Universidad Nacional Autónoma de México

Facultad de Química

Estudio sobre las Propiedades Electrónicas de Aleaciones

T E S I S

Que para obtener el título de:

Q U I M I C O

p r e s e n t a :

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LAT indica el tipo de malla, sus posibles valores son:

LAT = 1	FCC
LAT = 2	BCC
LAT = 3	Diamante
LAT = 4	HCP
LAT = 5	Estructuras Especiales
LAT = 6	Aleaciones

- (JRI(JJ),JJ=1,NJJ) FORMATO(6F10.0

JRI punto de la malla de APW(malla creada y descrita en CRYS) correspondiente al radio de la esfera.

- OMA, A, C, XALPHA FORMATO(6F10.6)

OMA volumen por átomo(unidades atómicas^3)

A, C parámetros de la malla(u. a.). En el caso de aleaciones y estructuras especiales A y C pueden ser=1.0 dependiendo de la forma en que se den las distancias.

XALPHA parámetro de intercambio cuando XALPHA no se especifica (XALPHA=0), el cálculo se efectua con los valores de $\alpha=2/3$ y $\beta=0.003$; de lo contrario α=XALPHA.

En el caso de aleaciones o de estructuras especiales se leen dentro de un DO de JJ=1,NJJ los siguientes datos:

- (XNA(I,JJ), I=1,14) FORMATO(8F10.6)
- (AAD(I,JJ), I=1,14) FORMATO(8F10.6)

XNA es el número de vecinos en cada capa; si LAT=5 será para las primeras 14 capas, si LAT=6 se da el número de vecinos de las 7 primeras capas del tipo del átomo central y de 8-14 el número de vecinos del otro tipo de átomo en èstas 7 capas.

Se lee primero cuando el átomo de tipo 1 es el central y luego cuando el átomo de tipo 2 es el central.

AAD son las distancias para cada capa de vecinos y se dan de la misma forma que XNA. Cuando es una aleación, la primera distancia para el átomo que no es el central debe de ser diferente de cero.

- MAXL, NE, ZVAL(1), ZVAL(2), NUMA(1), NUMA(2), BE, ES, DVINT(1), DVINT(2), IRESIS FORMATO(6I5, 4F10.5, 2I5)

MAXL máximo momento angular.

NE número de energías para el cálculo de las derivadas logarítmicas y corrimientos de fase, no debe de ser mayor de 60.

ZVAL(1), ZVAL(2) número de electrones de valencia para cada tipo de átomo.

NUMA(1), NUMA(2) número de dispersores de cada tipo de átomo.

BE valor de la energía inicial, BE $\neq$ 0, por lo general BE = 0.01.

ES intervalo de la malla de energías en LOGDER.

DVINT(1), DVINT(2) potencial intersticial adicional para cada tipo de átomo.

IRESIS ≠ 0 solo cuando se quiere calcular la resistividad. Cuando IRESIS ≠ 0 se lee:

- (AQUP(J),j=1,40) FORMATO(8F10.5)

AQUP tabla de factor de estructura.

Cuando IAL ≠ 0, o sea que se quiere calcular la densidad de estados se leen las siguientes tarjetas:

- TMAX, LLSS, IOPL, NPP, ATOCEL, NAME

FORMATO(I5,I3,2I2,F8.4,10A6)

TMAX tiempo máximo estimado para el cálculo en segundos.

LLSS ≠ 0 cuando se quiere variar el valor de LMAX procedente de LOGDER. LSS=(LMAX+1)-LLSS.

IOPL = 1 si se quieren tomar en cuenta para el cálculo los electrones p.

NPP número de puntos para la interpolación, si NPP=0 entonces NPP=4.

ATOCEL número de átomos dentro de la celda con parámetros A y C.

NAME título.

- PARA, EEMIN, EEMAX, EEDELT, FINT1, INUMA(1), INUMA(2)

FORMATO(I5,4F10.5,2I5)

PARA ≠ 0 cuando se quiere que la máquina perfore el valor de la última energía calculada y

el valor de la integral de la densidad de estados hasta esa energía.

EEMIN corrección para el valor de la energía mínima, si EEMIN ≠ 0, EMIN = EEMIN. Si EEMIN = 0 el programa utilizará como energía mínima la última del cálculo anterior, si es el primer cálculo usa la de LOGDER.

EEMAX corrección para el valor de la energía máxima, si EEMAX ≠ 0, EMAX = EEMAX.

EEDELT corrección al tamaño del intervalo, si EEDELT≠0 EDELTA = EEDELT.

FINT1 valor de la integral de la densidad de estados de del que parte la misma. si FINT1 = 0 empieza en 0 la primera vez y las siguientes ocasiones con el valor que guardó.

INUMA(1), INUMA(2) corrección para el número de dispersores para cada tipo de átomo; el número total de dispersores (NUMSC) será:

NUMSC=NUMA(1)+NUMA(2)+INUMA(1)+INUMA(2).

- (LX(I),LY(I),LZ(I),I=1,NUMSC) FORMATO(8F10.7)

Coordenadas para cada uno de los dispersores.

-((SCF(L,TN),L=1,LSS+1),TN=1,NJJ) FORMATO(8F10.7)

SCF escalamiento de los corrimientos de fase de momento angular l, se perfora una tarjeta para cada tipo de átomo.

Cuando unicamente se quiere hacer el cálculo de la densidad de estados y se parte de los datos guardados por el programa en disco

se necesitan: la primera tarjeta descrita, se omiten las siguientes hasta la tarjeta donde se lee TMAX, LLSS, etc.

Otra posibilidad es hacer el cálculo de la densidad de estados con corrimientos de fase no obtenidos en LOGDER para lo cual se da el siguiente instructivo, algunas tarjetas solamente se mencionan porque ya fueron descritas.

- ICALL FORMATO(2I5)
- A0, EMIN, EMAX, EDELTA, LSS, NPH, T, NUMA(1), ZVAL(1), NUMA(2), ZVAL(2) FORMATO(4F10.6,7I3)

  A0 parámetro de la malla.

  EMIN energía mínima, debe de ser diferente de cero.

  EMAX enrgía máxima.

  EDELTA tamaño del intervalo de malla.

  LSS máximo momento angular.

  NPH número de corrimientos de fase que tiene que leer el programa.

  T número de diferentes tipos de átomos.

  NUMA(1), ZVAL(1), NUMA(2), ZVAL(2) ya descritas.

- TMAX, LLSS, IOPL, NPP, ATOCFL, NAME FORMATO(I5,I3,2I2,F8.4,10A6)
- PARA, EEMIN, EEMAX, EEDELT, FINT1, INUMA(1), INUMA(2) FORMATO(I5,4F10.5,2I5)
- (LX(I),LY(I),LZ(I),I=1,NUMSC) FORMATO(8F10.7)
- ((SCF(L,TN),L=1,LSS+1),TN=1,T) FORMATO(8F10.8)
- ((E(I,TN),E(I+1,TN),E(I+2,TN),E(I+3,TN),E(I+4,TN),E(I+5,TN), E(I+6,TN),E(I+7,TN),I=1,NPH,8),TN=1,T) FORMATO(8F10.8)

energía correspondiente a cada corrimiento de fase.

