 35.817 -11.924 1.00 0.00 O
ATOM 262 I 262 -0.000 -33.202 -17.962 1.00 0.00 O
ATOM 263 I 263 -5.000 -24.575 -17.207 1.00 0.00 O
ATOM 264 I 264 -10.000 -15.947 -16.453 1.00 0.00 O
ATOM 265 I 265 -15.000 -7.320 -15.698 1.00 0.00 O
ATOM 266 I 266 -20.000 1.307 -14.943 1.00 0.00 O
ATOM 267 I 267 -25.000 9.935 -14.188 1.00 0.00 O
ATOM 268 I 268 -30.000 18.562 -13.433 1.00 0.00 O
ATOM 269 I 269 -35.000 27.189 -12.679 1.00 0.00 O
ATOM 270 I 270 -40.000 35.817 -11.924 1.00 0.00 O
ATOM 271 I 271 10.000 -33.202 -17.962 1.00 0.00 O
ATOM 272 I 272 5.000 -24.575 -17.207 1.00 0.00 O
ATOM 273 I 273 -0.000 -15.947 -16.453 1.00 0.00 O
ATOM 274 I 274 -5.000 -7.320 -15.698 1.00 0.00 O
ATOM 275 I 275 -10.000 1.307 -14.943 1.00 0.00 O

ATOM 276 I 276 -15.000 9.935 -14.188 1.00 0.00 O
ATOM 277 I 277 -20.000 18.562 -13.433 1.00 0.00 O
ATOM 278 I 278 -25.000 27.189 -12.679 1.00 0.00 O
ATOM 279 I 279 -30.000 35.817 -11.924 1.00 0.00 O
ATOM 280 I 280 20.000 -33.202 -17.962 1.00 0.00 O
ATOM 281 I 281 15.000 -24.575 -17.207 1.00 0.00 O
ATOM 282 I 282 10.000 -15.947 -16.453 1.00 0.00 O
ATOM 283 I 283 5.000 -7.320 -15.698 1.00 0.00 O
ATOM 284 I 284 -0.000 1.307 -14.943 1.00 0.00 O
ATOM 285 I 285 -5.000 9.935 -14.188 1.00 0.00 O
ATOM 286 I 286 -10.000 18.562 -13.433 1.00 0.00 O
ATOM 287 I 287 -15.000 27.189 -12.679 1.00 0.00 O
ATOM 288 I 288 -20.000 35.817 -11.924 1.00 0.00 O
ATOM 289 I 289 30.000 -33.202 -17.962 1.00 0.00 O
ATOM 290 I 290 25.000 -24.575 -17.207 1.00 0.00 O
ATOM 291 I 291 20.000 -15.947 -16.453 1.00 0.00 O
ATOM 292 I 292 15.000 -7.320 -15.698 1.00 0.00 O
ATOM 293 I 293 10.000 1.307 -14.943 1.00 0.00 O
ATOM 294 I 294 5.000 9.935 -14.188 1.00 0.00 O
ATOM 295 I 295 0.000 18.562 -13.433 1.00 0.00 O
ATOM 296 I 296 -5.000 27.189 -12.679 1.00 0.00 O
ATOM 297 I 297 -10.000 35.817 -11.924 1.00 0.00 O
ATOM 298 I 298 40.000 -33.202 -17.962 1.00 0.00 O
ATOM 299 I 299 35.000 -24.575 -17.207 1.00 0.00 O
ATOM 300 I 300 30.000 -15.947 -16.453 1.00 0.00 O
ATOM 301 I 301 25.000 -7.320 -15.698 1.00 0.00 O
ATOM 302 I 302 20.000 1.307 -14.943 1.00 0.00 O
ATOM 303 I 303 15.000 9.935 -14.188 1.00 0.00 O
ATOM 304 I 304 10.000 18.562 -13.433 1.00 0.00 O
ATOM 305 I 305 5.000 27.189 -12.679 1.00 0.00 O
ATOM 306 I 306 0.000 35.817 -11.924 1.00 0.00 O
ATOM 307 I 307 50.000 -33.202 -17.962 1.00 0.00 O
ATOM 308 I 308 45.000 -24.575 -17.207 1.00 0.00 O
ATOM 309 I 309 40.000 -15.947 -16.453 1.00 0.00 O
ATOM 310 I 310 35.000 -7.320 -15.698 1.00 0.00 O
ATOM 311 I 311 30.000 1.307 -14.943 1.00 0.00 O
ATOM 312 I 312 25.000 9.935 -14.188 1.00 0.00 O
ATOM 313 I 313 20.000 18.562 -13.433 1.00 0.00 O
ATOM 314 I 314 15.000 27.189 -12.679 1.00 0.00 O
ATOM 315 I 315 10.000 35.817 -11.924 1.00 0.00 O
ATOM 316 I 316 60.000 -33.202 -17.962 1.00 0.00 O
ATOM 317 I 317 55.000 -24.575 -17.207 1.00 0.00 O
ATOM 318 I 318 50.000 -15.947 -16.453 1.00 0.00 O
ATOM 319 I 319 45.000 -7.320 -15.698 1.00 0.00 O
ATOM 320 I 320 40.000 1.307 -14.943 1.00 0.00 O
ATOM 321 I 321 35.000 9.935 -14.188 1.00 0.00 O
ATOM 322 I 322 30.000 18.562 -13.433 1.00 0.00 O
ATOM 323 I 323 25.000 27.189 -12.679 1.00 0.00 O

ATOM 324 I 324 20.000 35.817 -11.924 1.00 0.00 O
ATOM 325 I 325 -20.000 -34.509 -3.019 1.00 0.00 O
ATOM 326 I 326 -25.000 -25.882 -2.264 1.00 0.00 O
ATOM 327 I 327 -30.000 -17.255 -1.510 1.00 0.00 O
ATOM 328 I 328 -35.000 -8.627 -0.755 1.00 0.00 O
ATOM 329 I 329 -40.000 0.000 0.000 1.00 0.00 O
ATOM 330 I 330 -45.000 8.627 0.755 1.00 0.00 O
ATOM 331 I 331 -50.000 17.255 1.510 1.00 0.00 O
ATOM 332 I 332 -55.000 25.882 2.264 1.00 0.00 O
ATOM 333 I 333 -60.000 34.509 3.019 1.00 0.00 O
ATOM 334 I 334 -10.000 -34.509 -3.019 1.00 0.00 O
ATOM 335 I 335 -15.000 -25.882 -2.264 1.00 0.00 O
ATOM 336 I 336 -20.000 -17.255 -1.510 1.00 0.00 O
ATOM 337 I 337 -25.000 -8.627 -0.755 1.00 0.00 O
ATOM 338 I 338 -30.000 0.000 0.000 1.00 0.00 O
ATOM 339 I 339 -35.000 8.627 0.755 1.00 0.00 O
ATOM 340 I 340 -40.000 17.255 1.510 1.00 0.00 O
ATOM 341 I 341 -45.000 25.882 2.264 1.00 0.00 O
ATOM 342 I 342 -50.000 34.509 3.019 1.00 0.00 O
ATOM 343 I 343 -0.000 -34.509 -3.019 1.00 0.00 O
ATOM 344 I 344 -5.000 -25.882 -2.264 1.00 0.00 O
ATOM 345 I 345 -10.000 -17.255 -1.510 1.00 0.00 O
ATOM 346 I 346 -15.000 -8.627 -0.755 1.00 0.00 O
ATOM 347 I 347 -20.000 0.000 0.000 1.00 0.00 O
ATOM 348 I 348 -25.000 8.627 0.755 1.00 0.00 O
ATOM 349 I 349 -30.000 17.255 1.510 1.00 0.00 O
ATOM 350 I 350 -35.000 25.882 2.264 1.00 0.00 O
ATOM 351 I 351 -40.000 34.509 3.019 1.00 0.00 O
ATOM 352 I 352 10.000 -34.509 -3.019 1.00 0.00 O
ATOM 353 I 353 5.000 -25.882 -2.264 1.00 0.00 O
ATOM 354 I 354 -0.000 -17.255 -1.510 1.00 0.00 O
ATOM 355 I 355 -5.000 -8.627 -0.755 1.00 0.00 O
ATOM 356 I 356 -10.000 0.000 0.000 1.00 0.00 O
ATOM 357 I 357 -15.000 8.627 0.755 1.00 0.00 O
ATOM 358 I 358 -20.000 17.255 1.510 1.00 0.00 O
ATOM 359 I 359 -25.000 25.882 2.264 1.00 0.00 O
ATOM 360 I 360 -30.000 34.509 3.019 1.00 0.00 O
ATOM 361 I 361 20.000 -34.509 -3.019 1.00 0.00 O
ATOM 362 I 362 15.000 -25.882 -2.264 1.00 0.00 O
ATOM 363 I 363 10.000 -17.255 -1.510 1.00 0.00 O
ATOM 364 I 364 5.000 -8.627 -0.755 1.00 0.00 O
ATOM 365 I 365 0.000 0.000 0.000 1.00 0.00 O
ATOM 366 I 366 -5.000 8.627 0.755 1.00 0.00 O
ATOM 367 I 367 -10.000 17.255 1.510 1.00 0.00 O
ATOM 368 I 368 -15.000 25.882 2.264 1.00 0.00 O
ATOM 369 I 369 -20.000 34.509 3.019 1.00 0.00 O
ATOM 370 I 370 30.000 -34.509 -3.019 1.00 0.00 O
ATOM 371 I 371 25.000 -25.882 -2.264 1.00 0.00 O

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ATOM    372  I       372      20.000 -17.255  -1.510  1.00  0.00          O
ATOM    373  I       373      15.000  -8.627  -0.755  1.00  0.00          O
ATOM    374  I       374      10.000   0.000   0.000  1.00  0.00          O
ATOM    375  I       375       5.000   8.627   0.755  1.00  0.00          O
ATOM    376  I       376       0.000  17.255   1.510  1.00  0.00          O
ATOM    377  I       377      -5.000  25.882   2.264  1.00  0.00          O
ATOM    378  I       378     -10.000  34.509   3.019  1.00  0.00          O
ATOM    379  I       379      40.000 -34.509  -3.019  1.00  0.00          O
ATOM    380  I       380      35.000 -25.882  -2.264  1.00  0.00          O
ATOM    381  I       381      30.000 -17.255  -1.510  1.00  0.00          O
ATOM    382  I       382      25.000  -8.627  -0.755  1.00  0.00          O
ATOM    383  I       383      20.000   0.000   0.000  1.00  0.00          O
ATOM    384  I       384      15.000   8.627   0.755  1.00  0.00          O
ATOM    385  I       385      10.000  17.255   1.510  1.00  0.00          O
ATOM    386  I       386       5.000  25.882   2.264  1.00  0.00          O
ATOM    387  I       387       0.000  34.509   3.019  1.00  0.00          O
ATOM    388  I       388      50.000 -34.509  -3.019  1.00  0.00          O
ATOM    389  I       389      45.000 -25.882  -2.264  1.00  0.00          O
ATOM    390  I       390      40.000 -17.255  -1.510  1.00  0.00          O
ATOM    391  I       391      35.000  -8.627  -0.755  1.00  0.00          O
ATOM    392  I       392      30.000   0.000   0.000  1.00  0.00          O
ATOM    393  I       393      25.000   8.627   0.755  1.00  0.00          O
ATOM    394  I       394      20.000  17.255   1.510  1.00  0.00          O
ATOM    395  I       395      15.000  25.882   2.264  1.00  0.00          O
ATOM    396  I       396      10.000  34.509   3.019  1.00  0.00          O
ATOM    397  I       397      60.000 -34.509  -3.019  1.00  0.00          O
ATOM    398  I       398      55.000 -25.882  -2.264  1.00  0.00          O
ATOM    399  I       399      50.000 -17.255  -1.510  1.00  0.00          O
ATOM    400  I       400      45.000  -8.627  -0.755  1.00  0.00          O
ATOM    401  I       401      40.000   0.000   0.000  1.00  0.00          O
ATOM    402  I       402      35.000   8.627   0.755  1.00  0.00          O
ATOM    403  I       403      30.000  17.255   1.510  1.00  0.00          O
ATOM    404  I       404      25.000  25.882   2.264  1.00  0.00          O
ATOM    405  I       405      20.000  34.509   3.019  1.00  0.00          O
ATOM    406  I       406     -20.000 -35.817  11.924  1.00  0.00          O
ATOM    407  I       407     -25.000 -27.189  12.679  1.00  0.00          O
ATOM    408  I       408     -30.000 -18.562  13.433  1.00  0.00          O
ATOM    409  I       409     -35.000  -9.935  14.188  1.00  0.00          O
ATOM    410  I       410     -40.000  -1.307  14.943  1.00  0.00          O
ATOM    411  I       411     -45.000   7.320  15.698  1.00  0.00          O
ATOM    412  I       412     -50.000  15.947  16.453  1.00  0.00          O
ATOM    413  I       413     -55.000  24.575  17.207  1.00  0.00          O
ATOM    414  I       414     -60.000  33.202  17.962  1.00  0.00          O
ATOM    415  I       415     -10.000 -35.817  11.924  1.00  0.00          O
ATOM    416  I       416     -15.000 -27.189  12.679  1.00  0.00          O
ATOM    417  I       417     -20.000 -18.562  13.433  1.00  0.00          O
ATOM    418  I       418     -25.000  -9.935  14.188  1.00  0.00          O
ATOM    419  I       419     -30.000  -1.307  14.943  1.00  0.00          O
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ATOM 420 I 420 -35.000 7.320 15.698 1.00 0.00 O
ATOM 421 I 421 -40.000 15.947 16.453 1.00 0.00 O
ATOM 422 I 422 -45.000 24.575 17.207 1.00 0.00 O
ATOM 423 I 423 -50.000 33.202 17.962 1.00 0.00 O
ATOM 424 I 424 -0.000 -35.817 11.924 1.00 0.00 O
ATOM 425 I 425 -5.000 -27.189 12.679 1.00 0.00 O
ATOM 426 I 426 -10.000 -18.562 13.433 1.00 0.00 O
ATOM 427 I 427 -15.000 -9.935 14.188 1.00 0.00 O
ATOM 428 I 428 -20.000 -1.307 14.943 1.00 0.00 O
ATOM 429 I 429 -25.000 7.320 15.698 1.00 0.00 O
ATOM 430 I 430 -30.000 15.947 16.453 1.00 0.00 O
ATOM 431 I 431 -35.000 24.575 17.207 1.00 0.00 O
ATOM 432 I 432 -40.000 33.202 17.962 1.00 0.00 O
ATOM 433 I 433 10.000 -35.817 11.924 1.00 0.00 O
ATOM 434 I 434 5.000 -27.189 12.679 1.00 0.00 O
ATOM 435 I 435 -0.000 -18.562 13.433 1.00 0.00 O
ATOM 436 I 436 -5.000 -9.935 14.188 1.00 0.00 O
ATOM 437 I 437 -10.000 -1.307 14.943 1.00 0.00 O
ATOM 438 I 438 -15.000 7.320 15.698 1.00 0.00 O
ATOM 439 I 439 -20.000 15.947 16.453 1.00 0.00 O
ATOM 440 I 440 -25.000 24.575 17.207 1.00 0.00 O
ATOM 441 I 441 -30.000 33.202 17.962 1.00 0.00 O
ATOM 442 I 442 20.000 -35.817 11.924 1.00 0.00 O
ATOM 443 I 443 15.000 -27.189 12.679 1.00 0.00 O
ATOM 444 I 444 10.000 -18.562 13.433 1.00 0.00 O
ATOM 445 I 445 5.000 -9.935 14.188 1.00 0.00 O
ATOM 446 I 446 0.000 -1.307 14.943 1.00 0.00 O
ATOM 447 I 447 -5.000 7.320 15.698 1.00 0.00 O
ATOM 448 I 448 -10.000 15.947 16.453 1.00 0.00 O
ATOM 449 I 449 -15.000 24.575 17.207 1.00 0.00 O
ATOM 450 I 450 -20.000 33.202 17.962 1.00 0.00 O
ATOM 451 I 451 30.000 -35.817 11.924 1.00 0.00 O
ATOM 452 I 452 25.000 -27.189 12.679 1.00 0.00 O
ATOM 453 I 453 20.000 -18.562 13.433 1.00 0.00 O
ATOM 454 I 454 15.000 -9.935 14.188 1.00 0.00 O
ATOM 455 I 455 10.000 -1.307 14.943 1.00 0.00 O
ATOM 456 I 456 5.000 7.320 15.698 1.00 0.00 O
ATOM 457 I 457 0.000 15.947 16.453 1.00 0.00 O
ATOM 458 I 458 -5.000 24.575 17.207 1.00 0.00 O
ATOM 459 I 459 -10.000 33.202 17.962 1.00 0.00 O
ATOM 460 I 460 40.000 -35.817 11.924 1.00 0.00 O
ATOM 461 I 461 35.000 -27.189 12.679 1.00 0.00 O
ATOM 462 I 462 30.000 -18.562 13.433 1.00 0.00 O
ATOM 463 I 463 25.000 -9.935 14.188 1.00 0.00 O
ATOM 464 I 464 20.000 -1.307 14.943 1.00 0.00 O
ATOM 465 I 465 15.000 7.320 15.698 1.00 0.00 O
ATOM 466 I 466 10.000 15.947 16.453 1.00 0.00 O
ATOM 467 I 467 5.000 24.575 17.207 1.00 0.00 O