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- ((PH(L,I,TN),PH(L,I+1,TN),PH(L,I+2,TN),PH(L,I+3,TN),PH(L,I+4,TN)
   PH(L,I+5,TN), PH(L,I+6,TN),PH(L,I+7,TN),L=1,NPH,8),TN=1,T)
                                   FORMATO(8F10.8)
```

corrimientos de fase.

APENDICE II. DESCRIPCION DE LOS RESULTADOS DEL CALCULO DE LA ALEACION Fe_4Ge.

Se presentan a continuación los resultados obtenidos en el cálculo de la aleación Fe_4Ge con una estructura FCC.

En la primera hoja se encuentran las distancias del centro a las primeras 14 capas de vecinos para las estructuras FCC, BCC y Diamante, se escriben también el número de vecinos para las estructuras anteriores y para la estructura HCP, las distancias para esta estructura se calculan en el programa.

A continuación se obtiene la tabla de radios de APW y las tablas de densidades electrónicas ya interpoladas a la malla de APW y las integrales de la densidad de carga para cada tipo de átomo. En este cálculo se ha legido al Fe como el átomo de tipo 1 y al Ge de tipo 2. Se encuentra después el tipo de malla (LAT) en este caso se indica con el número 6 por tratarse de una aleación(para otras estructuras ver el instructivo en el apéndice I), en seguida el punto de la malla correspondiente a la esfera de muffin-tin este dato recibe el nombre de JRI y en este caso tiene el mismo valor para los dos tipos de átomos

$$JRI = \frac{\ln R_{MT} + 8.85}{0.05} \qquad \ldots 29)$$

Se encuentran también el volumen por átomo, los parámetros de la

malla y por último los valores de α y β.

En la siguiente hoja se encuentran las distancias y número de vecinos para las primeras 7 capas de vecinos, primero cuando el Fe es el átomo central, en este caso los siete primeros números corresponden a las distancias que hay del Fe central a las primeras siete capas de Fe y los otros siete corresponden a al distancia que hay del Fe central a las siete primeras capas de Ge, en la misma forma aparecen el número de vecinos; en seguida cuando el Ge es el átomo central los primeros siete datos corresponden a las distancias y el número de átomos de Ge y las otras siete a los del Fe. En esta misma hoja encontramos la integral del potencial en la esfera de muffin-tin, la de $4\pi\rho$, la carga dentro de la esfera, el volumen de las esferas, el potencial de intercambio y el número de átomos de cada tipo considerando en este caso como átomos de tipo 1 a los del tipo del átomo central.

En esta parte el programa inicia el cálculo tomando primero al átomo de tipo 2 como central. Los valores que encontramos a continuación son: RI radio de la esfera de muffin-tin para cada tipo de átomo, como se dijo antes en este caso son iguales, RO es el redio de la esfera obtenido a partir del volumen por átomo, V BOUNDARY que es la integral del potencial final en un volumen por átomo, VINT que es el potencial promedio en la región intersticial(la región entre RI y RO), Z es el número átomico para este tipo de átomo, los dos valores de JRI, el tipo de malla(LAT) y los valores de α y β, la tabla que viene a continuación es la tabla del potencial en el cristal cuando el átomo de tipo 2 es el central

y en la siguiente hoja se encuentra este potencial multiplicado por el radio.

A continuación se encuentran los datos necesarios y los resultados de la subrutina LOGDER. Un vint adicional para esta subrutina que permite cambiar la posición del cero de energía(VINT), LMAX es el valor del máximo momento angular, en este caso no se han incluido electrones de tipo f en el cálculo, el número de energías, la enrgía inicial y el tamaño del intervalo de energías. A continuación aparecen las derivadas logarítmicas para cada l y los corrimientos de fase, la siguiente tabla CEP es

$$CEP_l = tan\,\eta_l - \frac{n_l}{j_l} \qquad \ldots 30)$$

donde n_l y j_l son las funciones de Neumann y Bessel respectivamente.

Al final de esta tabla se encuentra el nivel de Fermi, el número de electrones de valencia para el átomo de tipo 2 y el valor del corrimiento de fase s, p, d al nivel de Fermi.

A continuación se tiene la gráfica de corrimientos de fase vs. energía. La línea formada por * representa al corrimiento de fase de tipo s, la línea de + al de tipo p y la línea formada por - al de tipo d que en este caso es muy pequeño. La línea punteada vertical es el nivel de Fermi.

En la siguiente hoja se obtienen los resultados del cálculo cuando el átomo de tipo 1 es el central, se encuentra también el potencial, el potencial por el radio, aquí como se menciono en la pag. 7 es importante checar que el potencial intersticial (VINT)

no difiera en mas de 10^{-2}Ry del obtenido para el átomo de tipo 2. En seguida se obtienen los resultados de la subrutina LOGDER, en este caso además se obtiene un nivel de Fermi aproximado para la aleación, promediando los niveles de Fermi de cada tipo de átomo. En la gráfica se puede apreciar la resonancia d para el Fe.

En seguida se encuentran los datos necesarioa y resultados de la subrutina ASIL. En este caso se presenta el cálculo con solo 2 dispersores para poder mostrar una gráfica de la densidad de estados completa. La gráfica presentada en el cap. III se obtuvo haciendo el cálculo con 6 dispersores, pero ese cálculo se tuvo que efectuar en varias etapas.

Primero encontramos todos los datos que se le dieron a esta subrutina, como son l_{max}, el número de diferentes tipos de átomos, el número de átomos por celda, el parámetro de malla y el número de puntos para la interpolación. Esta parte del programa puede no tomar en cuenta a los electrones p para el cálculo, aunque en este caso si se incluyen por tener una contribución importante en el Ge. Se encuentra después la enrgía mínima y máxima y el tamaño del intervalo, los escalamientos s, p, d. Para el átomo de tipo 1 los electrones de valencia y el número de dispersores de este tipo y los corrimientos de fase, a continuación los escalamientos para el átomo de tipo 2, el número de electrones de valencia y el número de dispersores de este tipo y sus corrimientos de fase. Se tienen después las coordenadas de cada dispersor, primero las del átomo de tipo 1 y luego del tipo 2. En este caso con dos dispersores se consideró un dispersor de cada tipo. En seguida encontramos los resultados de la subrutina ASIL que son la densidad de estados, la

contribución de lectrones libres, el cambio en la densidad de estados y la densidad integrada de estados que como se mencionó en la descripción de la subrutina nos permite calcular el nivel de Fermi, como podemos observar en esta caso el nivel de Fermi se encontró a una energía de 0.985Ry. La densidad de estados y la parte de electrones libres se encuentran representados en la gráfica que aparece a continuación. En esta gráfica la curva fromada por * representa a la parte de electrones libres y la curva formada por + a la densidad de estados, la línea punteada vertical nos indica el nivel de Fermi, en este caso encontramos como punto importante un mínimo en la densidad de estados y el nivel de Fermi muy cerca de este, como se puede ver el fig. 5 del cálculo con 6 dispersores el nivel de Fermi se acerca mas al mínimo de la densidad de estados ya que la concentración se asemeja mas a la de formación del vidiro metálico y concuerda mejor con los resultados obtenidos con el modelo de electrones casi libres mencionado en el cap. III.

Abajo de la gráfica encontramos los valores para la suma de Friedel y la densidad de estados por volumen X 100, los números que no tienen paréntesis corresponden a los valores de confianza (faithful).

Cuando se efectua el cálculo de la densidad de estados aparece al principio del programa una serie de resultados que por seguir el orden en el que se efectua el cálculo aquí describimos e incluimos al final. Los valores que encontramos aquí para cada energía son: el valor de la matriz k para cada l y el corrimiento de fase correspondiente, el valor de la parte real y la parte imaginaria del determinante que como se vió en el capítulo II nos

permite calcular la densidad de estados, cuyo valor también aparece por unidad de volumen y multiplicado por 100 y encontramos también el tiempo de proceso al terminar el cálculo para cada valor de la energía.

DISTANCE/SIDE FOR FCC, BCC AND DIAMOND

0.000000	0.705000	1.000000	1.224700	1.414200	1.581100	1.732100	1.870800	
2.000000	2.121300	2.236100	2.345200	2.449500	2.549500			
0.000000	0.866050	1.000000	1.414200	1.658300	1.732100	2.000000	2.179400	
2.236100	2.449500	2.598100	2.738400	2.958000	3.000000			
0.000000	0.433020	0.707100	0.829100	1.000000	1.039700	1.224700	1.299000	
1.414200	1.479000	1.600700	1.639300	1.732100	1.785300			

NUMBER OF NEIGHBOUR ATOMS FOR FCC, BCC, DIAMOND AND HCP

1	12	6	24	12	24	8	48	6	36	24	24	24	72
1	8	6	12	24	8	6	24	24	24	32	12	48	50
1	4	12	12	6	12	24	16	12	24	24	12	8	24
1	6	6	6	2	12	6	12	6	12	12	6	6	12

MAXIMUM RADIUS FROM HEX= 60.00000 RECIPROCAL OF MESH INTERVAL FROM HEX= 32.00000

NUMBER OF MESH POINTS= 421 NUMBER OF TYPES OF ATOMS= 2 ATOMIC NUMBERS 26 32

TABLE OF APH RADIUS

.1507331E-03	.1584613E-03	.1665858E-03	.1751268E-03	.1841058E-03	.1935451E-03	.2034684E-03	.2139004E-03
.2248673E-03	.2363705E-03	.2485168E-03	.2612586E-03	.2746536E-03	.2887354E-03	.3035391E-03	.3191019E-03
.3354626E-03	.3526622E-03	.3707435E-03	.3897520E-03	.4097350E-03	.4307425E-03	.4528272E-03	.4760441E-03
.5004514E-03	.5261101E-03	.5530844E-03	.5814416E-03	.6112528E-03	.6425924E-03	.6755388E-03	.7101744E-03
.7465858E-03	.7848641E-03	.8251049E-03	.8674090E-03	.9118820E-03	.9586352E-03	.1007785E-02	.1059456E-02
.1113775E-02	.1170880E-02	.1230912E-02	.1294022E-02	.1360368E-02	.1430116E-02	.1503439E-02	.1580522E-02
.1661557E-02	.1746747E-02	.1836305E-02	.1930454E-02	.2029431E-02	.2133482E-02	.2242868E-02	.2357862E-02
.2478752E-02	.2605841E-02	.2739445E-02	.2879899E-02	.3027555E-02	.3182781E-02	.3345965E-02	.3517517E-02
.3697864E-02	.3887457E-02	.4086771E-02	.4296305E-02	.4516581E-02	.4748151E-02	.4991594E-02	.5247518E-02
.5516564E-02	.5799405E-02	.6096747E-02	.6409333E-02	.6737947E-02	.7083409E-02	.7446583E-02	.7828378E-02
.8229747E-02	.8651695E-02	.9095277E-02	.9561602E-02	.1005184E-01	.1056720E-01	.1110900E-01	.1167857E-01
.1227734E-01	.1290681E-01	.1356856E-01	.1426423E-01	.1499558E-01	.1576442E-01	.1657268E-01	.1742237E-01
.1831564E-01	.1925470E-01	.2024191E-01	.2127974E-01	.2237077E-01	.2351775E-01	.2472353E-01	.2599113E-01
.2732372E-01	.2872464E-01	.3019738E-01	.3174564E-01	.3337327E-01	.3508435E-01	.3688317E-01	.3877421E-01
.4076220E-01	.4285213E-01	.4504920E-01	.4735892E-01	.4978707E-01	.5233971E-01	.5502322E-01	.5784432E-01
.6081006E-01	.6392786E-01	.6720551E-01	.7065121E-01	.7427358E-01	.7808167E-01	.8208500E-01	.8629359E-01
.9071795E-01	.9536916E-01	.1002588E+00	.1053992E+00	.1108032E+00	.1164842E+00	.1224564E+00	.1287349E+00
.1353353E+00	.1422741E+00	.1495686E+00	.1572372E+00	.1652989E+00	.1737739E+00	.1826835E+00	.1920499E+00
.2018965E+00	.2122480E+00	.2231302E+00	.2345703E+00	.2465970E+00	.2592403E+00	.2725318E+00	.2865048E+00
.3011942E+00	.3166368E+00	.3328711E+00	.3499377E+00	.3678794E+00	.3867410E+00	.4065697E+00	.4274149E+00
.4493290E+00	.4723666E+00	.4965853E+00	.5220458E+00	.5488116E+00	.5769498E+00	.6065307E+00	.6376282E+00
.6703200E+00	.7046881E+00	.7408182E+00	.7788008E+00	.8187308E+00	.8607080E+00	.9048374E+00	.9512294E+00
.1000000E+01	.1051271E+01	.1105171E+01	.1161834E+01	.1221403E+01	.1284025E+01	.1349859E+01	.1419068E+01
.1491825E+01	.1568312E+01	.1648721E+01	.1733253E+01	.1822119E+01	.1915541E+01	.2013753E+01	.2117000E+01
.2225541E+01	.2339647E+01	.2459603E+01	.2585710E+01	.2718282E+01	.2857651E+01	.3004166E+01	.3158193E+01
.3320117E+01	.3490343E+01	.3669297E+01	.3857426E+01	.4055200E+01	.4263115E+01	.4481689E+01	.4711470E+01
.4953032E+01	.5206980E+01	.5473947E+01	.5754603E+01	.6049647E+01	.6359820E+01	.6685894E+01	.7028688E+01
.7389056E+01	.7767901E+01	.8166170E+01	.8584858E+01	.9025013E+01	.9487736E+01	.9974182E+01	.1048557E+02
.1102318E+02	.1158835E+02	.1218249E+02	.1280710E+02	.1346374E+02	.1415404E+02	.1487973E+02	.1564263E+02
.1644465E+02	.1728778E+02	.1817415E+02	.1910595E+02	.2008554E+02	.2111534E+02	.2219795E+02	.2333606E+02
.2453253E+02	.2579034E+02	.2711264E+02	.2850273E+02	.2996410E+02	.3150039E+02	.3311545E+02	.3481332E+02
.3659823E+02	.3847467E+02						

INTERPOLATED TABLE OF 4*PI*(R**2)*RHO FOR THIS PROGRAM, FOR THE 1 ATOM

.4178460E-02	.4007678E-02	.5080883E-02	.5002562E-02	.6177604E-02	.6811637E-02	.7510480E-02	.8280805E-02
.9129882E-02	.1006572E-01	.1109716E-01	.1222388E-01	.1340659E-01	.1480703E-01	.1038816E-01	.1306421E-01
.1991084E-01	.2194530E-01	.2418651E-01	.2665533E-01	.2937407E-01	.3230968E-01	.3566809E-01	.3930027E-01
.4329963E-01	.4770290E-01	.5255051E-01	.5786618E-01	.6375899E-01	.7022202E-01	.7733375E-01	.8515816E-01
.9370560E-01	.1032330E+00	.1136448E+00	.1250932E+00	.1370792E+00	.1515137E+00	.1067174E+00	.1834227E+00
.2017741E+00	.2219270E+00	.2440664E+00	.2683556E+00	.2950195E+00	.3242754E+00	.3563658E+00	.3915558E+00
.4301317E+00	.4724059E+00	.5187172E+00	.5674315E+00	.6249402E+00	.6856955E+00	.7521387E+00	.8247801E+00
.9041579E+00	.9908582E+00	.1085502E+01	.1186762E+01	.1301359E+01	.1424056E+01	.1557681E+01	.1703101E+01
.1861244E+01	.2033098E+01	.2219690E+01	.2422130E+01	.2641532E+01	.2879162E+01	.3136215E+01	.3413792E+01
.3713858E+01	.4037102E+01	.4385308E+01	.4759721E+01	.5161791E+01	.5592967E+01	.6054586E+01	.6547790E+01
.7074446E+01	.7035009E+01	.8230957E+01	.8862710E+01	.9531618E+01	.1023753E+02	.1098072E+02	.1176112E+02
.1257805E+02	.1343055E+02	.1431717E+02	.1523582E+02	.1010402E+02	.1715837E+02	.1815501E+02	.1910928E+02
.2019571E+02	.2122817E+02	.2225967E+02	.2328245E+02	.2428804E+02	.2526732E+02	.2621156E+02	.2710758E+02
.2794790E+02	.2872006E+02	.2941613E+02	.3002326E+02	.3053310E+02	.3093709E+02	.3122797E+02	.3140083E+02
.3145156E+02	.3138013E+02	.3118822E+02	.3083072E+02	.3040603E+02	.2995726E+02	.2930859E+02	.2871929E+02
.2803126E+02	.2733009E+02	.2664176E+02	.2599573E+02	.2542059E+02	.2494476E+02	.2459496E+02	.2439470E+02
.2436280E+02	.2451257E+02	.2485075E+02	.2537470E+02	.2607667E+02	.2693379E+02	.2792023E+02	.2399886E+02
.3012364E+02	.3124614E+02	.3230936E+02	.3325731E+02	.3403375E+02	.3458681E+02	.3487220E+02	.3484828E+02
.3449708E+02	.3380610E+02	.3270323E+02	.3144710E+02	.2983904E+02	.2801044E+02	.2602574E+02	.2396148E+02
.2189362E+02	.1990517E+02	.1617074E+02	.1645759E+02	.1511951E+02	.1409413E+02	.1339888E+02	.1303161E+02
.1297124E+02	.1317497E+02	.1359230E+02	.1415346E+02	.1478855E+02	.1542560E+02	.1599559E+02	.1044120E+02
.1671485E+02	.1078532E+02	.1063594E+02	.1626722E+02	.1560977E+02	.1493005E+02	.1401974E+02	.1299623E+02
.1190039E+02	.1076921E+02	.9639756E+01	.8541985E+01	.7500659E+01	.6533815E+01	.5054012E+01	.4366607E+01
.4172879E+01	.3570203E+01	.3052079E+01	.2611679E+01	.2239151E+01	.1925745E+01	.1662691E+01	.1441398E+01
.1255274E+01	.1097614E+01	.9035509E+00	.8490378E+00	.7503259E+00	.6640739E+00	.5893840E+00	.5226078E+00
.4629713E+00	.4093296E+00	.3609308E+00	.3171079E+00	.2774412E+00	.2415908E+00	.2092972E+00	.1804284E+00
.1540094E+00	.1323283E+00	.1128615E+00	.9626058E-01	.8241702E-01	.7097356E-01	.5921489E-01	.4910308E-01
.4101593E-01	.3465140E-01	.2907568E-01	.2583597E-01	.2280409E-01	.2034316E-01	.1827770E-01	.1645409E-01
.1477357E-01	.1317103E-01	.1161340E-01	.1009421E-01	.8624207E-02	.7225364E-02	.5923399E-02	.4742548E-02
.3702222E-02	.2812503E-02	.2076990E-02	.1489008E-02	.1033315E-02	.6941026E-03	.4497214E-03	.2807419E-03
.1680717E-03	.9099147E-04	.5563035E-04	.2825233E-04	.1419428E-04	.6797598E-05	.3063489E-05	.1322043E-05
.5333836E-06	.2031401E-06						

INTERPOLATED TABLE OF 4*PI*(R**2)*RHO FOR THIS PROGRAM, FOR THE 2 ATOM

.8696752E-02	.2580113E-02	.1055294E-01	.1162423E-01	.1280393E-01	.1410293E-01	.1553322E-01	.1710804E-01
.1884186E-01	.2075903E-01	.2285792E-01	.2516496E-01	.2771193E-01	.3051332E-01	.3358715E-01	.3696147E-01
.4072629E-01	.4488380E-01	.4943517E-01	.5443126E-01	.5992371E-01	.6596212E-01	.7260829E-01	.7992113E-01
.8797253E-01	.9682198E-01	.1065195E+00	.1172702E+00	.1290715E+00	.1420293E+00	.1563322E+00	.1721080E+00
.1897703E+00	.2088677E+00	.2297175E+00	.2526059E+00	.2778115E+00	.3056508E+00	.3364573E+00	.3706510E+00
.3996642E+00	.4388676E+00	.4814269E+00	.5280864E+00	.5794217E+00	.6368403E+00	.6990815E+00	.7661255E+00
.8399802E+00	.9207227E+00	.1008937E+01	.1105277E+01	.1210444E+01	.1325105E+01	.1450306E+01	.1586672E+01
.1735202E+01	.1896487E+01	.2072771E+01	.2265968E+01	.2477607E+01	.2709104E+01	.2961617E+01	.3236572E+01
.3534329E+01	.3856977E+01	.4206076E+01	.4583804E+01	.4992937E+01	.5434954E+01	.5911758E+01	.6424174E+01
.6976867E+01	.7570076E+01	.8204047E+01	.8880197E+01	.9599901E+01	.1036677E+02	.1118179E+02	.1204879E+02
.1297066E+02	.1395028E+02	.1499057E+02	.1609437E+02	.1726453E+02	.1850387E+02	.1981519E+02	.2120126E+02
.2266533E+02	.2420930E+02	.2583315E+02	.2753626E+02	.2931810E+02	.3117815E+02	.3311585E+02	.3513067E+02
.3722208E+02	.3938954E+02	.4163252E+02	.4395049E+02	.4634292E+02	.4880928E+02	.5134905E+02	.5396171E+02
.5664674E+02	.5940363E+02	.6223187E+02	.6513095E+02	.6810037E+02	.7113964E+02	.7424826E+02	.7742575E+02
.8067163E+02	.8398543E+02	.8736669E+02	.9081495E+02	.9432975E+02	.9791065E+02	.1015572E+03	.1052690E+03
.1090456E+03	.1128866E+03	.1167916E+03	.1207602E+03	.1247921E+03	.1288869E+03	.1330443E+03	.1372639E+03
.1415454E+03	.1458885E+03	.1502929E+03	.1547583E+03	.1592844E+03	.1638709E+03	.1685176E+03	.1732242E+03
.1779904E+03	.1828161E+03	.1877010E+03	.1926449E+03	.1976476E+03	.2027089E+03	.2078287E+03	.2130068E+03
.2182430E+03	.2235373E+03	.2288896E+03	.2342998E+03	.2397678E+03	.2452936E+03	.2508772E+03	.2565186E+03
.2622178E+03	.2679749E+03	.2737900E+03	.2796632E+03	.2855947E+03	.2915847E+03	.2976335E+03	.3037414E+03
.3099088E+03	.3161362E+03	.3224241E+03	.3287731E+03	.3351838E+03	.3416570E+03	.3481934E+03	.3547939E+03
.3614594E+03	.3681908E+03	.3749891E+03	.3818553E+03	.3887905E+03	.3957959E+03	.4028727E+03	.4100221E+03
.4172455E+03	.4245443E+03	.4319199E+03	.4393738E+03	.4469076E+03	.4545230E+03	.4622218E+03	.4700059E+03
.4778773E+03	.4858381E+03	.4938906E+03	.5020372E+03	.5102805E+03	.5186234E+03	.5270691E+03	.5356210E+03
.5442830E+03	.5530594E+03	.5619550E+03	.5709751E+03	.5801259E+03	.5894144E+03	.5988484E+03	.6084369E+03
.6181900E+03	.6281193E+03	.6382380E+03	.6485611E+03	.6591060E+03	.6698923E+03	.6809427E+03	.6922837E+03
.7039469E+03	.7159702E+03	.7284001E+03	.7412939E+03	.7547252E+03	.7687923E+03	.7836276E+03	.7994183E+03
.8164284E+03	.8350400E+03	.8557999E+03	.8795911E+03	.9078000E+03	.9435000E+03	.9935000E+03	.1000000E+04

INTEGRAL OF CHARGE DENSITY FOR THE 1 ATOM 25.93825116

INTEGRAL OF CHARGE DENSITY FOR THE 2 ATOM 31.99813193

LATTICE STRUCTURE= 6
MESH POINT CORRESPONDING TO THE APW ESPHERE RADIUS=194.850000
VOLUME PER ATOM(ATOMIC UNITS)= 87.740800
LATTICE CONSTANTS A AND C 7.053760 7.053760
EXCHANGE COEFICIENTS ALPHA AND BETA 0.080667 0.003000

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 NEIGHBOR DISTANCES AND NUMBER OF NEIGHBORS ---CENTRAL ATOM OF TYPE--- 1
 4.972901  7.053760  8.638740  9.975427 11.152700 12.217818  7.053760  4.972901
 1.000000  9.000000  3.000000 19.000000 10.000000 19.000000  6.000000  0.000000
 3.000000  1.000000  5.000000  2.000000  5.000000  2.000000

 NEIGHBOR DISTANCES AND NUMBER OF NEIGHBORS ---CENTRAL ATOM OF TYPE--- 2
 4.972901  7.053760  8.638740  9.975427 11.152700 12.217818  7.053760  4.972901
 1.000000  2.000000  1.000000  5.000000  2.000000  5.000000  2.000000  0.000000
10.000000  5.000000 19.000000 10.000000 19.000000  6.000000

 INTEGRAL OF POTENTIAL IN THE MUFFIN TIN SPHERE= -.606796E-01
 INTEGRAL OF4*PI*RHO=  .123986E+00
 CHARGE INTO THE SPHERE=  .254699E+02
 VOLUME=  .997414E+02
 EXCHANGE POTENTIAL=  .248548E+00
 NUMBER OF ATOMS OF TYPE 1=  .640000E+02
 NUMBER OF ATOMS OF TYPE 2=  .170000E+02

 INTEGRAL OF POTENTIAL IN THE MUFFIN TIN SPHERE= -.720954E-01
 INTEGRAL OF4*PI*RHO=  .140944E+00
 CHARGE INTO THE SPHERE=  .305762E+02
 VOLUME=  .997414E+02
 EXCHANGE POTENTIAL=  .967617E+00
 NUMBER OF ATOMS OF TYPE 1=  .170000E+02
 NUMBER OF ATOMS OF TYPE 2=  .660000E+02
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CENTRAL ATOM OF TYPE 2

RESULTS FOR MUFFIN TIN WITH RI(1)= 2.4412 RI(2)= 2.4412 RO= 2.7566 V BOUNDARY= -.6004959E+00
VINT= -.1488463E+01 Z= 32.00 JRI(1)=194.850000 JRI(2)=194.850000 LAT= 6
XALPHA= 0.6666667 XBETA= 0.0030000

-.42439722E+06	-.40368951E+06	-.38399171E+06	-.36525459E+06	-.34743127E+06
-.33047721E+06	-.31434999E+06	-.29900930E+06	-.28441678E+06	-.27053593E+06