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ATOM    468  I       468       0.000  33.202  17.962  1.00  0.00          O
ATOM    469  I       469      50.000 -35.817  11.924  1.00  0.00          O
ATOM    470  I       470      45.000 -27.189  12.679  1.00  0.00          O
ATOM    471  I       471      40.000 -18.562  13.433  1.00  0.00          O
ATOM    472  I       472      35.000  -9.935  14.188  1.00  0.00          O
ATOM    473  I       473      30.000  -1.307  14.943  1.00  0.00          O
ATOM    474  I       474      25.000   7.320  15.698  1.00  0.00          O
ATOM    475  I       475      20.000  15.947  16.453  1.00  0.00          O
ATOM    476  I       476      15.000  24.575  17.207  1.00  0.00          O
ATOM    477  I       477      10.000  33.202  17.962  1.00  0.00          O
ATOM    478  I       478      60.000 -35.817  11.924  1.00  0.00          O
ATOM    479  I       479      55.000 -27.189  12.679  1.00  0.00          O
ATOM    480  I       480      50.000 -18.562  13.433  1.00  0.00          O
ATOM    481  I       481      45.000  -9.935  14.188  1.00  0.00          O
ATOM    482  I       482      40.000  -1.307  14.943  1.00  0.00          O
ATOM    483  I       483      35.000   7.320  15.698  1.00  0.00          O
ATOM    484  I       484      30.000  15.947  16.453  1.00  0.00          O
ATOM    485  I       485      25.000  24.575  17.207  1.00  0.00          O
ATOM    486  I       486      20.000  33.202  17.962  1.00  0.00          O
ATOM    487  I       487     -20.000 -37.124  26.867  1.00  0.00          O
ATOM    488  I       488     -25.000 -28.497  27.621  1.00  0.00          O
ATOM    489  I       489     -30.000 -19.869  28.376  1.00  0.00          O
ATOM    490  I       490     -35.000 -11.242  29.131  1.00  0.00          O
ATOM    491  I       491     -40.000  -2.615  29.886  1.00  0.00          O
ATOM    492  I       492     -45.000   6.013  30.641  1.00  0.00          O
ATOM    493  I       493     -50.000  14.640  31.395  1.00  0.00          O
ATOM    494  I       494     -55.000  23.267  32.150  1.00  0.00          O
ATOM    495  I       495     -60.000  31.895  32.905  1.00  0.00          O
ATOM    496  I       496     -10.000 -37.124  26.867  1.00  0.00          O
ATOM    497  I       497     -15.000 -28.497  27.621  1.00  0.00          O
ATOM    498  I       498     -20.000 -19.869  28.376  1.00  0.00          O
ATOM    499  I       499     -25.000 -11.242  29.131  1.00  0.00          O
ATOM    500  I       500     -30.000  -2.615  29.886  1.00  0.00          O
ATOM    501  I       501     -35.000   6.013  30.641  1.00  0.00          O
ATOM    502  I       502     -40.000  14.640  31.395  1.00  0.00          O
ATOM    503  I       503     -45.000  23.267  32.150  1.00  0.00          O
ATOM    504  I       504     -50.000  31.895  32.905  1.00  0.00          O
ATOM    505  I       505      -0.000 -37.124  26.867  1.00  0.00          O
ATOM    506  I       506      -5.000 -28.497  27.621  1.00  0.00          O
ATOM    507  I       507     -10.000 -19.869  28.376  1.00  0.00          O
ATOM    508  I       508     -15.000 -11.242  29.131  1.00  0.00          O
ATOM    509  I       509     -20.000  -2.615  29.886  1.00  0.00          O
ATOM    510  I       510     -25.000   6.013  30.641  1.00  0.00          O
ATOM    511  I       511     -30.000  14.640  31.395  1.00  0.00          O
ATOM    512  I       512     -35.000  23.267  32.150  1.00  0.00          O
ATOM    513  I       513     -40.000  31.895  32.905  1.00  0.00          O
ATOM    514  I       514      10.000 -37.124  26.867  1.00  0.00          O
ATOM    515  I       515       5.000 -28.497  27.621  1.00  0.00          O
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ATOM 516 I 516 -0.000 -19.869 28.376 1.00 0.00 O
ATOM 517 I 517 -5.000 -11.242 29.131 1.00 0.00 O
ATOM 518 I 518 -10.000 -2.615 29.886 1.00 0.00 O
ATOM 519 I 519 -15.000 6.013 30.641 1.00 0.00 O
ATOM 520 I 520 -20.000 14.640 31.395 1.00 0.00 O
ATOM 521 I 521 -25.000 23.267 32.150 1.00 0.00 O
ATOM 522 I 522 -30.000 31.895 32.905 1.00 0.00 O
ATOM 523 I 523 20.000 -37.124 26.867 1.00 0.00 O
ATOM 524 I 524 15.000 -28.497 27.621 1.00 0.00 O
ATOM 525 I 525 10.000 -19.869 28.376 1.00 0.00 O
ATOM 526 I 526 5.000 -11.242 29.131 1.00 0.00 O
ATOM 527 I 527 0.000 -2.615 29.886 1.00 0.00 O
ATOM 528 I 528 -5.000 6.013 30.641 1.00 0.00 O
ATOM 529 I 529 -10.000 14.640 31.395 1.00 0.00 O
ATOM 530 I 530 -15.000 23.267 32.150 1.00 0.00 O
ATOM 531 I 531 -20.000 31.895 32.905 1.00 0.00 O
ATOM 532 I 532 30.000 -37.124 26.867 1.00 0.00 O
ATOM 533 I 533 25.000 -28.497 27.621 1.00 0.00 O
ATOM 534 I 534 20.000 -19.869 28.376 1.00 0.00 O
ATOM 535 I 535 15.000 -11.242 29.131 1.00 0.00 O
ATOM 536 I 536 10.000 -2.615 29.886 1.00 0.00 O
ATOM 537 I 537 5.000 6.013 30.641 1.00 0.00 O
ATOM 538 I 538 0.000 14.640 31.395 1.00 0.00 O
ATOM 539 I 539 -5.000 23.267 32.150 1.00 0.00 O
ATOM 540 I 540 -10.000 31.895 32.905 1.00 0.00 O
ATOM 541 I 541 40.000 -37.124 26.867 1.00 0.00 O
ATOM 542 I 542 35.000 -28.497 27.621 1.00 0.00 O
ATOM 543 I 543 30.000 -19.869 28.376 1.00 0.00 O
ATOM 544 I 544 25.000 -11.242 29.131 1.00 0.00 O
ATOM 545 I 545 20.000 -2.615 29.886 1.00 0.00 O
ATOM 546 I 546 15.000 6.013 30.641 1.00 0.00 O
ATOM 547 I 547 10.000 14.640 31.395 1.00 0.00 O
ATOM 548 I 548 5.000 23.267 32.150 1.00 0.00 O
ATOM 549 I 549 0.000 31.895 32.905 1.00 0.00 O
ATOM 550 I 550 50.000 -37.124 26.867 1.00 0.00 O
ATOM 551 I 551 45.000 -28.497 27.621 1.00 0.00 O
ATOM 552 I 552 40.000 -19.869 28.376 1.00 0.00 O
ATOM 553 I 553 35.000 -11.242 29.131 1.00 0.00 O
ATOM 554 I 554 30.000 -2.615 29.886 1.00 0.00 O
ATOM 555 I 555 25.000 6.013 30.641 1.00 0.00 O
ATOM 556 I 556 20.000 14.640 31.395 1.00 0.00 O
ATOM 557 I 557 15.000 23.267 32.150 1.00 0.00 O
ATOM 558 I 558 10.000 31.895 32.905 1.00 0.00 O
ATOM 559 I 559 60.000 -37.124 26.867 1.00 0.00 O
ATOM 560 I 560 55.000 -28.497 27.621 1.00 0.00 O
ATOM 561 I 561 50.000 -19.869 28.376 1.00 0.00 O
ATOM 562 I 562 45.000 -11.242 29.131 1.00 0.00 O
ATOM 563 I 563 40.000 -2.615 29.886 1.00 0.00 O

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ATOM    564  I       564      35.000   6.013  30.641  1.00  0.00          O
ATOM    565  I       565      30.000  14.640  31.395  1.00  0.00          O
ATOM    566  I       566      25.000  23.267  32.150  1.00  0.00          O
ATOM    567  I       567      20.000  31.895  32.905  1.00  0.00          O
ATOM    568  I       568     -20.000 -38.431  41.810  1.00  0.00          O
ATOM    569  I       569     -25.000 -29.804  42.564  1.00  0.00          O
ATOM    570  I       570     -30.000 -21.177  43.319  1.00  0.00          O
ATOM    571  I       571     -35.000 -12.549  44.074  1.00  0.00          O
ATOM    572  I       572     -40.000  -3.922  44.829  1.00  0.00          O
ATOM    573  I       573     -45.000   4.705  45.584  1.00  0.00          O
ATOM    574  I       574     -50.000  13.333  46.338  1.00  0.00          O
ATOM    575  I       575     -55.000  21.960  47.093  1.00  0.00          O
ATOM    576  I       576     -60.000  30.587  47.848  1.00  0.00          O
ATOM    577  I       577     -10.000 -38.431  41.810  1.00  0.00          O
ATOM    578  I       578     -15.000 -29.804  42.564  1.00  0.00          O
ATOM    579  I       579     -20.000 -21.177  43.319  1.00  0.00          O
ATOM    580  I       580     -25.000 -12.549  44.074  1.00  0.00          O
ATOM    581  I       581     -30.000  -3.922  44.829  1.00  0.00          O
ATOM    582  I       582     -35.000   4.705  45.584  1.00  0.00          O
ATOM    583  I       583     -40.000  13.333  46.338  1.00  0.00          O
ATOM    584  I       584     -45.000  21.960  47.093  1.00  0.00          O
ATOM    585  I       585     -50.000  30.587  47.848  1.00  0.00          O
ATOM    586  I       586      -0.000 -38.431  41.810  1.00  0.00          O
ATOM    587  I       587      -5.000 -29.804  42.564  1.00  0.00          O
ATOM    588  I       588     -10.000 -21.177  43.319  1.00  0.00          O
ATOM    589  I       589     -15.000 -12.549  44.074  1.00  0.00          O
ATOM    590  I       590     -20.000  -3.922  44.829  1.00  0.00          O
ATOM    591  I       591     -25.000   4.705  45.584  1.00  0.00          O
ATOM    592  I       592     -30.000  13.333  46.338  1.00  0.00          O
ATOM    593  I       593     -35.000  21.960  47.093  1.00  0.00          O
ATOM    594  I       594     -40.000  30.587  47.848  1.00  0.00          O
ATOM    595  I       595      10.000 -38.431  41.810  1.00  0.00          O
ATOM    596  I       596       5.000 -29.804  42.564  1.00  0.00          O
ATOM    597  I       597      -0.000 -21.177  43.319  1.00  0.00          O
ATOM    598  I       598      -5.000 -12.549  44.074  1.00  0.00          O
ATOM    599  I       599     -10.000  -3.922  44.829  1.00  0.00          O
ATOM    600  I       600     -15.000   4.705  45.584  1.00  0.00          O
ATOM    601  I       601     -20.000  13.333  46.338  1.00  0.00          O
ATOM    602  I       602     -25.000  21.960  47.093  1.00  0.00          O
ATOM    603  I       603     -30.000  30.587  47.848  1.00  0.00          O
ATOM    604  I       604      20.000 -38.431  41.810  1.00  0.00          O
ATOM    605  I       605      15.000 -29.804  42.564  1.00  0.00          O
ATOM    606  I       606      10.000 -21.177  43.319  1.00  0.00          O
ATOM    607  I       607       5.000 -12.549  44.074  1.00  0.00          O
ATOM    608  I       608       0.000  -3.922  44.829  1.00  0.00          O
ATOM    609  I       609      -5.000   4.705  45.584  1.00  0.00          O
ATOM    610  I       610     -10.000  13.333  46.338  1.00  0.00          O
ATOM    611  I       611     -15.000  21.960  47.093  1.00  0.00          O
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ATOM    612  I       612    -20.000  30.587  47.848  1.00  0.00          O
ATOM    613  I       613     30.000 -38.431  41.810  1.00  0.00          O
ATOM    614  I       614     25.000 -29.804  42.564  1.00  0.00          O
ATOM    615  I       615     20.000 -21.177  43.319  1.00  0.00          O
ATOM    616  I       616     15.000 -12.549  44.074  1.00  0.00          O
ATOM    617  I       617     10.000  -3.922  44.829  1.00  0.00          O
ATOM    618  I       618      5.000   4.705  45.584  1.00  0.00          O
ATOM    619  I       619      0.000  13.333  46.338  1.00  0.00          O
ATOM    620  I       620     -5.000  21.960  47.093  1.00  0.00          O
ATOM    621  I       621    -10.000  30.587  47.848  1.00  0.00          O
ATOM    622  I       622     40.000 -38.431  41.810  1.00  0.00          O
ATOM    623  I       623     35.000 -29.804  42.564  1.00  0.00          O
ATOM    624  I       624     30.000 -21.177  43.319  1.00  0.00          O
ATOM    625  I       625     25.000 -12.549  44.074  1.00  0.00          O
ATOM    626  I       626     20.000  -3.922  44.829  1.00  0.00          O
ATOM    627  I       627     15.000   4.705  45.584  1.00  0.00          O
ATOM    628  I       628     10.000  13.333  46.338  1.00  0.00          O
ATOM    629  I       629      5.000  21.960  47.093  1.00  0.00          O
ATOM    630  I       630      0.000  30.587  47.848  1.00  0.00          O
ATOM    631  I       631     50.000 -38.431  41.810  1.00  0.00          O
ATOM    632  I       632     45.000 -29.804  42.564  1.00  0.00          O
ATOM    633  I       633     40.000 -21.177  43.319  1.00  0.00          O
ATOM    634  I       634     35.000 -12.549  44.074  1.00  0.00          O
ATOM    635  I       635     30.000  -3.922  44.829  1.00  0.00          O
ATOM    636  I       636     25.000   4.705  45.584  1.00  0.00          O
ATOM    637  I       637     20.000  13.333  46.338  1.00  0.00          O
ATOM    638  I       638     15.000  21.960  47.093  1.00  0.00          O
ATOM    639  I       639     10.000  30.587  47.848  1.00  0.00          O
ATOM    640  I       640     60.000 -38.431  41.810  1.00  0.00          O
ATOM    641  I       641     55.000 -29.804  42.564  1.00  0.00          O
ATOM    642  I       642     50.000 -21.177  43.319  1.00  0.00          O
ATOM    643  I       643     45.000 -12.549  44.074  1.00  0.00          O
ATOM    644  I       644     40.000  -3.922  44.829  1.00  0.00          O
ATOM    645  I       645     35.000   4.705  45.584  1.00  0.00          O
ATOM    646  I       646     30.000  13.333  46.338  1.00  0.00          O
ATOM    647  I       647     25.000  21.960  47.093  1.00  0.00          O
ATOM    648  I       648     20.000  30.587  47.848  1.00  0.00          O
ATOM    649  I       649    -20.000 -39.739  56.753  1.00  0.00          O
ATOM    650  I       650    -25.000 -31.111  57.507  1.00  0.00          O
ATOM    651  I       651    -30.000 -22.484  58.262  1.00  0.00          O
ATOM    652  I       652    -35.000 -13.857  59.017  1.00  0.00          O
ATOM    653  I       653    -40.000  -5.229  59.772  1.00  0.00          O
ATOM    654  I       654    -45.000   3.398  60.526  1.00  0.00          O
ATOM    655  I       655    -50.000  12.025  61.281  1.00  0.00          O
ATOM    656  I       656    -55.000  20.653  62.036  1.00  0.00          O
ATOM    657  I       657    -60.000  29.280  62.791  1.00  0.00          O
ATOM    658  I       658    -10.000 -39.739  56.753  1.00  0.00          O
ATOM    659  I       659    -15.000 -31.111  57.507  1.00  0.00          O
```

```
ATOM    660  I       660     -20.000 -22.484  58.262  1.00  0.00          O
ATOM    661  I       661     -25.000 -13.857  59.017  1.00  0.00          O
ATOM    662  I       662     -30.000  -5.229  59.772  1.00  0.00          O
ATOM    663  I       663     -35.000   3.398  60.526  1.00  0.00          O
ATOM    664  I       664     -40.000  12.025  61.281  1.00  0.00          O
ATOM    665  I       665     -45.000  20.653  62.036  1.00  0.00          O
ATOM    666  I       666     -50.000  29.280  62.791  1.00  0.00          O
ATOM    667  I       667      -0.000 -39.739  56.753  1.00  0.00          O
ATOM    668  I       668      -5.000 -31.111  57.507  1.00  0.00          O
ATOM    669  I       669     -10.000 -22.484  58.262  1.00  0.00          O
ATOM    670  I       670     -15.000 -13.857  59.017  1.00  0.00          O
ATOM    671  I       671     -20.000  -5.229  59.772  1.00  0.00          O
ATOM    672  I       672     -25.000   3.398  60.526  1.00  0.00          O
ATOM    673  I       673     -30.000  12.025  61.281  1.00  0.00          O
ATOM    674  I       674     -35.000  20.653  62.036  1.00  0.00          O
ATOM    675  I       675     -40.000  29.280  62.791  1.00  0.00          O
ATOM    676  I       676      10.000 -39.739  56.753  1.00  0.00          O
ATOM    677  I       677       5.000 -31.111  57.507  1.00  0.00          O
ATOM    678  I       678       0.000 -22.484  58.262  1.00  0.00          O
ATOM    679  I       679      -5.000 -13.857  59.017  1.00  0.00          O
ATOM    680  I       680     -10.000  -5.229  59.772  1.00  0.00          O
ATOM    681  I       681     -15.000   3.398  60.526  1.00  0.00          O
ATOM    682  I       682     -20.000  12.025  61.281  1.00  0.00          O
ATOM    683  I       683     -25.000  20.653  62.036  1.00  0.00          O
ATOM    684  I       684     -30.000  29.280  62.791  1.00  0.00          O
ATOM    685  I       685      20.000 -39.739  56.753  1.00  0.00          O
ATOM    686  I       686      15.000 -31.111  57.507  1.00  0.00          O
ATOM    687  I       687      10.000 -22.484  58.262  1.00  0.00          O
ATOM    688  I       688       5.000 -13.857  59.017  1.00  0.00          O
ATOM    689  I       689       0.000  -5.229  59.772  1.00  0.00          O
ATOM    690  I       690      -5.000   3.398  60.526  1.00  0.00          O
ATOM    691  I       691     -10.000  12.025  61.281  1.00  0.00          O
ATOM    692  I       692     -15.000  20.653  62.036  1.00  0.00          O
ATOM    693  I       693     -20.000  29.280  62.791  1.00  0.00          O
ATOM    694  I       694      30.000 -39.739  56.753  1.00  0.00          O
ATOM    695  I       695      25.000 -31.111  57.507  1.00  0.00          O
ATOM    696  I       696      20.000 -22.484  58.262  1.00  0.00          O
ATOM    697  I       697      15.000 -13.857  59.017  1.00  0.00          O
ATOM    698  I       698      10.000  -5.229  59.772  1.00  0.00          O
ATOM    699  I       699       5.000   3.398  60.526  1.00  0.00          O
ATOM    700  I       700       0.000  12.025  61.281  1.00  0.00          O
ATOM    701  I       701      -5.000  20.653  62.036  1.00  0.00          O
ATOM    702  I       702     -10.000  29.280  62.791  1.00  0.00          O
ATOM    703  I       703      40.000 -39.739  56.753  1.00  0.00          O
ATOM    704  I       704      35.000 -31.111  57.507  1.00  0.00          O
ATOM    705  I       705      30.000 -22.484  58.262  1.00  0.00          O
ATOM    706  I       706      25.000 -13.857  59.017  1.00  0.00          O
ATOM    707  I       707      20.000  -5.229  59.772  1.00  0.00          O
```

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ATOM    708  I       708      15.000   3.398  60.526  1.00  0.00          O
ATOM    709  I       709      10.000  12.025  61.281  1.00  0.00          O
ATOM    710  I       710       5.000  20.653  62.036  1.00  0.00          O
ATOM    711  I       711       0.000  29.280  62.791  1.00  0.00          O
ATOM    712  I       712      50.000 -39.739  56.753  1.00  0.00          O
ATOM    713  I       713      45.000 -31.111  57.507  1.00  0.00          O
ATOM    714  I       714      40.000 -22.484  58.262  1.00  0.00          O
ATOM    715  I       715      35.000 -13.857  59.017  1.00  0.00          O
ATOM    716  I       716      30.000  -5.229  59.772  1.00  0.00          O
ATOM    717  I       717      25.000   3.398  60.526  1.00  0.00          O
ATOM    718  I       718      20.000  12.025  61.281  1.00  0.00          O
ATOM    719  I       719      15.000  20.653  62.036  1.00  0.00          O
ATOM    720  I       720      10.000  29.280  62.791  1.00  0.00          O
ATOM    721  I       721      60.000 -39.739  56.753  1.00  0.00          O
ATOM    722  I       722      55.000 -31.111  57.507  1.00  0.00          O
ATOM    723  I       723      50.000 -22.484  58.262  1.00  0.00          O
ATOM    724  I       724      45.000 -13.857  59.017  1.00  0.00          O
ATOM    725  I       725      40.000  -5.229  59.772  1.00  0.00          O
ATOM    726  I       726      35.000   3.398  60.526  1.00  0.00          O
ATOM    727  I       727      30.000  12.025  61.281  1.00  0.00          O
ATOM    728  I       728      25.000  20.653  62.036  1.00  0.00          O
ATOM    729  I       729      20.000  29.280  62.791  1.00  0.00          O
END
```

15.2.5 Archivo PDB Estructura Triclínica

Archivo PDB generado correspondiente a la estructura Triclínica de 4 celdas por lado; los parámetros de red con 10 Angstroms en a, 8 Angstroms en b y 5 Angstroms en c; con 80º en alfa, 100º en beta y 120º en gamma:

Campo1	Campo2	Campo3	Campo4	Campo5	Campo6	Campo7	Campo8	Campo9	Campo 10
Registro	serial	elemento	Numero de secuncia	Coordenadas otogonales para x	Coordenadas otogonales para y	Coordenadas otogonales para z	ocupancia	Factor de temperatura	Carga en el átomo

```
ATOM      1  I         1     -20.527 -27.897 -22.109  1.00  0.00          O
ATOM      2  I         2     -24.527 -20.995 -21.506  1.00  0.00          O
ATOM      3  I         3     -28.527 -14.093 -20.902  1.00  0.00          O
ATOM      4  I         4     -32.527  -7.192 -20.298  1.00  0.00          O
ATOM      5  I         5     -36.527  -0.290 -19.694  1.00  0.00          O
ATOM      6  I         6     -40.527   6.612 -19.090  1.00  0.00          O
ATOM      7  I         7     -44.527  13.514 -18.486  1.00  0.00          O
ATOM      8  I         8     -48.527  20.416 -17.883  1.00  0.00          O
ATOM      9  I         9     -52.527  27.318 -17.279  1.00  0.00          O
ATOM     10  I        10      -10.527 -27.897 -22.109  1.00  0.00          O
ATOM     11  I        11      -14.527 -20.995 -21.506  1.00  0.00          O
ATOM     12  I        12      -18.527 -14.093 -20.902  1.00  0.00          O
ATOM     13  I        13      -22.527  -7.192 -20.298  1.00  0.00          O
ATOM     14  I        14      -26.527  -0.290 -19.694  1.00  0.00          O
ATOM     15  I        15      -30.527   6.612 -19.090  1.00  0.00          O
ATOM     16  I        16      -34.527  13.514 -18.486  1.00  0.00          O
ATOM     17  I        17      -38.527  20.416 -17.883  1.00  0.00          O
ATOM     18  I        18      -42.527  27.318 -17.279  1.00  0.00          O
ATOM     19  I        19       -0.527 -27.897 -22.109  1.00  0.00          O
ATOM     20  I        20       -4.527 -20.995 -21.506  1.00  0.00          O
ATOM     21  I        21       -8.527 -14.093 -20.902  1.00  0.00          O
ATOM     22  I        22      -12.527  -7.192 -20.298  1.00  0.00          O
ATOM     23  I        23      -16.527  -0.290 -19.694  1.00  0.00          O
ATOM     24  I        24      -20.527   6.612 -19.090  1.00  0.00          O
ATOM     25  I        25      -24.527  13.514 -18.486  1.00  0.00          O
ATOM     26  I        26      -28.527  20.416 -17.883  1.00  0.00          O
ATOM     27  I        27      -32.527  27.318 -17.279  1.00  0.00          O
ATOM     28  I        28        9.473 -27.897 -22.109  1.00  0.00          O
ATOM     29  I        29        5.473 -20.995 -21.506  1.00  0.00          O
ATOM     30  I        30        1.473 -14.093 -20.902  1.00  0.00          O
ATOM     31  I        31       -2.527  -7.192 -20.298  1.00  0.00          O
ATOM     32  I        32       -6.527  -0.290 -19.694  1.00  0.00          O
ATOM     33  I        33      -10.527   6.612 -19.090  1.00  0.00          O
ATOM     34  I        34      -14.527  13.514 -18.486  1.00  0.00          O
ATOM     35  I        35      -18.527  20.416 -17.883  1.00  0.00          O
ATOM     36  I        36      -22.527  27.318 -17.279  1.00  0.00          O
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ATOM     37  I        37      19.473 -27.897 -22.109  1.00  0.00          O
ATOM     38  I        38      15.473 -20.995 -21.506  1.00  0.00          O
ATOM     39  I        39      11.473 -14.093 -20.902  1.00  0.00          O
ATOM     40  I        40       7.473  -7.192 -20.298  1.00  0.00          O
ATOM     41  I        41       3.473  -0.290 -19.694  1.00  0.00          O
ATOM     42  I        42      -0.527   6.612 -19.090  1.00  0.00          O
ATOM     43  I        43      -4.527  13.514 -18.486  1.00  0.00          O
ATOM     44  I        44      -8.527  20.416 -17.883  1.00  0.00          O
ATOM     45  I        45     -12.527  27.318 -17.279  1.00  0.00          O
ATOM     46  I        46      29.473 -27.897 -22.109  1.00  0.00          O
ATOM     47  I        47      25.473 -20.995 -21.506  1.00  0.00          O
ATOM     48  I        48      21.473 -14.093 -20.902  1.00  0.00          O
ATOM     49  I        49      17.473  -7.192 -20.298  1.00  0.00          O
ATOM     50  I        50      13.473  -0.290 -19.694  1.00  0.00          O
ATOM     51  I        51       9.473   6.612 -19.090  1.00  0.00          O
ATOM     52  I        52       5.473  13.514 -18.486  1.00  0.00          O
ATOM     53  I        53       1.473  20.416 -17.883  1.00  0.00          O
ATOM     54  I        54      -2.527  27.318 -17.279  1.00  0.00          O
ATOM     55  I        55      39.473 -27.897 -22.109  1.00  0.00          O
ATOM     56  I        56      35.473 -20.995 -21.506  1.00  0.00          O
ATOM     57  I        57      31.473 -14.093 -20.902  1.00  0.00          O
ATOM     58  I        58      27.473  -7.192 -20.298  1.00  0.00          O
ATOM     59  I        59      23.473  -0.290 -19.694  1.00  0.00          O
ATOM     60  I        60      19.473   6.612 -19.090  1.00  0.00          O
ATOM     61  I        61      15.473  13.514 -18.486  1.00  0.00          O
ATOM     62  I        62      11.473  20.416 -17.883  1.00  0.00          O
ATOM     63  I        63       7.473  27.318 -17.279  1.00  0.00          O
ATOM     64  I        64      49.473 -27.897 -22.109  1.00  0.00          O
ATOM     65  I        65      45.473 -20.995 -21.506  1.00  0.00          O
ATOM     66  I        66      41.473 -14.093 -20.902  1.00  0.00          O
ATOM     67  I        67      37.473  -7.192 -20.298  1.00  0.00          O
ATOM     68  I        68      33.473  -0.290 -19.694  1.00  0.00          O
ATOM     69  I        69      29.473   6.612 -19.090  1.00  0.00          O
ATOM     70  I        70      25.473  13.514 -18.486  1.00  0.00          O
ATOM     71  I        71      21.473  20.416 -17.883  1.00  0.00          O
ATOM     72  I        72      17.473  27.318 -17.279  1.00  0.00          O
ATOM     73  I        73      59.473 -27.897 -22.109  1.00  0.00          O
ATOM     74  I        74      55.473 -20.995 -21.506  1.00  0.00          O
ATOM     75  I        75      51.473 -14.093 -20.902  1.00  0.00          O
ATOM     76  I        76      47.473  -7.192 -20.298  1.00  0.00          O
ATOM     77  I        77      43.473  -0.290 -19.694  1.00  0.00          O
ATOM     78  I        78      39.473   6.612 -19.090  1.00  0.00          O
ATOM     79  I        79      35.473  13.514 -18.486  1.00  0.00          O
ATOM     80  I        80      31.473  20.416 -17.883  1.00  0.00          O
ATOM     81  I        81      27.473  27.318 -17.279  1.00  0.00          O
ATOM     82  I        82     -21.395 -27.825 -17.186  1.00  0.00          O
ATOM     83  I        83     -25.395 -20.923 -16.582  1.00  0.00          O
ATOM     84  I        84     -29.395 -14.021 -15.978  1.00  0.00          O
```