-.25733205E+06	-.24477213E+06	-.23282475E+06	-.22144600E+06	-.21060959E+06
-.20028636E+06	-.19045846E+06	-.18109997E+06	-.17218209E+06	-.16367986E+06
-.15557013E+06	-.14783317E+06	-.14044664E+06	-.13339268E+06	-.12665656E+06
-.12021493E+06	-.11404779E+06	-.10814199E+06	-.10248422E+06	-.99397543E+05
-.94533879E+05	-.89919907E+05	-.85543037E+05	-.81342351E+05	-.77364972E+05
-.73581478E+05	-.69982387E+05	-.66556720E+05	-.63301899E+05	-.60203775E+05
-.57256618E+05	-.54453037E+05	-.51786064E+05	-.49249021E+05	-.46835562E+05
-.44539609E+05	-.42355937E+05	-.40277011E+05	-.38301690E+05	-.36421461E+05
-.34632933E+05	-.32931530E+05	-.31313806E+05	-.29773452E+05	-.28306850E+05
-.26911563E+05	-.25585028E+05	-.24325685E+05	-.23130317E+05	-.21994490E+05
-.20914207E+05	-.19887196E+05	-.18908992E+05	-.17975808E+05	-.17067313E+05
-.16222074E+05	-.15411027E+05	-.14644205E+05	-.13925675E+05	-.13233611E+05
-.12576396E+05	-.11949908E+05	-.11353402E+05	-.10786825E+05	-.10247847E+05
-.97351689E+04	-.92474925E+04	-.87862209E+04	-.83423842E+04	-.79226821E+04
-.75234679E+04	-.71437393E+04	-.67825619E+04	-.64390026E+04	-.61122736E+04
-.58014945E+04	-.55059067E+04	-.52247822E+04	-.49571983E+04	-.47031385E+04
-.44613207E+04	-.42313562E+04	-.40126743E+04	-.38047311E+04	-.36070494E+04
-.34189966E+04	-.32400247E+04	-.30703074E+04	-.29088715E+04	-.27551747E+04
-.26091928E+04	-.24704409E+04	-.23385672E+04	-.22132415E+04	-.20991485E+04
-.19880843E+04	-.18734655E+04	-.17713137E+04	-.16742702E+04	-.15821887E+04
-.14945285E+04	-.14113693E+04	-.13333011E+04	-.12573025E+04	-.11861839E+04
-.11185793E+04	-.10544126E+04	-.99352054E+03	-.93575597E+03	-.88093054E+03
-.82907705E+03	-.77991502E+03	-.73338311E+03	-.68936697E+03	-.64775150E+03
-.60841809E+03	-.57124229E+03	-.53610606E+03	-.50288799E+03	-.47147439E+03
-.44176517E+03	-.41366431E+03	-.38707164E+03	-.36197097E+03	-.33823211E+03
-.31581354E+03	-.29465402E+03	-.27469591E+03	-.25588388E+03	-.23816296E+03
-.22147945E+03	-.20578178E+03	-.19101597E+03	-.17713177E+03	-.16408479E+03
-.15181298E+03	-.14026860E+03	-.12940625E+03	-.11922059E+03	-.10967454E+03
-.10068367E+03	-.92561974E+02	-.84863643E+02	-.77741300E+02	-.71158731E+02
-.65068849E+02	-.59418678E+02	-.54166021E+02	-.49276013E+02	-.44724310E+02
-.40496559E+02	-.36579609E+02	-.32962900E+02	-.29630043E+02	-.26568001E+02
-.23802886E+02	-.21272936E+02	-.18974575E+02	-.16884255E+02	-.15002924E+02
-.13326281E+02	-.11835492E+02	-.10480033E+02	-.92643599E+01	-.81743469E+01
-.71959342E+01	-.63173772E+01	-.55275506E+01	-.48178626E+01	-.41805470E+01
-.36111484E+01	-.31047417E+01	-.26596066E+01	-.22726640E+01	-.19397749E+01
-.16510946E+01	-.14031054E+01	-.11876925E+01	-.10018038E+01	-.84202260E+00
-.67641671E+00	-.54145024E+00	-.42195474E+00	-.31666473E+00	-.22325665E+00
-.14402371E+00	-.11522085E+00	-.69966190E-01	-.80629858E-01	-.97024350E-01
-.14247890E+00	-.25539677E+00	-.37319589E+00	-.63480804E+00	-.10717987E+01
-.19376693E+01	-.21009910E+01	-.42282200E+01	-.65864671E+01	-.43082922E+01
-.17258511E+01	-.11666919E+01	-.54113953E+00	-.30937754E+00	-.14313742E+01
-.22029610E+01	-.14933442E+01	-.65434658E+00	-.21105673E+01	-.42041330E+01
-.22033121E+01	-.11526228E+01	-.24779702E+01	-.11849535E+01	-.21447016E+01
-.89712802E+00	-.61157807E+00	0.	0.	0.
0.	0.	0.	0.	0.
0.	0.	0.	0.	0.
0.	0.	0.	0.	0.

R*V(R)

.63970473E+02	.63968938E+02	.63967333E+02	.63965624E+02	.63963837E+02
.63961956E+02	.63959977E+02	.63957895E+02	.63955705E+02	.63953400E+02
.63950976E+02	.63948424E+02	.63945740E+02	.63942915E+02	.63939943E+02
.63936816E+02	.63933525E+02	.63930063E+02	.63926419E+02	.63922585E+02
.63918553E+02	.63914303E+02	.63909834E+02	.63905130E+02	.63900178E+02
.63894968E+02	.63889479E+02	.63883694E+02	.63877582E+02	.63871145E+02
.63864348E+02	.63857164E+02	.63849567E+02	.63841521E+02	.63832991E+02
.63823942E+02	.63814320E+02	.63804102E+02	.63793231E+02	.63781655E+02
.63769340E+02	.63756208E+02	.63742230E+02	.63727395E+02	.63711577E+02
.63694775E+02	.63676887E+02	.63657837E+02	.63637829E+02	.63616483E+02
.63593807E+02	.63569934E+02	.63544670E+02	.63517941E+02	.63489666E+02
.63459842E+02	.63428313E+02	.63395139E+02	.63360150E+02	.63323228E+02
.63284306E+02	.63243367E+02	.63200232E+02	.63154903E+02	.63107093E+02
.63056833E+02	.63003871E+02	.62948238E+02	.62889714E+02	.62828118E+02
.62763390E+02	.62695261E+02	.62623726E+02	.62548529E+02	.62469450E+02
.62386494E+02	.62299085E+02	.62207403E+02	.62111243E+02	.62010794E+02
.61905908E+02	.61792577E+02	.61675742E+02	.61553175E+02	.61424630E+02
.61289788E+02	.61146056E+02	.61000566E+02	.60845611E+02	.60683315E+02
.60513097E+02	.60335423E+02	.60150045E+02	.59955864E+02	.59753774E+02
.59541107E+02	.59319947E+02	.59089193E+02	.58848569E+02	.58597718E+02
.58336300E+02	.58064197E+02	.57780820E+02	.57485958E+02	.57179261E+02
.56860394E+02	.56528040E+02	.56184220E+02	.55827195E+02	.55454324E+02
.55068016E+02	.54667012E+02	.54250523E+02	.53818147E+02	.53369206E+02
.52904219E+02	.52422005E+02	.51922667E+02	.51404406E+02	.50867394E+02
.50311525E+02	.49736145E+02	.49140183E+02	.48523745E+02	.47886744E+02
.47228605E+02	.46548934E+02	.45847455E+02	.45123930E+02	.44377284E+02
.43607502E+02	.42813603E+02	.41994691E+02	.41149936E+02	.40278644E+02
.39380203E+02	.38454064E+02	.37498744E+02	.36513800E+02	.35497824E+02
.34450414E+02	.33370161E+02	.32255624E+02	.31105316E+02	.29917679E+02
.28691123E+02	.27424953E+02	.26117350E+02	.24766345E+02	.23369741E+02
.21925078E+02	.20429579E+02	.18880108E+02	.17273016E+02	.15604102E+02
.13868553E+02	.12061000E+02	.10175447E+02	.82061000E+01	.60491030E+01
.37277539E+01	.11203230E+01	-.16605106E+00	-.30597491E+01	-.61915937E+01
-.94360684E+01	-.12693604E+02	-.16089623E+02	-.19468707E+02	-.22816249E+02
-.26125694E+02	-.29390483E+02	-.32604000E+02	-.35759774E+02	-.38849184E+02
-.41865000E+02	-.44799000E+02	-.47643000E+02	-.50388000E+02	-.53025000E+02
-.55544000E+02	-.57934000E+02	-.60183000E+02	-.62279000E+02	-.64208000E+02
-.65955000E+02	-.67504000E+02	-.68837000E+02	-.69934000E+02	-.70772000E+02
-.71324000E+02	-.71559000E+02	-.71440000E+02	-.70923000E+02	-.69960000E+02
-.68495000E+02	-.66464000E+02	-.63792000E+02	-.60394000E+02	-.56161000E+02
-.50950000E+02	-.44574000E+02	-.36775000E+02	-.27210000E+02	-.15400000E+02
-.00000000E+00	.17400000E+02	.37200000E+02	.59000000E+02	.82800000E+02
.10760000E+03	.13400000E+03	.16200000E+03	.19200000E+03	.22400000E+03
.25800000E+03	.29400000E+03	.33200000E+03	.37200000E+03	.41400000E+03
.45800000E+03	.50400000E+03	.55200000E+03	.60200000E+03	.65400000E+03
.70800000E+03	.76400000E+03	.82200000E+03	.88200000E+03	.94400000E+03
.10080000E+04	.10740000E+04	.11420000E+04	.12120000E+04	.12840000E+04
.13580000E+04	.14340000E+04	.15120000E+04	.15920000E+04	.16740000E+04
.17580000E+04	.18440000E+04	.19320000E+04	.20220000E+04	.21140000E+04
.22080000E+04	.23040000E+04	.24020000E+04	.25020000E+04	.26040000E+04
.27080000E+04	.28140000E+04	.29220000E+04	.30320000E+04	.31440000E+04
.32580000E+04	.33740000E+04	.34920000E+04	.36120000E+04	.37340000E+04
.38580000E+04	.39840000E+04	.41120000E+04	.42420000E+04	.43740000E+04
.45080000E+04	.46440000E+04	.47820000E+04	.49220000E+04	.50640000E+04
.52080000E+04	.53540000E+04	.55020000E+04	.56520000E+04	.58040000E+04
.59580000E+04	.61140000E+04	.62720000E+04	.64320000E+04	.65940000E+04
.67580000E+04	.69240000E+04	.70920000E+04	.72620000E+04	.74340000E+04
.76080000E+04	.77840000E+04	.79620000E+04	.81420000E+04	.83240000E+04
.85080000E+04	.86940000E+04	.88820000E+04	.90720000E+04	.92640000E+04
.94580000E+04	.96540000E+04	.98520000E+04	.10052000E+05	.10254000E+05
.10458000E+05	.10664000E+05	.10872000E+05	.11082000E+05	.11294000E+05
.11508000E+05	.11724000E+05	.11942000E+05	.12162000E+05	.12384000E+05
.12608000E+05	.12834000E+05	.13062000E+05	.13292000E+05	.13524000E+05
.13758000E+05	.13994000E+05	.14232000E+05	.14472000E+05	.14714000E+05
.14958000E+05	.15204000E+05	.15452000E+05	.15702000E+05	.15954000E+05
.16208000E+05	.16464000E+05	.16722000E+05	.16982000E+05	.17244000E+05
.17508000E+05	.17774000E+05	.18042000E+05	.18312000E+05	.18584000E+05
.18858000E+05	.19134000E+05	.19412000E+05	.19692000E+05	.19974000E+05
.20258000E+05	.20544000E+05	.20832000E+05	.21122000E+05	.21414000E+05
.21708000E+05	.22004000E+05	.22302000E+05	.22602000E+05	.22904000E+05
.23208000E+05	.23514000E+05	.23822000E+05	.24132000E+05	.24444000E+05
.24758000E+05	.25074000E+05	.25392000E+05	.25712000E+05	.26034000E+05
.26358000E+05	.26684000E+05	.27012000E+05	.27342000E+05	.27674000E+05
.28008000E+05	.28344000E+05	.28682000E+05	.29022000E+05	.29364000E+05
.29708000E+05	.30054000E+05	.30402000E+05	.30752000E+05	.31104000E+05
.31458000E+05	.31814000E+05	.32172000E+05	.32532000E+05	.32894000E+05
.33258000E+05	.33624000E+05	.33992000E+05	.34362000E+05	.34734000E+05
.35108000E+05	.35484000E+05	.35862000E+05	.36242000E+05	.36624000E+05
.37008000E+05	.37394000E+05	.37782000E+05	.38172000E+05	.38564000E+05
.38958000E+05	.39354000E+05	.39752000E+05	.40152000E+05	.40554000E+05
.40958000E+05	.41364000E+05	.41772000E+05	.42182000E+05	.42594000E+05
.43008000E+05	.43424000E+05	.43842000E+05	.44262000E+05	.44684000E+05
.45108000E+05	.45534000E+05	.45962000E+05	.46392000E+05	.46824000E+05
.47258000E+05	.47694000E+05	.48132000E+05	.48572000E+05	.49014000E+05
.49458000E+05	.49904000E+05	.50352000E+05	.50802000E+05	.51254000E+05
.51708000E+05	.52164000E+05	.52622000E+05	.53082000E+05	.53544000E+05
.54008000E+05	.54474000E+05	.54942000E+05	.55412000E+05	.55884000E+05
.56358000E+05	.56834000E+05	.57312000E+05	.57792000E+05	.58274000E+05
.58758000E+05	.59244000E+05	.59732000E+05	.60222000E+05	.60714000E+05
.61208000E+05	.61704000E+05	.62202000E+05	.62702000E+05	.63204000E+05
.63708000E+05	.64214000E+05	.64722000E+05	.65232000E+05	.65744000E+05
.66258000E+05	.66774000E+05	.67292000E+05	.67812000E+05	.68334000E+05
.68858000E+05	.69384000E+05	.69912000E+05	.70442000E+05	.70974000E+05
.71508000E+05	.72044000E+05	.72582000E+05	.73122000E+05	.73664000E+05
.74208000E+05	.74754000E+05	.75302000E+05	.75852000E+05	.76404000E+05
.76958000E+05	.77514000E+05	.78072000E+05	.78632000E+05	.79194000E+05
.79758000E+05	.80324000E+05	.80892000E+05	.81462000E+05	.82034000E+05
.82608000E+05	.83184000E+05	.83762000E+05	.84342000E+05	.84924000E+05
.85508000E+05	.86094000E+05	.86682000E+05	.87272000E+05	.87864000E+05
.88458000E+05	.89054000E+05	.89652000E+05	.90252000E+05	.90854000E+05
.91458000E+05	.92064000E+05	.92672000E+05	.93282000E+05	.93894000E+05
.94508000E+05	.95124000E+05	.95742000E+05	.96362000E+05	.96984000E+05
.97608000E+05	.98234000E+05	.98862000E+05	.99492000E+05	.10012400E+06
.10075800E+06	.10139400E+06	.10203200E+06	.10267200E+06	.10331400E+06
.10395800E+06	.10460400E+06	.10525200E+06	.10590200E+06	.10655400E+06
.10720800E+06	.10786400E+06	.10852200E+06	.10918200E+06	.10984400E+06
.11050800E+06	.11117400E+06	.11184200E+06	.11251200E+06	.11318400E+06
.11385800E+06	.11453400E+06	.11521200E+06	.11589200E+06	.11657400E+06
.11725800E+06	.11794400E+06	.11863200E+06	.11932200E+06	.12001400E+06
.12070800E+06	.12140400E+06	.12210200E+06	.12280200E+06	.12350400E+06
.12420800E+06	.12491400E+06	.12562200E+06	.12633200E+06	.12704400E+06
.12775800E+06	.12847400E+06	.12919200E+06	.12991200E+06	.13063400E+06
.13135800E+06	.13208400E+06	.13281200E+06	.13354200E+06	.13427400E+06
.13500800E+06	.13574400E+06	.13648200E+06	.13722200E+06	.13796400E+06
.13870800E+06	.13945400E+06	.14020200E+06	.14095200E+06	.14170400E+06
.14245800E+06	.14321400E+06	.14397200E+06	.14473200E+06	.14549400E+06
.14625800E+06	.14702400E+06	.14779200E+06	.14856200E+06	.14933400E+06
.15010800E+06	.15088400E+06	.15166200E+06	.15244200E+06	.15322400E+06
.15400800E+06	.15479400E+06	.15558200E+06	.15637200E+06	.15716400E+06
.15795800E+06	.15875400E+06	.15955200E+06	.16035200E+06	.16115400E+06
.16195800E+06	.16276400E+06	.16357200E+06	.16438200E+06	.16519400E+06
.16600800E+06	.16682400E+06	.16764200E+06	.16846200E+06	.16928400E+06
.17010800E+06	.17093400E+06	.17176200E+06	.17259200E+06	.17342400E+06
.17425800E+06	.17509400E+06	.17593200E+06	.17677200E+06	.17761400E+06
.17845800E+06	.17930400E+06	.18015200E+06	.18100200E+06	.18185400E+06
.18270800E+06	.18356400E+06	.18442200E+06	.18528200E+06	.18614400E+06
.18700800E+06	.18787400E+06	.18874200E+06	.18961200E+06	.19048400E+06
.19135800E+06	.19223400E+06	.19311200E+06	.19399200E+06	.19487400E+06
.19575800E+06	.19664400E+06	.19753200E+06	.19842200E+06	.19931400E+06
.20020800E+06	.20110400E+06	.20200200E+06	.20290200E+06	.20380400E+06
.20470800E+06	.20561400E+06	.20652200E+06	.20743200E+06	.20834400E+06
.20925800E+06	.21017400E+06	.21109200E+06	.21201200E+06	.21293400E+06
.21385800E+06	.21478400E+06	.21571200E+06	.21664200E+06	.21757400E+06
.21850800E+06	.21944400E+06	.22038200E+06	.22132200E+06	.22226400E+06
.22320800E+06	.22415400E+06	.22510200E+06	.22605200E+06	.22700400E+06
.22795800E+06	.22891400E+06	.22987200E+06	.23083200E+06	.23179400E+06
.23275800E+06	.23372400E+06	.23469200E+06	.23566200E+06	.23663400E+06
.23760800E+06	.23858400E+06	.23956200E+06	.24054200E+06	.24152400E+06
.24250800E+06	.24349400E+06	.24448200E+06	.24547200E+06	.24646400E+06
.24745800E+06	.24845400E+06	.24945200E+06	.25045200E+06	.25145400E+06
.25245800E+06	.25346400E+06	.25447200E+06	.25548200E+06	.25649400E+06
.25750800E+06	.25852400E+06	.25954200E+06	.26056200E+06	.26158400E+06
.26260800E+06	.26363400E+06	.26466200E+06	.26569200E+06	.26672400E+06
.26775800E+06	.26879400E+06	.26983200E+06	.27087200E+06	.27191400E+06
.27295800E+06	.27400400E+06	.27505200E+06	.27610200E+06	.27715400E+06
.27820800E+06	.27926400E+06	.28032200E+06	.28138200E+06	.28244400E+06
.28350800E+06	.28457400E+06	.28564200E+06	.28671200E+06	.28778400E+06
.28885800E+06	.28993400E+06	.29101200E+06	.29209200E+06	.29317400E+06
.29425800E+06	.29534400E+06	.29643200E+06	.29752200E+06	.29861400E+06
.29970800E+06	.30080400E+06	.30190200E+06	.30300200E+06	.30410400E+06
.30520800E+06	.30631400E+06	.30742200E+06	.30853200E+06	.30964400E+06
.31075800E+06	.31187400E+06	.31299200E+06	.31411200E+06	.31523400E+06
.31635800E+06	.31748400E+06	.31861200E+06	.31974200E+06	.32087400E+06
.32200800E+06	.32314400E+06	.32428200E+06	.32542200E+06	.32656400E+06
.32770800E+06	.32885400E+06	.32999200E+06	.33113200E+06	.33227400E+06
.33341800E+06	.33456400E+06	.33571200E+06	.33686200E+06	.33801400E+06
.33916800E+06	.34032400E+06	.34148200E+06	.34264200E+06	.34380400E+06
.34496800E+06	.34613400E+06	.34730200E+06	.34847200E+06	.34964400E+06
.35081800E+06	.35199400E+06	.35317200E+06	.35435200E+06	.35553400E+06
.35671800E+06	.35790400E+06	.35909200E+06	.36028200E+06	.36147400E+06
.36266800E+06	.36386400E+06	.36506200E+06	.36626200E+06	.36746400E+06
.36866800E+06	.36987400E+06	.37108200E+06	.37229200E+06	.37350400E+06
.37471800E+06	.37593400E+06	.37715200E+06	.37837200E+06	.37959400E+06
.38081800E+06	.38204400E+06	.38327200E+06	.38450200E+06	.38573400E+06
.38696800E+06	.38820400E+06	.38944200E+06	.39068200E+06	.39192400E+06
.39316800E+06	.39441400E+06	.39566200E+06	.39691200E+06	.39816400E+06
.39941800E+06	.40067400E+06	.40193200E+06	.40319200E+06	.40445400E+06
.40571800E+06	.40698400E+06	.40825200E+06	.40952200E+06	.41079400E+06
.41206800E+06	.41334400E+06	.41462200E+06	.41590200E+06	.41718400E+06
.41846800E+06	.41975400E+06	.42104200E+06	.42233200E+06	.42362400E+06
.42491800E+06	.42621400E+06	.42751200E+06	.42881200E+06	.43011400E+06
.43141800E+06	.43272400E+06	.43403200E+06	.43534200E+06	.43665400E+06
.43796800E+06	.43928400E+06	.44060200E+06	.44192200E+06	.44324400E+06
.44456800E+06	.44589400E+06	.44722200E+06	.44855200E+06	.44988400E+06
.45121800E+06	.45255400E+06	.45389200E+06	.45523200E+06	.45657400E+06
.45791800E+06	.45926400E+06	.46061200E+06	.46196200E+06	.46331400E+06
.46466800E+06	.46602400E+06	.46738200E+06	.46874200E+06	.47010400E+06
.47146800E+06	.47283400E+06	.47420200E+06	.47557200E+06	.47694400E+06
.47831800E+06	.47969400E+06	.48107200E+06	.48245200E+06	.48383400E+06
.48521800E+06	.48660400E+06	.48799200E+06	.48938200E+06	.49077400E+06
.49216800E+06	.49356400E+06	.49496200E+06	.49636200E+06	.49776400E+06
.49916800E+06	.50057400E+06	.50198200E+06	.50339200E+06	.50480400E+06
.50621800E+06	.50763400E+06	.50905200E+06	.51047200E+06	.51189400E+06
.51331800E+06	.51474400E+06	.51617200E+06	.51760200E+06	.51903400E+06
.52046800E+06	.52190400E+06	.52334200E+06	.52478200E+06	.52622400E+06
.52766800E+06	.52911400E+06	.53056200E+06	.53201200E+06	.53346400E+06
.53491800E+06	.53637400E+06	.53783200E+06	.53929200E+06	.54075400E+06
.54221800E+06	.54368400E+06	.54515200E+06	.54662200E+06	.54809400E+06
.54956800E+06	.55104400E+06	.55252200E+06	.55400200E+06	.55548400E+06
.55696800E+06	.55845400E+06	.55994200E+06	.56143200E+06	.56292400E+06
.56441800E+06	.56591400E+06	.56741200E+06	.56891200E+06	.57041400E+06
.57191800E+06	.57342400E+06	.57493200E+06	.57644200E+06	.57795400E+06
.57946800E+06	.58098400E+06	.58250200E+06	.58402200E+06	.58554400E+06
.58706800E+06	.58859400E+06	.59012200E+06	.59165200E+06	.59318400E+06
.59471800E+06	.59625400E+06	.59779200E+06	.59933200E+06	.60087400E+06
.60241800E+06	.60396400E+06	.60551200E+06	.60706200E+06	.60861400E+06
.61016800E+06	.61172400E+06	.61328200E+06	.61484200E+06	.61640400E+06
.61796800E+06	.61953400E+06	.62110200E+06	.62267200E+06	.62424400E+06
.62581800E+06	.62739400E+06	.62897200E+06	.63055200E+06	.63213400E+06
.63371800E+06	.63530400E+06	.63689200E+06	.63848200E+06	.64007400E+06
.64166800E+06	.64326400E+06	.64486200E+06	.64646200E+06	.64806400E+06
.64966800E+06	.65127400E+06	.65288200E+06	.65449200E+06	.65610400E+06
.65771800E+06	.65933400E+06	.66095200E+06	.66257200E+06	.66419400E+06
.66581800E+06	.66744400E+06	.66907200E+06	.67070200E+06	.67233400E+06
.67396800E+06	.67560400E+06	.67724200E+06	.67888200E+06	.68052400E+06
.68216800E+06	.68381400E+06	.68546200E+06	.68711200E+06	.68876400E+06
.69041800E+06	.69207400E+06	.69373200E+06	.69539200E+06	.69705400E+06
.69871800E+06	.70038400E+06	.70205200E+06	.70372200E+06	.70539400E+06
.70706800E+06	.70874400E+06	.71042200E+06	.71210200E+06	.71378400E+06
.71546800E+06	.71715400E+06	.71884200E+06	.72053200E+06	.72222400E+06
.72391800E+06	.72561400E+06	.72731200E+06	.72901200E+06	.73071400E+06
.73241800E+06	.73412400E+06	.73583200E+06	.73754200E+06	.73925400E+06
.74096800E+06	.74268400E+06	.74440200E+06	.74612200E+06	.74784400E+06
.74956800E+06	.75129400E+06	.75302200E+06	.75475200E+06	.75648400E+06
.75821800E+06	.75995400E+06	.76169200E+06	.76343200E+06	.76517400E+06
.76691800E+06	.76866400E+06	.77041200E+06	.77216200E+06	.77391400E+06
.77566800E+06	.77742400E+06	.77918200E+06	.78094200E+06	.78270400E+06
.78446800E+06	.78623400E+06	.78800200E+06	.78977200E+06	.79154400E+06
.79331800E+06	.79509400E+06	.79687200E+06	.79865200E+06	.80043400E+06
.80221800E+06	.80400400E+06	.80579200E+06	.80758200E+06	.80937400E+06
.81116800E+06	.81296400E+06	.81476200E+06	.81656200E+06	.81836400E+06
.82016800E+06	.82197400E+06	.82378200E+06	.82559200E+06	.82740400E+06
.82921800E+06	.83103400E+06	.83285200E+06	.83467200E+06	.83649400E+06
.83831800E+06	.84014400E+06	.84197200E+06	.84380200E+06	.84563400E+06
.84746800E+06	.84930400E+06	.85114200E+06	.85298200E+06	.85482400E+06
.85666800E+06	.85851400E+06	.86036200E+06	.86221200E+06	.86406400E+06
.86591800E+06	.86777400E+06	.86963200E+06	.87149200E+06	.87335400E+06
.87521800E+06	.87708400E+06	.87895200E+06	.88082200E+06	.88269400E+06
.88456800E+06	.88644400E+06	.88832200E+06	.89020200E+06	.89208400E+06
.89396800E+06	.89585400E+06	.89774200E+06	.89963200E+06	.90152400E+06
.90341800E+06	.90531400E+06	.90721200E+06	.90911200E+06	.91101400E+06
.91291800E+06	.91482400E+06	.91673200E+06	.91864200E+06	.92055400E+06
.92246800E+06	.92438400E+06	.92630200E+06	.92822200E+06	.93014400E+06
.93206800E+06	.93399400E+06	.93592200E+06	.93785200E+06	.93978400E+06
.94171800E+06	.94365400E+06	.94559200E+06	.94753200E+06	.94947400E+06
.95141800E+06	.95336400E+06	.95531200E+06	.95726200E+06	.95921400E+06
.96116800E+06	.96312400E+06	.96508200E+06	.96704200E+06	.96900400E+06
.97096800E+06	.97293400E+06	.97490200E+06	.97687200E+06	.97884400E+06
.98081800E+06	.98279400E+06	.98477200E+06	.98675200E+06	.98873400E+06
.99071800E+06	.99270400E+06	.99469200E+06	.99668200E+06	.99867400E+06

CRYS/DERI/ASIL FE(80%) - GE(20%) 18/7/77

ADDITIONAL VIBT FOR DERILOG= 0.0000
LMAX= 2
NUMBER OF ENERGIES= 60
BOTTOM ENERGY= 0.0100
STEP ENERGY= 0.0200

LOGARITHMIC DERIVATIVES FOR L=0 TO L=2

ENERGY	L=0	L=1	L=2
0.0100	-.7447466E+00	.1601873E-01	.7201751E+00
0.0300	-.7755524E+00	.1801869E-02	.7109542E+00
0.0500	-.8071238E+00	-.1259550E-01	.7017378E+00
0.0700	-.8394841E+00	-.2709483E-01	.6925232E+00
0.0900	-.8727085E+00	-.4178990E-01	.6833081E+00