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ATOM     85  I       85    -33.395  -7.119 -15.374  1.00  0.00          O
ATOM     86  I       86    -37.395  -0.217 -14.771  1.00  0.00          O
ATOM     87  I       87    -41.395   6.685 -14.167  1.00  0.00          O
ATOM     88  I       88    -45.395  13.586 -13.563  1.00  0.00          O
ATOM     89  I       89    -49.395  20.488 -12.959  1.00  0.00          O
ATOM     90  I       90    -53.395  27.390 -12.355  1.00  0.00          O
ATOM     91  I       91    -11.395 -27.825 -17.186  1.00  0.00          O
ATOM     92  I       92    -15.395 -20.923 -16.582  1.00  0.00          O
ATOM     93  I       93    -19.395 -14.021 -15.978  1.00  0.00          O
ATOM     94  I       94    -23.395  -7.119 -15.374  1.00  0.00          O
ATOM     95  I       95    -27.395  -0.217 -14.771  1.00  0.00          O
ATOM     96  I       96    -31.395   6.685 -14.167  1.00  0.00          O
ATOM     97  I       97    -35.395  13.586 -13.563  1.00  0.00          O
ATOM     98  I       98    -39.395  20.488 -12.959  1.00  0.00          O
ATOM     99  I       99    -43.395  27.390 -12.355  1.00  0.00          O
ATOM    100  I      100     -1.395 -27.825 -17.186  1.00  0.00          O
ATOM    101  I      101     -5.395 -20.923 -16.582  1.00  0.00          O
ATOM    102  I      102     -9.395 -14.021 -15.978  1.00  0.00          O
ATOM    103  I      103    -13.395  -7.119 -15.374  1.00  0.00          O
ATOM    104  I      104    -17.395  -0.217 -14.771  1.00  0.00          O
ATOM    105  I      105    -21.395   6.685 -14.167  1.00  0.00          O
ATOM    106  I      106    -25.395  13.586 -13.563  1.00  0.00          O
ATOM    107  I      107    -29.395  20.488 -12.959  1.00  0.00          O
ATOM    108  I      108    -33.395  27.390 -12.355  1.00  0.00          O
ATOM    109  I      109      8.605 -27.825 -17.186  1.00  0.00          O
ATOM    110  I      110      4.605 -20.923 -16.582  1.00  0.00          O
ATOM    111  I      111      0.605 -14.021 -15.978  1.00  0.00          O
ATOM    112  I      112     -3.395  -7.119 -15.374  1.00  0.00          O
ATOM    113  I      113     -7.395  -0.217 -14.771  1.00  0.00          O
ATOM    114  I      114    -11.395   6.685 -14.167  1.00  0.00          O
ATOM    115  I      115    -15.395  13.586 -13.563  1.00  0.00          O
ATOM    116  I      116    -19.395  20.488 -12.959  1.00  0.00          O
ATOM    117  I      117    -23.395  27.390 -12.355  1.00  0.00          O
ATOM    118  I      118     18.605 -27.825 -17.186  1.00  0.00          O
ATOM    119  I      119     14.605 -20.923 -16.582  1.00  0.00          O
ATOM    120  I      120     10.605 -14.021 -15.978  1.00  0.00          O
ATOM    121  I      121      6.605  -7.119 -15.374  1.00  0.00          O
ATOM    122  I      122      2.605  -0.217 -14.771  1.00  0.00          O
ATOM    123  I      123     -1.395   6.685 -14.167  1.00  0.00          O
ATOM    124  I      124     -5.395  13.586 -13.563  1.00  0.00          O
ATOM    125  I      125     -9.395  20.488 -12.959  1.00  0.00          O
ATOM    126  I      126    -13.395  27.390 -12.355  1.00  0.00          O
ATOM    127  I      127     28.605 -27.825 -17.186  1.00  0.00          O
ATOM    128  I      128     24.605 -20.923 -16.582  1.00  0.00          O
ATOM    129  I      129     20.605 -14.021 -15.978  1.00  0.00          O
ATOM    130  I      130     16.605  -7.119 -15.374  1.00  0.00          O
ATOM    131  I      131     12.605  -0.217 -14.771  1.00  0.00          O
ATOM    132  I      132      8.605   6.685 -14.167  1.00  0.00          O
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ATOM    133  I       133       4.605  13.586 -13.563  1.00  0.00           O
ATOM    134  I       134       0.605  20.488 -12.959  1.00  0.00           O
ATOM    135  I       135      -3.395  27.390 -12.355  1.00  0.00           O
ATOM    136  I       136      38.605 -27.825 -17.186  1.00  0.00           O
ATOM    137  I       137      34.605 -20.923 -16.582  1.00  0.00           O
ATOM    138  I       138      30.605 -14.021 -15.978  1.00  0.00           O
ATOM    139  I       139      26.605  -7.119 -15.374  1.00  0.00           O
ATOM    140  I       140      22.605  -0.217 -14.771  1.00  0.00           O
ATOM    141  I       141      18.605   6.685 -14.167  1.00  0.00           O
ATOM    142  I       142      14.605  13.586 -13.563  1.00  0.00           O
ATOM    143  I       143      10.605  20.488 -12.959  1.00  0.00           O
ATOM    144  I       144       6.605  27.390 -12.355  1.00  0.00           O
ATOM    145  I       145      48.605 -27.825 -17.186  1.00  0.00           O
ATOM    146  I       146      44.605 -20.923 -16.582  1.00  0.00           O
ATOM    147  I       147      40.605 -14.021 -15.978  1.00  0.00           O
ATOM    148  I       148      36.605  -7.119 -15.374  1.00  0.00           O
ATOM    149  I       149      32.605  -0.217 -14.771  1.00  0.00           O
ATOM    150  I       150      28.605   6.685 -14.167  1.00  0.00           O
ATOM    151  I       151      24.605  13.586 -13.563  1.00  0.00           O
ATOM    152  I       152      20.605  20.488 -12.959  1.00  0.00           O
ATOM    153  I       153      16.605  27.390 -12.355  1.00  0.00           O
ATOM    154  I       154      58.605 -27.825 -17.186  1.00  0.00           O
ATOM    155  I       155      54.605 -20.923 -16.582  1.00  0.00           O
ATOM    156  I       156      50.605 -14.021 -15.978  1.00  0.00           O
ATOM    157  I       157      46.605  -7.119 -15.374  1.00  0.00           O
ATOM    158  I       158      42.605  -0.217 -14.771  1.00  0.00           O
ATOM    159  I       159      38.605   6.685 -14.167  1.00  0.00           O
ATOM    160  I       160      34.605  13.586 -13.563  1.00  0.00           O
ATOM    161  I       161      30.605  20.488 -12.959  1.00  0.00           O
ATOM    162  I       162      26.605  27.390 -12.355  1.00  0.00           O
ATOM    163  I       163     -22.264 -27.752 -12.262  1.00  0.00           O
ATOM    164  I       164     -26.264 -20.850 -11.659  1.00  0.00           O
ATOM    165  I       165     -30.264 -13.949 -11.055  1.00  0.00           O
ATOM    166  I       166     -34.264  -7.047 -10.451  1.00  0.00           O
ATOM    167  I       167     -38.264  -0.145  -9.847  1.00  0.00           O
ATOM    168  I       168     -42.264   6.757  -9.243  1.00  0.00           O
ATOM    169  I       169     -46.264  13.659  -8.639  1.00  0.00           O
ATOM    170  I       170     -50.264  20.561  -8.036  1.00  0.00           O
ATOM    171  I       171     -54.264  27.462  -7.432  1.00  0.00           O
ATOM    172  I       172     -12.264 -27.752 -12.262  1.00  0.00           O
ATOM    173  I       173     -16.264 -20.850 -11.659  1.00  0.00           O
ATOM    174  I       174     -20.264 -13.949 -11.055  1.00  0.00           O
ATOM    175  I       175     -24.264  -7.047 -10.451  1.00  0.00           O
ATOM    176  I       176     -28.264  -0.145  -9.847  1.00  0.00           O
ATOM    177  I       177     -32.264   6.757  -9.243  1.00  0.00           O
ATOM    178  I       178     -36.264  13.659  -8.639  1.00  0.00           O
ATOM    179  I       179     -40.264  20.561  -8.036  1.00  0.00           O
ATOM    180  I       180     -44.264  27.462  -7.432  1.00  0.00           O
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ATOM    181  I       181      -2.264 -27.752 -12.262  1.00  0.00          O
ATOM    182  I       182      -6.264 -20.850 -11.659  1.00  0.00          O
ATOM    183  I       183     -10.264 -13.949 -11.055  1.00  0.00          O
ATOM    184  I       184     -14.264  -7.047 -10.451  1.00  0.00          O
ATOM    185  I       185     -18.264  -0.145  -9.847  1.00  0.00          O
ATOM    186  I       186     -22.264   6.757  -9.243  1.00  0.00          O
ATOM    187  I       187     -26.264  13.659  -8.639  1.00  0.00          O
ATOM    188  I       188     -30.264  20.561  -8.036  1.00  0.00          O
ATOM    189  I       189     -34.264  27.462  -7.432  1.00  0.00          O
ATOM    190  I       190       7.736 -27.752 -12.262  1.00  0.00          O
ATOM    191  I       191       3.736 -20.850 -11.659  1.00  0.00          O
ATOM    192  I       192      -0.264 -13.949 -11.055  1.00  0.00          O
ATOM    193  I       193      -4.264  -7.047 -10.451  1.00  0.00          O
ATOM    194  I       194      -8.264  -0.145  -9.847  1.00  0.00          O
ATOM    195  I       195     -12.264   6.757  -9.243  1.00  0.00          O
ATOM    196  I       196     -16.264  13.659  -8.639  1.00  0.00          O
ATOM    197  I       197     -20.264  20.561  -8.036  1.00  0.00          O
ATOM    198  I       198     -24.264  27.462  -7.432  1.00  0.00          O
ATOM    199  I       199      17.736 -27.752 -12.262  1.00  0.00          O
ATOM    200  I       200      13.736 -20.850 -11.659  1.00  0.00          O
ATOM    201  I       201       9.736 -13.949 -11.055  1.00  0.00          O
ATOM    202  I       202       5.736  -7.047 -10.451  1.00  0.00          O
ATOM    203  I       203       1.736  -0.145  -9.847  1.00  0.00          O
ATOM    204  I       204      -2.264   6.757  -9.243  1.00  0.00          O
ATOM    205  I       205      -6.264  13.659  -8.639  1.00  0.00          O
ATOM    206  I       206     -10.264  20.561  -8.036  1.00  0.00          O
ATOM    207  I       207     -14.264  27.462  -7.432  1.00  0.00          O
ATOM    208  I       208      27.736 -27.752 -12.262  1.00  0.00          O
ATOM    209  I       209      23.736 -20.850 -11.659  1.00  0.00          O
ATOM    210  I       210      19.736 -13.949 -11.055  1.00  0.00          O
ATOM    211  I       211      15.736  -7.047 -10.451  1.00  0.00          O
ATOM    212  I       212      11.736  -0.145  -9.847  1.00  0.00          O
ATOM    213  I       213       7.736   6.757  -9.243  1.00  0.00          O
ATOM    214  I       214       3.736  13.659  -8.639  1.00  0.00          O
ATOM    215  I       215      -0.264  20.561  -8.036  1.00  0.00          O
ATOM    216  I       216      -4.264  27.462  -7.432  1.00  0.00          O
ATOM    217  I       217      37.736 -27.752 -12.262  1.00  0.00          O
ATOM    218  I       218      33.736 -20.850 -11.659  1.00  0.00          O
ATOM    219  I       219      29.736 -13.949 -11.055  1.00  0.00          O
ATOM    220  I       220      25.736  -7.047 -10.451  1.00  0.00          O
ATOM    221  I       221      21.736  -0.145  -9.847  1.00  0.00          O
ATOM    222  I       222      17.736   6.757  -9.243  1.00  0.00          O
ATOM    223  I       223      13.736  13.659  -8.639  1.00  0.00          O
ATOM    224  I       224       9.736  20.561  -8.036  1.00  0.00          O
ATOM    225  I       225       5.736  27.462  -7.432  1.00  0.00          O
ATOM    226  I       226      47.736 -27.752 -12.262  1.00  0.00          O
ATOM    227  I       227      43.736 -20.850 -11.659  1.00  0.00          O
ATOM    228  I       228      39.736 -13.949 -11.055  1.00  0.00          O
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ATOM    229  I       229      35.736  -7.047 -10.451  1.00  0.00          O
ATOM    230  I       230      31.736  -0.145  -9.847  1.00  0.00          O
ATOM    231  I       231      27.736   6.757  -9.243  1.00  0.00          O
ATOM    232  I       232      23.736  13.659  -8.639  1.00  0.00          O
ATOM    233  I       233      19.736  20.561  -8.036  1.00  0.00          O
ATOM    234  I       234      15.736  27.462  -7.432  1.00  0.00          O
ATOM    235  I       235      57.736 -27.752 -12.262  1.00  0.00          O
ATOM    236  I       236      53.736 -20.850 -11.659  1.00  0.00          O
ATOM    237  I       237      49.736 -13.949 -11.055  1.00  0.00          O
ATOM    238  I       238      45.736  -7.047 -10.451  1.00  0.00          O
ATOM    239  I       239      41.736  -0.145  -9.847  1.00  0.00          O
ATOM    240  I       240      37.736   6.757  -9.243  1.00  0.00          O
ATOM    241  I       241      33.736  13.659  -8.639  1.00  0.00          O
ATOM    242  I       242      29.736  20.561  -8.036  1.00  0.00          O
ATOM    243  I       243      25.736  27.462  -7.432  1.00  0.00          O
ATOM    244  I       244     -23.132 -27.680  -7.339  1.00  0.00          O
ATOM    245  I       245     -27.132 -20.778  -6.735  1.00  0.00          O
ATOM    246  I       246     -31.132 -13.876  -6.131  1.00  0.00          O
ATOM    247  I       247     -35.132  -6.974  -5.527  1.00  0.00          O
ATOM    248  I       248     -39.132  -0.072  -4.924  1.00  0.00          O
ATOM    249  I       249     -43.132   6.829  -4.320  1.00  0.00          O
ATOM    250  I       250     -47.132  13.731  -3.716  1.00  0.00          O
ATOM    251  I       251     -51.132  20.633  -3.112  1.00  0.00          O
ATOM    252  I       252     -55.132  27.535  -2.508  1.00  0.00          O
ATOM    253  I       253     -13.132 -27.680  -7.339  1.00  0.00          O
ATOM    254  I       254     -17.132 -20.778  -6.735  1.00  0.00          O
ATOM    255  I       255     -21.132 -13.876  -6.131  1.00  0.00          O
ATOM    256  I       256     -25.132  -6.974  -5.527  1.00  0.00          O
ATOM    257  I       257     -29.132  -0.072  -4.924  1.00  0.00          O
ATOM    258  I       258     -33.132   6.829  -4.320  1.00  0.00          O
ATOM    259  I       259     -37.132  13.731  -3.716  1.00  0.00          O
ATOM    260  I       260     -41.132  20.633  -3.112  1.00  0.00          O
ATOM    261  I       261     -45.132  27.535  -2.508  1.00  0.00          O
ATOM    262  I       262      -3.132 -27.680  -7.339  1.00  0.00          O
ATOM    263  I       263      -7.132 -20.778  -6.735  1.00  0.00          O
ATOM    264  I       264     -11.132 -13.876  -6.131  1.00  0.00          O
ATOM    265  I       265     -15.132  -6.974  -5.527  1.00  0.00          O
ATOM    266  I       266     -19.132  -0.072  -4.924  1.00  0.00          O
ATOM    267  I       267     -23.132   6.829  -4.320  1.00  0.00          O
ATOM    268  I       268     -27.132  13.731  -3.716  1.00  0.00          O
ATOM    269  I       269     -31.132  20.633  -3.112  1.00  0.00          O
ATOM    270  I       270     -35.132  27.535  -2.508  1.00  0.00          O
ATOM    271  I       271       6.868 -27.680  -7.339  1.00  0.00          O
ATOM    272  I       272       2.868 -20.778  -6.735  1.00  0.00          O
ATOM    273  I       273      -1.132 -13.876  -6.131  1.00  0.00          O
ATOM    274  I       274      -5.132  -6.974  -5.527  1.00  0.00          O
ATOM    275  I       275      -9.132  -0.072  -4.924  1.00  0.00          O
ATOM    276  I       276     -13.132   6.829  -4.320  1.00  0.00          O
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ATOM    277  I       277    -17.132  13.731  -3.716  1.00  0.00          O
ATOM    278  I       278    -21.132  20.633  -3.112  1.00  0.00          O
ATOM    279  I       279    -25.132  27.535  -2.508  1.00  0.00          O
ATOM    280  I       280     16.868 -27.680  -7.339  1.00  0.00          O
ATOM    281  I       281     12.868 -20.778  -6.735  1.00  0.00          O
ATOM    282  I       282      8.868 -13.876  -6.131  1.00  0.00          O
ATOM    283  I       283      4.868  -6.974  -5.527  1.00  0.00          O
ATOM    284  I       284      0.868  -0.072  -4.924  1.00  0.00          O
ATOM    285  I       285     -3.132   6.829  -4.320  1.00  0.00          O
ATOM    286  I       286     -7.132  13.731  -3.716  1.00  0.00          O
ATOM    287  I       287    -11.132  20.633  -3.112  1.00  0.00          O
ATOM    288  I       288    -15.132  27.535  -2.508  1.00  0.00          O
ATOM    289  I       289     26.868 -27.680  -7.339  1.00  0.00          O
ATOM    290  I       290     22.868 -20.778  -6.735  1.00  0.00          O
ATOM    291  I       291     18.868 -13.876  -6.131  1.00  0.00          O
ATOM    292  I       292     14.868  -6.974  -5.527  1.00  0.00          O
ATOM    293  I       293     10.868  -0.072  -4.924  1.00  0.00          O
ATOM    294  I       294      6.868   6.829  -4.320  1.00  0.00          O
ATOM    295  I       295      2.868  13.731  -3.716  1.00  0.00          O
ATOM    296  I       296     -1.132  20.633  -3.112  1.00  0.00          O
ATOM    297  I       297     -5.132  27.535  -2.508  1.00  0.00          O
ATOM    298  I       298     36.868 -27.680  -7.339  1.00  0.00          O
ATOM    299  I       299     32.868 -20.778  -6.735  1.00  0.00          O
ATOM    300  I       300     28.868 -13.876  -6.131  1.00  0.00          O
ATOM    301  I       301     24.868  -6.974  -5.527  1.00  0.00          O
ATOM    302  I       302     20.868  -0.072  -4.924  1.00  0.00          O
ATOM    303  I       303     16.868   6.829  -4.320  1.00  0.00          O
ATOM    304  I       304     12.868  13.731  -3.716  1.00  0.00          O
ATOM    305  I       305      8.868  20.633  -3.112  1.00  0.00          O
ATOM    306  I       306      4.868  27.535  -2.508  1.00  0.00          O
ATOM    307  I       307     46.868 -27.680  -7.339  1.00  0.00          O
ATOM    308  I       308     42.868 -20.778  -6.735  1.00  0.00          O
ATOM    309  I       309     38.868 -13.876  -6.131  1.00  0.00          O
ATOM    310  I       310     34.868  -6.974  -5.527  1.00  0.00          O
ATOM    311  I       311     30.868  -0.072  -4.924  1.00  0.00          O
ATOM    312  I       312     26.868   6.829  -4.320  1.00  0.00          O
ATOM    313  I       313     22.868  13.731  -3.716  1.00  0.00          O
ATOM    314  I       314     18.868  20.633  -3.112  1.00  0.00          O
ATOM    315  I       315     14.868  27.535  -2.508  1.00  0.00          O
ATOM    316  I       316     56.868 -27.680  -7.339  1.00  0.00          O
ATOM    317  I       317     52.868 -20.778  -6.735  1.00  0.00          O
ATOM    318  I       318     48.868 -13.876  -6.131  1.00  0.00          O
ATOM    319  I       319     44.868  -6.974  -5.527  1.00  0.00          O
ATOM    320  I       320     40.868  -0.072  -4.924  1.00  0.00          O
ATOM    321  I       321     36.868   6.829  -4.320  1.00  0.00          O
ATOM    322  I       322     32.868  13.731  -3.716  1.00  0.00          O
ATOM    323  I       323     28.868  20.633  -3.112  1.00  0.00          O
ATOM    324  I       324     24.868  27.535  -2.508  1.00  0.00          O
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ATOM    325  I       325     -24.000 -27.607  -2.415  1.00  0.00          O
ATOM    326  I       326     -28.000 -20.706  -1.811  1.00  0.00          O
ATOM    327  I       327     -32.000 -13.804  -1.208  1.00  0.00          O
ATOM    328  I       328     -36.000  -6.902  -0.604  1.00  0.00          O
ATOM    329  I       329     -40.000   0.000   0.000  1.00  0.00          O
ATOM    330  I       330     -44.000   6.902   0.604  1.00  0.00          O
ATOM    331  I       331     -48.000  13.804   1.208  1.00  0.00          O
ATOM    332  I       332     -52.000  20.706   1.811  1.00  0.00          O
ATOM    333  I       333     -56.000  27.607   2.415  1.00  0.00          O
ATOM    334  I       334     -14.000 -27.607  -2.415  1.00  0.00          O
ATOM    335  I       335     -18.000 -20.706  -1.811  1.00  0.00          O
ATOM    336  I       336     -22.000 -13.804  -1.208  1.00  0.00          O
ATOM    337  I       337     -26.000  -6.902  -0.604  1.00  0.00          O
ATOM    338  I       338     -30.000   0.000   0.000  1.00  0.00          O
ATOM    339  I       339     -34.000   6.902   0.604  1.00  0.00          O