0.1100	-.9067947E+00	-.5665401E-01	.6740901E+00
0.1300	-.9417975E+00	-.7169300E-01	.6648670E+00
0.1500	-.9777605E+00	-.8690921E-01	.6556367E+00
0.1700	-.1014730E+01	-.1023070E+00	.6463973E+00
0.1900	-.1052756E+01	-.1179225E+00	.6371467E+00
0.2100	-.1091892E+01	-.1336606E+00	.6278831E+00
0.2300	-.1132192E+01	-.1496407E+00	.6186044E+00
0.2500	-.1173719E+01	-.1658135E+00	.6093100E+00
0.2700	-.1216530E+01	-.1821924E+00	.5999971E+00
0.2900	-.1260714E+01	-.1987424E+00	.5906644E+00
0.3100	-.1306326E+01	-.2155892E+00	.5813105E+00
0.3300	-.1353453E+01	-.2326402E+00	.5719337E+00
0.3500	-.1402180E+01	-.2499125E+00	.5625326E+00
0.3700	-.1452601E+01	-.2673670E+00	.5531059E+00
0.3900	-.1504816E+01	-.2850090E+00	.5436520E+00
0.4100	-.1558933E+01	-.3029702E+00	.5341697E+00
0.4300	-.1615069E+01	-.3213112E+00	.5246575E+00
0.4500	-.1673352E+01	-.3399051E+00	.5151142E+00
0.4700	-.1733921E+01	-.3588672E+00	.5055385E+00
0.4900	-.1796924E+01	-.3782051E+00	.4959291E+00
0.5100	-.1862537E+01	-.3979206E+00	.4862840E+00
0.5300	-.1930939E+01	-.4180400E+00	.4766043E+00
0.5500	-.2002285E+01	-.4386538E+00	.4668803E+00
0.5700	-.2076810E+01	-.4596769E+00	.4571298E+00
0.5900	-.2154781E+01	-.4772104E+00	.4473335E+00
0.6100	-.2236437E+01	-.4983479E+00	.4374962E+00
0.6300	-.2322006E+01	-.5199256E+00	.4276167E+00
0.6500	-.2411989E+01	-.5408517E+00	.4176939E+00
0.6700	-.2506556E+01	-.5627673E+00	.4077265E+00
0.6900	-.2606160E+01	-.5851535E+00	.3977134E+00
0.7100	-.2711241E+01	-.6077322E+00	.3876535E+00
0.7300	-.2822291E+01	-.6307858E+00	.3775455E+00
0.7500	-.2939861E+01	-.6542572E+00	.3673884E+00
0.7700	-.3064578E+01	-.6781498E+00	.3571809E+00
0.7900	-.3197139E+01	-.7024777E+00	.3469218E+00
0.8100	-.3338352E+01	-.7272557E+00	.3366100E+00
0.8300	-.3489120E+01	-.7524991E+00	.3262443E+00
0.8500	-.3650518E+01	-.7782241E+00	.3158235E+00
0.8700	-.3823726E+01	-.8044476E+00	.3053466E+00
0.8900	-.4010151E+01	-.8311873E+00	.2948118E+00
0.9100	-.4211419E+01	-.8584619E+00	.2842185E+00

0.9300	-.4429436E+01	-.8862907E+00	.2735652E+00
0.9500	-.4666450E+01	-.9148944E+00	.2628507E+00
0.9700	-.4925128E+01	-.9436944E+00	.2527738E+00
0.9900	-.5208664E+01	-.9733153E+00	.2412332E+00
1.0100	-.5520911E+01	-.1005575E+01	.2303276E+00
1.0300	-.5866562E+01	-.1031504E+01	.2193557E+00
1.0500	-.6251393E+01	-.1058128E+01	.2083191E+00
1.0700	-.6681594E+01	-.1084473E+01	.1972077E+00
1.0900	-.7169227E+01	-.1131570E+01	.1860205E+00
1.1100	-.7722809E+01	-.1159449E+01	.1747705E+00
1.1300	-.8350657E+01	-.1299143E+01	.1634550E+00
1.1500	-.9064429E+01	-.1233607E+01	.1520571E+00
1.1700	-.9875278E+01	-.1272117E+01	.1405832E+00
1.1900	-.1079651E+02	-.1309472E+01	.1290320E+00

PHASE SHIFTS

ENERGY.	L=0	L=1	L=2
0.0100	-.5341144E+00	.2241289E-02	.9355811E-06
0.0300	-.3504246E+00	.1181950E-01	.1469624E-04
0.0500	-.1056295E+01	.2573324E-01	.5306398E-04
0.0700	-.1197612E+01	.4394416E-01	.1238139E-03
0.0900	-.1307222E+01	.6331055E-01	.2333363E-03
0.1100	-.1397911E+01	.8620562E-01	.3871690E-03
0.1300	-.1475677E+01	.1115539E+00	.5903803E-03
0.1500	-.1543825E+01	.1387778E+00	.8473934E-03
0.1700	-.1539922E+01	.1677756E+00	.1162362E-02
0.1900	-.1481839E+01	.1985507E+00	.1539089E-02
0.2100	-.1431421E+01	.2301195E+00	.1980997E-02
0.2300	-.1384858E+01	.2629542E+00	.2491351E-02
0.2500	-.1341536E+01	.2951484E+00	.3073082E-02
0.2700	-.1300977E+01	.3279926E+00	.3728905E-02
0.2900	-.1262805E+01	.3629889E+00	.4461311E-02
0.3100	-.1226716E+01	.3969570E+00	.5272581E-02
0.3300	-.1192401E+01	.4285412E+00	.6164798E-02
0.3500	-.1159835E+01	.4602153E+00	.7139852E-02
0.3700	-.1128667E+01	.4900858E+00	.8199452E-02
0.3900	-.1098811E+01	.5203937E+00	.9345120E-02
0.4100	-.1070144E+01	.5486140E+00	.1057825E-01
0.4300	-.1042559E+01	.5751549E+00	.1190011E-01
0.4500	-.1015903E+01	.6008547E+00	.1331145E-01
0.4700	-.9902776E+00	.6247789E+00	.1481347E-01
0.4900	-.9654306E+00	.6472193E+00	.1640679E-01
0.5100	-.9413603E+00	.6681754E+00	.1809202E-01
0.5300	-.9180114E+00	.6879409E+00	.1986990E-01
0.5500	-.8953347E+00	.7057699E+00	.2173934E-01
0.5700	-.8732861E+00	.7224893E+00	.2370292E-01
0.5900	-.8518259E+00	.7378927E+00	.2575489E-01
0.6100	-.8309186E+00	.7522384E+00	.2790764E-01
0.6300	-.8105316E+00	.7649875E+00	.3014877E-01
0.6500	-.7906356E+00	.7768026E+00	.3248254E-01
0.6700	-.7712037E+00	.7875460E+00	.3490787E-01
0.6900	-.7522115E+00	.7972775E+00	.3742439E-01
0.7100	-.7336360E+00	.8059822E+00	.4003139E-01
0.7300	-.7154578E+00	.8137551E+00	.4272805E-01
0.7500	-.6976567E+00	.8210112E+00	.4551343E-01
0.7700	-.6802134E+00	.8272844E+00	.4838648E-01
0.7900	-.6631178E+00	.8329253E+00	.5134605E-01
0.8100	-.6463483E+00	.8378815E+00	.5439087E-01
0.8300	-.6298935E+00	.8421909E+00	.5751957E-01
0.8500	-.6137400E+00	.8455199E+00	.6073068E-01
0.8700	-.5978756E+00	.8483779E+00	.6402264E-01
0.8900	-.5822880E+00	.8511179E+00	.6739376E-01
0.9100	-.5669673E+00	.8531718E+00	.7084250E-01
0.9300	-.5519008E+00	.8547717E+00	.7436638E-01
0.9500	-.5370818E+00	.8559479E+00	.7796408E-01
0.9700	-.5225157E+00	.8567207E+00	.8163337E-01
0.9900	-.5081700E+00	.8571492E+00	.8537214E-01
1.0100	-.4940460E+00	.8572071E+00	.8917819E-01
1.0300	-.4801378E+00	.8569520E+00	.9304928E-01
1.0500	-.4664393E+00	.8563964E+00	.9698307E-01
1.0700	-.4529411E+00	.8555630E+00	.1009772E+00
1.0900	-.4396381E+00	.8544013E+00	.1050291E+00
1.1100	-.4265244E+00	.8531176E+00	.1091364E+00
1.1300	-.4135943E+00	.8515450E+00	.1132964E+00

1.1500	.4008424E+00	.8497585E+00	.1175066E+00
1.1700	.3882636E+00	.8477722E+00	.1217642E+00
1.1900	.3758530E+00	.8455990E+00	.1260666E+00

CEN
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0.0100	.7323865E+01	.6596985E+03	.1121592E+07
0.0300	.1369973E+01	.1285846E+03	.7152174E+05
0.0500	.1083597E+01	.6052069E+02	.1084407E+05
0.0700	.9351944E+00	.3796325E+02	.4520596E+04
0.0900	.8422592E+00	.2570670E+02	.2529891E+04
0.1100	.7786447E+00	.1926605E+02	.1735193E+04
0.1300	.7299380E+00	.1518696E+02	.1397475E+04
0.1500	.6949844E+00	.1249771E+02	.1254878E+04
0.1700	.6687785E+00	.1041389E+02	.9167609E+03
0.1900	.6482152E+00	.8921836E+01	.6936525E+03
0.2100	.6259158E+00	.7777496E+01	.5402388E+03
0.2300	.6109347E+00	.6870701E+01	.4305209E+03
0.2500	.5986001E+00	.6133964E+01	.3496969E+03
0.2700	.5884197E+00	.5533093E+01	.2889399E+03
0.2900	.5800239E+00	.5037274E+01	.2426606E+03
0.3100	.5731291E+00	.4614498E+01	.2059916E+03
0.3300	.5675134E+00	.4253606E+01	.1759917E+03
0.3500	.5630023E+00	.3942516E+01	.1523162E+03
0.3700	.5594530E+00	.3672030E+01	.1329478E+03
0.3900	.5567505E+00	.3435020E+01	.1169273E+03
0.4100	.5547996E+00	.3225933E+01	.1035443E+03
0.4300	.5535209E+00	.3040301E+01	.9226426E+02
0.4500	.5528477E+00	.2874569E+01	.8267932E+02
0.4700	.5527229E+00	.2725841E+01	.7447431E+02
0.4900	.5530978E+00	.2591744E+01	.6740287E+02
0.5100	.5539299E+00	.2470316E+01	.6127036E+02
0.5300	.5551821E+00	.2359921E+01	.5592152E+02
0.5500	.5568214E+00	.2259188E+01	.5123138E+02
0.5700	.5588101E+00	.2166956E+01	.4709852E+02
0.5900	.5611453E+00	.2082240E+01	.4344092E+02
0.6100	.5637781E+00	.2004195E+01	.4018755E+02
0.6300	.5666934E+00	.1932098E+01	.3728447E+02
0.6500	.5698686E+00	.1865321E+01	.3468355E+02
0.6700	.5732824E+00	.1803320E+01	.3234512E+02
0.6900	.5769132E+00	.1745620E+01	.3023573E+02
0.7100	.5807375E+00	.1691807E+01	.2832702E+02
0.7300	.5847391E+00	.1641513E+01	.2659479E+02
0.7500	.5888888E+00	.1594417E+01	.2501836E+02
0.7700	.5931639E+00	.1550233E+01	.2357092E+02
0.7900	.5975379E+00	.1508707E+01	.2224412E+02
0.8100	.6019817E+00	.1469612E+01	.2103568E+02
0.8300	.6064632E+00	.1432746E+01	.1994891E+02
0.8500	.6109464E+00	.1397927E+01	.1897280E+02
0.8700	.6153909E+00	.1364991E+01	.1809548E+02
0.8900	.6197519E+00	.1333792E+01	.1731415E+02
0.9100	.6239742E+00	.1304196E+01	.1663098E+02
0.9300	.6280005E+00	.1276081E+01	.1605789E+02
0.9500	.6317607E+00	.1249339E+01	.1558153E+02
0.9700	.6351744E+00	.1223859E+01	.1521312E+02
0.9900	.6381482E+00	.1199581E+01	.1494841E+02
1.0100	.6405732E+00	.1176389E+01	.1478301E+02
1.0300	.6423215E+00	.1154218E+01	.1471532E+02
1.0500	.6432432E+00	.1132998E+01	.1474205E+02
1.0700	.6431595E+00	.1112693E+01	.1485640E+02
1.0900	.6419612E+00	.1093154E+01	.1504055E+02

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1.1100   .6320972L+00   .1074415E+01   .1071074E+02
1.1300   .6345641L+00   .1053395E+01   .1032494E+02
1.1500   .6279142E+00   .1039046E+01   .9961325E+01
1.1700   .6187014L+00   .1022325E+01   .9618242E+01
1.1900   .6064032L+00   .1006190E+01   .9294184E+01


FERMI LEVEL=    1.16916      RYDBERGS
VALENCE=   4.000000
FOR L = 0   PHASESHIFT AT FERMI LEVEL= -2.75280175
FOR L = 1   PHASESHIFT AT FERMI LEVEL=  0.04785990
FOR L = 2   PHASESHIFT AT FERMI LEVEL=  0.12158353
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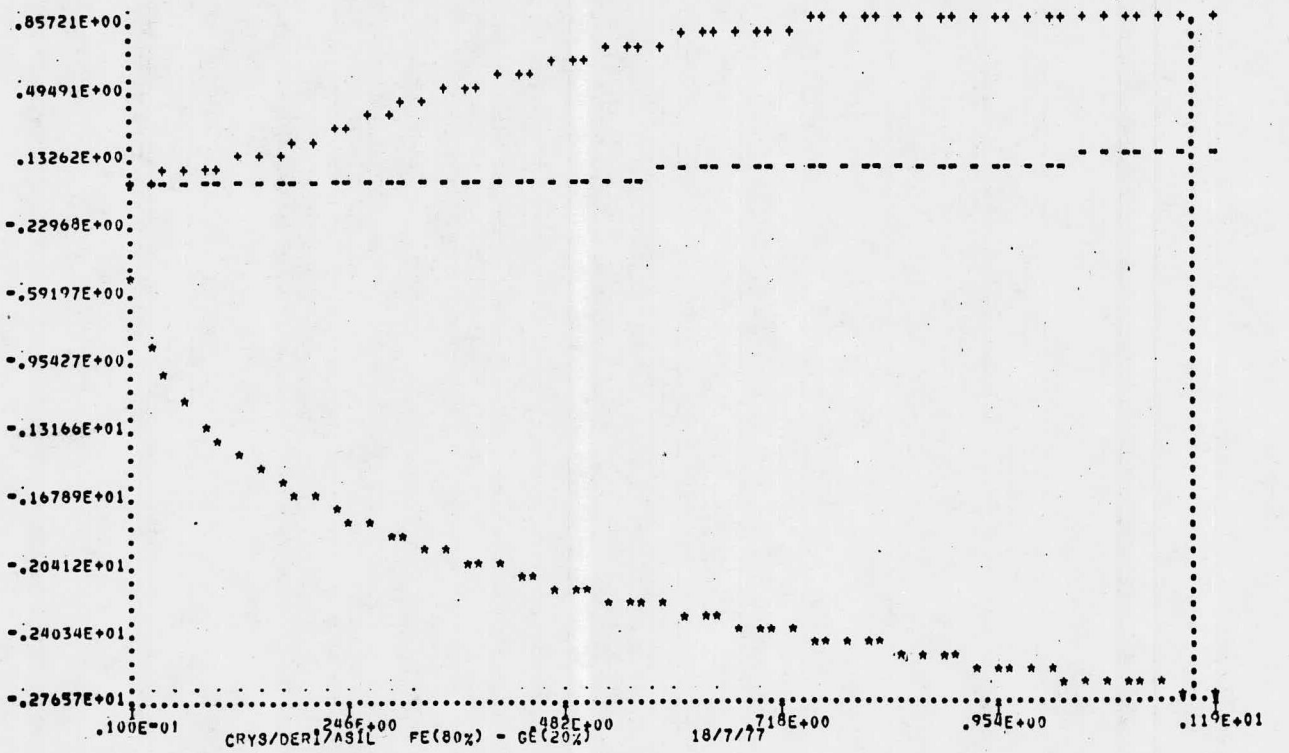
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-.27657E+01
.100E-01
.246E+00
.482E+00
.718E+00
.954E+00
.119E+01
CRYS/DERIVASIL FE(80%) - GE(20%)
18/7/77

CENTRAL ATOM OF TYPE 1

RESULTS FOR MUFFIN TIN WITH RI(1)= 2.4412 RI(2)= 2.4412 RO= 2.7566 V BOUNDARY= -.1050246E+01
VINT= -.1488658E+01 Z= 26.00 JRI(1)=194.850000 JRI(2)=194.850000 LAT= 6
XALPHA= 0.6666667 XBETA= 0.0030000

-.34484092E+06	-.32001594E+06	-.31201152E+06	-.29678764E+06	-.28230624E+06
-.26853194E+06	-.25542777E+06	-.24296350E+06	-.23110711E+06	-.21982856E+06
-.20911005E+06	-.19894554E+06	-.18931884E+06	-.17999496E+06	-.17117150E+06
-.16281842E+06	-.15488081E+06	-.14730881E+06	-.14011750E+06	-.13327692E+06
-.12676995E+06	-.12058032E+06	-.11469256E+06	-.10909194E+06	-.10376446E+06
-.98667975E+05	-.93787274E+05	-.89290444E+05	-.84929037E+05	-.80779945E+05
-.76833109E+05	-.73078397E+05	-.69503768E+05	-.66110600E+05	-.62879101E+05
-.59805277E+05	-.56881250E+05	-.54099773E+05	-.51453883E+05	-.48936954E+05
-.46542695E+05	-.44265104E+05	-.42098511E+05	-.40037485E+05	-.38076862E+05
-.36211704E+05	-.34437509E+05	-.32749706E+05	-.31144106E+05	-.29616708E+05
-.28163716E+05	-.26781485E+05	-.25466667E+05	-.24215773E+05	-.23025801E+05
-.21893920E+05	-.20817121E+05	-.19792806E+05	-.18818302E+05	-.17891429E+05
-.17009671E+05	-.16170450E+05	-.15372029E+05	-.14613897E+05	-.13891845E+05
-.13204097E+05	-.12548161E+05	-.11921705E+05	-.11323873E+05	-.10752462E+05
-.10205414E+05	-.97325659E+04	-.92824772E+04	-.88529926E+04	-.84429520E+04
-.80513328E+04	-.76771733E+04	-.73196591E+04	-.69780265E+04	-.66514612E+04
-.63391240E+04	-.60402526E+04	-.57540401E+04	-.54797933E+04	-.52168233E+04
-.49644578E+04	-.47220401E+04	-.44889933E+04	-.42647727E+04	-.40488470E+04
-.38406900E+04	-.36397922E+04	-.34457509E+04	-.32581470E+04	-.30765992E+04
-.29007555E+04	-.27302877E+04	-.25648859E+04	-.24042499E+04	-.22480877E+04
-.20961240E+04	-.19480900E+04	-.18037277E+04	-.16628205E+04	-.15251592E+04
-.13905182E+04	-.12586977E+04	-.11294040E+04	-.10024407E+04	-.87770048E+03
-.75502205E+03	-.63427185E+03	-.51532178E+03	-.39805332E+03	-.28234262E+03
-.16808127E+03	-.55332826E+02	-.55332826E+02	-.16808127E+03	-.28234262E+03
-.39805332E+03	-.51532178E+03	-.63427185E+03	-.75502205E+03	-.87770048E+03
-.10024407E+04	-.11294040E+04	-.12586977E+04	-.13905182E+04	-.15251592E+04
-.16628205E+04	-.18037277E+04	-.19480900E+04	-.20961240E+04	-.22480877E+04
-.24042499E+04	-.25648859E+04	-.27302877E+04	-.29007555E+04	-.30765992E+04
-.32581470E+04	-.34457509E+04	-.36397922E+04	-.38406900E+04	-.40488470E+04
-.42647727E+04	-.44889933E+04	-.47220401E+04	-.49644578E+04	-.52168233E+04
-.54797933E+04	-.57540401E+04	-.60402526E+04	-.63391240E+04	-.66514612E+04
-.69780265E+04	-.73196591E+04	-.76771733E+04	-.80513328E+04	-.84429520E+04
-.88529926E+04	-.92824772E+04	-.97325659E+04	-.10205414E+05	-.10752462E+05
-.11323873E+05	-.11921705E+05	-.12548161E+05	-.13204097E+05	-.13891845E+05
-.14613897E+05	-.15372029E+05	-.16170450E+05	-.17009671E+05	-.17891429E+05
-.18818302E+05	-.19792806E+05	-.20817121E+05	-.21893920E+05	-.23025801E+05
-.24215773E+05	-.25466667E+05	-.26781485E+05	-.28163716E+05	-.29616708E+05
-.31144106E+05	-.32749706E+05	-.34437509E+05	-.36211704E+05	-.38076862E+05
-.40037485E+05	-.42098511E+05	-.44265104E+05	-.46542695E+05	-.48936954E+05
-.51453883E+05	-.54099773E+05	-.56881250E+05	-.59805277E+05	-.62879101E+05
-.66110600E+05	-.69503768E+05	-.73078397E+05	-.76833109E+05	-.80779945E+05
-.84929037E+05	-.89290444E+05	-.93876274E+05	-.98667975E+05	-.10376446E+06
-.10909194E+06	-.11469256E+06	-.12058032E+06	-.12676995E+06	-.13327692E+06
-.14011750E+06	-.14730881E+06	-.15488081E+06	-.16281842E+06	-.17117150E+06
-.17999496E+06	-.18931884E+06	-.19894554E+06	-.20911005E+06	-.21982856E+06
-.23110711E+06	-.24296350E+06	-.25542777E+06	-.26853194E+06	-.28230624E+06
-.29678764E+06	-.31201152E+06	-.32001594E+06	-.34484092E+06	
0.	0.	0.	0.	0.
0.	0.	0.	0.	0.
0.	0.	0.	0.	0.
0.	0.	0.	0.	0.

CRYS/DERI/ASIL   FE(80%) - GE(20%)   18/7/77

R*V(R)

.51978707E+02	.51977604E+02	.51976444E+02	.51975224E+02	.51973940E+02
.51972589E+02	.51971169E+02	.51969674E+02	.51968103E+02	.51966449E+02
.51964709E+02	.51962879E+02	.51960954E+02	.51958929E+02	.51956798E+02
.51954557E+02	.51952199E+02	.51949718E+02	.51947108E+02	.51944362E+02
.51941472E+02	.51938432E+02	.51935234E+02	.51931868E+02	.51928326E+02
.51924599E+02	.51920676E+02	.51916547E+02	.51912199E+02	.51907619E+02
.51902793E+02	.51897704E+02	.51892336E+02	.51886667E+02	.51880677E+02
.51874341E+02	.51867628E+02	.51860517E+02	.51852973E+02	.51844958E+02
.51836437E+02	.51827366E+02	.51817726E+02	.51807464E+02	.51796522E+02
.51784880E+02	.51772463E+02	.51759274E+02	.51745242E+02	.51730300E+02
.51714433E+02	.51697555E+02	.51679691E+02	.51660734E+02	.51640621E+02
.51617350E+02	.51596795E+02	.51573015E+02	.51547840E+02	.51521224E+02
.51493204E+02	.51463534E+02	.51432308E+02	.51399391E+02	.51364645E+02
.51328079E+02	.51289484E+02	.51248926E+02	.51206215E+02	.51161199E+02
.51113875E+02	.51063996E+02	.51011608E+02	.50956493E+02	.50898465E+02
.50837497E+02	.50773319E+02	.50705930E+02	.50635097E+02	.50560607E+02
.50482382E+02	.50400139E+02	.50313835E+02	.50223206E+02	.50128012E+02
.50028142E+02	.49923291E+02	.49813374E+02	.49698102E+02	.49577197E+02
.49450534E+02	.49317806E+02	.49178856E+02	.49033400E+02	.48881155E+02
.48721956E+02	.48555501E+02	.48381581E+02	.48199937E+02	.48010294E+02
.47812436E+02	.47600091E+02	.47391008E+02	.47166942E+02	.46933624E+02
.46690798E+02	.46438230E+02	.46175572E+02	.45902589E+02	.45617013E+02
.45324470E+02	.45018750E+02	.44701350E+02	.44371969E+02	.44030313E+02
.43675809E+02	.43308225E+02	.42926713E+02	.42531509E+02	.42121809E+02
.41697284E+02	.41258926E+02	.40803929E+02	.40335398E+02	.39853367E+02
.39358717E+02	.38852967E+02	.38337644E+02	.37813945E+02	.37282771E+02
.36744352E+02	.36197914E+02	.35642637E+02	.35076820E+02	.34498790E+02
.33907600E+02	.33302123E+02	.32682388E+02	.32048460E+02	.31400678E+02
.30740118E+02	.30067630E+02	.29384233E+02	.28691022E+02	.27988857E+02
.27278419E+02	.26560386E+02	.25834536E+02	.25100728E+02	.24358575E+02
.23606495E+02	.22843528E+02	.22067660E+02	.21277581E+02	.20473904E+02
.19658628E+02	.18838488E+02	.18024428E+02	.17228044E+02	.16457491E+02
.15713791E+02	.14988005E+02	.14269881E+02	.13548211E+02	.12816403E+02
.12074273E+02	.11323295E+02	.10567693E+02	.98120987E+01	.99608929E+01
.83186466E+01	.75894525E+01	.68762495E+01	.61818912E+01	.55086979E+01
.48574539E+01	.42293011E+01	.36238929E+01	.30406678E+01	.24792657E+01
.19379420E+01	.14154472E+01	.91093483E+00	.42321681E+00	-.48971837E-01
-.50511636E+00	-.94562341E+00	-.13686778E+01	-.17730855E+01	-.21586470E+01
-.25223814E+01	-.28643955E+01	-.31822136E+01	-.34749972E+01	-.37415927E+01
-.39780894E+01	-.41625587E+01	-.43516870E+01	-.44801972E+01	-.45577827E+01
-.45027962E+01	-.44457322E+01	-.40929887E+01	-.32766828E+01	-.16555632E+01
.75027905E+00	.29593268E+01	.13192265E+02	.25733800E+02	.14992773E+02
.15418951E+01	-.20501763E+01	-.56616886E+01	-.73593008E+01	-.29011884E+02
.56464424E+01	.71120523E-01	-.64506372E+01	.50853940E+01	.23827667E+02
.69863538E+01	-.31952313E+01	.98592218E+01	-.31923254E+01	.72259515E+01

CRYS/DERI/ASIL FE(80%) - GE(20%) 18/7/77

ADDITIONAL VINT FOR DERILOG= 0.0000
LMAX= 2
NUMBER OF ENERGIES= 60
BOTTOM ENERGY= 0.0100
STEP ENERGY= 0.0200

LOGARITHMIC DERIVATIVES FOR L=0 TO L=2

ENERGY	L=0	L=1	L=2
0.0100	.1644287E+00	.5067206E+00	.5836278E+00
0.0300	.1529185E+00	.4976190E+00	.5716102E+00
0.0500	.1413185E+00	.4884678E+00	.5593770E+00
0.0700	.1296271E+00	.4792753E+00	.5469206E+00
0.0900	.1178429E+00	.4700378E+00	.5342270E+00
0.1100	.1059643E+00	.4607546E+00	.5212853E+00
0.1300	.9398952E-01	.4514251E+00	.5080837E+00
0.1500	.8191705E-01	.4420485E+00	.4946054E+00
0.1700	.6974508E-01	.4326241E+00	.4808387E+00
0.1900	.5747192E-01	.4231511E+00	.4667666E+00
0.2100	.4509576E-01	.4136287E+00	.4523715E+00
0.2300	.3261476E-01	.4040560E+00	.4376369E+00
0.2500	.2002708E-01	.3944322E+00	.4225459E+00
0.2700	.7320849E-02	.3847564E+00	.4070844E+00
0.2900	-.5417099E-01	.3750277E+00	.3912170E+00
0.3100	-.1810769E-01	.3652450E+00	.3749907E+00
0.3300	-.3100303E-01	.3554076E+00	.3584067E+00
0.3500	-.4401853E-01	.3455146E+00	.3414667E+00
0.3700	-.5705184E-01	.3355648E+00	.3241490E+00
0.3900	-.7124337E-01	.3255573E+00	.3064576E+00
0.4100	-.8475854E-01	.3154913E+00	.2883875E+00
0.4300	-.9839966E-01	.3053640E+00	.2699615E+00
0.4500	-.1121692E+00	.2951775E+00	.2511518E+00
0.4700	-.1260696E+00	.2849302E+00	.2319807E+00
0.4900	-.1401034E+00	.2746212E+00	.2124139E+00
0.5100	-.1542733E+00	.2642496E+00	.1924506E+00
0.5300	-.1685820E+00	.2538142E+00	.1720841E+00
0.5500	-.1830325E+00	.2433145E+00	.1513092E+00
0.5700	-.1976269E+00	.2327496E+00	.1301187E+00
0.5900	-.2123667E+00	.2221187E+00	.1085043E+00
0.6100	-.2272610E+00	.2114214E+00	.8645354E-01
0.6300	-.2423006E+00	.2006191E+00	.5002932E-01
0.6500	-.2575093E+00	.1899976E+00	.2000661E-01
0.6700	-.2728712E+00	.1791000E+00	-.1166610E-01
0.6900	-.2883907E+00	.1681431E+00	-.4523201E-01
0.7100	-.3040880E+00	.1571077E+00	-.8084279E-01
0.7300	-.3199514E+00	.1459988E+00	-.1187644E+00
0.7500	-.3359880E+00	.1348151E+00	-.1592841E+00
0.7700	-.3522024E+00	.1235554E+00	-.2027302E+00
0.7900	-.3685993E+00	.1122196E+00	-.2495279E+00
0.8100	-.3851802E+00	.1008032E+00	-.3001203E+00
0.8300	-.4019514E+00	.8930820E-01	-.3551050E+00
0.8500	-.4189176E+00	.7773213E-01	-.4151552E+00
0.8700	-.4360817E+00	.6607397E-01	-.4811255E+00
0.8900	-.4534493E+00	.5433153E-01	-.5535273E+00
0.9100	-.4710245E+00	.4250427E-01	-.7264279E+00

0.9300	-.4888123E+00	.3059048E-01	-.8296641E+00
0.9500	-.5068177E+00	.1853872E-01	-.9477949E+00
0.9700	-.5250459E+00	.6497513E-02	-.1084572E+01
0.9900	-.5435021E+00	-.5684661E-02	-.1245134E+01
1.0100	-.5621920E+00	-.1795934E-01	-.1436697E+01
1.0300	-.5811210E+00	-.3032811E-01	-.1669753E+01
1.0500	-.6002953E+00	-.4279257E-01	-.1960032E+01
1.0700	-.6197207E+00	-.5535439E-01	-.2332571E+01
1.0900	-.6394036E+00	-.6801524E-01	-.2829342E+01
1.1100	-.6593504E+00	-.8077636E-01	-.3526799E+01
1.1300	-.6795680E+00	-.9364101E-01	-.4580352E+01
1.1500	-.7000631E+00	-.1066095E+00	-.6361753E+01
1.1700	-.7208431E+00	-.1198842E+00	-.1003652E+02
1.1900	-.7419153E+00	-.1328669E+00	-.2210818E+02

PHASE SHIFTS

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ENERGY	L=0	L=1	L=2
0.0100	-.7105503E-01	-.3665408E-03	.2443808E-05
0.0300	-.1241500E+00	-.1063676E-02	.3842974E-04
0.0500	-.1603287E+00	-.3733741E-02	.1390998E-03
0.0700	-.1857651E+00	-.8387945E-02	.3257986E-03
0.0900	-.2152436E+00	-.1532746E-01	.6171453E-03
0.1100	-.2381338E+00	-.1210610E-01	.1030600E-02
0.1300	-.2548007E+00	-.1529350E-01	.1586366E-02
0.1500	-.2715139E+00	-.1957145E-01	.2293427E-02
0.1700	-.2952147E+00	-.2201332E-01	.3178017E-02
0.1900	-.3132590E+00	-.2553702E-01	.4256231E-02
0.2100	-.3294437E+00	-.2715742E-01	.5540801E-02
0.2300	-.3440901E+00	-.3284751E-01	.7074096E-02
0.2500	-.3509533E+00	-.3659580E-01	.8860137E-02
0.2700	-.3732956E+00	-.4039182E-01	.1092016E-01
0.2900	-.3870617E+00	-.4422662E-01	.1330900E-01
0.3100	-.4009412E+00	-.4809248E-01	.1603308E-01
0.3300	-.4158411E+00	-.5198275E-01	.1913350E-01
0.3500	-.4283195E+00	-.5589195E-01	.2264900E-01
0.3700	-.4331669E+00	-.5981106E-01	.2660000E-01
0.3900	-.4554150E+00	-.6374544E-01	.3111087E-01
0.4100	-.4616755E+00	-.6767338E-01	.3616138E-01
0.4300	-.4715926E+00	-.7160134E-01	.4184400E-01
0.4500	-.4811033E+00	-.7553001E-01	.4826700E-01
0.4700	-.4956012E+00	-.7947317E-01	.5540887E-01
0.4900	-.5050037E+00	-.8341352E-01	.6347054E-01
0.5100	-.5159911E+00	-.8733153E-01	.7255533E-01
0.5300	-.5261806E+00	-.9125194E-01	.8278495E-01
0.5500	-.5360000E+00	-.9512402E-01	.9433612E-01
0.5700	-.5460435E+00	-.9903755E-01	.1074021E+00
0.5900	-.5557247E+00	-.1029107E+00	.1222553E+00
0.6100	-.5652515E+00	-.1067603E+00	.1390976E+00
0.6300	-.5716321E+00	-.1106111E+00	.1583769E+00
0.6500	-.5833732E+00	-.1144369E+00	.1805043E+00
0.6700	-.5929810E+00	-.1182457E+00	.2060208E+00
0.6900	-.6019624E+00	-.1220308E+00	.2356305E+00
0.7100	-.6100223E+00	-.1258097E+00	.2702011E+00
0.7300	-.6195657E+00	-.1295041E+00	.3108142E+00
0.7500	-.6281974E+00	-.1332977E+00	.3588733E+00
0.7700	-.6367221E+00	-.1370191E+00	.4161535E+00
0.7900	-.6451438E+00	-.1407132E+00	.4848316E+00
0.8100	-.6534665E+00	-.1443908E+00	.5675408E+00
0.8300	-.6616937E+00	-.1480408E+00	.6672322E+00
0.8500	-.6698290E+00	-.1516872E+00	.7866524E+00
0.8700	-.6778755E+00	-.1553059E+00	.9273749E+00
0.8900	-.6858362E+00	-.1589049E+00	.1088124E+01
0.9100	-.6937141E+00	-.1624813E+00	.1263528E+01
0.9300	-.7015119E+00	-.1660441E+00	.1462693E+01
0.9500	-.7092329E+00	-.1695844E+00	.1686572E+01
0.9700	-.7168790E+00	-.1731054E+00	.1937042E+01
0.9900	-.7244499E+00	-.1766071E+00	.2214977E+01
1.0100	-.7319593E+00	-.1800876E+00	.2520562E+01
1.0300	-.7394080E+00	-.1835532E+00	.2851006E+01
1.0500	-.7467490E+00	-.1869900E+00	.3204577E+01
1.0700	-.7540591E+00	-.1904242E+00	.3580035E+01
1.0900	-.7612882E+00	-.1938320E+00	.3978515E+01
1.1100	-.7684649E+00	-.1972215E+00	.4398397E+01
1.1300	-.7755819E+00	-.2005931E+00	.4838376E+01

1.1500	-.7026407E+00	-.2039469E+00	-.7050315E+00
1.1700	-.7896428E+00	-.2172830E+00	-.6758866E+00
1.1900	-.7965895E+00	-.2100019E+00	-.6505855E+00

CEM

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0.0100	-.9917257E+01	-.2514622E+04	.4618203E+06
0.0300	-.5790999E+01	-.4921445E+03	.2949A65E+05
0.0500	-.4537408E+01	-.2332819E+03	.A187974E+04
0.0700	-.3879541E+01	-.1427504E+03	.3513366E+04
0.0900	-.3461816E+01	-.9955113E+02	.1864595E+04
0.1100	-.3168736E+01	-.7483357E+02	.1122775E+04
0.1300	-.2950061E+01	-.5925144E+02	.7351095E+03
0.1500	-.2779982E+01	-.4886041E+02	.5100172E+03
0.1700	-.2643718E+01	-.4092302E+02	.3711043E+03
0.1900	-.2532115E+01	-.3514420E+02	.2706572E+03
0.2100	-.2437171E+01	-.3077413E+02	.2156A45E+03
0.2300	-.2356765E+01	-.2727694E+02	.1704741E+03
0.2500	-.2287965E+01	-.2445176E+02	.1372651E+03
0.2700	-.2228623E+01	-.2212952E+02	.1122696E+03
0.2900	-.2176712E+01	-.2019163E+02	.9304007E+02
0.3100	-.2130998E+01	-.1855421E+02	.7799858E+02
0.3300	-.2090994E+01	-.1715504E+02	.6604033E+02
0.3500	-.2054625E+01	-.1594779E+02	.5640236E+02
0.3700	-.2021539E+01	-.1489732E+02	.4853903E+02
0.3900	-.1992259E+01	-.1397600E+02	.4205505E+02
0.4100	-.1965125E+01	-.1316217E+02	.3665808E+02
0.4300	-.1940345E+01	-.1243977E+02	.3212017E+02
0.4500	-.1917819E+01	-.1179393E+02	.2827913E+02
0.4700	-.1896576E+01	-.1121402E+02	.2500300E+02
0.4900	-.1876300E+01	-.1069004E+02	.2220116E+02
0.5100	-.1857210E+01	-.1021693E+02	.1976102E+02
0.5300	-.1839117E+01	-.9785670E+01	.1765159E+02
0.5500	-.1822078E+01	-.9392096E+01	.1580906E+02
0.5700	-.1806033E+01	-.9031613E+01	.1419251E+02
0.5900	-.1790838E+01	-.8700425E+01	.1276708E+02
0.6100	-.1776565E+01	-.8395276E+01	.1150714E+02
0.6300	-.1763060E+01	-.8113306E+01	.1038707E+02
0.6500	-.1750215E+01	-.7852278E+01	.9388344E+01
0.6700	-.1738056E+01	-.7609908E+01	.8494745E+01
0.6900	-.1726322E+01	-.7384425E+01	.7692620E+01
0.7100	-.1715817E+01	-.7174224E+01	.6970405E+01
0.7300	-.1705951E+01	-.6977872E+01	.6318200E+01
0.7500	-.1696744E+01	-.6793185E+01	.5727776E+01
0.7700	-.1687523E+01	-.6622000E+01	.5191735E+01
0.7900	-.2011468E+01	-.6460357E+01	.4703914E+01
0.8100	-.2029486E+01	-.6308303E+01	.4258934E+01
0.8300	-.2049369E+01	-.6165297E+01	.3852121E+01
0.8500	-.2071104E+01	-.6030399E+01	.3479405E+01
0.8700	-.2094988E+01	-.5903003E+01	.3137228E+01
0.8900	-.2120935E+01	-.5782721E+01	.2822470E+01
0.9100	-.2149124E+01	-.5668652E+01	.2532384E+01
0.9300	-.2179688E+01	-.5561023E+01	.2264504E+01
0.9500	-.2212785E+01	-.5458706E+01	.2016858E+01
0.9700	-.2248538E+01	-.5361747E+01	.1787372E+01
0.9900	-.2287299E+01	-.5269622E+01	.1574422E+01
1.0100	-.2329145E+01	-.5182031E+01	.1376505E+01
1.0300	-.2374388E+01	-.5098706E+01	.1192281E+01
1.0500	-.2423334E+01	-.5019302E+01	.1020550E+01
1.0700	-.2476294E+01	-.4943816E+01	.8602347E+00
1.0900	-.2533688E+01	-.4871705E+01	.7103690E+00

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1.1100 -.2595958E+01 -.4803083E+01  .5700820E+00
1.1300 -.2693625E+01 -.4737521E+01  .4385802E+00
1.1500 -.2737294E+01 -.4674926E+01  .3151781E+00
1.1700 -.2817674E+01 -.4615136E+01  .1992092E+00
1.1900 -.2905595E+01 -.4558002E+01  .9009873E-01


FERMI LEVEL=    0.98222     RYDBERGS
APROXIMATE FERMI LEVLL FOR THE ALLOY=    1.07569
VALENCE=  8.000000
FOR L = 0  PHASESHIFT AT FERMI LEVEL= -0.72151014
FOR L = 1  PHASESHIFT AT FERMI LEVEL= -0.17524632
FOR L = 2  PHASESHIFT AT FERMI LEVEL=  1.85636612
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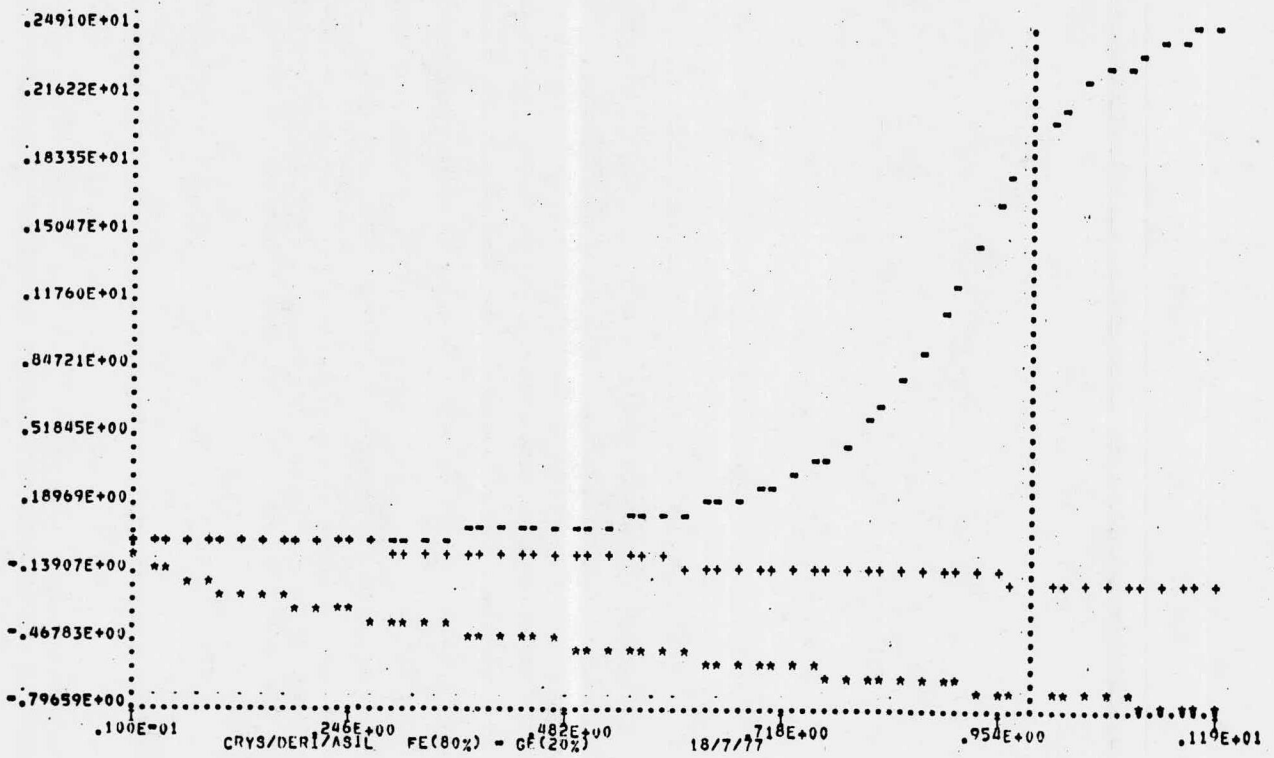
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-.46783E+00
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.100E-01
.246E+00
.482E+00
.718E+00
.954E+00
.119E+01
CRYS/DERI/ASIL FE(80%) - GE(20%)
18/7/77

FE-GE 10/8/77

CALCULATION OF THE DENSITY OF STATES FOR COMPLEX OF 2 SCATTERERS IN FE-GE

MAXIMUM SINGLE SITE PHASESHIFT= 2

NUMBER OF TYPES OF ATOMS 2

ATOMS PER UNIT CELL= 4.00000 LATTICE PARAMETER A= 7.05376 POINTS FOR THE INTERPOLATING FUNCTION= 4

**P ELECTRONS ACCOUNTED

ENERGY REGION: EMIN= 0.11500000 EMAX= 1.39869100 WITH STEP EDELTA= 0.03000000

PHASESHIFT USED IN CALCULATION WITH SSCF= 1.00000 PSCF= 1.00000

ATOMS TYPE 1 ; VALENCE ELECTRONS= 8 NUMBER OF ATOMS= 1

ENERGIES AND PHASESHIFTS:

ENERGY	S	ENERGY	P	ENERGY	D
0.01000	-0.07166	0.01000	-0.00037	0.01000	0.00000
0.03000	-0.12415	0.03000	-0.00187	0.03000	0.00004
0.05000	-0.16033	0.05000	-0.00393	0.05000	0.00014
0.07000	-0.18977	0.07000	-0.00639	0.07000	0.00033
0.09000	-0.21524	0.09000	-0.00913	0.09000	0.00062
0.11000	-0.23804	0.11000	-0.01211	0.11000	0.00103
0.13000	-0.25886	0.13000	-0.01526	0.13000	0.00158
0.15000	-0.27815	0.15000	-0.01857	0.15000	0.00229
0.17000	-0.29621	0.17000	-0.02200	0.17000	0.00318
0.19000	-0.31326	0.19000	-0.02554	0.19000	0.00426
0.21000	-0.32944	0.21000	-0.02916	0.21000	0.00555
0.23000	-0.34489	0.23000	-0.03285	0.23000	0.00708
0.25000	-0.35969	0.25000	-0.03660	0.25000	0.00886
0.27000	-0.37393	0.27000	-0.04039	0.27000	0.01093
0.29000	-0.38766	0.29000	-0.04423	0.29000	0.01331
0.31000	-0.40094	0.31000	-0.04809	0.31000	0.01603
0.33000	-0.41381	0.33000	-0.05198	0.33000	0.01913
0.35000	-0.42631	0.35000	-0.05589	0.35000	0.02265
0.37000	-0.43847	0.37000	-0.05981	0.37000	0.02663
0.39000	-0.45032	0.39000	-0.06375	0.39000	0.03111
0.41000	-0.46187	0.41000	-0.06768	0.41000	0.03616
0.43000	-0.47316	0.43000	-0.07162	0.43000	0.04184
0.45000	-0.48420	0.45000	-0.07556	0.45000	0.04823
0.47000	-0.49501	0.47000	-0.07949	0.47000	0.05540
0.49000	-0.50560	0.49000	-0.08342	0.49000	0.06347
0.51000	-0.51599	0.51000	-0.08734	0.51000	0.07256
0.53000	-0.52619	0.53000	-0.09125	0.53000	0.08279
0.55000	-0.53620	0.55000	-0.09515	0.55000	0.09434
0.57000	-0.54604	0.57000	-0.09904	0.57000	0.10740
0.59000	-0.55572	0.59000	-0.10291	0.59000	0.12223
0.61000	-0.56525	0.61000	-0.10677	0.61000	0.13910
0.63000	-0.57463	0.63000	-0.11061	0.63000	0.15838
0.65000	-0.58387	0.65000	-0.11444	0.65000	0.18050
0.67000	-0.59298	0.67000	-0.11825	0.67000	0.20603
0.69000	-0.60196	0.69000	-0.12204	0.69000	0.23564

0.71000	-0.61082	0.71000	-0.12581	0.71000	0.27020
0.73000	-0.61957	0.73000	-0.12956	0.73000	0.31082
0.75000	-0.62830	0.75000	-0.13330	0.75000	0.35208
0.77000	-0.63672	0.77000	-0.13702	0.77000	0.41615
0.79000	-0.64514	0.79000	-0.14071	0.79000	0.48433
0.81000	-0.65347	0.81000	-0.14439	0.81000	0.56755
0.83000	-0.66169	0.83000	-0.14805	0.83000	0.66723
0.85000	-0.66983	0.85000	-0.15169	0.85000	0.78695
0.87000	-0.67788	0.87000	-0.15531	0.87000	0.92737
0.89000	-0.68584	0.89000	-0.15890	0.89000	1.08812
0.91000	-0.69371	0.91000	-0.16248	0.91000	1.26323
0.93000	-0.70151	0.93000	-0.16604	0.93000	1.44209
0.95000	-0.70923	0.95000	-0.16958	0.95000	1.61502
0.97000	-0.71688	0.97000	-0.17311	0.97000	1.77115
0.99000	-0.72445	0.99000	-0.17661	0.99000	1.90061
1.01000	-0.73195	1.01000	-0.18009	1.01000	2.02103
1.03000	-0.73938	1.03000	-0.18355	1.03000	2.11641
1.05000	-0.74675	1.05000	-0.18700	1.05000	2.19502
1.07000	-0.75405	1.07000	-0.19042	1.07000	2.26156
1.09000	-0.76129	1.09000	-0.19383	1.09000	2.31674
1.11000	-0.76846	1.11000	-0.19722	1.11000	2.36325
1.13000	-0.77558	1.13000	-0.20059	1.13000	2.40276
1.15000	-0.78264	1.15000	-0.20395	1.15000	2.43656
1.17000	-0.78964	1.17000	-0.20728	1.17000	2.46571
1.19000	-0.79659	1.19000	-0.21060	1.19000	2.49101

ENERGY REGION: EMIN= 0.11500000 EMAX= 1.39869100 WITH STEP EDELTA= 0.03000000

PHASESHIFT USED IN CALCULATION WITH SSCF= 1.00000 PSCF= 1.00000

ATOMS TYPE 2 ; VALENCE ELECTRONS= 4 NUMBER OF ATOMS= 1
ENERGIES AND PHASESHIFTS:

ENERGY	S	ENERGY	P	ENERGY	D
0.01000	-0.53411	0.01000	0.00224	0.01000	0.00000
0.03000	-0.80492	0.03000	0.01120	0.03000	0.00001
0.05000	-1.05829	0.05000	0.02570	0.05000	0.00005
0.07000	-1.19761	0.07000	0.04304	0.07000	0.00012
0.09000	-1.30722	0.09000	0.06325	0.09000	0.00023
0.11000	-1.39797	0.11000	0.08629	0.11000	0.00039
0.13000	-1.47568	0.13000	0.11155	0.13000	0.00059
0.15000	-1.54383	0.15000	0.13808	0.15000	0.00085
0.17000	-1.60467	0.17000	0.16798	0.17000	0.00116
0.19000	-1.66975	0.19000	0.19856	0.19000	0.00154
0.21000	-1.71017	0.21000	0.23032	0.21000	0.00198
0.23000	-1.75673	0.23000	0.26295	0.23000	0.00249
0.25000	-1.80006	0.25000	0.29615	0.25000	0.00307
0.27000	-1.84062	0.27000	0.32959	0.27000	0.00373
0.29000	-1.87879	0.29000	0.36299	0.29000	0.00446
0.31000	-1.91488	0.31000	0.39606	0.31000	0.00527
0.33000	-1.94913	0.33000	0.42854	0.33000	0.00616
0.35000	-1.98176	0.35000	0.46022	0.35000	0.00714
0.37000	-2.01293	0.37000	0.49089	0.37000	0.00820
0.39000	-2.04278	0.39000	0.52039	0.39000	0.00935
0.41000	-2.07145	0.41000	0.54861	0.41000	0.01058
0.43000	-2.09903	0.43000	0.57545	0.43000	0.01190
0.45000	-2.12563	0.45000	0.60085	0.45000	0.01331

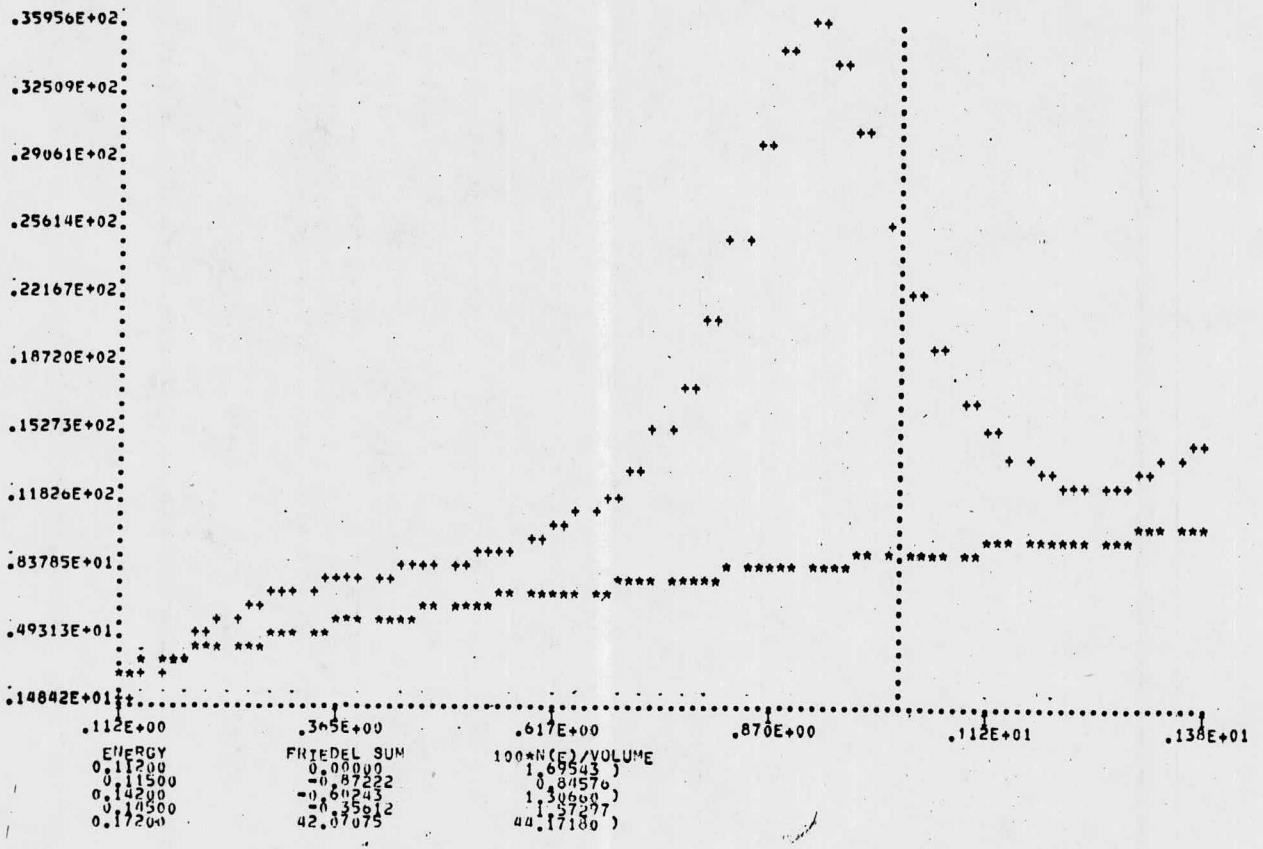
0.47000	-2.15132	0.47000	0.62478	0.47000	0.01481
0.49000	-2.17616	0.49000	0.64722	0.49000	0.01641
0.51000	-2.20023	0.51000	0.66818	0.51000	0.01809
0.53000	-2.22358	0.53000	0.68768	0.53000	0.01987
0.55000	-2.24626	0.55000	0.70577	0.55000	0.02174
0.57000	-2.26831	0.57000	0.72249	0.57000	0.02370
0.59000	-2.28977	0.59000	0.73789	0.59000	0.02576
0.61000	-2.31067	0.61000	0.75204	0.61000	0.02791
0.63000	-2.33106	0.63000	0.76499	0.63000	0.03015
0.65000	-2.35098	0.65000	0.77680	0.65000	0.03248
0.67000	-2.37039	0.67000	0.78755	0.67000	0.03491
0.69000	-2.38938	0.69000	0.79728	0.69000	0.03742
0.71000	-2.40796	0.71000	0.80606	0.71000	0.04003
0.73000	-2.42614	0.73000	0.81396	0.73000	0.04273
0.75000	-2.44394	0.75000	0.82101	0.75000	0.04551
0.77000	-2.46138	0.77000	0.82728	0.77000	0.04839
0.79000	-2.47848	0.79000	0.83283	0.79000	0.05135
0.81000	-2.49524	0.81000	0.83768	0.81000	0.05439
0.83000	-2.51170	0.83000	0.84190	0.83000	0.05752
0.85000	-2.52785	0.85000	0.84552	0.85000	0.06073
0.87000	-2.54372	0.87000	0.84858	0.87000	0.06402
0.89000	-2.55930	0.89000	0.85112	0.89000	0.06739
0.91000	-2.57462	0.91000	0.85317	0.91000	0.07084
0.93000	-2.58969	0.93000	0.85477	0.93000	0.07437
0.95000	-2.60450	0.95000	0.85595	0.95000	0.07796
0.97000	-2.61908	0.97000	0.85673	0.97000	0.08163
0.99000	-2.63342	0.99000	0.85714	0.99000	0.08537
1.01000	-2.64755	1.01000	0.85721	1.01000	0.08918
1.03000	-2.66145	1.03000	0.85695	1.03000	0.09305
1.05000	-2.67515	1.05000	0.85640	1.05000	0.09698
1.07000	-2.68865	1.07000	0.85556	1.07000	0.10098
1.09000	-2.70195	1.09000	0.85446	1.09000	0.10503
1.11000	-2.71507	1.11000	0.85312	1.11000	0.10914
1.13000	-2.72800	1.13000	0.85155	1.13000	0.11330
1.15000	-2.74075	1.15000	0.84976	1.15000	0.11751
1.17000	-2.75333	1.17000	0.84777	1.17000	0.12176
1.19000	-2.76574	1.19000	0.84560	1.19000	0.12607

LX= 0.00000 LY= 0.00000 LZ= 0.00000

LX= 0.00000 LY= 3.52688 LZ= 3.52688

ENERGY	CLUSTER CHANGE IN U(E)	FREE ELECTRON	DENSITY OF STATES	INTEGRATED DENS. OF STATES
0.11200	0.00000	2.97517	2.97517	0.00000
0.11500	-1.53359	3.01475	1.48416-	0.00445
0.14200	-1.65716	3.35001	2.29285	0.00445
0.14500	-0.62493	3.38521	2.70028-	0.00872
0.17200	73.62651	3.68644	77.51345	0.08758
0.17500	0.10392	3.71896	3.02288-	0.09165
0.20200	0.41764	3.99556	4.41320	0.20195
0.20500	0.70986	4.02512	4.73498-	0.34400
0.23200	0.96687	4.28209	5.24886	0.34400
0.23500	1.20423	4.30959	5.51383-	0.50941
0.26200	1.40925	4.55043	5.99968	0.50941
0.26500	1.59535	4.57641	6.17177-	0.69456
0.29200	1.74941	4.80390	6.55331	0.69456
0.29500	1.88551	4.82851	6.71402-	0.89598
0.32200	1.99295	5.04464	7.03759	0.89599
0.32500	2.08444	5.06800	7.15253-	1.11056
0.35200	2.15059	5.27441	7.42499	1.11056
0.35500	2.20355	5.29683	7.50038-	1.33557
0.38200	2.23803	5.49457	7.73260	1.33557
0.38500	2.26333	5.51611	7.77940-	1.56895
0.41200	2.27609	5.70625	7.98234	1.56895
0.41500	2.28581	5.72699	8.01079-	1.80928
0.44200	2.28752	5.91035	8.19787	1.80928
0.44500	2.29061	5.93038	8.22098-	2.05591
0.47200	2.29687	6.10764	8.40371	2.05591
0.47500	2.30493	6.12702	8.43195-	2.30887
0.50200	2.32417	6.29975	8.62292	2.30887
0.50500	2.35090	6.31754	8.66844-	2.56892
0.53200	2.39559	6.48422	8.87782	2.56892
0.53500	2.44737	6.50248	8.94980-	2.83741
0.56200	2.52518	6.66454	9.18972	2.83741
0.56500	2.61044	6.68231	9.30075-	3.11644
0.59200	2.74187	6.84911	9.58198	3.11644
0.59500	2.88511	6.86702	9.74253-	3.40871
0.62200	3.07919	7.03128	10.01147	3.40871
0.62500	3.28201	7.02817	10.31018-	3.71802
0.65200	3.54604	7.17837	10.72441	3.71802
0.65500	3.84465	7.19487	11.03952-	4.04920
0.68200	4.21836	7.34166	11.55986	4.04920
0.68500	4.64052	7.35779	11.90831-	4.40915
0.71200	5.16021	7.50140	12.66149	4.40915
0.71500	5.74524	7.51713	13.26243-	4.80703
0.74200	6.47669	7.65789	14.13449	4.80703
0.74500	7.30431	7.67327	14.97761-	5.25635
0.77200	8.32599	7.81108	16.13707	5.25635
0.77500	9.48048	7.82624	17.30672-	5.77556
0.80200	10.91623	7.96140	18.87763	5.77556
0.80500	12.52729	7.97628	20.30357-	6.39066
0.83200	14.47085	8.10894	22.57978	6.39066
0.83500	16.82094	8.12354	24.74448-	7.13300
0.86200	19.80817	8.25384	27.26201	7.13300
0.86500	21.45187	8.26819	29.72006-	8.02466
0.89200	23.78501	8.39624	32.18124	8.02466
0.89500	25.84473	8.41034	34.25507-	9.05225
0.92200	26.93642	8.53626	35.47268	9.05225
0.92500	27.40563	8.55014	35.95581-	10.13093
0.95200	-47.39194	8.67403	-38.71791	10.13093
0.95500	25.34132	8.68768	34.02901-	11.15180

FERMI LEVEL	0.98200	23.42498	8.80964	32.23462	11.15180
	0.98500	21.28252	8.82308	30.10561-	12.05496
	1.01200	19.11819	8.94319	27.96120	12.05496
	1.01500	16.80922	8.95644	25.76565-	12.05496
	1.04200	14.70273	9.07478	23.67751	12.05496
	1.04500	12.92080	9.08783	22.01764-	12.05496
	1.07200	11.32114	9.20949	20.52563	12.05496
	1.07500	9.86499	9.21736	19.08235-	12.05496
	1.10200	8.63045	9.33239	17.97084	12.05496
	1.10500	7.53041	9.34509	16.88353-	12.05496
	1.13200	6.63108	9.45857	16.08965	12.05496
	1.13500	5.81919	9.47109	15.29028-	12.05496
	1.16200	5.14479	9.58208	14.72687	12.05496
	1.16500	4.53213	9.59545	14.12758-	12.05496
	1.19200	4.03626	9.70930	13.73227	12.05496
	1.19500	3.58024	9.71921	13.29041-	12.05496
	1.22200	3.23597	9.82736	13.06335	12.05496
	1.22500	2.94977	9.83904	12.78920-	12.05496
	1.25200	2.76219	9.94728	12.70947	12.05496
	1.25500	2.63082	9.95919	12.59001-	12.05496
	1.28200	2.59513	10.06575	12.66088	12.05496
	1.28500	2.61409	10.07752	12.69161-	12.05496
	1.31200	2.72635	10.18244	12.90910	12.05496
	1.31500	2.89205	10.19448	13.08653-	12.05496
	1.34200	3.14926	10.29861	13.44787	12.05496
	1.34500	3.45904	10.31011	13.76915-	12.05496
	1.37200	3.85911	10.41300	14.27220	12.05496
	1.37500	4.31125	10.42446	14.73571-	12.05496



ENERGY	FRIEDEL SUM	100*N(E)/VOLUME
0.11200	0.00000	1.69543)
0.11500	-0.87222	0.84576
0.14200	-0.60243	1.30600)
0.14500	-0.35612	1.57277
0.17200	42.07075	44.17180)

0.17500	0.05922	2.17850)
0.20200	0.23800	2.51491)
0.20500	0.40452	2.89827)
0.23200	0.55098	2.99112)
0.23500	0.68624	3.14211)
0.26200	0.80307	3.39618)
0.26500	0.90913	3.51704)
0.29200	0.99692	3.73447)
0.29500	1.07448	3.82605)
0.32200	1.13570	4.01044)
0.32500	1.18784	4.07594)
0.35200	1.22553	4.23121)
0.35500	1.25571	4.27417)
0.38200	1.27539	4.40650)
0.38500	1.28976	4.44117)
0.41200	1.29705	4.54081)
0.41500	1.30145	4.56503)
0.44200	1.30327	4.67104)
0.44500	1.30532	4.69481)
0.47200	1.30844	4.78893)
0.47500	1.31349	4.80503)
0.50200	1.32445	4.91385)
0.50500	1.33968	4.93979)
0.53200	1.36401	5.05911)
0.53500	1.39466	5.10016)
0.56200	1.43900	5.23685)
0.56500	1.49214	5.30012)
0.59200	1.56248	5.40038)
0.59500	1.64411	5.55188)
0.62200	1.74954	5.74502)
0.62500	1.87029	5.87536)
0.65200	2.02074	6.11141)
0.65500	2.19091	6.22098)
0.68200	2.40378	6.50750)
0.68500	2.64445	6.83736)
0.71200	2.94048	7.21522)
0.71500	3.27398	7.55772)
0.74200	3.69081	8.05408)
0.74500	4.16245	8.53513)
0.77200	4.74465	9.19586)
0.77500	5.40254	9.86240)
0.80200	6.22072	10.75760)
0.80500	7.13080	11.88410)
0.83200	8.24635	12.80731)
0.83500	9.47180	14.10088)
0.86200	10.83198	15.53552)
0.86500	12.22456	16.93926)
0.89200	13.55412	18.33879)
0.89500	14.72787	19.52059)
0.92200	15.34998	20.21445)
0.92500	15.61739	20.48977)
0.95200	-27.00676	-22.00378)
0.95500	14.44100	19.39176)
0.98200	13.34895	18.30931)
0.98500	12.12805	17.15597)
1.01200	10.83765	15.93401)
1.01500	9.57890	14.68281)
1.04200	8.43548	13.56083)
1.04500	7.36817	12.58090)
1.07200	6.45146	11.69673)

1.07500	5.62166	10.87426
1.10000	4.92270	10.24086)
1.10500	4.29585	9.62124
1.11000	3.77879	9.19804)
1.11500	3.31612	8.71331
1.16000	2.92953	8.39054)
1.16500	2.58268	8.05074
1.17000	2.29441	7.82547)
1.17500	2.04021	7.57023
1.22000	1.84405	7.44428)
1.22500	1.68095	7.28805
1.23000	1.57446	7.24262)
1.25500	1.49920	7.17454
1.28000	1.47888	7.21492)
1.28500	1.48966	7.23324
1.31000	1.55363	7.35643)
1.31500	1.64807	7.45749
1.34000	1.79464	7.60340)
1.34500	1.97117	7.83648
1.37000	2.19915	8.11315)
1.37500	2.45681	8.33729

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 BEGIN CALCULATION

FOR L=  0 SINGLE SITE PHASESHIFT=-1.40627 K-MATRIX=17.99761

FOR L=  1 SINGLE SITE PHASESHIFT= 0.08871 K-MATRIX=-0.26578

FOR L=  2 SINGLE SITE PHASESHIFT= 0.00041 K-MATRIX=-0.00121
REAL PART OF DET=  0.21559     IMAG PART DET 0.97648
FOR ENERGY= 0.11200 RYDBERGS
DENSITY OF STATES PER UNIT VOLUME*100 IS                0.00000
                                                ** PROCESS TIME=133.6667  SECONDS **

FOR L=  0 SINGLE SITE PHASESHIFT=-1.41848 K-MATRIX=19.21055

FOR L=  1 SINGLE SITE PHASESHIFT= 0.09239 K-MATRIX=-0.27324

FOR L=  2 SINGLE SITE PHASESHIFT= 0.00043 K-MATRIX=-0.00128
REAL PART OF DET=  0.20854     IMAG PART DET 0.97801
FOR ENERGY= 0.11500 RYDBERGS
CHANGE IN DENSITY OF STATES IS          -1.53059
DENSITY OF STATES PER UNIT VOLUME*100 IS                0.84570
                                                ** PROCESS TIME=139.4167  SECONDS **

FOR L=  0 SINGLE SITE PHASESHIFT=-1.51757 K-MATRIX=49.80804

FOR L=  1 SINGLE SITE PHASESHIFT= 0.12772 K-MATRIX=-0.34079

FOR L=  2 SINGLE SITE PHASESHIFT= 0.00074 K-MATRIX=-0.00196
REAL PART OF DET=  0.16450     IMAG PART DET 0.98638
FOR ENERGY= 0.14200 RYDBERGS
CHANGE IN DENSITY OF STATES IS          -1.05716
DENSITY OF STATES PER UNIT VOLUME*100 IS                1.30660
                                                ** PROCESS TIME=145.2167  SECONDS **

FOR L=  0 SINGLE SITE PHASESHIFT=-1.52756 K-MATRIX=60.70236

FOR L=  1 SINGLE SITE PHASESHIFT= 0.13187 K-MATRIX=-0.34833

FOR L=  2 SINGLE SITE PHASESHIFT= 0.00078 K-MATRIX=-0.00204
REAL PART OF DET=  0.16159     IMAG PART DET 0.98686
FOR ENERGY= 0.14500 RYDBERGS
CHANGE IN DENSITY OF STATES IS          -0.62493
DENSITY OF STATES PER UNIT VOLUME*100 IS                1.57297
                                                ** PROCESS TIME=151.0000  SECONDS **
```

```
FOR L=  0 SINGLE SITE PHASESHIFT=-2.87178 K-MATRIX=-0.23611

FOR L=  1 SINGLE SITE PHASESHIFT= 0.81943 K-MATRIX=-0.91391

FOR L=  2 SINGLE SITE PHASESHIFT= 0.16684 K-MATRIX=-0.14377

REAL PART OF DET=  0.96210      IMAG PART DET 0.24668
FOR ENERGY= 1.37200 RYDBERGS
CHANGE IN DENSITY OF STATES IS                3.85911
DENSITY OF STATES PER UNIT VOLUME*100 IS                  8.13315
                                                  ** PROCESS TIME=657.5167  SECONDS **

FOR L=  0 SINGLE SITE PHASESHIFT=-2.87344 K-MATRIX=-0.23433

FOR L=  1 SINGLE SITE PHASESHIFT= 0.81893 K-MATRIX=-0.91200

FOR L=  2 SINGLE SITE PHASESHIFT= 0.16753 K-MATRIX=-0.14422

REAL PART OF DET=  0.97391      IMAG PART DET 0.22694
FOR ENERGY= 1.37500 RYDBERGS
CHANGE IN DENSITY OF STATES IS                4.31125
DENSITY OF STATES PER UNIT VOLUME*100 IS                  8.39729
                                                  ** PROCESS TIME=664.2167  SECONDS **
```