ATOM    340  I       340     -38.000  13.804   1.208  1.00  0.00          O
ATOM    341  I       341     -42.000  20.706   1.811  1.00  0.00          O
ATOM    342  I       342     -46.000  27.607   2.415  1.00  0.00          O
ATOM    343  I       343      -4.000 -27.607  -2.415  1.00  0.00          O
ATOM    344  I       344      -8.000 -20.706  -1.811  1.00  0.00          O
ATOM    345  I       345     -12.000 -13.804  -1.208  1.00  0.00          O
ATOM    346  I       346     -16.000  -6.902  -0.604  1.00  0.00          O
ATOM    347  I       347     -20.000   0.000   0.000  1.00  0.00          O
ATOM    348  I       348     -24.000   6.902   0.604  1.00  0.00          O
ATOM    349  I       349     -28.000  13.804   1.208  1.00  0.00          O
ATOM    350  I       350     -32.000  20.706   1.811  1.00  0.00          O
ATOM    351  I       351     -36.000  27.607   2.415  1.00  0.00          O
ATOM    352  I       352       6.000 -27.607  -2.415  1.00  0.00          O
ATOM    353  I       353       2.000 -20.706  -1.811  1.00  0.00          O
ATOM    354  I       354      -2.000 -13.804  -1.208  1.00  0.00          O
ATOM    355  I       355      -6.000  -6.902  -0.604  1.00  0.00          O
ATOM    356  I       356     -10.000   0.000   0.000  1.00  0.00          O
ATOM    357  I       357     -14.000   6.902   0.604  1.00  0.00          O
ATOM    358  I       358     -18.000  13.804   1.208  1.00  0.00          O
ATOM    359  I       359     -22.000  20.706   1.811  1.00  0.00          O
ATOM    360  I       360     -26.000  27.607   2.415  1.00  0.00          O
ATOM    361  I       361      16.000 -27.607  -2.415  1.00  0.00          O
ATOM    362  I       362      12.000 -20.706  -1.811  1.00  0.00          O
ATOM    363  I       363       8.000 -13.804  -1.208  1.00  0.00          O
ATOM    364  I       364       4.000  -6.902  -0.604  1.00  0.00          O
ATOM    365  I       365       0.000   0.000   0.000  1.00  0.00          O
ATOM    366  I       366      -4.000   6.902   0.604  1.00  0.00          O
ATOM    367  I       367      -8.000  13.804   1.208  1.00  0.00          O
ATOM    368  I       368     -12.000  20.706   1.811  1.00  0.00          O
ATOM    369  I       369     -16.000  27.607   2.415  1.00  0.00          O
ATOM    370  I       370      26.000 -27.607  -2.415  1.00  0.00          O
ATOM    371  I       371      22.000 -20.706  -1.811  1.00  0.00          O
ATOM    372  I       372      18.000 -13.804  -1.208  1.00  0.00          O
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ATOM    373  I       373      14.000  -6.902  -0.604  1.00  0.00          O
ATOM    374  I       374      10.000   0.000   0.000  1.00  0.00          O
ATOM    375  I       375       6.000   6.902   0.604  1.00  0.00          O
ATOM    376  I       376       2.000  13.804   1.208  1.00  0.00          O
ATOM    377  I       377      -2.000  20.706   1.811  1.00  0.00          O
ATOM    378  I       378      -6.000  27.607   2.415  1.00  0.00          O
ATOM    379  I       379      36.000 -27.607  -2.415  1.00  0.00          O
ATOM    380  I       380      32.000 -20.706  -1.811  1.00  0.00          O
ATOM    381  I       381      28.000 -13.804  -1.208  1.00  0.00          O
ATOM    382  I       382      24.000  -6.902  -0.604  1.00  0.00          O
ATOM    383  I       383      20.000   0.000   0.000  1.00  0.00          O
ATOM    384  I       384      16.000   6.902   0.604  1.00  0.00          O
ATOM    385  I       385      12.000  13.804   1.208  1.00  0.00          O
ATOM    386  I       386       8.000  20.706   1.811  1.00  0.00          O
ATOM    387  I       387       4.000  27.607   2.415  1.00  0.00          O
ATOM    388  I       388      46.000 -27.607  -2.415  1.00  0.00          O
ATOM    389  I       389      42.000 -20.706  -1.811  1.00  0.00          O
ATOM    390  I       390      38.000 -13.804  -1.208  1.00  0.00          O
ATOM    391  I       391      34.000  -6.902  -0.604  1.00  0.00          O
ATOM    392  I       392      30.000   0.000   0.000  1.00  0.00          O
ATOM    393  I       393      26.000   6.902   0.604  1.00  0.00          O
ATOM    394  I       394      22.000  13.804   1.208  1.00  0.00          O
ATOM    395  I       395      18.000  20.706   1.811  1.00  0.00          O
ATOM    396  I       396      14.000  27.607   2.415  1.00  0.00          O
ATOM    397  I       397      56.000 -27.607  -2.415  1.00  0.00          O
ATOM    398  I       398      52.000 -20.706  -1.811  1.00  0.00          O
ATOM    399  I       399      48.000 -13.804  -1.208  1.00  0.00          O
ATOM    400  I       400      44.000  -6.902  -0.604  1.00  0.00          O
ATOM    401  I       401      40.000   0.000   0.000  1.00  0.00          O
ATOM    402  I       402      36.000   6.902   0.604  1.00  0.00          O
ATOM    403  I       403      32.000  13.804   1.208  1.00  0.00          O
ATOM    404  I       404      28.000  20.706   1.811  1.00  0.00          O
ATOM    405  I       405      24.000  27.607   2.415  1.00  0.00          O
ATOM    406  I       406     -24.868 -27.535   2.508  1.00  0.00          O
ATOM    407  I       407     -28.868 -20.633   3.112  1.00  0.00          O
ATOM    408  I       408     -32.868 -13.731   3.716  1.00  0.00          O
ATOM    409  I       409     -36.868  -6.829   4.320  1.00  0.00          O
ATOM    410  I       410     -40.868   0.072   4.924  1.00  0.00          O
ATOM    411  I       411     -44.868   6.974   5.527  1.00  0.00          O
ATOM    412  I       412     -48.868  13.876   6.131  1.00  0.00          O
ATOM    413  I       413     -52.868  20.778   6.735  1.00  0.00          O
ATOM    414  I       414     -56.868  27.680   7.339  1.00  0.00          O
ATOM    415  I       415     -14.868 -27.535   2.508  1.00  0.00          O
ATOM    416  I       416     -18.868 -20.633   3.112  1.00  0.00          O
ATOM    417  I       417     -22.868 -13.731   3.716  1.00  0.00          O
ATOM    418  I       418     -26.868  -6.829   4.320  1.00  0.00          O
ATOM    419  I       419     -30.868   0.072   4.924  1.00  0.00          O
ATOM    420  I       420     -34.868   6.974   5.527  1.00  0.00          O
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ATOM    421  I       421    -38.868  13.876   6.131  1.00  0.00          O
ATOM    422  I       422    -42.868  20.778   6.735  1.00  0.00          O
ATOM    423  I       423    -46.868  27.680   7.339  1.00  0.00          O
ATOM    424  I       424     -4.868 -27.535   2.508  1.00  0.00          O
ATOM    425  I       425     -8.868 -20.633   3.112  1.00  0.00          O
ATOM    426  I       426    -12.868 -13.731   3.716  1.00  0.00          O
ATOM    427  I       427    -16.868  -6.829   4.320  1.00  0.00          O
ATOM    428  I       428    -20.868   0.072   4.924  1.00  0.00          O
ATOM    429  I       429    -24.868   6.974   5.527  1.00  0.00          O
ATOM    430  I       430    -28.868  13.876   6.131  1.00  0.00          O
ATOM    431  I       431    -32.868  20.778   6.735  1.00  0.00          O
ATOM    432  I       432    -36.868  27.680   7.339  1.00  0.00          O
ATOM    433  I       433      5.132 -27.535   2.508  1.00  0.00          O
ATOM    434  I       434      1.132 -20.633   3.112  1.00  0.00          O
ATOM    435  I       435     -2.868 -13.731   3.716  1.00  0.00          O
ATOM    436  I       436     -6.868  -6.829   4.320  1.00  0.00          O
ATOM    437  I       437    -10.868   0.072   4.924  1.00  0.00          O
ATOM    438  I       438    -14.868   6.974   5.527  1.00  0.00          O
ATOM    439  I       439    -18.868  13.876   6.131  1.00  0.00          O
ATOM    440  I       440    -22.868  20.778   6.735  1.00  0.00          O
ATOM    441  I       441    -26.868  27.680   7.339  1.00  0.00          O
ATOM    442  I       442     15.132 -27.535   2.508  1.00  0.00          O
ATOM    443  I       443     11.132 -20.633   3.112  1.00  0.00          O
ATOM    444  I       444      7.132 -13.731   3.716  1.00  0.00          O
ATOM    445  I       445      3.132  -6.829   4.320  1.00  0.00          O
ATOM    446  I       446     -0.868   0.072   4.924  1.00  0.00          O
ATOM    447  I       447     -4.868   6.974   5.527  1.00  0.00          O
ATOM    448  I       448     -8.868  13.876   6.131  1.00  0.00          O
ATOM    449  I       449    -12.868  20.778   6.735  1.00  0.00          O
ATOM    450  I       450    -16.868  27.680   7.339  1.00  0.00          O
ATOM    451  I       451     25.132 -27.535   2.508  1.00  0.00          O
ATOM    452  I       452     21.132 -20.633   3.112  1.00  0.00          O
ATOM    453  I       453     17.132 -13.731   3.716  1.00  0.00          O
ATOM    454  I       454     13.132  -6.829   4.320  1.00  0.00          O
ATOM    455  I       455      9.132   0.072   4.924  1.00  0.00          O
ATOM    456  I       456      5.132   6.974   5.527  1.00  0.00          O
ATOM    457  I       457      1.132  13.876   6.131  1.00  0.00          O
ATOM    458  I       458     -2.868  20.778   6.735  1.00  0.00          O
ATOM    459  I       459     -6.868  27.680   7.339  1.00  0.00          O
ATOM    460  I       460     35.132 -27.535   2.508  1.00  0.00          O
ATOM    461  I       461     31.132 -20.633   3.112  1.00  0.00          O
ATOM    462  I       462     27.132 -13.731   3.716  1.00  0.00          O
ATOM    463  I       463     23.132  -6.829   4.320  1.00  0.00          O
ATOM    464  I       464     19.132   0.072   4.924  1.00  0.00          O
ATOM    465  I       465     15.132   6.974   5.527  1.00  0.00          O
ATOM    466  I       466     11.132  13.876   6.131  1.00  0.00          O
ATOM    467  I       467      7.132  20.778   6.735  1.00  0.00          O
ATOM    468  I       468      3.132  27.680   7.339  1.00  0.00          O
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ATOM    469  I       469      45.132 -27.535   2.508  1.00  0.00          O
ATOM    470  I       470      41.132 -20.633   3.112  1.00  0.00          O
ATOM    471  I       471      37.132 -13.731   3.716  1.00  0.00          O
ATOM    472  I       472      33.132  -6.829   4.320  1.00  0.00          O
ATOM    473  I       473      29.132   0.072   4.924  1.00  0.00          O
ATOM    474  I       474      25.132   6.974   5.527  1.00  0.00          O
ATOM    475  I       475      21.132  13.876   6.131  1.00  0.00          O
ATOM    476  I       476      17.132  20.778   6.735  1.00  0.00          O
ATOM    477  I       477      13.132  27.680   7.339  1.00  0.00          O
ATOM    478  I       478      55.132 -27.535   2.508  1.00  0.00          O
ATOM    479  I       479      51.132 -20.633   3.112  1.00  0.00          O
ATOM    480  I       480      47.132 -13.731   3.716  1.00  0.00          O
ATOM    481  I       481      43.132  -6.829   4.320  1.00  0.00          O
ATOM    482  I       482      39.132   0.072   4.924  1.00  0.00          O
ATOM    483  I       483      35.132   6.974   5.527  1.00  0.00          O
ATOM    484  I       484      31.132  13.876   6.131  1.00  0.00          O
ATOM    485  I       485      27.132  20.778   6.735  1.00  0.00          O
ATOM    486  I       486      23.132  27.680   7.339  1.00  0.00          O
ATOM    487  I       487     -25.736 -27.462   7.432  1.00  0.00          O
ATOM    488  I       488     -29.736 -20.561   8.036  1.00  0.00          O
ATOM    489  I       489     -33.736 -13.659   8.639  1.00  0.00          O
ATOM    490  I       490     -37.736  -6.757   9.243  1.00  0.00          O
ATOM    491  I       491     -41.736   0.145   9.847  1.00  0.00          O
ATOM    492  I       492     -45.736   7.047  10.451  1.00  0.00          O
ATOM    493  I       493     -49.736  13.949  11.055  1.00  0.00          O
ATOM    494  I       494     -53.736  20.850  11.659  1.00  0.00          O
ATOM    495  I       495     -57.736  27.752  12.262  1.00  0.00          O
ATOM    496  I       496     -15.736 -27.462   7.432  1.00  0.00          O
ATOM    497  I       497     -19.736 -20.561   8.036  1.00  0.00          O
ATOM    498  I       498     -23.736 -13.659   8.639  1.00  0.00          O
ATOM    499  I       499     -27.736  -6.757   9.243  1.00  0.00          O
ATOM    500  I       500     -31.736   0.145   9.847  1.00  0.00          O
ATOM    501  I       501     -35.736   7.047  10.451  1.00  0.00          O
ATOM    502  I       502     -39.736  13.949  11.055  1.00  0.00          O
ATOM    503  I       503     -43.736  20.850  11.659  1.00  0.00          O
ATOM    504  I       504     -47.736  27.752  12.262  1.00  0.00          O
ATOM    505  I       505      -5.736 -27.462   7.432  1.00  0.00          O
ATOM    506  I       506      -9.736 -20.561   8.036  1.00  0.00          O
ATOM    507  I       507     -13.736 -13.659   8.639  1.00  0.00          O
ATOM    508  I       508     -17.736  -6.757   9.243  1.00  0.00          O
ATOM    509  I       509     -21.736   0.145   9.847  1.00  0.00          O
ATOM    510  I       510     -25.736   7.047  10.451  1.00  0.00          O
ATOM    511  I       511     -29.736  13.949  11.055  1.00  0.00          O
ATOM    512  I       512     -33.736  20.850  11.659  1.00  0.00          O
ATOM    513  I       513     -37.736  27.752  12.262  1.00  0.00          O
ATOM    514  I       514       4.264 -27.462   7.432  1.00  0.00          O
ATOM    515  I       515       0.264 -20.561   8.036  1.00  0.00          O
ATOM    516  I       516      -3.736 -13.659   8.639  1.00  0.00          O
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ATOM    517  I       517     -7.736  -6.757   9.243  1.00  0.00          O
ATOM    518  I       518    -11.736   0.145   9.847  1.00  0.00          O
ATOM    519  I       519    -15.736   7.047  10.451  1.00  0.00          O
ATOM    520  I       520    -19.736  13.949  11.055  1.00  0.00          O
ATOM    521  I       521    -23.736  20.850  11.659  1.00  0.00          O
ATOM    522  I       522    -27.736  27.752  12.262  1.00  0.00          O
ATOM    523  I       523     14.264 -27.462   7.432  1.00  0.00          O
ATOM    524  I       524     10.264 -20.561   8.036  1.00  0.00          O
ATOM    525  I       525      6.264 -13.659   8.639  1.00  0.00          O
ATOM    526  I       526      2.264  -6.757   9.243  1.00  0.00          O
ATOM    527  I       527     -1.736   0.145   9.847  1.00  0.00          O
ATOM    528  I       528     -5.736   7.047  10.451  1.00  0.00          O
ATOM    529  I       529     -9.736  13.949  11.055  1.00  0.00          O
ATOM    530  I       530    -13.736  20.850  11.659  1.00  0.00          O
ATOM    531  I       531    -17.736  27.752  12.262  1.00  0.00          O
ATOM    532  I       532     24.264 -27.462   7.432  1.00  0.00          O
ATOM    533  I       533     20.264 -20.561   8.036  1.00  0.00          O
ATOM    534  I       534     16.264 -13.659   8.639  1.00  0.00          O
ATOM    535  I       535     12.264  -6.757   9.243  1.00  0.00          O
ATOM    536  I       536      8.264   0.145   9.847  1.00  0.00          O
ATOM    537  I       537      4.264   7.047  10.451  1.00  0.00          O
ATOM    538  I       538      0.264  13.949  11.055  1.00  0.00          O
ATOM    539  I       539     -3.736  20.850  11.659  1.00  0.00          O
ATOM    540  I       540     -7.736  27.752  12.262  1.00  0.00          O
ATOM    541  I       541     34.264 -27.462   7.432  1.00  0.00          O
ATOM    542  I       542     30.264 -20.561   8.036  1.00  0.00          O
ATOM    543  I       543     26.264 -13.659   8.639  1.00  0.00          O
ATOM    544  I       544     22.264  -6.757   9.243  1.00  0.00          O
ATOM    545  I       545     18.264   0.145   9.847  1.00  0.00          O
ATOM    546  I       546     14.264   7.047  10.451  1.00  0.00          O
ATOM    547  I       547     10.264  13.949  11.055  1.00  0.00          O
ATOM    548  I       548      6.264  20.850  11.659  1.00  0.00          O
ATOM    549  I       549      2.264  27.752  12.262  1.00  0.00          O
ATOM    550  I       550     44.264 -27.462   7.432  1.00  0.00          O
ATOM    551  I       551     40.264 -20.561   8.036  1.00  0.00          O
ATOM    552  I       552     36.264 -13.659   8.639  1.00  0.00          O
ATOM    553  I       553     32.264  -6.757   9.243  1.00  0.00          O
ATOM    554  I       554     28.264   0.145   9.847  1.00  0.00          O
ATOM    555  I       555     24.264   7.047  10.451  1.00  0.00          O
ATOM    556  I       556     20.264  13.949  11.055  1.00  0.00          O
ATOM    557  I       557     16.264  20.850  11.659  1.00  0.00          O
ATOM    558  I       558     12.264  27.752  12.262  1.00  0.00          O
ATOM    559  I       559     54.264 -27.462   7.432  1.00  0.00          O
ATOM    560  I       560     50.264 -20.561   8.036  1.00  0.00          O
ATOM    561  I       561     46.264 -13.659   8.639  1.00  0.00          O
ATOM    562  I       562     42.264  -6.757   9.243  1.00  0.00          O
ATOM    563  I       563     38.264   0.145   9.847  1.00  0.00          O
ATOM    564  I       564     34.264   7.047  10.451  1.00  0.00          O
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ATOM 565 I 565 30.264 13.949 11.055 1.00 0.00 O
ATOM 566 I 566 26.264 20.850 11.659 1.00 0.00 O
ATOM 567 I 567 22.264 27.752 12.262 1.00 0.00 O
ATOM 568 I 568 -26.605 -27.390 12.355 1.00 0.00 O
ATOM 569 I 569 -30.605 -20.488 12.959 1.00 0.00 O
ATOM 570 I 570 -34.605 -13.586 13.563 1.00 0.00 O
ATOM 571 I 571 -38.605 -6.685 14.167 1.00 0.00 O
ATOM 572 I 572 -42.605 0.217 14.771 1.00 0.00 O
ATOM 573 I 573 -46.605 7.119 15.374 1.00 0.00 O
ATOM 574 I 574 -50.605 14.021 15.978 1.00 0.00 O
ATOM 575 I 575 -54.605 20.923 16.582 1.00 0.00 O
ATOM 576 I 576 -58.605 27.825 17.186 1.00 0.00 O
ATOM 577 I 577 -16.605 -27.390 12.355 1.00 0.00 O
ATOM 578 I 578 -20.605 -20.488 12.959 1.00 0.00 O
ATOM 579 I 579 -24.605 -13.586 13.563 1.00 0.00 O
ATOM 580 I 580 -28.605 -6.685 14.167 1.00 0.00 O
ATOM 581 I 581 -32.605 0.217 14.771 1.00 0.00 O
ATOM 582 I 582 -36.605 7.119 15.374 1.00 0.00 O
ATOM 583 I 583 -40.605 14.021 15.978 1.00 0.00 O
ATOM 584 I 584 -44.605 20.923 16.582 1.00 0.00 O
ATOM 585 I 585 -48.605 27.825 17.186 1.00 0.00 O
ATOM 586 I 586 -6.605 -27.390 12.355 1.00 0.00 O
ATOM 587 I 587 -10.605 -20.488 12.959 1.00 0.00 O
ATOM 588 I 588 -14.605 -13.586 13.563 1.00 0.00 O
ATOM 589 I 589 -18.605 -6.685 14.167 1.00 0.00 O
ATOM 590 I 590 -22.605 0.217 14.771 1.00 0.00 O
ATOM 591 I 591 -26.605 7.119 15.374 1.00 0.00 O
ATOM 592 I 592 -30.605 14.021 15.978 1.00 0.00 O
ATOM 593 I 593 -34.605 20.923 16.582 1.00 0.00 O
ATOM 594 I 594 -38.605 27.825 17.186 1.00 0.00 O
ATOM 595 I 595 3.395 -27.390 12.355 1.00 0.00 O
ATOM 596 I 596 -0.605 -20.488 12.959 1.00 0.00 O
ATOM 597 I 597 -4.605 -13.586 13.563 1.00 0.00 O
ATOM 598 I 598 -8.605 -6.685 14.167 1.00 0.00 O
ATOM 599 I 599 -12.605 0.217 14.771 1.00 0.00 O
ATOM 600 I 600 -16.605 7.119 15.374 1.00 0.00 O
ATOM 601 I 601 -20.605 14.021 15.978 1.00 0.00 O
ATOM 602 I 602 -24.605 20.923 16.582 1.00 0.00 O
ATOM 603 I 603 -28.605 27.825 17.186 1.00 0.00 O
ATOM 604 I 604 13.395 -27.390 12.355 1.00 0.00 O
ATOM 605 I 605 9.395 -20.488 12.959 1.00 0.00 O
ATOM 606 I 606 5.395 -13.586 13.563 1.00 0.00 O
ATOM 607 I 607 1.395 -6.685 14.167 1.00 0.00 O
ATOM 608 I 608 -2.605 0.217 14.771 1.00 0.00 O
ATOM 609 I 609 -6.605 7.119 15.374 1.00 0.00 O
ATOM 610 I 610 -10.605 14.021 15.978 1.00 0.00 O
ATOM 611 I 611 -14.605 20.923 16.582 1.00 0.00 O
ATOM 612 I 612 -18.605 27.825 17.186 1.00 0.00 O