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TABLA I

	Vint	E_f-Vint	E_f	$\delta_2(E_f)$	$\frac{10\delta_2(E_f)}{\pi}$
γ-Fe($4s^2 3d^6$)	-1.56654	0.33177	-1.2348	2.16463	6.89
Co($4s^2 3d^7$)	-1.20163	0.22072	-0.9809	1.79127	5.702
Co($4s^{1.2} 3d^{7.8}$)	-1.1007	0.39178	-0.70892	2.54519	8.101
Ni($4s^2 3d^8$)	-1.87469	0.8400	-1.03469	2.48024	7.895
Ni($4s^{0.5} 3d^{9.5}$)	-1.73218	1.27769	-0.4545	2.38156	7.581
Ni($4s^{1.1} 3d^{8.9}$)	-1.75294	1.1977	-0.55524	2.45791	7.824
Cu($4s^1 3d^{10}$)	-1.03169	0.60801	-0.4237	2.96977	9.453
Rh($5s^1 4d^8$)	-1.31644	0.56726	-0.74918	2.5804	8.214
Ag($5s^1 4d^{10}$)	-1.28978	0.97301	-0.3168	2.68937	8.561
Nd($6s^2 4f^3 5d^1$)	-0.59364	0.09765	-0.49599	0.31623	1.007
Eu($6s^2 4f^6 5d^1$)	-0.52504	0.26204	-0.263	0.31956	1.017
Cd(BCC)($6s^2 4f^7 5d^1$)	-0.70768	0.22315	-0.48453	0.32006	1.019
Cd(HCP)	-0.58137	0.15863	-0.4227	0.3074	0.979
Lu($6s^2 4f^{1.4} 5d^1$)	-0.70568	0.26963	-0.43605	0.32673	1.04
Os($6s^2 5d^6$)	-1.15239	0.59506	-0.5573	2.31636	7.373
Ir($6s^2 5d^7$)	-1.17929	0.69577	-0.4835	2.51113	7.993
Pt($6s^1 5d^3$)	-1.75704	1.540	-0.2170	1.8947	6.031
Au($6s^1 5d^{10}$)	-1.29552	1.18999	-0.1055	2.42109	7.707

TABLA II

	$E_{max\delta_2}$	$max\delta_2(E)$	$\frac{10\delta_2(E)}{\pi}$	Carácter d deslocalizado
γ-Fe($4s^2 3d^6$)	0.75	2.97063	9.456	0.544
Co($4s^2 3d^{7.8}$)	0.43	3.04212	9.683	0.317
Co($4s^{1.2} 3d^{7.8}$)	0.99	2.9810	9.489	0.511
Ni($4s^2 3d^8$)	1.4	2.86412	9.1168	0.883
Ni($4s^{0.5} 3d^{9.5}$)	1.78	2.71532	8.643	1.357
Ni($4s^{1.1} 3d^{8.9}$)	1.30	2.77482	8.83252	1.16748
Cu($4s^1 3d^{10}$)	0.75	2.98933	9.515	0.485
Rh($5s^1 4d^8$)	0.85	2.69862	8.590	1.41
Ag($5s^1 4d^{10}$)	1.03	2.69203	8.569	1.431
Nd($6s^2 4f^3 5d^1$)	0.23	2.80740	8.936	1.064
Eu($6s^2 4f^6 5d^1$)	0.60	2.08798	6.646	3.354
Gd(BCC) ($6s^2 4f^7 5d^1$)	0.63	2.33133	7.421	2.579
Gd(HCP)	0.41	2.55707	8.139	1.861
Lu($6s^2 4f^{14} 5d^1$)	0.81	2.29097	7.292	2.708
Os($6s^2 5d^6$)	0.89	2.49638	7.946	2.054
Ir($6s^2 5d^7$)	0.89	2.54975	8.116	1.884
Pt($6s^1 5d^9$)	1.78	2.02806	6.456	3.544
Au($6s^1 5d^{10}$)	1.33	2.42919	7.732	2.268

TABLA III

RAZON DE OCUPACION.

$$\frac{10\delta_2(F_f)}{\pi} \Big/ \frac{10\delta_2(E)}{\pi}$$

γ-Fe($4s^2 3d^6$)	0.72864
Co($4s^2 3d^7$)	0.58887
Co($4s^{1.2} 3d^{7.8}$)	0.85373
Ni($4s^2 3d^8$)	0.86598
Ni($4s^{0.5} 3d^{9.5}$)	0.87713
Ni($4s^{1.1} 3d^{8.9}$)	0.88582
Cu($4s^1 3d^{10}$)	0.99348
Rh($5s^1 4d^8$)	0.95623
Ag($5s^1$4d10)	0.99907
Nd($6s^2 4f^3 5d^1$)	0.11269
Eu($6s^2 4f^6 5d^1$)	0.15302
Cd(BCC) ($6s^2 4f^7 5d^1$)	0.13731
Cd(HCP)	0.12029
Lu($6s^2 4f^{14} 5d^1$)	0.14262
Os($6s^2 5d^6$)	0.92788
Ir($6s^2 5d^7$)	0.98484
Pt($6s^2 5d^8$)	0.93417
Au($6s^1 5d^{10}$)	0.99677

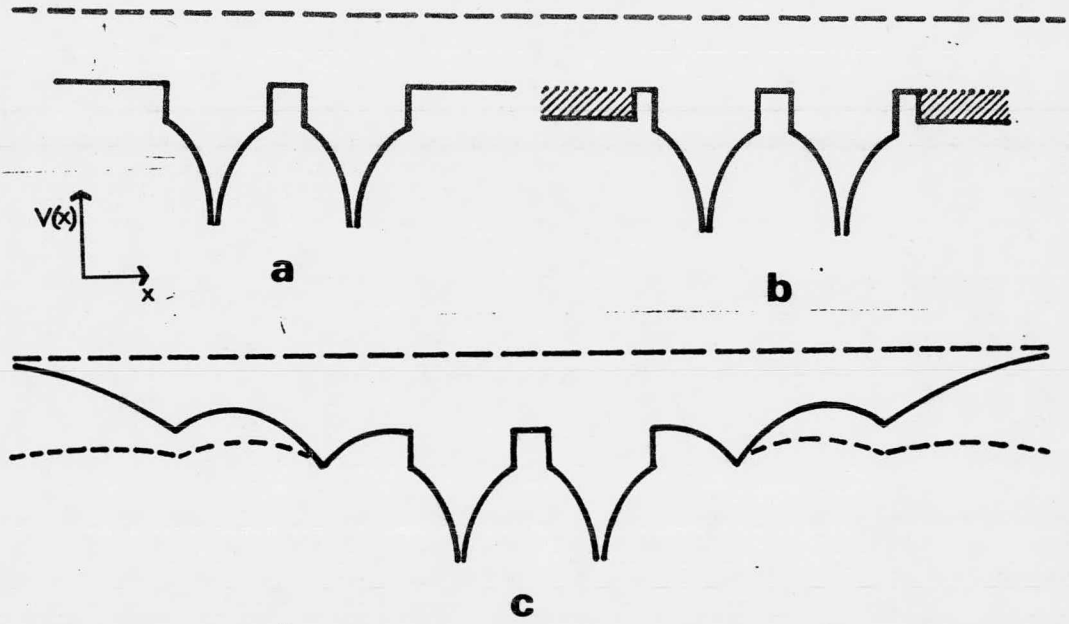

FIGURA 1

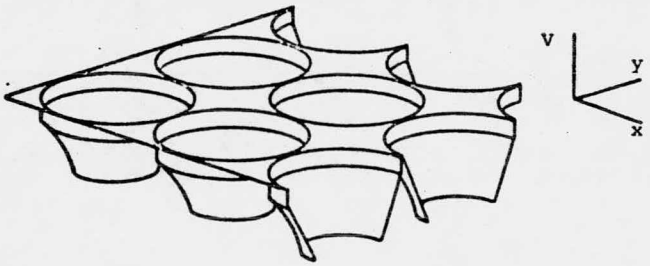

FIGURA 2

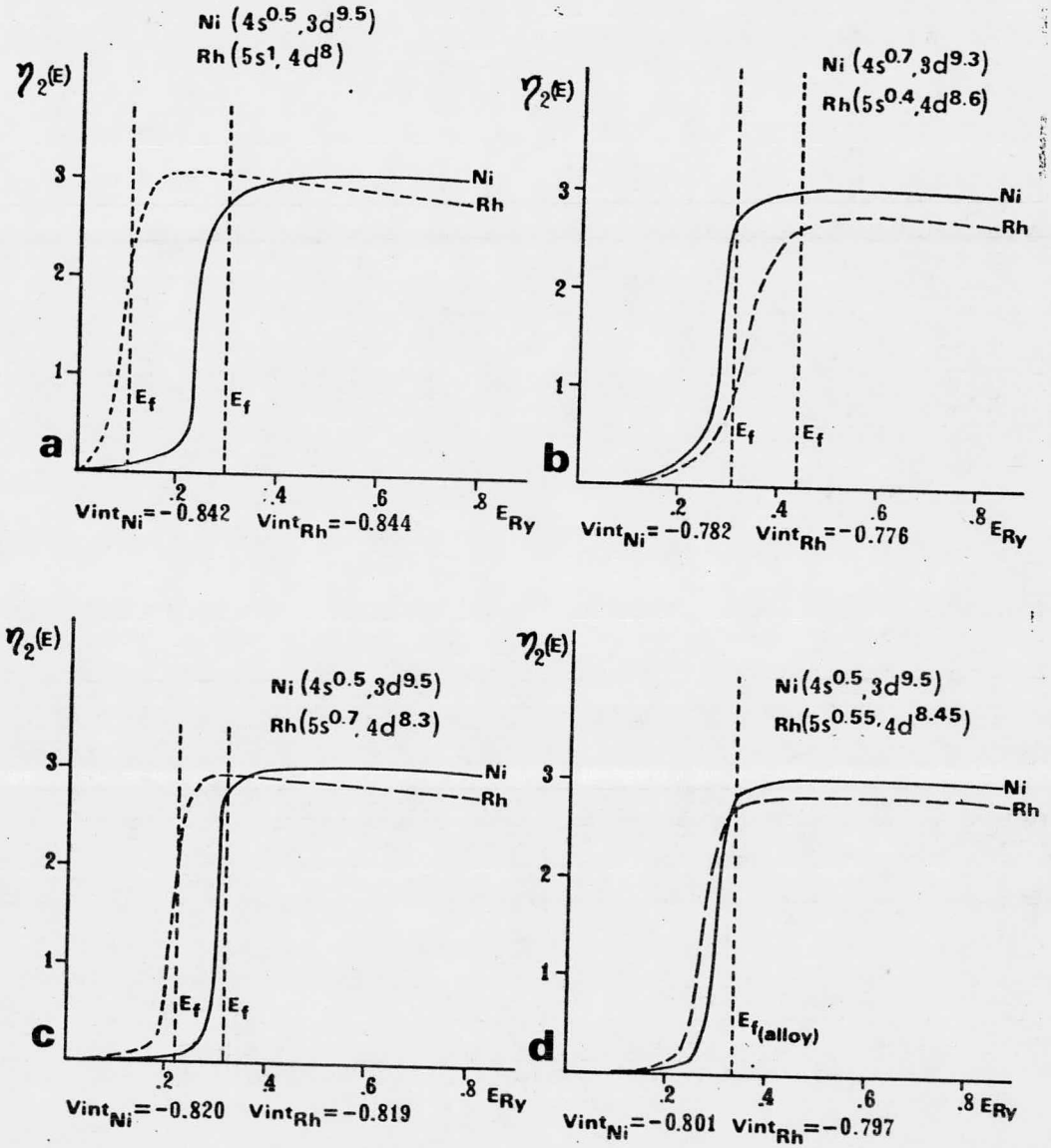
Ni (4s^0.5, 3d^9.5)
Rh (5s^1, 4d^8)
η2(E)
Ni
Rh
Ef
Ef
a
Vint_Ni = −0.842
Vint_Rh = −0.844
ERy
Ni (4s^0.7, 3d^9.3)
Rh(5s^0.4, 4d^8.6)
b
Vint_Ni = −0.782
Vint_Rh = −0.776
Ni (4s^0.5, 3d^9.5)
Rh(5s^0.7, 4d^8.3)
c
Vint_Ni = −0.820
Vint_Rh = −0.819
Ni(4s^0.5, 3d^9.5)
Rh(5s^0.55, 4d^8.45)
Ef(alloy)
d
Vint_Ni = −0.801
Vint_Rh = −0.797

FIGURA 3

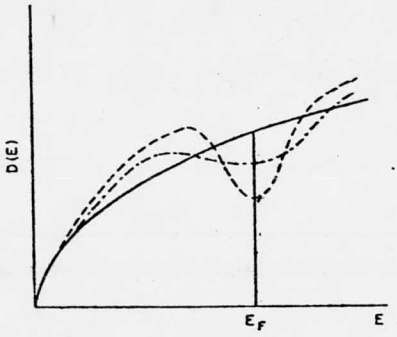

FIGURA 4

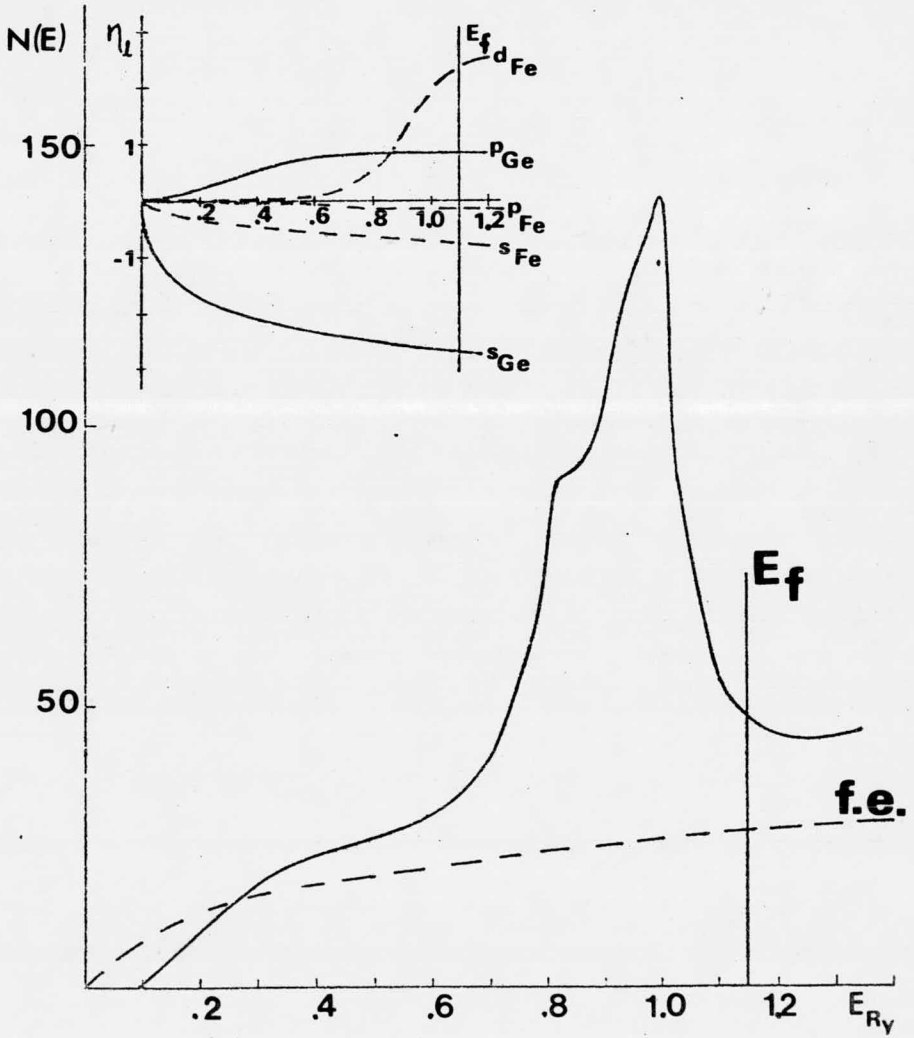

FIGURA 5

DESCRIPCION DE LAS FIGURAS.

FIG. 1.- Esta es la representación para tres aproximaciones de las condiciones a la frontera de un cúmulo de átomos en materia condensada. a) Representa a un cúmulo en el potencial intersticial V_{int}. b) Un cúmulo rodeado por el potencial promedio del resto del sistema. c) El cúmulo rodeado por el promedio esférico del resto del sistema, la línea continua es el potencial en un sistema finito y la línea punteada en un sistema extendido.

FIG. 2.- Potencial de muffin-tin para un cristal bidimensional.

FIG. 3.- Estudio de los corrimientos de fase de la aleación Ni-Rh (50%-50% atómico). Partiendo de la ocupación óptima del Ni y del estado basal del Rh los niveles de Fermi para el Ni y el Rh son inconsistentes (a). Una disminución del carácter 3d para el Ni y un aumento del carácter 4d para el Rh no resuelve la discrepancia (b). Solo el incremento de carácter 4d en el Rh da un nivel de Fermi consistente para ambos componentes (c) y (d).

FIG. 4.- Diagrama esquemático de la densidad de estados presentado por Nagel y Tauc [32] para 3 casos: La curva contínua es para el modelo de electrones libres, la curva a rayas es para el vidrio en el modelo de electrones casi libres que presentan y la de la curva punteada-rayas es para un vidrio perturbado con un factor de estructura no esferica-

mente simétrico.

FIG. 5.- Densidad de estados para la aleación Fe-Ge con un contenido de 20% atómico de Ge, la línea punteada es la contribución de electrones libres. En la parte superior izquierda se presentan los corrimientos de fase para cada especie en la aleación.

```
      86700/87700   F O R T R A N   C O M P I L A T I O N   M A R K   2.8.060
FILE  4=PERF ,UNIT=PUNCH                                                    00001000
FILE  5= DATOS ,UNIT =READER                                                00002000
FILE  6=PAPEL,UNIT=PRINTER                                                  00003000
FILE  7=TARJ,UNIT=PRINTER                                                   00004000
FILE  8=HEXD,UNIT=DISK,RECORD=14,BLOCKING=15,AREA=150*1                     00005000
FILE  9=HEXD1,UNIT=DISK,RECORD=14,BLOCKING=15,AREA=150*1                    00006000
FILE  10=HEXD2,UNIT=DISK,RECORD=14,BLOCKING=15,AREA=150*1                   00007000
FILE  11=HEXD3,UNIT=DISK,RECORD=14,BLOCKING=15,AREA=150*1                   00008000
FILE  12=HEXD4,UNIT=DISK,RECORD=14,BLOCKING=15,AREA=150*1                   00009000

      COMMON/CRYDER/BGXIT(250),NAME(20),JRI(2),JMA,A,NJJ,EFE,IAL,IZZ        00010000
      DIMENSION        SIGA(5,2),B5(250,2),W(250,2),AA(250,14),           00011000
     1AB(250,14),AACR(250),ABCR(250),          XNA(14,2),AD(14,2),          00012000
     2NA(4,15),R(15),XAD(3,15),          SH(500,2),AAD(14,2),FAP(250),     00013000
     3XNB(14),BD(14),IZZ(2),RHSX(421),RAP(250),JEC(14),XRI(2)               00014000
      DIMENSION GE(250),GRAD(250),GRAD2(250),SCP(250),AA1(250),AB1(250)     00015000
     1,AC(250,2),AC(250,2),R1(2)                                            00016000
      REAL JRI                                                              00017000
      FU(A,B,C,D,T)=(A*(D-T)-B*(C-T))/(D-C)                                 00018000
                                                                            00019000
C                                                                           00020000
C       FORMAT                                                              00021000
    6 FORMAT(6E14.7)                                                        00022000
   28 FORMAT(1H1,30X,20A4,//,30X,30('*'))                                   00023000
   29 FORMAT(1H ,10X,'NUMBER OF MESH POINTS= ',I4,10X,'NUMBER OF TYPES O   00024000
     1F ATOMS= ',I4,10X,'ATOMIC NUMBERS',/2I5)                              00025000
   30 FORMAT(1H ,15X,'NUMBER OF NEIGHBOUR ATOMS FOR FCC, BCC, DIAMOND AN   00026000
     1D HCP')                                                               00027000
   32 FORMAT(1H ,30X,'DISTANCE/SIDE FOR FCC,BCC AND DIAMOND')               00028000
   33 FORMAT(10X,6F10.6)                                                    00029000
   51 FORMAT (8F10.6)                                                       00030000
   61 FORMAT(20A4)                                                          00031000
   80 FORMAT(2I5)                                                           00032000
   81 FORMAT (14I5)                                                         00033000
  115 FORMAT (5E20.8)                                                       00034000
  117 FORMAT(2X,'VINT=',E17.8,'     Z=',F10.2,'     JRI(1)=',F10.6,'   JR   00035000
     1I(2)=',F10.6,'     LAT=',I3,//,' XALPHA=',F10.7,'     XBETA=',F10.7,  00036000
     2//)                                                                   00037000
  130 FORMAT(1H ,5X,' NEIGHBOR DISTANCES AND NUMBER OF NEIGHBORS ---CENT   00038000
     1RAL ATOM OF TYPE---',I2)                                              00039000
  141 FORMAT(2F10.5)                                                        00040000
  147 FORMAT(8E14.7)                                                        00041000
  148 FORMAT(1H1,30X,'TABLE OF APW RADIUS')                                 00042000
  151 FORMAT(1H1,30X,'INTERPOLATED TABLE OF 4*PI*(R**2)*RHO FOR THIS PRO   00043000
     1GRAM, FOR THE',I3,' ATOM')                                            00044000
  312 FORMAT(2X,'CENTRAL ATOM OF TYPE 1',/,2X,22('='))                      00045000
  314 FORMAT(2X,'CENTRAL ATOM OF TYPE 2',/,2X,22('='))                      00046000
  350 FORMAT(3(2E15.6,3X))                                                  00047000
                                                                            00048000
  800 FORMAT(' INTEGRAL OF CHARGE DENSITY FOR THE',I2,' ATOM',F16.8)        00049000
  801 FORMAT(1H ,10X,'MAXIMUM RADIUS FROM HEX=',F10.5,10X,'RECIPROCAL OF   00050000
     1 MESH INTERVAL FROM HEX=',F10.5,/)                                    00051000
 1001 FORMAT(1H ,10X,'LATTICE STRUCTURE= ',I4,/,20X,'MESH POINT CORRESPO   00052000
     1NDING TO THE APW SPHERE RADIUS=',F10.6,/,20X,'VOLUME PER ATOM(ATO    00053000
     2MIC UNITS)=',F10.5,/,20X,'LATTICE CONSTANTS A AND C',2F10.6,//,19X,  00054000
     3'EXCHANGE COEFFICIENTS ALPHA AND BETA',2F10.6,//)                      00055000
 1170 FORMAT(2X,' RESULTS FOR BUFFIN TIN WITH  RI(1)=',F7.4,5X,'RI(2       00056000
     1)=',F7.4,5X,'RO=',F7.4,3X,'V BOUNDARY=',E14.7)                        00057000
 1180 FORMAT(////)                                                          00058000
 9997 FORMAT(20X,'R*V(R)')                                                  00059000
C                                                                           00060000
C       START                                                               00061000
    3  READ(5,80,END=310,DATA=310)ICALL,KIND                                00062000
       IF(ICALL.GT.0.0) CALL ASIL(ICALL)                                    00063000
       DO 50 I=1,3                                                          00064000
   50  READ(5,51,DATA=3,END=3)(XAD(I,J),J=1,14)                            00065000
       DO 75 I=1,4                                                          00066000
   75  READ (5,81)(NA(I,J),J=1,14)                                         00067000
       READ(5,51,END=310)DUMY                                               00068000
C                                                                           00069000
C       STOPS IF A CARD WITH END (PUNCHED ON 2ND COLUMN) IS FOUND            00070000
```

```
C
      IF(JAJES1).EQ.4HEND) GO TO 8                                      00069000
      READ(5,2) JAL                                                     00070000
      IF(JAL.EQ.4H) JAL=4H                                              00071000
      IF(JAL.EQ.4H) JAL=4H                                              00072000
C                                                                       00073000
C        RMAX=MAXIMUM RADIUS FROM NUCLEUS                               00074000
C        H=RECIPROCAL OF THE GRID INTERVAL FROM HEX                     00075000
C        NSIG=NUMBER OF SIGNIFICANT POINTS FROM HEX                     00076000
C        NJJ=NUMBER OF TYPES OF ATOMS                                   00077000
C        IZZ(JJ)=ATOMIC NUMBER OF EACH TYPE OF ATOM                     00078000
      READ(5,141)RMAX,H                                                 00079000
      READ(5,81) NSIG,NJJ                                               00080000
      READ(5,81)(IZZ(JJ),JJ=1,NJJ)                                      00081000
      WRITE(6,28)(JAL(I),I=1,20)                                        00082000
      WRITE(6,1180)                                                     00083000
      WRITE(6,32)                                                       00084000
      DO 31 I=1,3                                                       00085000
   31 WRITE(6,33)(XMAD(I,J),J=1,14)                                     00086000
      WRITE(6,1180)                                                     00087000
      WRITE(6,30)                                                       00088000
      DO 751 I=1,4                                                      00089000
  751 WRITE(6,81)(NA(I,J),J=1,14)                                       00090000
      WRITE(6,1180)                                                     00091000
      WRITE(6,301)RMAX,H                                                00092000
      WRITE(6,29)NSIG,NJJ,(IZZ(JJ),JJ=1,NJJ)                            00093000
C                                                                       00094000
C        CALCULUS OF HEX AND A.P.A. MESHES                              00095000
C                                                                       00096000
      XHEX=-(NSIG/H)                                                    00097000
      DXHEX=1./H                                                        00098000
      DO 142 K=1,NSIG                                                   00099000
  142 RHEX(K)=RMAX*EXP(XHEX+K*DXHEX)                                    00100000
      DO 143 K=1,250                                                    00101000
  143 RAPW(K)=EXP(-8.8+(K-1)*0.05)                                      00102000
      WRITE(6,148)                                                      00103000
      WRITE(6,1180)                                                     00104000
      WRITE(6,147)(RAPW(K),K=1,250)                                     00105000
      DO 998 JJ=1,NJJ                                                   00106000
      IF(JJ.EQ.2) NM=NM+KIND                                            00107000
C                                                                       00108000
C        STGW(J,JJ)= TABLE OF 4*PI*(R**2)*RHO FROM HEX                  00109000
      READ(NM,6) (STGW(J,JJ),J=1,NSIG)                                  00110000
      DO 144 K=1,250                                                    00111000
      DO 145 KK=1,NSIG                                                  00112000
      IF(RHEX(KK)-RAPW(K))145,146,146                                   00113000
  145 CONTINUE                                                          00114000
  146 FU1=FU(STGW(KK,JJ),STGW(KK-1,JJ),RHEX(KK),RHEX(KK-1),RAPW(K))     00115000
      FU2=FU(STGW(KK+1,JJ),STGW(KK,JJ),RHEX(KK+1),RHEX(KK),RAPW(K))     00116000
  144 PSQ(K,JJ)=FU(FU2,FU1,RHEX(KK+1),RHEX(KK-1),RAPW(K))               00117000
  998 CONTINUE                                                          00118000
      DO 149 JJ=1,NJJ                                                   00119000
      WRITE(6,151)JJ                                                    00120000
      WRITE(6,1180)                                                     00121000
      WRITE(6,147)(PSQ(J,JJ),J=1,250)                                   00122000
  149 CONTINUE                                                          00123000
      DO 996 JJ=1,NJJ                                                   00124000
      SUMA=0.0                                                          00125000
      ZZ=IZZ(JJ)                                                        00126000
      DO 92 JL=1,224,2                                                  00127000
      TSC=EXP(0.05)                                                     00128000
      TSC2=EXP((JL-1)*0.05-8.8)                                         00129000
   92 SUMA=SUMA+TSC2*(2.0*PSQ(JL,JJ)+TSC*PSQ(JL+1,JJ))                  00130000
      SUMA=SUMA*0.033333                                                00131000
      WRITE(6,809)JJ,SUMA                                               00132000
      WRITE(6,1180)                                                     00133000
      DO 93 JL=1,224                                                    00134000
   93 PSQ(JL,JJ)=PSQ(JL,JJ)*ZZ/SUMA                                    00135000
      DO 94 JL=225,250                                                  00136000
   94 PSQ(JL,JJ)=0.0                                                    00137000
  996 CONTINUE                                                          00138000
C                                                                       00139000
C     LATTICE CALCULATIONS                                              00140000
C                                                                       00141000
C        LAT=1      FCC                                                00142000
C        LAT=2      BCC                                                00143000
C        LAT=3      DIAMOND STRUCTURE                                  00144000
C        LAT=4      HCP                                                00145000
C        LAT=5      SPECIAL STRUCTURES OF ELEMENTS                     00146000
C        LAT=6      ALLOYS                                             00147000
C                                                                       00148000
      READ(5,81)LAT                                                     00149000
      READ(5,99)(JRI(JJ),JJ=1,NJJ)                                      00150000
   99 FORMAT(8E10.6)                                                    00151000
      READ (5,51)JMA,A,C,XALPHA                                         00152000
```

```
C
C       IF A IS SET TO 0.0 THEN A=1.0 IS TAKEN AND THE DISTANCES GIVEN
C       IN AAD ARE NO MORE RELATIVE DISTANCES
C
C
C     IF XALPHA IS NOT SPECIFIED, XALPHA-BETA EXCHANGE POTENCIAL IS CALC
C     WITH ALPHA=2/3 AND BETA=0.003
C     IF XALPHA IS GIVEN, XALPHA EXCHANGE POTENCIAL IS CALCULATED WITH T
C     SPECIFIED VALUE OF XALPHA
C
      IF(XALPHA.LT.0.01) GO TO 1
      XBETA=0.0
      GO TO 4
    1 XBETA=0.003
      XALPHA=0.666667
    4 IF(A.LT.0.01) A=1.0
      WRITE(6,1001)LAT,JRI(1),DMA,A,C,XALPHA,XBETA
      IF (LAT-4)82,400,101
C
C     HCP CRYSTAL STRUCTURE
C
  400 B=C/A
      BS=B*B
      R(1)=0.
      R(2)=1./3.+BS/4.
      R(3)=1.
      R(4)=4./3.+BS/4.
      R(5)=BS
      R(6)=7./3.+BS/4.
      R(7)=3.
      R(8)=1.+BS
      R(9)=4.
      R(10)=10./3.+BS/4.
      R(11)=3.+BS
      R(12)=13./3.+(3.*BS)/4.
      R(13)=10./3.+BS/4.
      R(14)=4.+BS
      DO 2 I=1,14
    2 AD(I,1)=SQRT(R(I))
      GO TO 82
C
C         FCC,BCC, AND DIAMOND STRUCTURES
C
   82 DO 83 I=1,14
   83 AD(I,1)=XAD(LAT,I)
      DO 83 I=1,14
   83 XNA(I,1)=NA(LAT,I)
      DS=A
      DO 21 I=2,14
   21 AD(I,1)=DS*AD(I,1)
      GO TO 85
C
C         SPECIAL CRYSTAL STRUCTURES
C
C       XNA(I,1) FOR I=1,7 ARE THE NUMBER OF NEIGHBORS OF TYPE 1.
C       (CENTRAL ATOM) IN SEVEN SHELLS. FOR I=8,14  ARE THE NUMBER OF
C       NEIGHBORS OF TYPE 2 IN SEVEN SHELLS(MAY BE DIFFERENT OF THOSE
C       OF THE FIRST TYPE.    THERE IS A RESTRICTION, SEE NEXT COMMENT.
C                             ****************************************
C
C       AAD(I,1) FOR I=1,7 ARE THE RELATIVE DISTANCES OF THE SEVEN
C       SHELLS OF NEIGHBORS OF TYPE ONE WHICH NUMBER WAS GIVEN BEFORE.
C       FOR I=8,14 ARE THE DISTANCES OF SECOND TYPE ATOMS
C       RESTRICTION--    AAD(I,7)=AAD(I,14)
C       **********
C       LAST SHELL MUST BE THE SAME FOR BOTH TYPE OF ATOMS.
C
C       FOR XNA(I,2) AND AAD(I,2) CENTRAL ATOM IS OF TYPE 2. IN THE FOR
C       MER INSTANCE NA(I) AND AD(I) MUST BE INTERCHANGED
C
  101 DO 9999 JJ=1,JJ
      READ(5,51)(XNA(I,JJ),I=1,14)
      READ (5,51)(AD(I,JJ),I=1,14)
      DO 1111 I=1,14
 1111 AD(I,JJ)=AD(I,JJ)*A
 9999 CONTINUE
      IF(LAT-2)5,6,7
    5 DO 9998 JJ=1,JJ
      WRITE(6,1100)
      WRITE(6,1500)JJ
      WRITE (6,51)(XNA(I,JJ),I=1,14)
      WRITE(6,1102)
```

```
      WRITE (6,911)(XMA(I,JJ),I=1,14)                                   00237000
 9000 WRITE(6,1100)                                                     00238000
      GO TO 206                                                         00239000
C                                                                       00240000
C     MUFFIN TIN SEGMENT                                                00241000
C                                                                       00242000
   65 DO 1020 JJ=1,JJ                                                   00243000
      DO 1020 K=1,14                                                    00244000
      XMB(K,JJ)=XMA(K,JJ)                                               00245000
 1020 BD(K)=AD(K,1)                                                     00246000
      WRITE(6,1500)MJJ                                                  00247000
      WRITE(6,911)(BD(K),K=1,14)                                        00248000
      WRITE(6,1100)                                                     00249000
  206 DO 407 JJ=1,MJJ                                                   00250000
      Z=IZZ(JJ)                                                         00251000
      JJCHI=225                                                         00252000
      CALL POISJJ (PSJ,Z,JJCHI,.,JJ)                                    00253000
      X=-8.8                                                            00254000
      DO 409 J=1,JJCHI                                                  00255000
      CE=EXP(-.5*X)                                                     00256000
      AC(J,JJ)=CE*(-2.*Z*CF+M(I,JJ))                                    00257000
C                                                                       00258000
CCC                 (ATOMIC ELECTROSTATIC POTENTIAL)                    00259000
C                                                                       00260000
      AE(J,JJ)=PSJ(J,JJ)*EXP(-2.*X)                                     00261000
C                    (1*PI*ATOMIC ELECTRONIC DENSITY)                   00262000
  409 X=X+.05                                                           00263000
      CONTINUE                                                          00264000
      IF(LAT-3)160,160,161                                              00265000
  161 DO 207 JJ=1,MJJ                                                   00266000
      IK=-1                                                             00267000
      IF(JJ.EQ.1) IK=1                                                  00268000
      DO 209 J=1,JJCHI                                                  00269000
      DO 208 K=1,7                                                      00270000
      AA(J,K)=AC(J,JJ)                                                  00271000
  208 AB(J,K)=AE(J,JJ)                                                  00272000
      DO 210 K=8,14                                                     00273000
      AA(J,K)=AC(J,JJ+IK)                                               00274000
  210 AB(J,K)=AE(J,JJ+IK)                                               00275000
  209 CONTINUE                                                          00276000
      DO 213 K=1,14                                                     00277000
      BD(K)=AD(K,JJ)                                                    00278000
  213 XNB(K)=XMA(K,JJ)                                                  00279000
      TNA1=0.0                                                          00280000
      TNA2=0.0                                                          00281000
      DO 215 K=1,6                                                      00282000
      TNA1=TNA1+XNB(K)                                                  00283000
  215 TNA2=TNA2+XNB(K+7)                                                00284000
      TNA1=TNA1+0.5*XNB(7)                                              00285000
      TNA2=TNA2+0.5*XNB(14)                                             00286000
      GO TO 192                                                         00287000
  160 DO 163 J=1,250                                                    00288000
      DO 163 KJ=1,14                                                    00289000
      AA(J,KJ)=AC(J,1)                                                  00290000
  163 AB(J,KJ)=AE(J,1)                                                  00291000
      MMM=0                                                             00292000
      JJ=1                                                              00293000
  192 Z=IZZ(JJ)                                                         00294000
      IF(JJ.EQ.2) GO TO 212                                             00295000
      DO 71 J=1,2                                                       00296000
      XRI(J)=(-8.8+.05*(JRI(J)-1.))                                     00297000
   71 RI(J)=EXP(XRI(J))                                                 00298000
      RD=((3./4.)*OMA/3.141593)**(1./3.)                                00299000
      IF(LAT.GT.5) GO TO 212                                            00300000
C                                                                       00301000
CCC   NEXT CARD MUST BE CHANGED IF DIFFERENT AVERAGE POTENCIAL IS WANTED 00302000
C                                                                       00303000
      JTOP=JJCHI                                                        00304000
      XJTOP=-8.8+.05*(XJJCHI-1.)                                        00305000
      RTOP=EXP(XJTOP)                                                   00306000
      TNOMA=((4./3.)*3.141593*RTOP**3)/OMA                              00307000
      CI=3./(RTOP**3-TNOMA*RI(1)**3)                                    00308000
      GO TO 211                                                         00309000
C                                                                       00310000
C                                                                       00311000
C        FOR SPECIAL CRYSTAL STRUCTURES THE INTERSTITIAL POTENTIAL IS   00312000
C        CALCULATED BY AN INTEGRATION  UP  TO  THE SEVEN SHELL OF NEIGH 00313000
C        BOURS SPECIFIED IN AAD.                                        00314000
C        THAT IS WHY BD(7) IS USED IN NEXT CARD.                        00315000
C                                                                       00316000
  212 JTOP=20.*(ALOG(BD(7))+8.85)                                       00317000
      RTOP=BD(7)                                                        00318000
      CI=3./(RTOP**3-(TNA1*RI(1)**3+TNA2*RI(2)**3))                     00319000
                                                                        00320000
                                                                        00321000
```

```
  211 CP=2.*(2./(2.*3.141593))**2)**(1./3.)                                00322000
  503 CALL SUMAX(AA,AACR,JJCHI,XMB,BD,JTOP)                               00323000
C**     WRITE(6,11234)(AACR(I),I=1,JJCHI)                                 00324000
      CALL SUMAX(AB,ABCR,JJCHI,XMB,BD,JTOP)                               00325000
C**     WRITE(6,11234)(ABCR(I),I=1,JJCHI)                                 00326000
C**34 FORMAT(10X,8E14.7)                                                  00327000
C                                                                         00328000
C       BEGIN CALCULUS OF AVERAGE POTENCIAL                               00329000
C                                                                         00330000
      IF(LAT.LE.5) GO TO 411                                              00331000
      ARTOP=FU(AACR(JTOP),AACR(JTOP+1),RAPW(JTOP),RAPW(JTOP+1),RTOP)      00332000
      BRTOP=FU(ABCR(JTOP),ABCR(JTOP+1),RAPW(JTOP),RAPW(JTOP+1),RTOP)      00333000
      FRC=CI*RTOP**3*ARTOP                                                00334000
      FRD=CI*RTOP**3*BRTOP                                                00335000
      FLC=CI*RAPW(JTOP)**3*AACR(JTOP)                                     00336000
      FLD=CI*RAPW(JTOP)**3*ABCR(JTOP)                                     00337000
      VINU1=0.025*(FRC+FLC)                                               00338000
      VINU2=0.025*(FRD+FLD)                                               00339000
C**     WRITE(6,1132)VINU1,VINU2,LAT                                      00340000
C**     WRITE(6,1125)ARTOP,BRTOP,JTOP                                     00341000
C**22 FORMAT(10X,2F14.7,2X,I4)                                            00342000
  411 VINT1=0.0                                                           00343000
      VINT2=0.0                                                           00344000
      JXB=0                                                               00345000
      XJXB=-8.85                                                          00346000
    7 JXB=JXB+1                                                           00347000
      JJRI=IFIX(JRI(JJ))                                                  00348000
      IF(JXB-JJRI)5,118,5                                                 00349000
    5 XJXB=XJXB+0.05                                                      00350000
      IF(JXB-JTOP)120,119,119                                             00351000
                                                                          00352000
  120 FRC=CI*EXP(3.*(XJXB+.05))*AACR(JXB+1)                               00353000
      FRD=CI*EXP(3.*(XJXB+.05))*ABCR(JXB+1)                               00354000
      FLC=CI*EXP(3.*XJXB)*AACR(JXB)                                       00355000
      FLD=CI*EXP(3.*XJXB)*ABCR(JXB)                                       00356000
      VINT1=VINT1+0.025*(FRC+FLC)                                         00357000
      VINT2=VINT2+0.025*(FRD+FLD)                                         00358000
C**   VINT3=VINT1/CI                                                      00359000
C**   VINT4=VINT2/CI                                                      00360000
C**   WRITE(6,1123)VINT3,VINT4                                            00361000
      GO TO 7                                                             00362000
  118 GGE=(AACR(JJRI+1)-AACR(JJRI))*(JRI(JJ)-JJRI)                        00363000
      FLC=(AACR(JJRI)+GGE)*CI*EXP(3*XRI(JJ))                              00364000
      PFIN1=(FRC+FLC)*(XRI(JJ)-(XJXB+0.05))/2.                            00365000
      PI1C=VINT1+PFIN1                                                    00366000
      GGE=(ABCR(JJRI+1)-ABCR(JJRI))*(JRI(JJ)-JJRI)                        00367000
      FLD=(ABCR(JJRI)+GGE)*CI*EXP(3*XRI(JJ))                              00368000
      PFIN2=(FRD+FLD)*(XRI(JJ)-(XJXB+0.05))/2.                            00369000
      PI1C=VINT2+PFIN2                                                    00370000
      QRI=PI1C/CI                                                         00371000
      VRI=(4./3.)*3.141593*(RI(JJ)**3)                                    00372000
      VEX=4.*3.141593*(Z-QRI)/(OMA-VRI)                                   00373000
C**   WRITE(6,1123)PI1C,PI1E,QRI,VRI,VEX,CI,CP,TNA1,TNA2                 00374000
      WRITE(6,1124)PI1C,PI1E,QRI,VRI,VEX,TNA1,TNA2                        00375000
 1124 FORMAT(20X,'INTEGRAL OF POTENTIAL IN THE MUFFIN TIN SPHERE=',E13.6  00376000
     1,/,20X,'INTEGRAL OF 4*PI*RHO=',E13.6,/,20X,'CHARGE INTO THE SPHERE=  00377000
     2,E13.6,/,20X,'VOLUME=',E13.6,/,20X,'EXCHANGE POTENTIAL=',E13.6,/,    00378000
     320X,'NUMBER OF ATOMS OF TYPE 1=',E15.6,/,20X,'NUMBER OF ATOMS OF T  00379000
     4YPE 2=',E13.6)                                                      00380000
      WRITE(6,1180)                                                       00381000
C**23 FORMAT(9E13.6)                                                      00382000
 1123 FORMAT(9E13.6)                                                      00383000
      GO TO 5                                                             00384000
  119 IF(LAT.GT.5) GO TO 214                                              00385000
      VINT=VINT1-TNOMA*PI1C-CP*XALPHA*VEX**(1./3.)                        00386000
      GO TO 216                                                           00387000
  214 VINT1=VINT1+VINU1                                                   00388000
      VINT2=VINT2+VINU2                                                   00389000
      IF(JJ.EQ.2)GO TO 220                                                00390000
C                                                                         00391000
C         STORAGE OF THE DATA OBTAINED WHEN THE CENTRAL ATOM IS OF TYPE 1 00392000
C                                                                         00393000
      P1=PI1C                                                             00394000
      VINC=VINT1-TNA1*P1                                                  00395000
      TN2=TNA2                                                            00396000
      VEX1=VEX                                                            00397000
      DO 219 J=1,JJCHI                                                    00398000
      AA1(J)=AACR(J)                                                      00399000
  219 AB1(J)=ABCR(J)                                                      00400000
      GO TO 227                                                           00401000
  220 VEXO=(VEX+VEX1)/2.                                                  00402000
      SIGN=1.0                                                            00403000
      IF(VEXO.LE.0.0)SIGN=-1.0                                            00404000
      IF(SIGN.EQ.-1.0)WRITE(6,4441)                                       00405000
 4441 FORMAT(2X,'EXCHANGE PART OF THE INTERSTITIAL POTENCIAL NEG          00406000
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     1ATIVE')                                                                   00407000
       VEXC=(SIGN*VEXO)**(1./3.)                                               00408000
       VINTA1=VINC-TM2*PI1C-CP*XALPHA*VEXC*SIGN                                00409000
       VINT  =VINT1-TMA2*P1-TMA1*PI1C-CP*XALPHA*VEXC*SIGN                      00410000
   207 MMM=1                                                                   00411000
C                                                                              00412000
CCC    BEGIN XALPHA-BETA                                                       00413000
C                                                                              00414000
   216 N=1                                                                     00415000
       DO 413 J=1,JTOP                                                         00416000
   413 ABCR(J)=ABCR(J)/(4.*3.141593)                                           00417000
       IF(XBETA.LT.1.0E-05)GO TO 203                                           00418000
       CALL DGT3(RAPW,ABCR,GRAD,JTOP,CON1)                                     00419000
       CALL DGT3(RAPW,GRAD,GRAD2,JTOP,CON2)                                    00420000
   203 DO 201 K=1,JTOP                                                         00421000
       G=RAPW(K)                                                               00422000
       RJ=ABCP(K)                                                              00423000
       IF(RJ.GT.1.0E-06.OR.XBETA.GT.1.E-05) GO TO 202                          00424000
       ALPALP=1.                                                               00425000
       GO TO 201                                                               00426000
   202 GR=GRAD(K)/RJ                                                           00427000
       QB=RJ**(1./3.)                                                          00428000
       GE(K)=((4./3.)*GR*GR-2.0*(GRAD2(K)+2.*GR*RJ/G)/RJ)/(QB*QB)              00429000
       ALPALP=1.+TAN1((XBETA/XALPHA)*GE(K))                                    00430000
C**    WRITE(6,123)G,RJ,GRAD(K),GRAD2(K),GE(K),ALPALP                          00431000
   201 SCP(K)=CP*XALPHA*ALPALP                                                 00432000
       DO 112 J=1,JTOP                                                         00433000
       ABCR(J)=ABCR(J)*4.*3.141593                                             00434000
   112 BGXMT(J)= AACR(J)-SCP(J)*ABCP(J)**(1./3.)-VINT                          00435000
       WRITE(6,28)(NAME(I),I=1,20)                                             00436000
C                                                                              00437000
CCC    CALCULUS OF V BOUNDARY BY INTEGRATION OF THE FINAL POTENTIAL            00438000
C      IN A VOLUME PER ATOM                                                    00439000
       CALL TRAPEZ(RO,BGXMT,VB)                                                00440000
       VBOUND=VB/(4*3.141593*RO**3)                                            00441000
C                                                                              00442000
       IF(LAT.LE.5) GO TO 313                                                  00443000
       IF(MMM.EQ.1) GO TO 311                                                  00444000
       WRITE(6,312)                                                            00445000
       GO TO 313                                                               00446000
   311 WRITE(6,314)                                                            00447000
   313 WRITE(6,117)RI,RO,VBOUND                                                00448000
       WRITE(6,117)VINT,Z,(JRI(JJ),JJ=1,2),LAT,XALPHA,XBETA                   00449000
       WRITE (6,115)BGXMT                                                      00450000
       DO 72 K=1,250                                                           00451000
    72 BGXMT(K)=-BGXMT(K)                                                      00452000
       WRITE (6,28)NAME                                                        00453000
       WRITE (7,28)NAME                                                        00454000
C      DO 73 K=1,234,18                                                        00455000
CCC 73 WRITE(7,74)BGXMT(K),BGXMT(K+3),BGXMT(K+6),BGXMT(K+9),BGXMT(K+12),B      00456000
C     1GXMT(K+15)                                                              00457000
C  74 FORMAT(10X,6F13.5)                                                       00458000
       WRITE(6,9997)                                                           00459000
       DO 1133 J=1,225                                                         00460000
 1133  FAP(J)=(BGXMT(J)+VINT)*RAPW(J)                                          00461000
       WRITE (6,115) (FAP(J),J=1,225)                                          00462000
       WRITE(6,1180)                                                           00463000
       IF(LAT.LE.5) GO TO 315                                                  00464000
       DO 221 J=1,JJCHI                                                        00465000
       AACR(J)=AA1(J)                                                          00466000
   221 ABCR(J)=AB1(J)                                                          00467000
       IF(MMM.EQ.1) N=2                                                        00468000
       VINT =VINTA1                                                            00469000
       Z=IZZ(1)                                                                00470000
                                                                               00471000
   315 CALL LOGDER(N)                                                          00472000
       MMM=MMM+1                                                               00473000
        IF(MMM.EQ.2) GO TO 216                                                 00474000
       GO TO 3                                                                 00475000
   316 STOP                                                                    00476000
CCC        THESE FINAL CARDS MAKE ZERO THE NUMBER OF NEIGHBOURS AND, IF        00477000
CCC        THE COMMENT ON CARD ME=-1 (BEFORE LABEL 503) IS RELEASED, THEN      00478000
CCCCC      A CALCULUS IS MADE FOR THE ATOM ALONE.  THIS CALCULUS OF POTEN      00479000
CCCCC      TIAL MUST BE SIMILAR TO ONE MADE BY HARTEE-FOCK OR HEX.             00480000
C                                                                              00481000
       END                                                                     00482000
       SUBROUTINE POISON(PSO,Z,J,N,JJ)                                         00483000
       DIMENSION PSO(250,2),A(250,2),B(250),F(250)                             00484000
       A=1.-.0025/48.                                                          00485000
       B=-2.-.0025/48.                                                         00486000
       FDL=EXP(.025)                                                           00487000
       C=.0025/6.                                                              00488000
       C2=B/A                                                                  00489000
                                                                               00490000
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      F(1)=2.
      F(I)=EXP(.5*S)                                                    00491000
      X=-8.8                                                            00492000
      ITOP=50                                                           00493000
      DO 5 I=2,ITOP                                                     00494000
      K1=I-1                                                            00495000
      K2=I-2                                                            00496000
      S=0.*EXP(-.5*X)*(CBL*PSO(K1,JJ)+10.*PSO(I,JJ)+PSO(K2,JJ))/EBL     00497000
      F(I)=S2-1./F(K2)                                                  00498000
      P(I)=(I/A+F(K2))/F(I)                                             00499000
    5 X=X+.05                                                           00500000
      W(J,JJ)=2.*Z*EXP(-.5*X)                                           00501000
      DO 6 I=1,ITOP                                                     00502000
      JV=J-I                                                            00503000
      JV1=JV+1                                                          00504000
    6 R(JV,JJ)=E(JV)+W(JV1,JJ)/F(JV)                                    00505000
      RETURN                                                            00506000
      END                                                               00507000
      SUBROUTINE SUMAX(CHIAT,CHICRY,JJCHI,XNA,AD,JTOP)                  00508000
      DIMENSION CHIAT(250,14),CHICRY(250),XNA(15),AD(15),STOR(250,15)   00509000
C           SUMS OVER 14 LARGEST SHELLS OF ATOMS                        00510000
      XJJCHI=JJCHI                                                      00511000
      TOPX=.05*(XJJCHI-1.)-8.8                                          00512000
      DO 8 J=1,JTOP                                                     00513000
    8 STOR(J,1)=CHIAT(J,1)                                              00514000
      JA=2                                                              00515000
    7 X=-8.8                                                            00516000
      I=1                                                               00517000
    8 XINT=0                                                            00518000
      ET=EXP(X)                                                         00519000
      BLX=ALOG(ABS(AD(JA)-ET))                                          00520000
      IF (BLX-TOPX)9,50,50                                              00521000
    9 JBL=2.+20.*(BLX+8.8)                                              00522000
      XJBL=JBL                                                          00523000
      XBL=.05*(XJBL-1.)-8.8                                             00524000
      G=XBL-BLX                                                         00525000
      XINT=XINT+.5*G*(CHIAT(JBL,JA)*(2.-20.*G)*EXP(2.*XBL)+20.*G*CHIAT( 00526000
     1JBL-1,JA)*EXP(2.*(XBL-.05)))                                      00527000
      TLX=ALOG(ABS(JA)+ET)                                              00528000
      IF (TLX-TOPX)10,11,11                                             00529000
   11 JTL=JJCHI                                                         00530000
      GO TO 40                                                          00531000
   10 JTL=1.+20.*(TLX+8.8)                                              00532000
      IF (JTL-JBL)12,13,13                                              00533000
   12 FZ0=CHIAT(JTL,JA)*EXP(2.*(XBL-.05))                               00534000
      FZ3=CHIAT(JBL,JA)*EXP(5.*XBL)                                     00535000
      FZ2=FZ0+20.*(FZ3-FZ0)*(TLX-XBL+.05)                               00536000
      FZ1=FZ0+20.*(FZ3-FZ0)*(BLX-XBL+.05)                               00537000
      XINT=.5*(FZ1+FZ2)*(TLX-BLX)                                       00538000
      GO TO 50                                                          00539000
   13 XJTL=JTL                                                          00540000
      XTL=.05*(XJTL-1.)-8.8                                             00541000
      C=TLX-XTL                                                         00542000
      K3=JTL+                                                           00543000
      XINT=XINT+.5*C*(CHIAT(JTL,JA)*(2.-20.*C)*EXP(2.*XTL)+CHIAT(K3,JA)* 00544000
     120.*C*EXP(5.*(XTL+.05)))                                          00545000
   40 IF (JTL-JBL)55,30,14                                              00546000
   14 XINT=XINT+.5*(CHIAT(JBL,JA)*EXP(2.*XBL)+CHIAT(JBL+1,JA)*EXP(2.*   00547000
     1(XBL+.05)))*.05                                                   00548000
      JBL=JBL+1                                                         00549000
      IF (JBL-JTL)15,30,55                                              00550000
   15 XBL=XBL+.05                                                       00551000
      GO TO 14                                                          00552000
   55 STOR(I,JA)=.5*XINT*XNA(JA)/(AD(JA)*ET)                            00553000
      IF (I-JTOP)16,17,17                                               00554000
   16 I=I+1                                                             00555000
      X=X+.05                                                           00556000
      GO TO 8                                                           00557000
   17 IF (JA-14)19,20,20                                                00558000
   19 JA=JA+1                                                           00559000
      GO TO 7                                                           00560000
   20 I=1                                                               00561000
   21 JA=1                                                              00562000
      CHICRY(I)=0.                                                      00563000
   22 CHICRY(I)=CHICRY(I)+STOR(I,JA)                                    00564000
      IF (JA-14)23,24,24                                                00565000
   23 JA=JA+1                                                           00566000
      GO TO 22                                                          00567000
   24 IF (I-JTOP)25,26,26                                               00568000
   25 I=I+1                                                             00569000
      II=I-1                                                            00570000
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      GO TO 21                                                          00575000
   20 RETURN                                                            00576000
      END                                                               00577000
      SUBROUTINE DGT3(X,Y,Z,NDIM,IER)                                   00578000
      DIMENSION X(1),Y(1),Z(1)                                          00579000
      IER=-1                                                            00580000
      IF(NDIM-3)3,1,1                                                   00581000
    1 A=X(1)                                                            00582000
      B=Y(1)                                                            00583000
      I=2                                                               00584000
      DY2=X(2)-A                                                        00585000
      IF(DY2)2,9,2                                                      00586000
    2 DY2=(Y(2)-B)/DY2                                                  00587000
      DO 6 I=3,NDIM                                                     00588000
      A=X(I)-A                                                          00589000
      IF(A)3,9,3                                                        00590000
    3 A=(Y(I)-B)/A                                                      00591000
      B=X(I)-X(I-1)                                                     00592000
      IF(B)4,9,4                                                        00593000
    4 DY1=DY2                                                           00594000
      DY2=(Y(I)-Y(I-1))/B                                               00595000
      DY3=A                                                             00596000
      A=X(I-1)                                                          00597000
      B=Y(I-1)                                                          00598000
      IF(I-3)5,5,6                                                      00599000
    5 Z(I-2)=DY1+DY3-DY2                                                00600000
    6 Z(I-1)=DY1+DY2-DY3                                                00601000
      IER=0                                                             00602000
      I=NDIM                                                            00603000
    7 Z(I)=DY2+DY3-DY1                                                  00604000
    8 RETURN                                                            00605000
    9 IER=I                                                             00606000
      I=I-1                                                             00607000
      IF(I-2)8,8,7                                                      00608000
      END                                                               00609000
$SET CAM                                                                00610000
                                                                        00611000
      SUBROUTINE LOGDER(I)                                              00612000
C                                                                       00613000
C  LOGARITHMIC DERIVATIVES SUBROUTINE.ALSO COMPUTES PHASE SHIFTS.       00614000
C  SIMPLIFIED VERSION.                                                  00615000
      COMMON/CRYDER/AGX(250),TEXT(20),JRI(2),UMA,A0,NJJ,EFE,IAL,IZZ     00616000
      DIMENSION ISTER(6),EN(60),P(5,90),PP(5,90),Y(250),AN(5,90),       00617000
     1FFG(5),CLD(5),FLD(5),CFG(5),ELIA(5,90),CEP(5,90)                  00618000
      DIMENSION BESTA(60),SZI(60),DVINT(2),CF(4)                        00619000
      REAL JRI,JRI                                                      00620000
      INTEGER NUMA(2),ZVAL(2)                                           00621000
C                                                                       00622000
C     SYMBOLS TO PLOT                                                   00623000
      DATA ISTER/'.',' ','*','+','-','='/                               00624000
C                                                                       00625000
C        MAXL=MAXIMUM ANGULAR MOMENT                                    00626000
C        NE=NUMBER OF ENERGIES                                          00627000
C        BE=BOTTOM ENERGY                                               00628000
C        ES=STEP ENERGY                                                 00629000
C        DVINT=ADDITIONAL V INTERSTITIAL                                00630000
C        ZVAL=NUMBER OF VALENCE ELECTRONS                               00631000
      FUC(A,B,C,D,T)=(A*(D-T)-B*(C-T))/(D-C)                            00632000
                          IF(NJJ.EQ.1.OR.N.EQ.2)                        00633000
     *READ(5,1)MAXL,NE,ZVAL(1),ZVAL(2),NUMA(1),NUMA(2),BE,ES,DVINT(1),  00634000
     1DVINT(2),IRESIS                                                   00635000
    1 FORMAT(6I5,4F10.5,2I5)                                            00636000
C                                                                       00637000
C        AGX=CONDENSED MATTER POTENTIAL (MUFFIN-TIN)                    00638000
      DO 2 I=1,250                                                      00639000
    2 AGX(I)=-(AGX(I)+DVINT(1))                                         00640000
      WRITE(6,3)TEXT                                                    00641000
    3 FORMAT(1H1,20X,20A4)                                              00642000
      WRITE(6,4)DVINT(1),MAXL,NE,BE,ES                                  00643000
    4 FORMAT(///,20X,'ADDITIONAL VINT FOR OVERLOG=',F10.4,//,20X,'LMAX=',00644000
     1I2,/,20X,'NUMBER OF ENERGIES=',I4,/,20X,'BOTTOM ENERGY=',F10.4,//,2 00645000
     2OX,'STEP ENERGY=',F10.4)                                          00646000
C                                                                       00647000
C        NUMERICAL SOLUTION OF SCHRODINGER EQUATION. MILNE'S METHOD     00648000
      JRI=JRI(1)                                                        00649000
      DAC=2.0333333E-04                                                 00650000
      DB=DAC*10.0                                                       00651000
      NL=MAXL+1                                                         00652000
      DO 5 I=1,NL                                                       00653000
      WL=I-1                                                            00654000
      CE(WL+0.5)**2                                                     00655000
      E=BE-ES                                                           00656000
                                                                        00657000
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      DO 5 J=1,NE                                                       00658000
      E=E+ES                                                            00659000
      EN(J)=E                                                           00660000
      YJM1=A.E-20                                                       00661000
      YJ=EXP(.05*(NL+.5))*YJM1                                          00662000
      SGM1=0+EXP(-17.5)*(AGX(1)-E)                                      00663000
      SG=0+EXP(-17.5)*(AGX(2)-E)                                        00664000
      X=-8.0                                                            00665000
      Y(1)=YJM1                                                         00666000
      Y(2)=YJ                                                           00667000
      JJRI=IFIX(JRI)                                                    00668000
      DO 6 K=1,JJRI+1                                                   00669000
      X=X+0.05                                                          00670000
      EEF=EXP(2.*(X+.05))                                               00671000
      SGP1=0+EEF*(AGX(K+2)-E)                                           00672000
      A=1.-DAC*SGP1                                                     00673000
      B=-2.-DD*SG                                                       00674000
      C=1.-DAC*SGM1                                                     00675000
      YJP1=-(B*YJ+C*YJM1)/A                                             00676000
      Y(K+2)=YJP1                                                       00677000
      YJM1=YJ                                                           00678000
      YJ=YJP1                                                           00679000
      SGM1=SG                                                           00680000
    6 SG=SGP1                                                           00681000
      XJ=X-0.05                                                         00682000
C                                                                       00683000
C        R=RADIAL PART OF THE WAVE FUNCTION                             00684000
C        RP=DERIVATIVE OF R                                             00685000
      YJRI=FU(Y(JJRI),Y(JJRI+1),JJRI,JJRI+1,JRI)                        00686000
      R(I,J)=EXP(-0.5*(-8.85+0.05*JRI))*YJRI                            00687000
      YP1=(Y(JJRI-2)-8.0*Y(JJRI-1)+8.0*Y(JJRI+1)-Y(JJRI+2))/0.6         00688000
      YP2=(Y(JJRI-1)-8.0*Y(JJRI)+8.0*Y(JJRI+2)-Y(JJRI+3))/0.6           00689000
      YP=FU(YP1,YP2,JJRI,JJRI+1,JRI)                                    00690000
      RP(I,J)=EXP(-1.5*(-8.85+0.05*JRI))*(YP-0.5*YJRI)                  00691000
C                                                                       00692000
C        AN=LOGARITHMIC DERIVATIVES                                     00693000
    5 AN(I,J)=RP(I,J)/R(I,J)                                            00694000
      WRITE(6,7)MAXL                                                    00695000
    7 FORMAT(4(/),20X,'LOGARITHMIC DERIVATIVES FOR L=0 TO L=',I1)       00696000
      WRITE(6,8)                                                        00697000
    8 FORMAT(13X,'ENERGY',8X,'L=0',11X,'L=1',11X,'L=2',11X,'L=3')       00698000
      DO 9 J=1,NE                                                       00699000
    9 WRITE(6,10)EN(J),(AN(I,J),I=1,NL)                                 00700000
   10 FORMAT(10X,F10.4,4D14.7)                                          00701000
      WRITE(6,13)                                                       00702000
   13 FORMAT(1H1,20X,'PHASE SHIFTS ',/,21X,12('*'))                     00703000
      WRITE(6,8)                                                        00704000
      DO 14 J=1,NE                                                      00705000
      DO 12 I=1,NL                                                      00706000
      E=EN(J)                                                           00707000
      CALL OLDASH(E,JRI,MAXL,CLD,CFG,FLD,FFG)                           00708000
      TETA=CFG(I)*(CLD(I)-AN(I,J))/(FFG(I)*(FLD(I)-AN(I,J)))            00709000
C                                                                       00710000
C        ELTA=PHASESHIFTS                                               00711000
      ELTA(I,J)=ATAN(TETA)                                              00712000
      CET      =COS(ELTA(I,J))/SIN(ELTA(1,J))                           00713000
   12 CEP(I,J)=CET      *FFG(I)/CFG(I)                                  00714000
   14 WRITE(6,10)EN(J),(ELTA(I,J),I=1,NL)                               00715000
      WRITE(6,282)                                                      00716000
  282 FORMAT(20X,'CEP',/,21X,3('*'))                                    00717000
      DO 11 J=1,NE                                                      00718000
   11 WRITE(6,10) EN(J),(CEP(I,J),I=1,NL)                               00719000
  281 FORMAT(1H1,20X,'ENERGY',8X,'L=0',11X,'L=1',11X,'L=2',11X,'L=3')   00720000
C                                                                       00721000
C       THIS PART OF THE PROGRAM MAKES THE PHASESHIFTS CONTINUOUS       00722000
      DO 21  K=1,NL                                                     00723000
      ISIGN=1                                                           00724000
      ID=1                                                              00725000
      DO 21 J=1,NE                                                      00726000
      IF(J.LT.NE)DIF=ABS(ELTA(K,J+1)-ELTA(K,J))                         00727000
      GO TO(20,19,21),ID                                                00728000
   19 ELTA(K,J)=ELTA(K,J)+ISIGN*3.141593                                00729000
   20 IF(DIF.LT.1.0) GO TO21                                            00730000
      ID=ID+1                                                           00731000
      IF(ELTA(K,J).LT.0.0) ISIGN=-1                                     00732000
   21 CONTINUE                                                          00733000
  227 FORMAT(20X,'VALENCE=',F10.6)                                      00734000
C                                                                       00735000
C                                                                       00736000
C       CALCULUS OF THE FLUX LEVEL BY FRIEDEL SUM                       00737000
      FFE2=EFG*(NUM-Z)                                                  00738000
      IOUT=1                                                            00739000
      DO 22 J=1,NE                                                      00740000
                                                                        00741000
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      OMEGA=OMA*(EN(J)**(3./2.))/(3*3.141593**2)                        00742000
      SUMA=0.0                                                          00743000
      DO 23 K=1,NL                                                      00744000
      IF(K.EQ.4)GO TO 23                                                00745000
      SUMA=2*(2*(K-1)+1)*ELTA(K,J)/3.141593+SUMA                        00746000
   23 CONTINUE                                                          00747000
      SIGMA=OMEGA+SUMA                                                  00748000
      RESTA(J)=SIGMA-ZVAL(N)                                            00749000