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ATOM    613  I       613      23.395 -27.390  12.355  1.00  0.00          O
ATOM    614  I       614      19.395 -20.488  12.959  1.00  0.00          O
ATOM    615  I       615      15.395 -13.586  13.563  1.00  0.00          O
ATOM    616  I       616      11.395  -6.685  14.167  1.00  0.00          O
ATOM    617  I       617       7.395   0.217  14.771  1.00  0.00          O
ATOM    618  I       618       3.395   7.119  15.374  1.00  0.00          O
ATOM    619  I       619      -0.605  14.021  15.978  1.00  0.00          O
ATOM    620  I       620      -4.605  20.923  16.582  1.00  0.00          O
ATOM    621  I       621      -8.605  27.825  17.186  1.00  0.00          O
ATOM    622  I       622      33.395 -27.390  12.355  1.00  0.00          O
ATOM    623  I       623      29.395 -20.488  12.959  1.00  0.00          O
ATOM    624  I       624      25.395 -13.586  13.563  1.00  0.00          O
ATOM    625  I       625      21.395  -6.685  14.167  1.00  0.00          O
ATOM    626  I       626      17.395   0.217  14.771  1.00  0.00          O
ATOM    627  I       627      13.395   7.119  15.374  1.00  0.00          O
ATOM    628  I       628       9.395  14.021  15.978  1.00  0.00          O
ATOM    629  I       629       5.395  20.923  16.582  1.00  0.00          O
ATOM    630  I       630       1.395  27.825  17.186  1.00  0.00          O
ATOM    631  I       631      43.395 -27.390  12.355  1.00  0.00          O
ATOM    632  I       632      39.395 -20.488  12.959  1.00  0.00          O
ATOM    633  I       633      35.395 -13.586  13.563  1.00  0.00          O
ATOM    634  I       634      31.395  -6.685  14.167  1.00  0.00          O
ATOM    635  I       635      27.395   0.217  14.771  1.00  0.00          O
ATOM    636  I       636      23.395   7.119  15.374  1.00  0.00          O
ATOM    637  I       637      19.395  14.021  15.978  1.00  0.00          O
ATOM    638  I       638      15.395  20.923  16.582  1.00  0.00          O
ATOM    639  I       639      11.395  27.825  17.186  1.00  0.00          O
ATOM    640  I       640      53.395 -27.390  12.355  1.00  0.00          O
ATOM    641  I       641      49.395 -20.488  12.959  1.00  0.00          O
ATOM    642  I       642      45.395 -13.586  13.563  1.00  0.00          O
ATOM    643  I       643      41.395  -6.685  14.167  1.00  0.00          O
ATOM    644  I       644      37.395   0.217  14.771  1.00  0.00          O
ATOM    645  I       645      33.395   7.119  15.374  1.00  0.00          O
ATOM    646  I       646      29.395  14.021  15.978  1.00  0.00          O
ATOM    647  I       647      25.395  20.923  16.582  1.00  0.00          O
ATOM    648  I       648      21.395  27.825  17.186  1.00  0.00          O
ATOM    649  I       649     -27.473 -27.318  17.279  1.00  0.00          O
ATOM    650  I       650     -31.473 -20.416  17.883  1.00  0.00          O
ATOM    651  I       651     -35.473 -13.514  18.486  1.00  0.00          O
ATOM    652  I       652     -39.473  -6.612  19.090  1.00  0.00          O
ATOM    653  I       653     -43.473   0.290  19.694  1.00  0.00          O
ATOM    654  I       654     -47.473   7.192  20.298  1.00  0.00          O
ATOM    655  I       655     -51.473  14.093  20.902  1.00  0.00          O
ATOM    656  I       656     -55.473  20.995  21.506  1.00  0.00          O
ATOM    657  I       657     -59.473  27.897  22.109  1.00  0.00          O
ATOM    658  I       658     -17.473 -27.318  17.279  1.00  0.00          O
ATOM    659  I       659     -21.473 -20.416  17.883  1.00  0.00          O
ATOM    660  I       660     -25.473 -13.514  18.486  1.00  0.00          O
```

```
ATOM    661  I       661    -29.473  -6.612  19.090  1.00  0.00          O
ATOM    662  I       662    -33.473   0.290  19.694  1.00  0.00          O
ATOM    663  I       663    -37.473   7.192  20.298  1.00  0.00          O
ATOM    664  I       664    -41.473  14.093  20.902  1.00  0.00          O
ATOM    665  I       665    -45.473  20.995  21.506  1.00  0.00          O
ATOM    666  I       666    -49.473  27.897  22.109  1.00  0.00          O
ATOM    667  I       667     -7.473 -27.318  17.279  1.00  0.00          O
ATOM    668  I       668    -11.473 -20.416  17.883  1.00  0.00          O
ATOM    669  I       669    -15.473 -13.514  18.486  1.00  0.00          O
ATOM    670  I       670    -19.473  -6.612  19.090  1.00  0.00          O
ATOM    671  I       671    -23.473   0.290  19.694  1.00  0.00          O
ATOM    672  I       672    -27.473   7.192  20.298  1.00  0.00          O
ATOM    673  I       673    -31.473  14.093  20.902  1.00  0.00          O
ATOM    674  I       674    -35.473  20.995  21.506  1.00  0.00          O
ATOM    675  I       675    -39.473  27.897  22.109  1.00  0.00          O
ATOM    676  I       676      2.527 -27.318  17.279  1.00  0.00          O
ATOM    677  I       677     -1.473 -20.416  17.883  1.00  0.00          O
ATOM    678  I       678     -5.473 -13.514  18.486  1.00  0.00          O
ATOM    679  I       679     -9.473  -6.612  19.090  1.00  0.00          O
ATOM    680  I       680    -13.473   0.290  19.694  1.00  0.00          O
ATOM    681  I       681    -17.473   7.192  20.298  1.00  0.00          O
ATOM    682  I       682    -21.473  14.093  20.902  1.00  0.00          O
ATOM    683  I       683    -25.473  20.995  21.506  1.00  0.00          O
ATOM    684  I       684    -29.473  27.897  22.109  1.00  0.00          O
ATOM    685  I       685     12.527 -27.318  17.279  1.00  0.00          O
ATOM    686  I       686      8.527 -20.416  17.883  1.00  0.00          O
ATOM    687  I       687      4.527 -13.514  18.486  1.00  0.00          O
ATOM    688  I       688      0.527  -6.612  19.090  1.00  0.00          O
ATOM    689  I       689     -3.473   0.290  19.694  1.00  0.00          O
ATOM    690  I       690     -7.473   7.192  20.298  1.00  0.00          O
ATOM    691  I       691    -11.473  14.093  20.902  1.00  0.00          O
ATOM    692  I       692    -15.473  20.995  21.506  1.00  0.00          O
ATOM    693  I       693    -19.473  27.897  22.109  1.00  0.00          O
ATOM    694  I       694     22.527 -27.318  17.279  1.00  0.00          O
ATOM    695  I       695     18.527 -20.416  17.883  1.00  0.00          O
ATOM    696  I       696     14.527 -13.514  18.486  1.00  0.00          O
ATOM    697  I       697     10.527  -6.612  19.090  1.00  0.00          O
ATOM    698  I       698      6.527   0.290  19.694  1.00  0.00          O
ATOM    699  I       699      2.527   7.192  20.298  1.00  0.00          O
ATOM    700  I       700     -1.473  14.093  20.902  1.00  0.00          O
ATOM    701  I       701     -5.473  20.995  21.506  1.00  0.00          O
ATOM    702  I       702     -9.473  27.897  22.109  1.00  0.00          O
ATOM    703  I       703     32.527 -27.318  17.279  1.00  0.00          O
ATOM    704  I       704     28.527 -20.416  17.883  1.00  0.00          O
ATOM    705  I       705     24.527 -13.514  18.486  1.00  0.00          O
ATOM    706  I       706     20.527  -6.612  19.090  1.00  0.00          O
ATOM    707  I       707     16.527   0.290  19.694  1.00  0.00          O
ATOM    708  I       708     12.527   7.192  20.298  1.00  0.00          O
```

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ATOM    709  I       709       8.527  14.093  20.902  1.00  0.00          O
ATOM    710  I       710       4.527  20.995  21.506  1.00  0.00          O
ATOM    711  I       711       0.527  27.897  22.109  1.00  0.00          O
ATOM    712  I       712      42.527 -27.318  17.279  1.00  0.00          O
ATOM    713  I       713      38.527 -20.416  17.883  1.00  0.00          O
ATOM    714  I       714      34.527 -13.514  18.486  1.00  0.00          O
ATOM    715  I       715      30.527  -6.612  19.090  1.00  0.00          O
ATOM    716  I       716      26.527   0.290  19.694  1.00  0.00          O
ATOM    717  I       717      22.527   7.192  20.298  1.00  0.00          O
ATOM    718  I       718      18.527  14.093  20.902  1.00  0.00          O
ATOM    719  I       719      14.527  20.995  21.506  1.00  0.00          O
ATOM    720  I       720      10.527  27.897  22.109  1.00  0.00          O
ATOM    721  I       721      52.527 -27.318  17.279  1.00  0.00          O
ATOM    722  I       722      48.527 -20.416  17.883  1.00  0.00          O
ATOM    723  I       723      44.527 -13.514  18.486  1.00  0.00          O
ATOM    724  I       724      40.527  -6.612  19.090  1.00  0.00          O
ATOM    725  I       725      36.527   0.290  19.694  1.00  0.00          O
ATOM    726  I       726      32.527   7.192  20.298  1.00  0.00          O
ATOM    727  I       727      28.527  14.093  20.902  1.00  0.00          O
ATOM    728  I       728      24.527  20.995  21.506  1.00  0.00          O
ATOM    729  I       729      20.527  27.897  22.109  1.00  0.00          O
END
```

15.2.6 Archivo PDB Estructura Ortorrómbica

Archivo PDB generado correspondiente a la estructura Ortorrómbica de 4 celdas por lado, los parámetros de red con 10 Angstroms en a, 8 Angstroms en b y 5 Angstroms en c:

Campo1	Campo2	Campo3	Campo4	Campo5	Campo6	Campo7	Campo8	Campo9	Campo 10
Registro	serial	elemento	Numero de secuncia	Coordenadas otogonales para x	Coordenadas otogonales para y	Coordenadas otogonales para z	ocupancia	Factor de temperatura	Carga en el átomo

```
ATOM      1  I         1     -40.000 -30.135 -22.713  1.00  0.00          O
ATOM      2  I         2     -40.000 -22.166 -22.016  1.00  0.00          O
ATOM      3  I         3     -40.000 -14.196 -21.318  1.00  0.00          O
ATOM      4  I         4     -40.000  -6.226 -20.621  1.00  0.00          O
ATOM      5  I         5     -40.000   1.743 -19.924  1.00  0.00          O
ATOM      6  I         6     -40.000   9.713 -19.227  1.00  0.00          O
ATOM      7  I         7     -40.000  17.682 -18.529  1.00  0.00          O
ATOM      8  I         8     -40.000  25.652 -17.832  1.00  0.00          O
ATOM      9  I         9     -40.000  33.621 -17.135  1.00  0.00          O
ATOM     10  I        10     -30.000 -30.135 -22.713  1.00  0.00          O
ATOM     11  I        11     -30.000 -22.166 -22.016  1.00  0.00          O
ATOM     12  I        12     -30.000 -14.196 -21.318  1.00  0.00          O
ATOM     13  I        13     -30.000  -6.226 -20.621  1.00  0.00          O
ATOM     14  I        14     -30.000   1.743 -19.924  1.00  0.00          O
ATOM     15  I        15     -30.000   9.713 -19.227  1.00  0.00          O
ATOM     16  I        16     -30.000  17.682 -18.529  1.00  0.00          O
ATOM     17  I        17     -30.000  25.652 -17.832  1.00  0.00          O
ATOM     18  I        18     -30.000  33.621 -17.135  1.00  0.00          O
ATOM     19  I        19     -20.000 -30.135 -22.713  1.00  0.00          O
ATOM     20  I        20     -20.000 -22.166 -22.016  1.00  0.00          O
ATOM     21  I        21     -20.000 -14.196 -21.318  1.00  0.00          O
ATOM     22  I        22     -20.000  -6.226 -20.621  1.00  0.00          O
ATOM     23  I        23     -20.000   1.743 -19.924  1.00  0.00          O
ATOM     24  I        24     -20.000   9.713 -19.227  1.00  0.00          O
ATOM     25  I        25     -20.000  17.682 -18.529  1.00  0.00          O
ATOM     26  I        26     -20.000  25.652 -17.832  1.00  0.00          O
ATOM     27  I        27     -20.000  33.621 -17.135  1.00  0.00          O
ATOM     28  I        28     -10.000 -30.135 -22.713  1.00  0.00          O
ATOM     29  I        29     -10.000 -22.166 -22.016  1.00  0.00          O
ATOM     30  I        30     -10.000 -14.196 -21.318  1.00  0.00          O
ATOM     31  I        31     -10.000  -6.226 -20.621  1.00  0.00          O
ATOM     32  I        32     -10.000   1.743 -19.924  1.00  0.00          O
ATOM     33  I        33     -10.000   9.713 -19.227  1.00  0.00          O
ATOM     34  I        34     -10.000  17.682 -18.529  1.00  0.00          O
ATOM     35  I        35     -10.000  25.652 -17.832  1.00  0.00          O
ATOM     36  I        36     -10.000  33.621 -17.135  1.00  0.00          O
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ATOM     37  I         37     -0.000 -30.135 -22.713  1.00  0.00           O
ATOM     38  I         38     -0.000 -22.166 -22.016  1.00  0.00           O
ATOM     39  I         39     -0.000 -14.196 -21.318  1.00  0.00           O
ATOM     40  I         40     -0.000  -6.226 -20.621  1.00  0.00           O
ATOM     41  I         41     -0.000   1.743 -19.924  1.00  0.00           O
ATOM     42  I         42     -0.000   9.713 -19.227  1.00  0.00           O
ATOM     43  I         43     -0.000  17.682 -18.529  1.00  0.00           O
ATOM     44  I         44      0.000  25.652 -17.832  1.00  0.00           O
ATOM     45  I         45      0.000  33.621 -17.135  1.00  0.00           O
ATOM     46  I         46     10.000 -30.135 -22.713  1.00  0.00           O
ATOM     47  I         47     10.000 -22.166 -22.016  1.00  0.00           O
ATOM     48  I         48     10.000 -14.196 -21.318  1.00  0.00           O
ATOM     49  I         49     10.000  -6.226 -20.621  1.00  0.00           O
ATOM     50  I         50     10.000   1.743 -19.924  1.00  0.00           O
ATOM     51  I         51     10.000   9.713 -19.227  1.00  0.00           O
ATOM     52  I         52     10.000  17.682 -18.529  1.00  0.00           O
ATOM     53  I         53     10.000  25.652 -17.832  1.00  0.00           O
ATOM     54  I         54     10.000  33.621 -17.135  1.00  0.00           O
ATOM     55  I         55     20.000 -30.135 -22.713  1.00  0.00           O
ATOM     56  I         56     20.000 -22.166 -22.016  1.00  0.00           O
ATOM     57  I         57     20.000 -14.196 -21.318  1.00  0.00           O
ATOM     58  I         58     20.000  -6.226 -20.621  1.00  0.00           O
ATOM     59  I         59     20.000   1.743 -19.924  1.00  0.00           O
ATOM     60  I         60     20.000   9.713 -19.227  1.00  0.00           O
ATOM     61  I         61     20.000  17.682 -18.529  1.00  0.00           O
ATOM     62  I         62     20.000  25.652 -17.832  1.00  0.00           O
ATOM     63  I         63     20.000  33.621 -17.135  1.00  0.00           O
ATOM     64  I         64     30.000 -30.135 -22.713  1.00  0.00           O
ATOM     65  I         65     30.000 -22.166 -22.016  1.00  0.00           O
ATOM     66  I         66     30.000 -14.196 -21.318  1.00  0.00           O
ATOM     67  I         67     30.000  -6.226 -20.621  1.00  0.00           O
ATOM     68  I         68     30.000   1.743 -19.924  1.00  0.00           O
ATOM     69  I         69     30.000   9.713 -19.227  1.00  0.00           O
ATOM     70  I         70     30.000  17.682 -18.529  1.00  0.00           O
ATOM     71  I         71     30.000  25.652 -17.832  1.00  0.00           O
ATOM     72  I         72     30.000  33.621 -17.135  1.00  0.00           O
ATOM     73  I         73     40.000 -30.135 -22.713  1.00  0.00           O
ATOM     74  I         74     40.000 -22.166 -22.016  1.00  0.00           O
ATOM     75  I         75     40.000 -14.196 -21.318  1.00  0.00           O
ATOM     76  I         76     40.000  -6.226 -20.621  1.00  0.00           O
ATOM     77  I         77     40.000   1.743 -19.924  1.00  0.00           O
ATOM     78  I         78     40.000   9.713 -19.227  1.00  0.00           O
ATOM     79  I         79     40.000  17.682 -18.529  1.00  0.00           O
ATOM     80  I         80     40.000  25.652 -17.832  1.00  0.00           O
ATOM     81  I         81     40.000  33.621 -17.135  1.00  0.00           O
ATOM     82  I         82    -40.000 -30.571 -17.732  1.00  0.00           O
ATOM     83  I         83    -40.000 -22.601 -17.035  1.00  0.00           O
ATOM     84  I         84    -40.000 -14.632 -16.337  1.00  0.00           O
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ATOM     85  I        85    -40.000  -6.662 -15.640  1.00  0.00          O
ATOM     86  I        86    -40.000   1.307 -14.943  1.00  0.00          O
ATOM     87  I        87    -40.000   9.277 -14.246  1.00  0.00          O
ATOM     88  I        88    -40.000  17.246 -13.548  1.00  0.00          O
ATOM     89  I        89    -40.000  25.216 -12.851  1.00  0.00          O
ATOM     90  I        90    -40.000  33.186 -12.154  1.00  0.00          O
ATOM     91  I        91    -30.000 -30.571 -17.732  1.00  0.00          O
ATOM     92  I        92    -30.000 -22.601 -17.035  1.00  0.00          O
ATOM     93  I        93    -30.000 -14.632 -16.337  1.00  0.00          O
ATOM     94  I        94    -30.000  -6.662 -15.640  1.00  0.00          O
ATOM     95  I        95    -30.000   1.307 -14.943  1.00  0.00          O
ATOM     96  I        96    -30.000   9.277 -14.246  1.00  0.00          O
ATOM     97  I        97    -30.000  17.246 -13.548  1.00  0.00          O
ATOM     98  I        98    -30.000  25.216 -12.851  1.00  0.00          O
ATOM     99  I        99    -30.000  33.186 -12.154  1.00  0.00          O
ATOM    100  I       100    -20.000 -30.571 -17.732  1.00  0.00          O
ATOM    101  I       101    -20.000 -22.601 -17.035  1.00  0.00          O
ATOM    102  I       102    -20.000 -14.632 -16.337  1.00  0.00          O
ATOM    103  I       103    -20.000  -6.662 -15.640  1.00  0.00          O
ATOM    104  I       104    -20.000   1.307 -14.943  1.00  0.00          O
ATOM    105  I       105    -20.000   9.277 -14.246  1.00  0.00          O
ATOM    106  I       106    -20.000  17.246 -13.548  1.00  0.00          O
ATOM    107  I       107    -20.000  25.216 -12.851  1.00  0.00          O
ATOM    108  I       108    -20.000  33.186 -12.154  1.00  0.00          O
ATOM    109  I       109    -10.000 -30.571 -17.732  1.00  0.00          O
ATOM    110  I       110    -10.000 -22.601 -17.035  1.00  0.00          O
ATOM    111  I       111    -10.000 -14.632 -16.337  1.00  0.00          O
ATOM    112  I       112    -10.000  -6.662 -15.640  1.00  0.00          O
ATOM    113  I       113    -10.000   1.307 -14.943  1.00  0.00          O
ATOM    114  I       114    -10.000   9.277 -14.246  1.00  0.00          O
ATOM    115  I       115    -10.000  17.246 -13.548  1.00  0.00          O
ATOM    116  I       116    -10.000  25.216 -12.851  1.00  0.00          O
ATOM    117  I       117    -10.000  33.186 -12.154  1.00  0.00          O
ATOM    118  I       118     -0.000 -30.571 -17.732  1.00  0.00          O
ATOM    119  I       119     -0.000 -22.601 -17.035  1.00  0.00          O
ATOM    120  I       120     -0.000 -14.632 -16.337  1.00  0.00          O
ATOM    121  I       121     -0.000  -6.662 -15.640  1.00  0.00          O
ATOM    122  I       122     -0.000   1.307 -14.943  1.00  0.00          O
ATOM    123  I       123     -0.000   9.277 -14.246  1.00  0.00          O
ATOM    124  I       124      0.000  17.246 -13.548  1.00  0.00          O
ATOM    125  I       125      0.000  25.216 -12.851  1.00  0.00          O
ATOM    126  I       126      0.000  33.186 -12.154  1.00  0.00          O
ATOM    127  I       127     10.000 -30.571 -17.732  1.00  0.00          O
ATOM    128  I       128     10.000 -22.601 -17.035  1.00  0.00          O
ATOM    129  I       129     10.000 -14.632 -16.337  1.00  0.00          O
ATOM    130  I       130     10.000  -6.662 -15.640  1.00  0.00          O
ATOM    131  I       131     10.000   1.307 -14.943  1.00  0.00          O
ATOM    132  I       132     10.000   9.277 -14.246  1.00  0.00          O
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ATOM    133  I       133      10.000  17.246 -13.548  1.00  0.00          O
ATOM    134  I       134      10.000  25.216 -12.851  1.00  0.00          O
ATOM    135  I       135      10.000  33.186 -12.154  1.00  0.00          O
ATOM    136  I       136      20.000 -30.571 -17.732  1.00  0.00          O
ATOM    137  I       137      20.000 -22.601 -17.035  1.00  0.00          O
ATOM    138  I       138      20.000 -14.632 -16.337  1.00  0.00          O
ATOM    139  I       139      20.000  -6.662 -15.640  1.00  0.00          O
ATOM    140  I       140      20.000   1.307 -14.943  1.00  0.00          O
ATOM    141  I       141      20.000   9.277 -14.246  1.00  0.00          O
ATOM    142  I       142      20.000  17.246 -13.548  1.00  0.00          O
ATOM    143  I       143      20.000  25.216 -12.851  1.00  0.00          O
ATOM    144  I       144      20.000  33.186 -12.154  1.00  0.00          O
ATOM    145  I       145      30.000 -30.571 -17.732  1.00  0.00          O
ATOM    146  I       146      30.000 -22.601 -17.035  1.00  0.00          O
ATOM    147  I       147      30.000 -14.632 -16.337  1.00  0.00          O
ATOM    148  I       148      30.000  -6.662 -15.640  1.00  0.00          O
ATOM    149  I       149      30.000   1.307 -14.943  1.00  0.00          O
ATOM    150  I       150      30.000   9.277 -14.246  1.00  0.00          O
ATOM    151  I       151      30.000  17.246 -13.548  1.00  0.00          O
ATOM    152  I       152      30.000  25.216 -12.851  1.00  0.00          O
ATOM    153  I       153      30.000  33.186 -12.154  1.00  0.00          O
ATOM    154  I       154      40.000 -30.571 -17.732  1.00  0.00          O
ATOM    155  I       155      40.000 -22.601 -17.035  1.00  0.00          O
ATOM    156  I       156      40.000 -14.632 -16.337  1.00  0.00          O
ATOM    157  I       157      40.000  -6.662 -15.640  1.00  0.00          O
ATOM    158  I       158      40.000   1.307 -14.943  1.00  0.00          O
ATOM    159  I       159      40.000   9.277 -14.246  1.00  0.00          O
ATOM    160  I       160      40.000  17.246 -13.548  1.00  0.00          O
ATOM    161  I       161      40.000  25.216 -12.851  1.00  0.00          O
ATOM    162  I       162      40.000  33.186 -12.154  1.00  0.00          O
ATOM    163  I       163     -40.000 -31.007 -12.751  1.00  0.00          O
ATOM    164  I       164     -40.000 -23.037 -12.054  1.00  0.00          O
ATOM    165  I       165     -40.000 -15.068 -11.356  1.00  0.00          O
ATOM    166  I       166     -40.000  -7.098 -10.659  1.00  0.00          O
ATOM    167  I       167     -40.000   0.872  -9.962  1.00  0.00          O
ATOM    168  I       168     -40.000   8.841  -9.265  1.00  0.00          O
ATOM    169  I       169     -40.000  16.811  -8.567  1.00  0.00          O
ATOM    170  I       170     -40.000  24.780  -7.870  1.00  0.00          O
ATOM    171  I       171     -40.000  32.750  -7.173  1.00  0.00          O
ATOM    172  I       172     -30.000 -31.007 -12.751  1.00  0.00          O
ATOM    173  I       173     -30.000 -23.037 -12.054  1.00  0.00          O
ATOM    174  I       174     -30.000 -15.068 -11.356  1.00  0.00          O
ATOM    175  I       175     -30.000  -7.098 -10.659  1.00  0.00          O
ATOM    176  I       176     -30.000   0.872  -9.962  1.00  0.00          O
ATOM    177  I       177     -30.000   8.841  -9.265  1.00  0.00          O
ATOM    178  I       178     -30.000  16.811  -8.567  1.00  0.00          O
ATOM    179  I       179     -30.000  24.780  -7.870  1.00  0.00          O
ATOM    180  I       180     -30.000  32.750  -7.173  1.00  0.00          O
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ATOM    181  I       181     -20.000 -31.007 -12.751  1.00  0.00          O
ATOM    182  I       182     -20.000 -23.037 -12.054  1.00  0.00          O
ATOM    183  I       183     -20.000 -15.068 -11.356  1.00  0.00          O
ATOM    184  I       184     -20.000  -7.098 -10.659  1.00  0.00          O
ATOM    185  I       185     -20.000   0.872  -9.962  1.00  0.00          O
ATOM    186  I       186     -20.000   8.841  -9.265  1.00  0.00          O
ATOM    187  I       187     -20.000  16.811  -8.567  1.00  0.00          O
ATOM    188  I       188     -20.000  24.780  -7.870  1.00  0.00          O
ATOM    189  I       189     -20.000  32.750  -7.173  1.00  0.00          O
ATOM    190  I       190     -10.000 -31.007 -12.751  1.00  0.00          O
ATOM    191  I       191     -10.000 -23.037 -12.054  1.00  0.00          O
ATOM    192  I       192     -10.000 -15.068 -11.356  1.00  0.00          O
ATOM    193  I       193     -10.000  -7.098 -10.659  1.00  0.00          O
ATOM    194  I       194     -10.000   0.872  -9.962  1.00  0.00          O
ATOM    195  I       195     -10.000   8.841  -9.265  1.00  0.00          O
ATOM    196  I       196     -10.000  16.811  -8.567  1.00  0.00          O
ATOM    197  I       197     -10.000  24.780  -7.870  1.00  0.00          O
ATOM    198  I       198     -10.000  32.750  -7.173  1.00  0.00          O
ATOM    199  I       199      -0.000 -31.007 -12.751  1.00  0.00          O
ATOM    200  I       200      -0.000 -23.037 -12.054  1.00  0.00          O
ATOM    201  I       201      -0.000 -15.068 -11.356  1.00  0.00          O
ATOM    202  I       202      -0.000  -7.098 -10.659  1.00  0.00          O
ATOM    203  I       203      -0.000   0.872  -9.962  1.00  0.00          O
ATOM    204  I       204      -0.000   8.841  -9.265  1.00  0.00          O
ATOM    205  I       205       0.000  16.811  -8.567  1.00  0.00          O
ATOM    206  I       206       0.000  24.780  -7.870  1.00  0.00          O
ATOM    207  I       207       0.000  32.750  -7.173  1.00  0.00          O
ATOM    208  I       208      10.000 -31.007 -12.751  1.00  0.00          O
ATOM    209  I       209      10.000 -23.037 -12.054  1.00  0.00          O
ATOM    210  I       210      10.000 -15.068 -11.356  1.00  0.00          O
ATOM    211  I       211      10.000  -7.098 -10.659  1.00  0.00          O
ATOM    212  I       212      10.000   0.872  -9.962  1.00  0.00          O
ATOM    213  I       213      10.000   8.841  -9.265  1.00  0.00          O
ATOM    214  I       214      10.000  16.811  -8.567  1.00  0.00          O
ATOM    215  I       215      10.000  24.780  -7.870  1.00  0.00          O
ATOM    216  I       216      10.000  32.750  -7.173  1.00  0.00          O
ATOM    217  I       217      20.000 -31.007 -12.751  1.00  0.00          O
ATOM    218  I       218      20.000 -23.037 -12.054  1.00  0.00          O
ATOM    219  I       219      20.000 -15.068 -11.356  1.00  0.00          O
ATOM    220  I       220      20.000  -7.098 -10.659  1.00  0.00          O
ATOM    221  I       221      20.000   0.872  -9.962  1.00  0.00          O
ATOM    222  I       222      20.000   8.841  -9.265  1.00  0.00          O
ATOM    223  I       223      20.000  16.811  -8.567  1.00  0.00          O
ATOM    224  I       224      20.000  24.780  -7.870  1.00  0.00          O
ATOM    225  I       225      20.000  32.750  -7.173  1.00  0.00          O
ATOM    226  I       226      30.000 -31.007 -12.751  1.00  0.00          O
ATOM    227  I       227      30.000 -23.037 -12.054  1.00  0.00          O
ATOM    228  I       228      30.000 -15.068 -11.356  1.00  0.00          O
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ATOM 229 I 229 30.000 -7.098 -10.659 1.00 0.00 O
ATOM 230 I 230 30.000 0.872 -9.962 1.00 0.00 O
ATOM 231 I 231 30.000 8.841 -9.265 1.00 0.00 O
ATOM 232 I 232 30.000 16.811 -8.567 1.00 0.00 O
ATOM 233 I 233 30.000 24.780 -7.870 1.00 0.00 O
ATOM 234 I 234 30.000 32.750 -7.173 1.00 0.00 O
ATOM 235 I 235 40.000 -31.007 -12.751 1.00 0.00 O
ATOM 236 I 236 40.000 -23.037 -12.054 1.00 0.00 O
ATOM 237 I 237 40.000 -15.068 -11.356 1.00 0.00 O
ATOM 238 I 238 40.000 -7.098 -10.659 1.00 0.00 O
ATOM 239 I 239 40.000 0.872 -9.962 1.00 0.00 O
ATOM 240 I 240 40.000 8.841 -9.265 1.00 0.00 O
ATOM 241 I 241 40.000 16.811 -8.567 1.00 0.00 O
ATOM 242 I 242 40.000 24.780 -7.870 1.00 0.00 O
ATOM 243 I 243 40.000 32.750 -7.173 1.00 0.00 O
ATOM 244 I 244 -40.000 -31.442 -7.770 1.00 0.00 O
ATOM 245 I 245 -40.000 -23.473 -7.073 1.00 0.00 O
ATOM 246 I 246 -40.000 -15.503 -6.375 1.00 0.00 O
ATOM 247 I 247 -40.000 -7.534 -5.678 1.00 0.00 O
ATOM 248 I 248 -40.000 0.436 -4.981 1.00 0.00 O
ATOM 249 I 249 -40.000 8.405 -4.284 1.00 0.00 O
ATOM 250 I 250 -40.000 16.375 -3.586 1.00 0.00 O
ATOM 251 I 251 -40.000 24.344 -2.889 1.00 0.00 O
ATOM 252 I 252 -40.000 32.314 -2.192 1.00 0.00 O
ATOM 253 I 253 -30.000 -31.442 -7.770 1.00 0.00 O
ATOM 254 I 254 -30.000 -23.473 -7.073 1.00 0.00 O
ATOM 255 I 255 -30.000 -15.503 -6.375 1.00 0.00 O
ATOM 256 I 256 -30.000 -7.534 -5.678 1.00 0.00 O
ATOM 257 I 257 -30.000 0.436 -4.981 1.00 0.00 O
ATOM 258 I 258 -30.000 8.405 -4.284 1.00 0.00 O
ATOM 259 I 259 -30.000 16.375 -3.586 1.00 0.00 O
ATOM 260 I 260 -30.000 24.344 -2.889 1.00 0.00 O
ATOM 261 I 261 -30.000 32.314 -2.192 1.00 0.00 O
ATOM 262 I 262 -20.000 -31.442 -7.770 1.00 0.00 O
ATOM 263 I 263 -20.000 -23.473 -7.073 1.00 0.00 O
ATOM 264 I 264 -20.000 -15.503 -6.375 1.00 0.00 O
ATOM 265 I 265 -20.000 -7.534 -5.678 1.00 0.00 O
ATOM 266 I 266 -20.000 0.436 -4.981 1.00 0.00 O
ATOM 267 I 267 -20.000 8.405 -4.284 1.00 0.00 O
ATOM 268 I 268 -20.000 16.375 -3.586 1.00 0.00 O
ATOM 269 I 269 -20.000 24.344 -2.889 1.00 0.00 O
ATOM 270 I 270 -20.000 32.314 -2.192 1.00 0.00 O
ATOM 271 I 271 -10.000 -31.442 -7.770 1.00 0.00 O
ATOM 272 I 272 -10.000 -23.473 -7.073 1.00 0.00 O
ATOM 273 I 273 -10.000 -15.503 -6.375 1.00 0.00 O
ATOM 274 I 274 -10.000 -7.534 -5.678 1.00 0.00 O
ATOM 275 I 275 -10.000 0.436 -4.981 1.00 0.00 O
ATOM 276 I 276 -10.000 8.405 -4.284 1.00 0.00 O

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ATOM    277  I       277    -10.000  16.375  -3.586  1.00  0.00          O
ATOM    278  I       278    -10.000  24.344  -2.889  1.00  0.00          O
ATOM    279  I       279    -10.000  32.314  -2.192  1.00  0.00          O
ATOM    280  I       280     -0.000 -31.442  -7.770  1.00  0.00          O
ATOM    281  I       281     -0.000 -23.473  -7.073  1.00  0.00          O
ATOM    282  I       282     -0.000 -15.503  -6.375  1.00  0.00          O
ATOM    283  I       283     -0.000  -7.534  -5.678  1.00  0.00          O
ATOM    284  I       284     -0.000   0.436  -4.981  1.00  0.00          O
ATOM    285  I       285      0.000   8.405  -4.284  1.00  0.00          O
ATOM    286  I       286      0.000  16.375  -3.586  1.00  0.00          O
ATOM    287  I       287      0.000  24.344  -2.889  1.00  0.00          O
ATOM    288  I       288      0.000  32.314  -2.192  1.00  0.00          O
ATOM    289  I       289     10.000 -31.442  -7.770  1.00  0.00          O
ATOM    290  I       290     10.000 -23.473  -7.073  1.00  0.00          O
ATOM    291  I       291     10.000 -15.503  -6.375  1.00  0.00          O
ATOM    292  I       292     10.000  -7.534  -5.678  1.00  0.00          O
ATOM    293  I       293     10.000   0.436  -4.981  1.00  0.00          O
ATOM    294  I       294     10.000   8.405  -4.284  1.00  0.00          O
ATOM    295  I       295     10.000  16.375  -3.586  1.00  0.00          O
ATOM    296  I       296     10.000  24.344  -2.889  1.00  0.00          O
ATOM    297  I       297     10.000  32.314  -2.192  1.00  0.00          O
ATOM    298  I       298     20.000 -31.442  -7.770  1.00  0.00          O
ATOM    299  I       299     20.000 -23.473  -7.073  1.00  0.00          O
ATOM    300  I       300     20.000 -15.503  -6.375  1.00  0.00          O
ATOM    301  I       301     20.000  -7.534  -5.678  1.00  0.00          O
ATOM    302  I       302     20.000   0.436  -4.981  1.00  0.00          O
ATOM    303  I       303     20.000   8.405  -4.284  1.00  0.00          O
ATOM    304  I       304     20.000  16.375  -3.586  1.00  0.00          O
ATOM    305  I       305     20.000  24.344  -2.889  1.00  0.00          O
ATOM    306  I       306     20.000  32.314  -2.192  1.00  0.00          O
ATOM    307  I       307     30.000 -31.442  -7.770  1.00  0.00          O
ATOM    308  I       308     30.000 -23.473  -7.073  1.00  0.00          O
ATOM    309  I       309     30.000 -15.503  -6.375  1.00  0.00          O
ATOM    310  I       310     30.000  -7.534  -5.678  1.00  0.00          O
ATOM    311  I       311     30.000   0.436  -4.981  1.00  0.00          O
ATOM    312  I       312     30.000   8.405  -4.284  1.00  0.00          O
ATOM    313  I       313     30.000  16.375  -3.586  1.00  0.00          O
ATOM    314  I       314     30.000  24.344  -2.889  1.00  0.00          O
ATOM    315  I       315     30.000  32.314  -2.192  1.00  0.00          O
ATOM    316  I       316     40.000 -31.442  -7.770  1.00  0.00          O
ATOM    317  I       317     40.000 -23.473  -7.073  1.00  0.00          O
ATOM    318  I       318     40.000 -15.503  -6.375  1.00  0.00          O
ATOM    319  I       319     40.000  -7.534  -5.678  1.00  0.00          O
ATOM    320  I       320     40.000   0.436  -4.981  1.00  0.00          O
ATOM    321  I       321     40.000   8.405  -4.284  1.00  0.00          O
ATOM    322  I       322     40.000  16.375  -3.586  1.00  0.00          O
ATOM    323  I       323     40.000  24.344  -2.889  1.00  0.00          O
ATOM    324  I       324     40.000  32.314  -2.192  1.00  0.00          O
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ATOM    325  I       325     -40.000 -31.878  -2.789  1.00  0.00          O
ATOM    326  I       326     -40.000 -23.909  -2.092  1.00  0.00          O
ATOM    327  I       327     -40.000 -15.939  -1.394  1.00  0.00          O
ATOM    328  I       328     -40.000  -7.970  -0.697  1.00  0.00          O
ATOM    329  I       329     -40.000   0.000   0.000  1.00  0.00          O
ATOM    330  I       330     -40.000   7.970   0.697  1.00  0.00          O
ATOM    331  I       331     -40.000  15.939   1.394  1.00  0.00          O
ATOM    332  I       332     -40.000  23.909   2.092  1.00  0.00          O
ATOM    333  I       333     -40.000  31.878   2.789  1.00  0.00          O
ATOM    334  I       334     -30.000 -31.878  -2.789  1.00  0.00          O
ATOM    335  I       335     -30.000 -23.909  -2.092  1.00  0.00          O
ATOM    336  I       336     -30.000 -15.939  -1.394  1.00  0.00          O
ATOM    337  I       337     -30.000  -7.970  -0.697  1.00  0.00          O
ATOM    338  I       338     -30.000   0.000   0.000  1.00  0.00          O
ATOM    339  I       339     -30.000   7.970   0.697  1.00  0.00          O
ATOM    340  I       340     -30.000  15.939   1.394  1.00  0.00          O
ATOM    341  I       341     -30.000  23.909   2.092  1.00  0.00          O
ATOM    342  I       342     -30.000  31.878   2.789  1.00  0.00          O
ATOM    343  I       343     -20.000 -31.878  -2.789  1.00  0.00          O
ATOM    344  I       344     -20.000 -23.909  -2.092  1.00  0.00          O
ATOM    345  I       345     -20.000 -15.939  -1.394  1.00  0.00          O
ATOM    346  I       346     -20.000  -7.970  -0.697  1.00  0.00          O
ATOM    347  I       347     -20.000   0.000   0.000  1.00  0.00          O
ATOM    348  I       348     -20.000   7.970   0.697  1.00  0.00          O
ATOM    349  I       349     -20.000  15.939   1.394  1.00  0.00          O
ATOM    350  I       350     -20.000  23.909   2.092  1.00  0.00          O
ATOM    351  I       351     -20.000  31.878   2.789  1.00  0.00          O
ATOM    352  I       352     -10.000 -31.878  -2.789  1.00  0.00          O
ATOM    353  I       353     -10.000 -23.909  -2.092  1.00  0.00          O
ATOM    354  I       354     -10.000 -15.939  -1.394  1.00  0.00          O
ATOM    355  I       355     -10.000  -7.970  -0.697  1.00  0.00          O
ATOM    356  I       356     -10.000   0.000   0.000  1.00  0.00          O
ATOM    357  I       357     -10.000   7.970   0.697  1.00  0.00          O
ATOM    358  I       358     -10.000  15.939   1.394  1.00  0.00          O
ATOM    359  I       359     -10.000  23.909   2.092  1.00  0.00          O
ATOM    360  I       360     -10.000  31.878   2.789  1.00  0.00          O
ATOM    361  I       361      -0.000 -31.878  -2.789  1.00  0.00          O
ATOM    362  I       362      -0.000 -23.909  -2.092  1.00  0.00          O
ATOM    363  I       363      -0.000 -15.939  -1.394  1.00  0.00          O
ATOM    364  I       364      -0.000  -7.970  -0.697  1.00  0.00          O
ATOM    365  I       365       0.000   0.000   0.000  1.00  0.00          O
ATOM    366  I       366       0.000   7.970   0.697  1.00  0.00          O
ATOM    367  I       367       0.000  15.939   1.394  1.00  0.00          O
ATOM    368  I       368       0.000  23.909   2.092  1.00  0.00          O
ATOM    369  I       369       0.000  31.878   2.789  1.00  0.00          O
ATOM    370  I       370      10.000 -31.878  -2.789  1.00  0.00          O
ATOM    371  I       371      10.000 -23.909  -2.092  1.00  0.00          O
ATOM    372  I       372      10.000 -15.939  -1.394  1.00  0.00          O
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ATOM 373 I 373 10.000 -7.970 -0.697 1.00 0.00 O
ATOM 374 I 374 10.000 0.000 0.000 1.00 0.00 O
ATOM 375 I 375 10.000 7.970 0.697 1.00 0.00 O
ATOM 376 I 376 10.000 15.939 1.394 1.00 0.00 O
ATOM 377 I 377 10.000 23.909 2.092 1.00 0.00 O
ATOM 378 I 378 10.000 31.878 2.789 1.00 0.00 O
ATOM 379 I 379 20.000 -31.878 -2.789 1.00 0.00 O
ATOM 380 I 380 20.000 -23.909 -2.092 1.00 0.00 O
ATOM 381 I 381 20.000 -15.939 -1.394 1.00 0.00 O
ATOM 382 I 382 20.000 -7.970 -0.697 1.00 0.00 O
ATOM 383 I 383 20.000 0.000 0.000 1.00 0.00 O
ATOM 384 I 384 20.000 7.970 0.697 1.00 0.00 O
ATOM 385 I 385 20.000 15.939 1.394 1.00 0.00 O
ATOM 386 I 386 20.000 23.909 2.092 1.00 0.00 O
ATOM 387 I 387 20.000 31.878 2.789 1.00 0.00 O
ATOM 388 I 388 30.000 -31.878 -2.789 1.00 0.00 O
ATOM 389 I 389 30.000 -23.909 -2.092 1.00 0.00 O
ATOM 390 I 390 30.000 -15.939 -1.394 1.00 0.00 O
ATOM 391 I 391 30.000 -7.970 -0.697 1.00 0.00 O
ATOM 392 I 392 30.000 0.000 0.000 1.00 0.00 O
ATOM 393 I 393 30.000 7.970 0.697 1.00 0.00 O
ATOM 394 I 394 30.000 15.939 1.394 1.00 0.00 O
ATOM 395 I 395 30.000 23.909 2.092 1.00 0.00 O
ATOM 396 I 396 30.000 31.878 2.789 1.00 0.00 O
ATOM 397 I 397 40.000 -31.878 -2.789 1.00 0.00 O
ATOM 398 I 398 40.000 -23.909 -2.092 1.00 0.00 O
ATOM 399 I 399 40.000 -15.939 -1.394 1.00 0.00 O
ATOM 400 I 400 40.000 -7.970 -0.697 1.00 0.00 O
ATOM 401 I 401 40.000 0.000 0.000 1.00 0.00 O
ATOM 402 I 402 40.000 7.970 0.697 1.00 0.00 O
ATOM 403 I 403 40.000 15.939 1.394 1.00 0.00 O
ATOM 404 I 404 40.000 23.909 2.092 1.00 0.00 O
ATOM 405 I 405 40.000 31.878 2.789 1.00 0.00 O
ATOM 406 I 406 -40.000 -32.314 2.192 1.00 0.00 O
ATOM 407 I 407 -40.000 -24.344 2.889 1.00 0.00 O
ATOM 408 I 408 -40.000 -16.375 3.586 1.00 0.00 O
ATOM 409 I 409 -40.000 -8.405 4.284 1.00 0.00 O
ATOM 410 I 410 -40.000 -0.436 4.981 1.00 0.00 O
ATOM 411 I 411 -40.000 7.534 5.678 1.00 0.00 O
ATOM 412 I 412 -40.000 15.503 6.375 1.00 0.00 O
ATOM 413 I 413 -40.000 23.473 7.073 1.00 0.00 O
ATOM 414 I 414 -40.000 31.442 7.770 1.00 0.00 O
ATOM 415 I 415 -30.000 -32.314 2.192 1.00 0.00 O
ATOM 416 I 416 -30.000 -24.344 2.889 1.00 0.00 O
ATOM 417 I 417 -30.000 -16.375 3.586 1.00 0.00 O
ATOM 418 I 418 -30.000 -8.405 4.284 1.00 0.00 O
ATOM 419 I 419 -30.000 -0.436 4.981 1.00 0.00 O
ATOM 420 I 420 -30.000 7.534 5.678 1.00 0.00 O

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ATOM    421  I       421     -30.000  15.503   6.375  1.00  0.00          O
ATOM    422  I       422     -30.000  23.473   7.073  1.00  0.00          O
ATOM    423  I       423     -30.000  31.442   7.770  1.00  0.00          O
ATOM    424  I       424     -20.000 -32.314   2.192  1.00  0.00          O
ATOM    425  I       425     -20.000 -24.344   2.889  1.00  0.00          O
ATOM    426  I       426     -20.000 -16.375   3.586  1.00  0.00          O
ATOM    427  I       427     -20.000  -8.405   4.284  1.00  0.00          O
ATOM    428  I       428     -20.000  -0.436   4.981  1.00  0.00          O
ATOM    429  I       429     -20.000   7.534   5.678  1.00  0.00          O
ATOM    430  I       430     -20.000  15.503   6.375  1.00  0.00          O
ATOM    431  I       431     -20.000  23.473   7.073  1.00  0.00          O
ATOM    432  I       432     -20.000  31.442   7.770  1.00  0.00          O
ATOM    433  I       433     -10.000 -32.314   2.192  1.00  0.00          O
ATOM    434  I       434     -10.000 -24.344   2.889  1.00  0.00          O
ATOM    435  I       435     -10.000 -16.375   3.586  1.00  0.00          O
ATOM    436  I       436     -10.000  -8.405   4.284  1.00  0.00          O
ATOM    437  I       437     -10.000  -0.436   4.981  1.00  0.00          O
ATOM    438  I       438     -10.000   7.534   5.678  1.00  0.00          O
ATOM    439  I       439     -10.000  15.503   6.375  1.00  0.00          O
ATOM    440  I       440     -10.000  23.473   7.073  1.00  0.00          O
ATOM    441  I       441     -10.000  31.442   7.770  1.00  0.00          O
ATOM    442  I       442      -0.000 -32.314   2.192  1.00  0.00          O
ATOM    443  I       443      -0.000 -24.344   2.889  1.00  0.00          O
ATOM    444  I       444      -0.000 -16.375   3.586  1.00  0.00          O
ATOM    445  I       445      -0.000  -8.405   4.284  1.00  0.00          O
ATOM    446  I       446       0.000  -0.436   4.981  1.00  0.00          O
ATOM    447  I       447       0.000   7.534   5.678  1.00  0.00          O
ATOM    448  I       448       0.000  15.503   6.375  1.00  0.00          O
ATOM    449  I       449       0.000  23.473   7.073  1.00  0.00          O
ATOM    450  I       450       0.000  31.442   7.770  1.00  0.00          O
ATOM    451  I       451      10.000 -32.314   2.192  1.00  0.00          O
ATOM    452  I       452      10.000 -24.344   2.889  1.00  0.00          O
ATOM    453  I       453      10.000 -16.375   3.586  1.00  0.00          O
ATOM    454  I       454      10.000  -8.405   4.284  1.00  0.00          O
ATOM    455  I       455      10.000  -0.436   4.981  1.00  0.00          O
ATOM    456  I       456      10.000   7.534   5.678  1.00  0.00          O
ATOM    457  I       457      10.000  15.503   6.375  1.00  0.00          O
ATOM    458  I       458      10.000  23.473   7.073  1.00  0.00          O
ATOM    459  I       459      10.000  31.442   7.770  1.00  0.00          O
ATOM    460  I       460      20.000 -32.314   2.192  1.00  0.00          O
ATOM    461  I       461      20.000 -24.344   2.889  1.00  0.00          O
ATOM    462  I       462      20.000 -16.375   3.586  1.00  0.00          O
ATOM    463  I       463      20.000  -8.405   4.284  1.00  0.00          O
ATOM    464  I       464      20.000  -0.436   4.981  1.00  0.00          O
ATOM    465  I       465      20.000   7.534   5.678  1.00  0.00          O
ATOM    466  I       466      20.000  15.503   6.375  1.00  0.00          O
ATOM    467  I       467      20.000  23.473   7.073  1.00  0.00          O
ATOM    468  I       468      20.000  31.442   7.770  1.00  0.00          O
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ATOM 469 I 469 30.000 -32.314 2.192 1.00 0.00 O
ATOM 470 I 470 30.000 -24.344 2.889 1.00 0.00 O
ATOM 471 I 471 30.000 -16.375 3.586 1.00 0.00 O
ATOM 472 I 472 30.000 -8.405 4.284 1.00 0.00 O
ATOM 473 I 473 30.000 -0.436 4.981 1.00 0.00 O
ATOM 474 I 474 30.000 7.534 5.678 1.00 0.00 O
ATOM 475 I 475 30.000 15.503 6.375 1.00 0.00 O
ATOM 476 I 476 30.000 23.473 7.073 1.00 0.00 O
ATOM 477 I 477 30.000 31.442 7.770 1.00 0.00 O
ATOM 478 I 478 40.000 -32.314 2.192 1.00 0.00 O
ATOM 479 I 479 40.000 -24.344 2.889 1.00 0.00 O
ATOM 480 I 480 40.000 -16.375 3.586 1.00 0.00 O
ATOM 481 I 481 40.000 -8.405 4.284 1.00 0.00 O
ATOM 482 I 482 40.000 -0.436 4.981 1.00 0.00 O
ATOM 483 I 483 40.000 7.534 5.678 1.00 0.00 O
ATOM 484 I 484 40.000 15.503 6.375 1.00 0.00 O
ATOM 485 I 485 40.000 23.473 7.073 1.00 0.00 O
ATOM 486 I 486 40.000 31.442 7.770 1.00 0.00 O
ATOM 487 I 487 -40.000 -32.750 7.173 1.00 0.00 O
ATOM 488 I 488 -40.000 -24.780 7.870 1.00 0.00 O
ATOM 489 I 489 -40.000 -16.811 8.567 1.00 0.00 O
ATOM 490 I 490 -40.000 -8.841 9.265 1.00 0.00 O
ATOM 491 I 491 -40.000 -0.872 9.962 1.00 0.00 O
ATOM 492 I 492 -40.000 7.098 10.659 1.00 0.00 O
ATOM 493 I 493 -40.000 15.068 11.356 1.00 0.00 O
ATOM 494 I 494 -40.000 23.037 12.054 1.00 0.00 O
ATOM 495 I 495 -40.000 31.007 12.751 1.00 0.00 O
ATOM 496 I 496 -30.000 -32.750 7.173 1.00 0.00 O
ATOM 497 I 497 -30.000 -24.780 7.870 1.00 0.00 O
ATOM 498 I 498 -30.000 -16.811 8.567 1.00 0.00 O
ATOM 499 I 499 -30.000 -8.841 9.265 1.00 0.00 O
ATOM 500 I 500 -30.000 -0.872 9.962 1.00 0.00 O
ATOM 501 I 501 -30.000 7.098 10.659 1.00 0.00 O
ATOM 502 I 502 -30.000 15.068 11.356 1.00 0.00 O
ATOM 503 I 503 -30.000 23.037 12.054 1.00 0.00 O
ATOM 504 I 504 -30.000 31.007 12.751 1.00 0.00 O
ATOM 505 I 505 -20.000 -32.750 7.173 1.00 0.00 O
ATOM 506 I 506 -20.000 -24.780 7.870 1.00 0.00 O
ATOM 507 I 507 -20.000 -16.811 8.567 1.00 0.00 O
ATOM 508 I 508 -20.000 -8.841 9.265 1.00 0.00 O
ATOM 509 I 509 -20.000 -0.872 9.962 1.00 0.00 O
ATOM 510 I 510 -20.000 7.098 10.659 1.00 0.00 O
ATOM 511 I 511 -20.000 15.068 11.356 1.00 0.00 O
ATOM 512 I 512 -20.000 23.037 12.054 1.00 0.00 O
ATOM 513 I 513 -20.000 31.007 12.751 1.00 0.00 O
ATOM 514 I 514 -10.000 -32.750 7.173 1.00 0.00 O
ATOM 515 I 515 -10.000 -24.780 7.870 1.00 0.00 O
ATOM 516 I 516 -10.000 -16.811 8.567 1.00 0.00 O

ATOM 517 I 517 -10.000 -8.841 9.265 1.00 0.00 O
ATOM 518 I 518 -10.000 -0.872 9.962 1.00 0.00 O
ATOM 519 I 519 -10.000 7.098 10.659 1.00 0.00 O
ATOM 520 I 520 -10.000 15.068 11.356 1.00 0.00 O
ATOM 521 I 521 -10.000 23.037 12.054 1.00 0.00 O
ATOM 522 I 522 -10.000 31.007 12.751 1.00 0.00 O
ATOM 523 I 523 -0.000 -32.750 7.173 1.00 0.00 O
ATOM 524 I 524 -0.000 -24.780 7.870 1.00 0.00 O
ATOM 525 I 525 -0.000 -16.811 8.567 1.00 0.00 O
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ATOM 527 I 527 0.000 -0.872 9.962 1.00 0.00 O
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ATOM 530 I 530 0.000 23.037 12.054 1.00 0.00 O
ATOM 531 I 531 0.000 31.007 12.751 1.00 0.00 O
ATOM 532 I 532 10.000 -32.750 7.173 1.00 0.00 O
ATOM 533 I 533 10.000 -24.780 7.870 1.00 0.00 O
ATOM 534 I 534 10.000 -16.811 8.567 1.00 0.00 O
ATOM 535 I 535 10.000 -8.841 9.265 1.00 0.00 O
ATOM 536 I 536 10.000 -0.872 9.962 1.00 0.00 O
ATOM 537 I 537 10.000 7.098 10.659 1.00 0.00 O
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ATOM 539 I 539 10.000 23.037 12.054 1.00 0.00 O
ATOM 540 I 540 10.000 31.007 12.751 1.00 0.00 O
ATOM 541 I 541 20.000 -32.750 7.173 1.00 0.00 O
ATOM 542 I 542 20.000 -24.780 7.870 1.00 0.00 O
ATOM 543 I 543 20.000 -16.811 8.567 1.00 0.00 O
ATOM 544 I 544 20.000 -8.841 9.265 1.00 0.00 O
ATOM 545 I 545 20.000 -0.872 9.962 1.00 0.00 O
ATOM 546 I 546 20.000 7.098 10.659 1.00 0.00 O
ATOM 547 I 547 20.000 15.068 11.356 1.00 0.00 O
ATOM 548 I 548 20.000 23.037 12.054 1.00 0.00 O
ATOM 549 I 549 20.000 31.007 12.751 1.00 0.00 O
ATOM 550 I 550 30.000 -32.750 7.173 1.00 0.00 O
ATOM 551 I 551 30.000 -24.780 7.870 1.00 0.00 O
ATOM 552 I 552 30.000 -16.811 8.567 1.00 0.00 O
ATOM 553 I 553 30.000 -8.841 9.265 1.00 0.00 O
ATOM 554 I 554 30.000 -0.872 9.962 1.00 0.00 O
ATOM 555 I 555 30.000 7.098 10.659 1.00 0.00 O
ATOM 556 I 556 30.000 15.068 11.356 1.00 0.00 O
ATOM 557 I 557 30.000 23.037 12.054 1.00 0.00 O
ATOM 558 I 558 30.000 31.007 12.751 1.00 0.00 O
ATOM 559 I 559 40.000 -32.750 7.173 1.00 0.00 O
ATOM 560 I 560 40.000 -24.780 7.870 1.00 0.00 O
ATOM 561 I 561 40.000 -16.811 8.567 1.00 0.00 O
ATOM 562 I 562 40.000 -8.841 9.265 1.00 0.00 O
ATOM 563 I 563 40.000 -0.872 9.962 1.00 0.00 O
ATOM 564 I 564 40.000 7.098 10.659 1.00 0.00 O

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ATOM    565  I       565      40.000  15.068  11.356  1.00  0.00          O
ATOM    566  I       566      40.000  23.037  12.054  1.00  0.00          O
ATOM    567  I       567      40.000  31.007  12.751  1.00  0.00          O
ATOM    568  I       568     -40.000 -33.186  12.154  1.00  0.00          O
ATOM    569  I       569     -40.000 -25.216  12.851  1.00  0.00          O
ATOM    570  I       570     -40.000 -17.246  13.548  1.00  0.00          O
ATOM    571  I       571     -40.000  -9.277  14.246  1.00  0.00          O
ATOM    572  I       572     -40.000  -1.307  14.943  1.00  0.00          O
ATOM    573  I       573     -40.000   6.662  15.640  1.00  0.00          O
ATOM    574  I       574     -40.000  14.632  16.337  1.00  0.00          O
ATOM    575  I       575     -40.000  22.601  17.035  1.00  0.00          O
ATOM    576  I       576     -40.000  30.571  17.732  1.00  0.00          O
ATOM    577  I       577     -30.000 -33.186  12.154  1.00  0.00          O
ATOM    578  I       578     -30.000 -25.216  12.851  1.00  0.00          O
ATOM    579  I       579     -30.000 -17.246  13.548  1.00  0.00          O
ATOM    580  I       580     -30.000  -9.277  14.246  1.00  0.00          O
ATOM    581  I       581     -30.000  -1.307  14.943  1.00  0.00          O
ATOM    582  I       582     -30.000   6.662  15.640  1.00  0.00          O
ATOM    583  I       583     -30.000  14.632  16.337  1.00  0.00          O
ATOM    584  I       584     -30.000  22.601  17.035  1.00  0.00          O
ATOM    585  I       585     -30.000  30.571  17.732  1.00  0.00          O
ATOM    586  I       586     -20.000 -33.186  12.154  1.00  0.00          O
ATOM    587  I       587     -20.000 -25.216  12.851  1.00  0.00          O
ATOM    588  I       588     -20.000 -17.246  13.548  1.00  0.00          O
ATOM    589  I       589     -20.000  -9.277  14.246  1.00  0.00          O
ATOM    590  I       590     -20.000  -1.307  14.943  1.00  0.00          O
ATOM    591  I       591     -20.000   6.662  15.640  1.00  0.00          O
ATOM    592  I       592     -20.000  14.632  16.337  1.00  0.00          O
ATOM    593  I       593     -20.000  22.601  17.035  1.00  0.00          O
ATOM    594  I       594     -20.000  30.571  17.732  1.00  0.00          O
ATOM    595  I       595     -10.000 -33.186  12.154  1.00  0.00          O
ATOM    596  I       596     -10.000 -25.216  12.851  1.00  0.00          O
ATOM    597  I       597     -10.000 -17.246  13.548  1.00  0.00          O
ATOM    598  I       598     -10.000  -9.277  14.246  1.00  0.00          O
ATOM    599  I       599     -10.000  -1.307  14.943  1.00  0.00          O
ATOM    600  I       600     -10.000   6.662  15.640  1.00  0.00          O
ATOM    601  I       601     -10.000  14.632  16.337  1.00  0.00          O
ATOM    602  I       602     -10.000  22.601  17.035  1.00  0.00          O
ATOM    603  I       603     -10.000  30.571  17.732  1.00  0.00          O
ATOM    604  I       604      -0.000 -33.186  12.154  1.00  0.00          O
ATOM    605  I       605      -0.000 -25.216  12.851  1.00  0.00          O
ATOM    606  I       606      -0.000 -17.246  13.548  1.00  0.00          O
ATOM    607  I       607       0.000  -9.277  14.246  1.00  0.00          O
ATOM    608  I       608       0.000  -1.307  14.943  1.00  0.00          O
ATOM    609  I       609       0.000   6.662  15.640  1.00  0.00          O
ATOM    610  I       610       0.000  14.632  16.337  1.00  0.00          O
ATOM    611  I       611       0.000  22.601  17.035  1.00  0.00          O
ATOM    612  I       612       0.000  30.571  17.732  1.00  0.00          O
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ATOM 613 I 613 10.000 -33.186 12.154 1.00 0.00 O
ATOM 614 I 614 10.000 -25.216 12.851 1.00 0.00 O
ATOM 615 I 615 10.000 -17.246 13.548 1.00 0.00 O
ATOM 616 I 616 10.000 -9.277 14.246 1.00 0.00 O
ATOM 617 I 617 10.000 -1.307 14.943 1.00 0.00 O
ATOM 618 I 618 10.000 6.662 15.640 1.00 0.00 O
ATOM 619 I 619 10.000 14.632 16.337 1.00 0.00 O
ATOM 620 I 620 10.000 22.601 17.035 1.00 0.00 O
ATOM 621 I 621 10.000 30.571 17.732 1.00 0.00 O
ATOM 622 I 622 20.000 -33.186 12.154 1.00 0.00 O
ATOM 623 I 623 20.000 -25.216 12.851 1.00 0.00 O
ATOM 624 I 624 20.000 -17.246 13.548 1.00 0.00 O
ATOM 625 I 625 20.000 -9.277 14.246 1.00 0.00 O
ATOM 626 I 626 20.000 -1.307 14.943 1.00 0.00 O
ATOM 627 I 627 20.000 6.662 15.640 1.00 0.00 O
ATOM 628 I 628 20.000 14.632 16.337 1.00 0.00 O
ATOM 629 I 629 20.000 22.601 17.035 1.00 0.00 O
ATOM 630 I 630 20.000 30.571 17.732 1.00 0.00 O
ATOM 631 I 631 30.000 -33.186 12.154 1.00 0.00 O
ATOM 632 I 632 30.000 -25.216 12.851 1.00 0.00 O
ATOM 633 I 633 30.000 -17.246 13.548 1.00 0.00 O
ATOM 634 I 634 30.000 -9.277 14.246 1.00 0.00 O
ATOM 635 I 635 30.000 -1.307 14.943 1.00 0.00 O
ATOM 636 I 636 30.000 6.662 15.640 1.00 0.00 O
ATOM 637 I 637 30.000 14.632 16.337 1.00 0.00 O
ATOM 638 I 638 30.000 22.601 17.035 1.00 0.00 O
ATOM 639 I 639 30.000 30.571 17.732 1.00 0.00 O
ATOM 640 I 640 40.000 -33.186 12.154 1.00 0.00 O
ATOM 641 I 641 40.000 -25.216 12.851 1.00 0.00 O
ATOM 642 I 642 40.000 -17.246 13.548 1.00 0.00 O
ATOM 643 I 643 40.000 -9.277 14.246 1.00 0.00 O
ATOM 644 I 644 40.000 -1.307 14.943 1.00 0.00 O
ATOM 645 I 645 40.000 6.662 15.640 1.00 0.00 O
ATOM 646 I 646 40.000 14.632 16.337 1.00 0.00 O
ATOM 647 I 647 40.000 22.601 17.035 1.00 0.00 O
ATOM 648 I 648 40.000 30.571 17.732 1.00 0.00 O
ATOM 649 I 649 -40.000 -33.621 17.135 1.00 0.00 O
ATOM 650 I 650 -40.000 -25.652 17.832 1.00 0.00 O
ATOM 651 I 651 -40.000 -17.682 18.529 1.00 0.00 O
ATOM 652 I 652 -40.000 -9.713 19.227 1.00 0.00 O
ATOM 653 I 653 -40.000 -1.743 19.924 1.00 0.00 O
ATOM 654 I 654 -40.000 6.226 20.621 1.00 0.00 O
ATOM 655 I 655 -40.000 14.196 21.318 1.00 0.00 O
ATOM 656 I 656 -40.000 22.166 22.016 1.00 0.00 O
ATOM 657 I 657 -40.000 30.135 22.713 1.00 0.00 O
ATOM 658 I 658 -30.000 -33.621 17.135 1.00 0.00 O
ATOM 659 I 659 -30.000 -25.652 17.832 1.00 0.00 O
ATOM 660 I 660 -30.000 -17.682 18.529 1.00 0.00 O

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ATOM 662 I 662 -30.000 -1.743 19.924 1.00 0.00 O
ATOM 663 I 663 -30.000 6.226 20.621 1.00 0.00 O
ATOM 664 I 664 -30.000 14.196 21.318 1.00 0.00 O
ATOM 665 I 665 -30.000 22.166 22.016 1.00 0.00 O
ATOM 666 I 666 -30.000 30.135 22.713 1.00 0.00 O
ATOM 667 I 667 -20.000 -33.621 17.135 1.00 0.00 O
ATOM 668 I 668 -20.000 -25.652 17.832 1.00 0.00 O
ATOM 669 I 669 -20.000 -17.682 18.529 1.00 0.00 O
ATOM 670 I 670 -20.000 -9.713 19.227 1.00 0.00 O
ATOM 671 I 671 -20.000 -1.743 19.924 1.00 0.00 O
ATOM 672 I 672 -20.000 6.226 20.621 1.00 0.00 O
ATOM 673 I 673 -20.000 14.196 21.318 1.00 0.00 O
ATOM 674 I 674 -20.000 22.166 22.016 1.00 0.00 O
ATOM 675 I 675 -20.000 30.135 22.713 1.00 0.00 O
ATOM 676 I 676 -10.000 -33.621 17.135 1.00 0.00 O
ATOM 677 I 677 -10.000 -25.652 17.832 1.00 0.00 O
ATOM 678 I 678 -10.000 -17.682 18.529 1.00 0.00 O
ATOM 679 I 679 -10.000 -9.713 19.227 1.00 0.00 O
ATOM 680 I 680 -10.000 -1.743 19.924 1.00 0.00 O
ATOM 681 I 681 -10.000 6.226 20.621 1.00 0.00 O
ATOM 682 I 682 -10.000 14.196 21.318 1.00 0.00 O
ATOM 683 I 683 -10.000 22.166 22.016 1.00 0.00 O
ATOM 684 I 684 -10.000 30.135 22.713 1.00 0.00 O
ATOM 685 I 685 -0.000 -33.621 17.135 1.00 0.00 O
ATOM 686 I 686 -0.000 -25.652 17.832 1.00 0.00 O
ATOM 687 I 687 0.000 -17.682 18.529 1.00 0.00 O
ATOM 688 I 688 0.000 -9.713 19.227 1.00 0.00 O
ATOM 689 I 689 0.000 -1.743 19.924 1.00 0.00 O
ATOM 690 I 690 0.000 6.226 20.621 1.00 0.00 O
ATOM 691 I 691 0.000 14.196 21.318 1.00 0.00 O
ATOM 692 I 692 0.000 22.166 22.016 1.00 0.00 O
ATOM 693 I 693 0.000 30.135 22.713 1.00 0.00 O
ATOM 694 I 694 10.000 -33.621 17.135 1.00 0.00 O
ATOM 695 I 695 10.000 -25.652 17.832 1.00 0.00 O
ATOM 696 I 696 10.000 -17.682 18.529 1.00 0.00 O
ATOM 697 I 697 10.000 -9.713 19.227 1.00 0.00 O
ATOM 698 I 698 10.000 -1.743 19.924 1.00 0.00 O
ATOM 699 I 699 10.000 6.226 20.621 1.00 0.00 O
ATOM 700 I 700 10.000 14.196 21.318 1.00 0.00 O
ATOM 701 I 701 10.000 22.166 22.016 1.00 0.00 O
ATOM 702 I 702 10.000 30.135 22.713 1.00 0.00 O
ATOM 703 I 703 20.000 -33.621 17.135 1.00 0.00 O
ATOM 704 I 704 20.000 -25.652 17.832 1.00 0.00 O
ATOM 705 I 705 20.000 -17.682 18.529 1.00 0.00 O
ATOM 706 I 706 20.000 -9.713 19.227 1.00 0.00 O
ATOM 707 I 707 20.000 -1.743 19.924 1.00 0.00 O
ATOM 708 I 708 20.000 6.226 20.621 1.00 0.00 O

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ATOM    709  I       709      20.000  14.196  21.318  1.00  0.00          O
ATOM    710  I       710      20.000  22.166  22.016  1.00  0.00          O
ATOM    711  I       711      20.000  30.135  22.713  1.00  0.00          O
ATOM    712  I       712      30.000 -33.621  17.135  1.00  0.00          O
ATOM    713  I       713      30.000 -25.652  17.832  1.00  0.00          O
ATOM    714  I       714      30.000 -17.682  18.529  1.00  0.00          O
ATOM    715  I       715      30.000  -9.713  19.227  1.00  0.00          O
ATOM    716  I       716      30.000  -1.743  19.924  1.00  0.00          O
ATOM    717  I       717      30.000   6.226  20.621  1.00  0.00          O
ATOM    718  I       718      30.000  14.196  21.318  1.00  0.00          O
ATOM    719  I       719      30.000  22.166  22.016  1.00  0.00          O
ATOM    720  I       720      30.000  30.135  22.713  1.00  0.00          O
ATOM    721  I       721      40.000 -33.621  17.135  1.00  0.00          O
ATOM    722  I       722      40.000 -25.652  17.832  1.00  0.00          O
ATOM    723  I       723      40.000 -17.682  18.529  1.00  0.00          O
ATOM    724  I       724      40.000  -9.713  19.227  1.00  0.00          O
ATOM    725  I       725      40.000  -1.743  19.924  1.00  0.00          O
ATOM    726  I       726      40.000   6.226  20.621  1.00  0.00          O
ATOM    727  I       727      40.000  14.196  21.318  1.00  0.00          O
ATOM    728  I       728      40.000  22.166  22.016  1.00  0.00          O
ATOM    729  I       729      40.000  30.135  22.713  1.00  0.00          O
END
```