      IF(RESTA(J).GE.0.0) IOUT=-3                                       00750000
      IF(J.GT.2) IOUT=IOUT+1                                            00751000
      IF(IOUT.EQ.0) GO TO 24                                            00752000
   22 CONTINUE                                                          00753000
   24 EFE=INTER(EN,RESTA,NE,0.0,4)                                      00754000
      WRITE(6,279) EFE                                                  00755000
      EFE2=(EFE2+EFE)*N/FLOAT(NJJ)                                      00756000
      IF(N.EQ.1.AND.NJJ.EQ.2) WRITE(6,283) EFE2                         00757000
      WRITE(6,227) ZVAL(N)                                              00758000
C                                                                       00759000
      DO 25 IN=1,NL                                                     00760000
      DO 26 INE=1,NE                                                    00761000
   26 ZZI(INE)=ELTA(IN,INE)                                             00762000
      CF(IN)=INTER(ZZI,EN,NE,EFE,4)                                     00763000
   25 WRITE(6,280) IN,CF(IN)                                            00764000
      IF(RESIS.GT.0) CALL RESIS(OMA,EFE,IZZ,CF,N)                       00765000
C        PLOTTING PHASESHIFTS                                           00766000
      CALL CARTE(NE,ELTA,EN,ISTER,NL,EFE)                               00767000
      WRITE(6,15)TEXT                                                   00768000
      IF(IAL.EQ.0) RETURN                                               00769000
      NPH=NE                                                            00770000
      IF(N.EQ.2) GO TO 29                                               00771000
      EMAX=EFE*1.3                                                      00772000
C                                                                       00773000
      NPH= (EMAX-BF)/ES+1                                               00774000
      NPH=MIN0(NPH,NE)                                                  00775000
      IF(NJJ.EQ.1) GO TO 28                                             00776000
      REWIND IAL                                                        00777000
      DO 27 I=1,NL                                                      00778000
      DO 27 J=1,NE,8                                                    00779000
   27 READ(IAL,278) AN(I,J),AN(I,J+1),AN(I,J+2),AN(I,J+3),AN(I,J+4),AN(I 00780000
     *,J+5),AN(I,J+6),AN(I,J+7)                                         00781000
   28 REWIND IAL                                                        00782000
      WRITE(IAL,277) A0,BE,EMAX,ES,MAXL,NPH,NJJ,NUMA(1),ZVAL(1),NUMA(2), 00783000
     *ZVAL(2)                                                           00784000
  277 FORMAT(4F10.6,7I3)                                                00785000
      WRITE(IAL,278) (EN(K),K=1,NPH)                                    00786000
   29 DO 30 K=1,NL                                                      00787000
   30 WRITE(IAL,278) (ELTA(K,J),J=1,NPH)                                00788000
         IF(NJJ.EQ.1) CALL ASIL(IAL)                                    00789000
         IF(N.EQ.2.OR.IAL.EQ.0)        RETURN                           00790000
      WRITE(IAL,278)    (EN(K),K=1,NPH)                                 00791000
      DO 31 K=1,NL                                                      00792000
   31 WRITE(IAL,278) (AN(K,J),J=1,NPH)                                  00793000
      CALL ASIL(IAL)                                                    00794000
  278 FORMAT(8F10.7)                                                    00795000
  279 FORMAT(////20X,'FERMI LEVEL=',F10.5,'     RYDBERGS')              00796000
  280 FORMAT(20X,'FOR L =',I3,'  PHASESHIFT AT FERMI LEVEL='F12.8)      00797000
  283 FORMAT(20X,'APPROXIMATE FERMI LEVEL FOR THE ALLOY='F10.5)         00798000
C                                                                       00799000
   15 FORMAT(1H ,20X,20A4)                                              00800000
C                                                                       00801000
      RETURN                                                            00802000
 $RESET OWN                                                             00803000
      END                                                               00804000
      SUBROUTINE TRAPEZ(RO,BGXMT,VINT)                                  00805000
      DIMENSION BGXMT(250)                                              00806000
      ARO=20*(8.85+ALOG(RO))                                            00807000
      JRO=ARO                                                           00808000
      PI4=4.*3.141593                                                   00809000
      JXB=0                                                             00810000
      XJXB=-8.85                                                        00811000
    7 JXB=JXB+1                                                         00812000
      IF(JXB-JRO)5,6,6                                                  00813000
    5 XJXB=XJXB+0.05                                                    00814000
      FR=PI4*EXP((XJXB+0.05)*3.)*BGXMT(JXB+1)                           00815000
      FL=PI4*EXP(3.*XJXB)*BGXMT(JXB)                                    00816000
      VINT=VINT+0.025*(FR+FL)                                           00817000
      GO TO 7                                                           00818000
    6 BGRO=BGXMT(JRO)+(BGXMT(JRO)+BGXMT(JRO+1))*(ARO-JRO)               00819000
      FL=PI4*EXP(3.*ALOG(RO))*BGRO                                      00820000
      END=0.025*(FR+FL)                                                 00821000
      VINT=VINT+END                                                     00822000
      RETURN                                                            00823000
      END                                                               00824000
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      SUBROUTINE BLDASH(E,JRI,LMAX,CLD,CFG,FLD,FFG)                     00825000
      DIMENSION BLD(10),BFG(10),CLD(10),CFG(10),FLD(10),FFG(10),ELD(10),00826000
     1EFG(10)                                                           00827000
      DOUBLE PRECISION BLD,BFG,EN,A,RS,X,BJMO,BJZ,Z,P,Q,ZMULT,ZC,ELD,   00828000
     1FFG,XJRI,XI                                                       00829000
      REAL JRI                                                          00830000
      EN=E                                                              00831000
      XJRI=JRI                                                          00832000
                                                                        00833000
      XI=0.05*(XJRI-1.)-8.8                                             00834000
      RS=DEXP(XI)                                                       00835000
      MLD=LMAX+2                                                        00836000
      MMM=MLD-1                                                         00837000
      P=2.                                                              00838000
      Q=1.0                                                             00839000
      A=DSQRT(DABS(EN))                                                 00840000
      X=A*RS                                                            00841000
      IF(EN)5,27,51                                                     00842000
C     BJMO =  IMAGINAGY , BJZ = REAL                                    00843000
    5 BJMO=0.5*(DEXP(-X)+DEXP(X))/X                                     00844000
      BJZ=-0.5*(DEXP(-X)-DEXP(X))/X                                     00845000
      C=-1.0                                                            00846000
      GO TO 52                                                          00847000
   51 BJMO=DCOS(X)/X                                                    00848000
      BJZ=DSIN(X)/X                                                     00849000
      C=1.0                                                             00850000
   52 ZC=C                                                              00851000
      BFG(1)=BJZ                                                        00852000
      BFG(2)=ZC*(BJZ/X-BJMO)                                            00853000
      EFG(1)=-BJMO                                                      00854000
      EFG(2)=-ZC*(BJMO/X+BJZ)                                           00855000
      DO 70 I=2,MLD                                                     00856000
      Z=I                                                               00857000
      ZMULT=C**I                                                        00858000
      BFG(I+1)=ZMULT*(P*Z-Q)*BFG(I)/X-BFG(I-1)                          00859000
   70 EFG(I+1)=ZMULT*(P*Z-Q)*EFG(I)/X-EFG(I-1)                          00860000
      BLD(1)=-BFG(2)                                                    00861000
      ELD(1)=-EFG(2)                                                    00862000
      DO 71 I=1,MMM                                                     00863000
      Z=I                                                               00864000
      BLD(I+1)=(Z*BFG(I)-(Z+Q)*BFG(I+2))/(P*Z+Q)                        00865000
   71 ELD(I+1)=(Z*EFG(I)-(Z+Q)*EFG(I+2))/(P*Z+Q)                        00866000
      DO 72 I=1,MLD                                                     00867000
      Z=I                                                               00868000
      ZMULT=C**I                                                        00869000
      BLD(I)=(BLD(I)/BFG(I))*A*ZMULT                                    00870000
      ELD(I)=(ELD(I)/EFG(I))*A*ZMULT                                    00871000
      CLD(I)=BLD(I)                                                     00872000
      CFG(I)=BFG(I)                                                     00873000
      FLD(I)=ELD(I)                                                     00874000
   72 FFG(I)=EFG(I)                                                     00875000
      GO TO 28                                                          00876000
   27 WRITE (6,73)                                                      00877000
   73 FORMAT (14H ZERO ENERGY  )                                        00878000
   28 RETURN                                                            00879000
      END                                                               00880000
      REAL FUNCTION INTEP(Y,X,N,Z,NPP)                                  00881000
      DIMENSION Y(60),X(60),FU1(10)                                     00882000
      FO(A,B,C,D,T)=(A*(D-T)-B*(C-T))/(D-C)                             00883000
      DO 1 KUAL=1,N                                                     00884000
      IF(Z-X(KUAL))2,2,1                                                00885000
    1 CONTINUE                                                          00886000
    2 IU=KUAL-NPP/2                                                     00887000
      IF(IU.LT.1) IU=1                                                  00888000
      IF(NPP+IU.GT.N) IU=N-NPP+1                                        00889000
      L=IU                                                              00890000
      DO 3 J=1,NPP                                                      00891000
      FU1(J)=Y(L)                                                       00892000
                                                                        00893000
    3 L=L+1                                                             00894000
      IX=1                                                              00895000
    4 DO 5 K=1,NPP-IX                                                   00896000
      FU1(K)=FO(FU1(K),FU1(K+1),X(IU),X(IU+IX),Z)                       00897000
    5 IU=IU+1                                                           00898000
      IU=L-NPP                                                          00899000
      IX=IX+1                                                           00900000
      IF(IX.LT.NPP) GO TO 4                                             00901000
      INTEP=FU1(1)                                                      00902000
      RETURN                                                            00903000
      END                                                               00904000
      SUBROUTINE CARTE(I,X,T,IS,N,EF)                                   00905000
      DIMENSION X(5,100),T(100),IS(6),XPL(100),XPLO(100),IG(5,100),     00906000
     1L(101),A(6)                                                       00907000
   20 FORMAT(I4,E14.5)                                                  00908000
   21 FORMAT(2X)                                                        00909000
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   22 FORMAT(1H1)                                                                  00910000
   23 FORMAT(15X,5('I                    '),'I')                                   00911000
   24 FORMAT(6(1PE                  ))                                             00912000
   25 FORMAT(1H+,14X,101('-'))                                                     00913000
   30 FORMAT(1H+,14X,101A1)                                                        00914000
      WRITE(6,22)                                                                  00915000
      CALL MIMAX(T,T0,TF,I)                                                        00916000
      DO 1 K=1,N                                                                   00917000
      DO 2 J=1,I                                                                   00918000
    2 XPL(J)=X(K,J)                                                                00919000
      CALL MIMAX(XPL,XMIN,XMAX,I)                                                  00920000
      XPLO(K)=XMIN                                                                 00921000
      KK=K+N                                                                       00922000
    1 XPLO(KK)=XMAX                                                                00923000
      KK=2.*N                                                                      00924000
      CALL MIMAX(XPLO,XMIN,XMAX,KK)                                                00925000
      DO 3 K=1,N                                                                   00926000
      DO 3 J=1,I                                                                   00927000
    3 IG(K,J)=50.*(1.-(X(K,J)-XMIN)/(XMAX-XMIN))+1.5                               00928000
      DO 4 K=1,51                                                                  00929000
      L(1)=IS(1)                                                                   00930000
      DO 5 J=2,101                                                                 00931000
    5 L(J)=IS(2)                                                                   00932000
      DO 6 II=1,N                                                                  00933000
      DO 7 III=1,I                                                                 00934000
      IF(IG(II,III)-K)7,8,7                                                        00935000
    8 SJ=100.*(III-1)/(I-1)+1.5                                                    00936000
      JJ=SJ                                                                        00937000
      L(JJ)=IS(II+2)                                                               00938000
    7 CONTINUE                                                                     00939000
      JKL=((ET-T0)/(TF-T0))*100+1.5                                                00940000
      IF(JKL.GT.101) GO TO 77                                                      00941000
      L(JKL)=IS(1)                                                                 00942000
   77 WRITE(6,30) (L(KK),KK=1,101)                                                 00943000
      DO 6 KK=1,101                                                                00944000
      L(KK)=IS(2)                                                                  00945000
    6 CONTINUE                                                                     00946000
      IF(K-51)17,18,17                                                             00947000
   17 SJ=(K+4)/5.                                                                  00948000
      JK=SJ                                                                        00949000
      IF(JK-SJ)9,10,9                                                              00950000
   10 SJ=XMAX-(K-1)*(XMAX-XMIN)/50.                                                00951000
      WRITE(6,20)SJ                                                                00952000
                                                                                   00953000
    9 WRITE(6,21)                                                                  00954000
      IF(K-50)4,14,4                                                               00955000
   14 DO 11 J=1,101                                                                00956000
   11 L(J)=IS(1)                                                                   00957000
      WRITE(6,25)                                                                  00958000
   18 WRITE(6,20)XMIN                                                              00959000
    4 CONTINUE                                                                     00960000
      WRITE(6,23)                                                                  00961000
      DO 12 J=1,6                                                                  00962000
   12 A(J)=T0+(J-1)*(TF-T0)/5.                                                     00963000
      WRITE(6,24)(A(J),J=1,6)                                                      00964000
      RETURN                                                                       00965000
      END                                                                          00966000
      SUBROUTINE MIMAX(V,VMIN,VMAX,N)                                              00967000
      DIMENSION V(100)                                                             00968000
      VMAX=V(1)                                                                    00969000
      VMIN=V(1)                                                                    00970000
      DO 1 I=2,N                                                                   00971000
      IF(V(I)-VMAX)2,2,3                                                           00972000
    3 VMAX=V(I)                                                                    00973000
      GO TO 1                                                                      00974000
    2 IF(VMIN-V(I))1,1,4                                                           00975000
    4 VMIN=V(I)                                                                    00976000
    1 CONTINUE                                                                     00977000
      RETURN                                                                       00978000
      END                                                                          00979000
$SET OWN                                                                           00980000
      SUBROUTINE ASIL(IAL)                                                         00981000
                                                                                   00982000
      REAL KAPA,INTER,LX(24),LY(24),LZ(24),RSS(8)                                  00983000
                                                                                   00984000
      INTEGER C1,C2,SL,TN,TN1,PARA,FSIGN,FJUMP,TMAX,TPROM,SEG,ZVAL(2),CC           00985000
     1,Z,T                                                                         00986000
                                                                                   00987000
                                                                                   00988000
      DIMENSION NAME(10),VENERG(100),QNTER(5,100),IS(6),INUMA(2),DENSST(           00989000
     1200),PSHIFT(8),SCF(8,2),POM(60),E(60,2),PH(4,60,2),AKSS(140),AE(60           00990000
     2),COSTHE(20),R12(290),APHI(290),NUMA(3)                                      00991000
```

```
      COMPLEX KAPC,ENERGC,COMDET,KSC(20,4),POTC(20),G(140,140),DETC
      COMMON/VCOMPL/G,KSC,KAPC,ENERGC,POTC
      COMMON/VARRE/LX,LY,LZ,KSS,PSHIFT,JCF,E,POM,PH,AKSS,COSTHE,R12,APHI
      COMMON/VSIMP/KAPA,DETRE,DETIM,OFRSUM,PI,ENERGY,FSIGN,FJUMP,N1,NE,L
     1SS1,NUMSC,IOPL
      DATA IS/' ','.',':','*','+','-','0'/
C     ASIL ALLOYS PROGRAM TO COMPUTE DENSITY OF STATES OF ALLOYS (1-3 TY
C     ACCORDING TO CLUSTER METHOD. DEFINITIONS AS IN J. KELLER PAPER IN
C     COMPUTATIONAL METHODS FOR LARGE MOLECULES AND LOCALIZED STATES IN
C     PLENUM PRESS 1973)
  100 FORMAT(5F8.5)
  201 FORMAT(' CALCULATION OF THE DENSITY OF STATES FOR COMPLEX OF'
     1,I10,' SCATTERERS IN ')
  500 FORMAT(1H+,82X,3A6)
  600 FORMAT(//,' MAXIMUM SINGLE SITE PHASESHIFT=',I10)
  700 FORMAT(///,' ENERGY REGION: EMIN= ',F12.8,' EMAX= ',F12.8,' WITH
     1STEP EDELTA= ',F12.8)
      IF(IAL.NE.5)REWIND IAL
C     INPUT=  Z= ATOMIC NUMBER AS REFERENCE,  A0= LATTICE PARAMETER OF
C     CRYSTALLINE EQUIVALENT,  LSS= MAXIMUM ANGULAR MOMENT,  NPH= NUMBER
C     PHASESHIFTS AND ENERGIES GIVEN TO CARACTHERIZE SCATTERERS (SAME F
C     ALL TYPES),  NUMSC= TOTAL NUMBER OF SCATTERERS,  EMIN,EMAX, AND E
C     LOWER,HIGHER AND STEP OF THE ENERGY MESH OF THE CALCULATION
      READ(IAL,74)A0,EMIN,EMAX,EDELTA,LSS,NPH,T,NUMA(1),ZVAL(1),NUMA(2
     *),ZVAL(2)
      READ(5,75) TMAX,LLSS,IOPL,NPP,ATOCEL,NAME
      READ(5,73)PARA,EEMIN,EEMAX,EEDELT,FINT1,INUMA(1),INUMA(2)
      FINT=0.5
      IF(EEMIN.NE.0.) EMIN=EEMIN
      IF(EEMAX.NE.0.) EMAX=EEMAX
      IF(EEDELT.NE.0.) EDELTA=EEDELT
      IF(FINT1.NE.0.) FINT=FINT1
   73 FORMAT(I5,4F10.5,2I5)
      TMAX=TMAX-(TIME(2)/60)
      NUMSC=NUMA(1)+NUMA(2)+INUMA(2)+INUMA(1)+INUMA(2)
   74 FORMAT(4F10.6,7I3)
   75 FORMAT(I5,I3,2I2,F8.4,10A6)
      IF(NPP.EQ.0) NPP=4
C      ATOCEL=ATOMS IN A0**3
C     IOPL=1 IF P ELECTRONS ACCOUNTED
      WRITE(6,77) NAME
   77 FORMAT(1H1,20X,10A6,/)
C
C
      WRITE(6,201)NUMSC
      WRITE(6,500)NAME(1),NAME(2),NAME(3)
      WRITE(6,600)LSS
C
      EMAX=EMAX+0.01*EDELTA
      NE=(EMAX-EMIN)/EDELTA+1
      NE=2*NE
C     NUMBER OF POINTS DOUBLE OF GIVEN BY EDELTA TO
C     AVOID UNFAITHFUL PHASE.
 1100 FORMAT(3F10.8)
C     LX, LY AND LZ = CARTESIAN COORDINATES OF SCATTERERS IN THE ALLOY
   10 READ(5,1101)(LX(I),LY(I),LZ(I),I=1,NUMSC)
      LSS1=LSS+1
      PI=3.141593
C     T=NUMBER OF TYPES OF SCATTERERS IN THE ALLOY
      WRITE(6,3500)T
 3500 FORMAT(//,' NUMBER OF TYPES OF ATOMS',I5)
C     NUMA(TN) = NUMBER OF SCATTERERS OF EACH TYPE
 3003 FORMAT(3I5)
      WRITE(6,501)ATOCEL,A0,NPP
  501 FORMAT(//,' ATOMS PER UNIT CELL=',F10.5,5X,' LATTICE PARAMETER A='
     1F9.5,5X,' POINTS FOR THE INTERPOLATING FUNCTION=',I5)
      BLK='
      IF(IOPL.LT.1)BLK='*NOT'
      WRITE(6,502)BLK
  502 FORMAT(//'***P ELECTRONS',A4,' ACCOUNTED')
      TN=1
      LSS=LSS1-LLSS
      GO TO 3004
```

```
 1101 FORMAT(3F10.7)                                                    01076000
 3000 TN=2                                                              01077000
      GO TO 3004                                                        01078000
 3001 TN=3                                                              01079000
 3004 TN1=TN+1                                                          01080000
                                                                        01081000
C       SCF(L,TN) = SCALING OF (PHASE SHIFTS, ANGULAR MOMENTUM L  FOR TYPE  T 01082000
C       DESIRED, IF NOT VALUE 1.0 SHOULD BE GIVEN                       01083000
   20   READ(5,1100)(SCF(L,TN),L=1,LSS1)                                01084000
C       ENERGIES AND PHASESHIFTS FOR ATOM TYPE TN                       01085000
   30   READ(IAL,1100)(E(I,TN),E(I+1,TN),E(I+2,TN),E(I+3,TN),E(I+4,TN),  01086000
       *E(I+5,TN),E(I+6,TN),E(I+7,TN),I=1,NPH,8)                        01087000
        DO 40 L=1,LSS1                                                  01088000
        DO 40 I=1,NPH,8                                                 01089000
   40   READ(IAL,1100) PH(L,I,TN),PH(L,I+1,TN),PH(L,I+2,TN),PH(L,I+3,TN), 01090000
       *PH(L,I+4,TN),PH(L,I+5,TN),PH(L,I+6,TN),PH(L,I+7,TN)             01091000
        DO 60 L=1,LSS1                                                  01092000
        DO 60 I=1,NPH                                                   01093000
   60   PH(L,I,TN)=PH(L,I,TN)*SCF(L,TN)                                 01094000
        IF(TN.NE.T) GO TO 59                                            01095000
        READ(IAL,76,END=59) EMIN,FINT                                   01096000
   76   FORMAT(4F10.5,215)                                              01097000
        WRITE(6,6664) EMIN                                              01098000
        IF(FINT1.NE.0.0) FINT=FINT1                                     01099000
        IF(EEMIN.NE.0.0) EMIN=EEMIN                                     01100000
        EMIN=EMIN+(0.1*EDELTA)                                          01101000
        BACKSPACE IAL                                                   01102000
   59   CONTINUE                                                        01103000
                                                                        01104000
                                                                        01105000
        WRITE(6,700) EMIN,EMAX,EDELTA                                   01106000
 1200   FORMAT(//' PHASESHIFT USED IN CALCULATION WITH SSCF= ',F8.5)    01107000
        WRITE(6,1200)SCF(1,TN)                                          01108000
        IF(LSS1.GT.1) WRITE(6,1300)SCF(2,TN)                            01109000
        NUMA(TN)=NOMA(TN)+NUMA(TN)                                      01110000
        WRITE(6,505)T,ZVAL(TN),NUMA(TN)                                 01111000
  505   FORMAT(/' ATOMS TYPE ',I2,' : VALENCE ELECTRONS=',I3,10X,' NUMBER 01112000
      1OF ATOMS=',I3/' ENERGIES AND PHASESHIFTS:'/)                     01113000
 1300   FORMAT(4H+,60X,' PSCF=',F8.5)                                   01114000
 1400   FORMAT(5X,'ENERGY',6X,' S',8X,'ENERGY',7X,'P')                  01115000
 1488   FORMAT(1H+,T49,' ENERGY',7X,' D')                               01116000
        WRITE(6,1400)                                                   01117000
        IF(LSS.GT.1)WRITE(6,1488)                                       01118000
 1500   FORMAT(9F11.5)                                                  01119000
        DO 61 I=1,NPH                                                   01120000
   61   WRITE(6,1500)(E(I,TN),PH(L,I,TN),L=1,LSS)                       01121000
        IF(TN.EQ.T)GO TO 3002                                           01122000
        IF(TN-2)3000,3001,3002                                          01123000
 3002   ELAST=EMIN                                                      01124000
        DENSST(T)=0.0                                                   01125000
        IF(NAME(10).EQ.6H PUNCH) CALL PUNCH(PARA,IAL)                   01126000
        LSS1=LSS                                                        01127000
   62   N1=NUMSC*(LSS*LSS-3)                                            01128000
        IF(IOPL.EQ.1)N1=N1+3.0*NUMSC                                    01129000
        DELTAS=0.0                                                      01130000
        CH=0.0                                                          01131000
        OLDEL=EDELTA                                                    01132000
        K=1                                                             01133000
                                                                        01134000
        FJUMP=0                                                         01135000
        DO 3600 I=1,NUMSC                                               01136000
        LX(I)=AU*LX(I)                                                  01137000
        LY(I)=AU*LY(I)                                                  01138000
 3600   LZ(I)=AU*LZ(I)                                                  01139000
        WRITE(6,350)(LX(I),LY(I),LZ(I),I=1,NUMSC)                       01140000
 3501   FORMAT(/,' LX=',F10.5,' LY=',F10.5,' LZ=',F10.5)                01141000
        CALL ANGLE(LX,LY,LZ,NUMSC,COSTHE,R12,APHI)                      01142000
        ENERGY=EMIN                                                     01143000
 4000   ENERGY=ENERGY-0.1*OLDEL                                         01144000
C       IF ENERGY MESH TOO BROAD CHANGE THIS STEP TO SMALLER VALUE, SEE 01145000
C       LABELS 4000, 4001, 123, 4002, 4003, 333, 4005 AND 949           01146000
C       BEGIN CALCULATION                                               01147000
        WRITE(7,400)                                                    01148000
  400   FORMAT(1H1,' BEGIN CALCULATION')                                01149000
        NCOUNT=1                                                        01150000
    99  IF(ENERGY.GT.EMAX) GOTO 998                                     01151000
        KAPA=SQRT(ENERGY)                                               01152000
        J=0                                                             01153000
        DO 80 L=1,LSS1                                                  01154000
        IF(IOPL.EQ.1) GO TO 801                                         01155000
        IF (L.EQ.2) GO TO 80                                            01156000
  801   KK=2*(L-1)+1                                                    01157000
        DO 3005 KKK=1,KK                                                01158000
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      DO 3005 TN=1,3                                                    01159000
      IF (TN.GT.T)GO TO 3005                                            01160000
C     CALCULATION OF K-MATRICES                                         01161000
      DO 90 I=1,NPW                                                     01162000
      AE(I)=E(I,TN)                                                     01163000
                                                                        01164000
   90 PH(I)=PH(L,I,TN)                                                  01165000
      PSHIFT(L)=INTER(PH,AE,NPW,ENERGY,NPP)                             01166000
      KSS(L)=-(SIN(PSHIFT(L))/COS(PSHIFT(L)))/KAPA                      01167000
      I=NUMA(TN)                                                        01168000
      DO 3005 KXYZ=1,I                                                  01169000
      J=J+1                                                             01170000
      AKSS(J)=KSS(L)                                                    01171000
 3005 CONTINUE                                                          01172000
      LMIN1=L-1                                                         01173000
      WRITE(7,1700)LMIN1,PSHIFT(L),KSS(L)                               01174000
 1700 FORMAT(//,'  FOR L=',I3,' SINGLE SITE PHASESHIFT=',F8.5,          01175000
     1' K-MATRIX=',F8.5)                                                01176000
   80 CONTINUE                                                          01177000
C     CONSTRUCTION OF DETERMINANT                                       01178000
      CALL GMTRIX                                                       01179000
      COMDET=DETC(G,N1)                                                 01180000
 1800 FORMAT(//' REAL PART OF DET= ',F8.5,5X,'IMAG PART DET',F8.5)      01181000
    4 WRITE(7,1800)COMDET                                               01182000
C**** CALCULATION OF THE IMAGINARY PART OF LOG(DET)                     01183000
    2 DETRE=REAL(COMDET)                                                01184000
    3 DETIM=AIMAG(COMDET)                                               01185000
      IF(DETRE) 160,120,170                                             01186000
  120 IF(DETIM) 140,150,130                                             01187000
  130 ERSUM=0.5*PI                                                      01188000
      GOTO 180                                                          01189000
  140 ERSUM=1.5*PI                                                      01190000
      GOTO 180                                                          01191000
  150 ERSUM=0.0                                                         01192000
      GOTO 180                                                          01193000
                                                                        01194000
  160 ERSUM=ATAN(DETIM/DETRE)                                           01195000
      ERSUM=ERSUM+PI                                                    01196000
      GOTO 180                                                          01197000
  170 ERSUM=ATAN(DETIM/DETRE)                                           01198000
  180 ERSUM=-ERSUM                                                      01199000
 1900 FORMAT(' FOR ENERGY=',F8.5,' RYDBERGS')                           01200000
      WRITE(7,1900)ENERGY                                               01201000
      IF(K.EQ.1)GO TO 190                                               01202000
      DELTAS=ERSUM-OERSUM                                               01203000
      FSIGN=-SIGN(1.0,DELTAS)                                           01204000
      IF(ABS(DELTAS).GT.PI)DELTAS=DELTAS+FSIGN*2.0*PI                   01205000
  200 DENSST(K)=DELTAS*2.0/(PI*EDELTA)                                  01206000
 2000 FORMAT(' CHANGE IN DENSITY OF STATES IS ',F20.5)                  01207000
      WRITE(7,2000)DENSST(K)                                            01208000
      DEST=(DENSST(K)*100.*ATOCEL/((A0**3)*NUMSC))+100*(SQRT(ENERGY)/(2* 01209000
     1PI*PI))                                                           01210000
      IF(EDELTA.GT.0.5*OLDEL.OR.DEST.GT.0.0)GO TO 190                   01211000
      IF(SEG+(TIME(21)/60).GT.TMAX)GO TO 190                            01212000
      NCOUNT=NCOUNT+1                                                   01213000
      ENER=ENERGY-EDELTA                                                01214000
      EDELTA=EDELTA/FLOAT(NCOUNT)                                       01215000
      ENERGY=ENER+EDELTA                                                01216000
      IF(NCOUNT.EQ.4)GO TO 190                                          01217000
      GO TO 99                                                          01218000
  190 IF(NCOUNT.GT.1)NCOUNT=1                                           01219000
      VENERG(K)=ENERGY                                                  01220000
 2100 FORMAT(' DENSITY OF STATES PER UNIT VOLUME*100 IS',F20.5)         01221000
      WRITE(7,2100)DEST                                                 01222000
      TIEMPO=TIME(2)/60.                                                01223000
      WRITE(7,2200)TIEMPO                                               01224000
 2200 FORMAT(60X, '** PROCESS TIME='F8.4,'  SECONDS **')                01225000
      ELAST=ENERGY                                                      01226000
      IF(K.EQ.99) GO TO 999                                             01227000
      TPROM=TIEMPO/K                                                    01228000
      SEG=TPROM+1.0                                                     01229000
      IF(SEG+TIEMPO.GT.TMAX) GO TO 999                                  01230000
      OERSUM=ERSUM                                                      01231000
      IF(2*(K/2).NE.K) GO TO 123                                        01232000
 4001 EDELTA=OLDEL*0.9                                                  01233000
      GO TO 124                                                         01234000
  123 EDELTA=OLDEL*0.1                                                  01235000
  124 CONTINUE                                                          01236000
      K=K+1                                                             01237000
      ENERGY=ENERGY+EDELTA                                              01238000
      GOTO 99                                                           01239000
  998 K=K-1                                                             01240000
  999 CC =NUMA(1)*ZVAL(1)+NUMA(2)*ZVAL(2)                               01241000
```

```
      FEL=0.0                                                           01242000
      ENI=VENERG(1)                                                     01243000
 2400 FORMAT(1HI,3X,'CLUSTER CHANGE',10X,'FREF',14X,'DENSITY',12X,'INTE 01244000
     1GRATED',/,14X,'ENERGY',13X,'IN  N(E)',12X,'ELECTRONY',11X,'OF STATE 01245000
     1S',9X,'DENS. OF STATES')                                          01246000
      WRITE(6,2400)                                                     01247000
C4002 ENERGY=EMIN-0.9*OLDEL-0.1*OLDEL                                   01248000
      DO 210 I=1,K                                                      01249000
C     IF(2*(I/2).NE.I) GO TO 333                                        01250000
C4003 EDELTA=OLDEL*0.1                                                  01251000
C     GO TO 334                                                         01252000
C                                                                       01253000
C 333 EDELTA=OLDEL*0.9                                                  01254000
C 334 CONTINUE                                                          01255000
C     ENERGY=ENERGY+EDELTA                                              01256000
      ENERGY= VENERG(I)                                                 01257000
      QNTER(1,I)=(A0**3)*SQRT(ENERGY)*NUMSC/(2.0*ATOCEL*PI*PI)          01258000
      QNTER(2,I)=QNTER(1,I)+DENSST(I)                                   01259000
      IF(2*(I/2).NE.I.OR.FEL.NE.0.0) GO TO 210                          01260000
      ENI=ENERGY-ENI                                                    01261000
      FINT=QNTER(2,I)*ENI+FINT                                          01262000
      ENI=ENERGY                                                        01263000
      IF(FINT-CC)210,335,335                                            01264000
  335 WRITE(6,2401)                                                     01265000
      FEL=ENERGY                                                        01266000
 2401 FORMAT(1H+,' FERMI LEVEL')                                        01267000
  210 WRITE(6,2500) ENERGY,DENSST(I),QNTER(1,I),QNTER(2,I),FINT         01268000
 2600 FORMAT(/,14X,'ENERGY',11X,'FRIEDEL SUM',8X,'100*N(E)/VOLUME')     01269000
 2500 FORMAT(1H ,5F20.5)                                                01270000
C4004 ENERGY=EMIN-1.0*OLDEL                                             01271000
C                                                                       01272000
      DO 4004 I=1,K                                                     01273000
      IF(2*(I/2).EQ.I) GO TO 4004                                       01274000
      QNTER(2,I)=QNTER(2,I+1)                                           01275000
 4004 CONTINUE                                                          01276000
      CALL CARTE(K,QNTER,VENERG,IS,2,FEL)                               01277000
      WRITE(6,2600)                                                     01278000
      DO 220 I=1,K                                                      01279000
C     IF(2*(I/2).NE.I)  GO TO 949                                       01280000
C4005 EDELTA=OLDEL*0.1                                                  01281000
C     GO TO 950                                                         01282000
C 949 EDELTA=OLDEL*0.9                                                  01283000
C 950 CONTINUE                                                          01284000
      ENERGY= VENERG(I)                                                 01285000
C     ENERGY=ENERGY+EDELTA                                              01286000
      DENSST(I)=DENSST(I)*100.0*ATOCEL/((A0**3)*NUMSC)                  01287000
      RNTER=DENSST(I)+(SQRT(ENERGY)/(2*PI**2))*100                      01288000
      IF(2*(I/2).NE.I) WRITE(6,2501)ENERGY,DENSST(I),RNTER              01289000
      IF(2*(I/2).EQ.I) WRITE(6,2500)ENERGY,DENSST(I),RNTER              01290000
  220 CONTINUE                                                          01291000
C                                                                       01292000
      IF(ENERGY+OLDEL.LT.EMAX) GO TO 621                                01293000
      IAL=0                                                             01294000
      RETURN                                                            01295000
C     INTEGRATED DENSITY OF STATES NOT USED                             01296000
C     A INTEGRATION IS MADE WHEN REQUIRED                               01297000
 2501 FORMAT(3F20.5,' ')                                                01298000
C     IF NEW CONFIGURATION WANTED FOR SAME SCATTERERS                   01299000
      READ(5,1100)(LX(I),LY(I),LZ(I),I=1,NUMSC)                         01300000
      XXX=(LX(1)-LX(2))*(LX(1)-LX(2))                                   01301000
      YYY=(LY(1)-LY(2))*(LY(1)-LY(2))                                   01302000
      ZZZ=(LZ(1)-LZ(2))*(LZ(1)-LZ(2))                                   01303000
      RXYZ=XXX+YYY+ZZZ                                                  01304000
      IF(RXYZ.EQ.0.0) GO TO 620                                         01305000
      GO TO 62                                                          01306000
  621 WRITE(6,60)                                                       01307000
      IF(IAL.NE.5) WRITE(IAL,6665) ELAST,FINT                           01308000
 6665 FORMAT(2F10.7)                                                    01309000
      IF(IAL.NE.5)LOCK IAL                                              01310000
      IF(NAME(10).EQ.8H  LOCK),          GO TO 62)                      01311000
   66 FORMAT(///,10X,5('*'),'  WORK ENDED BECAUSE TIME IS NEARLY UP')   01312000
      WRITE(6,6666) TIEMPO,ELAST                                        01313000
 6666 FORMAT(//,10X,'TOTAL PROCESS TIME='F10.5,9X,'LAST ENERGY ACCOUNTED 01314000
     *=',F10.7)                                                         01315000
 6664 FORMAT(//10('*')//,10X,'ENERGY REGION FROM EMIN TO',F10.7,' HAS BE 01316000
     *EN ALREADY CALCULATED IN PREVIOUS JOB'//110('*'))                  01317000
C                                                                       01318000
  620 CONTINUE                                                          01319000
      IAL=0                                                             01320000
      RETURN                                                            01321000
      RETURN                                                            01322000
$RESET 0,NN                                                             01323000
      END                                                               01324000
                                                                        01325000
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      SUBROUTINE GMTRIX                                                 01326000
                                                                        01327000
                                                                        01328000
      REAL KAPA,LX(24),LY(24),LZ(24),KSS(8),ML,JL                       01329000
                                                                        01330000
      INTEGER C1,C2,SL,FSIGN,FJUMP,Z                                    01331000
                                                                        01332000
      DIMENSION AKSS(140),PSHIFT(8),SCF(8,2),E(60,2),POM(60),PH(4,60,2),01333000
     1COSTHE(290),R12(290),APHI(290)                                    01334000
                                                                        01335000
      COMPLEX KSC(20,4),PUTC(20),KAPC,ENERGC,BTH(20),VHTH,YC,CONDET,G(14 01336000
     16,140),AUC,SUC1,SUC2,APC,S2C1,S2C2,ZERO                           01337000
                                                                        01338000
                                                                        01339000
                                                                        01340000
                                                                        01341000
      COMMON/VCOMPL/G,KSC,KAPC,ENERGC,PUTC                              01342000
      COMMON/VARREZ/LX,LY,LZ,KSS,PSHIFT,SCF,E,POM,PH,AKSS,COSTHE,R12,APHI 01343000
                                                                        01344000
                                                                        01345000
      COMMON/VSIMP/KAPA,DETRE,DETIM,OFRSUM,PI,ENERGY,FSIGN,FJUMP,N1,NE,L 01346000
     1SS1,NUMSC,IOPL                                                    01347000
                                                                        01348000
                                                                        01349000
  899 ZERO=CMPLX(0.0,0.0)                                               01350000
      LSS=LSS1-1                                                        01351000
      DO 10 I=1,N1                                                      01352000
      DO 10 J=1,N1                                                      01353000
   10 G(I,J)=CMPLX(0.0,0.0)                                             01354000
      C1=0                                                              01355000
      C2=0                                                              01356000
      CONST=4.0*PI*KAPA                                                 01357000
      L1=0                                                              01358000
   21 CONTINUE                                                          01359000
      IF(L1.EQ.1.AND.IOPL.NE.1) GO TO 23                                01360000
      M1=-L1                                                            01361000
   22 CONTINUE                                                          01362000
      L2=L1                                                             01363000
   31 CONTINUE                                                          01364000
      IF(IOPL.EQ.1) GO TO 801                                           01365000
      IF(L2.EQ.1) GO TO 40                                              01366000
  801 IF(L2.EQ.L1)ML=M1                                                 01367000
      IF(L2.NE.L1)ML=-L2                                                01368000
      LMAX=L1+L2                                                        01369000
      LMIN=L2-L1                                                        01370000
      M2=ML                                                             01371000
   41 DO 50 I=1,NUMSC                                                   01372000
      J1=I                                                              01373000
      IF((M1.EQ.M2).AND.(L1.EQ.L2)) J1=I+1                              01374000
      IF(J1.GT.NUMSC) GOTO 50                                           01375000
      DO 50 J=J1,NUMSC                                                  01376000
                                                                        01377000
      IF(J.EQ.I)GOTO 100                                                01378000
      IF(J.GT.I)  GO TO 101                                             01379000
      KK=(J-1)*NUMSC+1-J*(J+1)/2                                        01380000
      R=R12(KK)                                                         01381000
      THETA=-COSTHE(KK)                                                 01382000
      FI=APHI(KK)+PI                                                    01383000
      GO TO 102                                                         01384000
  101 KK=J-I+(I-1)*NUMSC-(I*I-I)/2                                      01385000
      R=R12(KK)                                                         01386000
      THETA=COSTHE(KK)                                                  01387000
      FI=APHI(KK)                                                       01388000
  102 CONTINUE                                                          01389000
 1090 RI=KAPA*R                                                         01390000
  299 S2C1=CMPLX(0.0,0.0)                                               01391000
  399 S2C2=S2C1                                                         01392000
  499 SUC1=S2C1                                                         01393000
  599 SUC2=SUC1                                                         01394000
      L3=LMIN                                                           01395000
   72 CONTINUE                                                          01396000
      M3=-L3                                                            01397000
   71 X=C(L2,M2,L1,M1,L3,M3)                                            01398000
      AUX=C(L1,M1,L2,M2,L3,M3)                                          01399000
      IF(ABS(X).LT.0.001) GOTO 1699                                     01400000
  699 AUC=YC(L3,M3,THETA,FI)*CONST*X                                    01401000
      SUC1=SUC1+JL(L3,RI)*AUC*(ZERO)**L3                                01402000
      SUC2=SUC2+JL(L3,RI)*AUC*(ZERO)**L3                                01403000
 1699 IF(ABS(AUX).LT.0.001) GOTO 73                                     01404000
  799 A2C=YC(L3,M3,-THETA,FI+3.1416)*CONST*AUX                          01405000
      S2C1=S2C1+JL(L3,RI)*A2C*(ZERO)**L3                                01406000
      S2C2=S2C2+JL(L3,RI)*A2C*(ZERO)**L3                                01407000
   73 CONTINUE                                                          01408000
                                                                        01409000
```

```
      M3=M3+1                                                           01410000
      IF(M3.GT.L3) GOTO 81                                              01411000
      GOTO 71                                                           01412000
   81 L3=L3+1                                                           01413000
      IF(L3.GT.LMAX) GOTO 70                                            01414000
      GOTO 72                                                           01415000
   70 CONTINUE                                                          01416000
      IC1=C1+I                                                          01417000
      JC2=C2+J                                                          01418000
    5 G(IC1,JC2)=-SC1+SC2*ZERO                                          01419000
    6 G(JC2,IC1)=-S2C1+S2C2*ZERO                                        01420000
  100 CONTINUE                                                          01421000
   60 CONTINUE                                                          01422000
   50 CONTINUE                                                          01423000
      C2=C2+NUMSC                                                       01424000
      M2=M2+1                                                           01425000
      IF(M2.GT.L2)GOTO 40                                               01426000
      GOTO 41                                                           01427000
   40 CONTINUE                                                          01428000
      L2=L2+1                                                           01429000
      IF(L2.GT.LSS)GOTO 24                                              01430000
      GOTO 31                                                           01431000
   24 CONTINUE                                                          01432000
   30 CONTINUE                                                          01433000
      C1=C1+NUMSC                                                       01434000
      C2=C1                                                             01435000
      M1=M1+1                                                           01436000
      IF(M1.GT.L1) GOTO 23                                              01437000
                                                                        01438000
      GOTO 22                                                           01439000
   23 L1=L1+1                                                           01440000
      IF(L1.GT.LSS)GOTO 20                                              01441000
      GOTO 21                                                           01442000
   20 CONTINUE                                                          01443000
      DO 90 I=1,N1                                                      01444000
   90 G(I,I)=                KAPA*ZERO                                  01445000
      DO 120 I=1,N1                                                     01446000
      DO 120 J=1,N1                                                     01447000
  120 G(I,J)=G(I,J)*AKSS(J)                                             01448000
      DO 130 I=1,N1                                                     01449000
  199 G(I,I)=1.0+G(I,I)                                                 01450000
 2500 FORMAT(/3X,10F11.4)                                               01451000
 2501 FORMAT(6I4,2F8.4)                                                 01452000
  130 CONTINUE                                                          01453000
      RETURN                                                            01454000
      END                                                               01455000
      COMPLEX FUNCTION YC(L,N,CTH,PH)                                   01456000
C**** EVALUATES COMPLEX SPHERICAL HARMONICS Y(L,M),CTH=COS(THETA)        01457000
C**** PH=PHI                                                            01458000
      M=N                                                               01459000
      Z=(2.0*L+1.0)/12.5663753                                          01460000
      IF (M) 1000,1010,1060                                             01461000
 1000 A=1.0                                                             01462000
      B=-1.0                                                            01463000
      M=-M                                                              01464000
      C=M*PH                                                            01465000
      Z=Z*F(L-M)/F(L+M)                                                 01466000
      IF (Z) 1070,1090,1100                                             01467000
 1010 IF (Z) 1020,1090,1040                                             01468000
 1020 Z=SQRT(-1.0*Z)*P(L,0,CTH)                                         01469000
 1030 YC=CMPLX(0.0,Z)                                                   01470000
      RETURN                                                            01471000
 1040 Z=SQRT(Z)*P(L,0,CTH)                                              01472000
 1050 YC=CMPLX(Z,0.0)                                                   01473000
      RETURN                                                            01474000
 1060 A=(-1.0)**M                                                       01475000
      B=A                                                               01476000
      C=M*PH                                                            01477000
      Z=Z*F(L-M)/F(L+M)                                                 01478000
      IF (Z) 1070,1090,1100                                             01479000
 1070 Z=SQRT(-1.0*Z)*P(L,M,CTH)                                         01480000
      X=Z*SIN(C)*A                                                      01481000
      Y=Z*COS(C)*B                                                      01482000
 1080 YC=CMPLX(X,Y)                                                     01483000
      RETURN                                                            01484000
 1090 YC=CMPLX(0.0,0.0)                                                 01485000
      RETURN                                                            01486000
 1100 Z=SQRT(Z)*P(L,M,CTH)                                              01487000
      X=Z*COS(C)*A                                                      01488000
      Y=Z*SIN(C)*B                                                      01489000
 1110 YC=CMPLX(X,Y)                                                     01490000
      RETURN                                                            01491000
      END                                                               01492000
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      SUBROUTINE ANGLE(LX,LY,LZ,NUMSC,COSTHE,R12,APHI)                  01493000
      REAL COSTHE(300),R12(300),APHI(300)                               01494000
      REAL LX(24),LY(24),LZ(24)                                         01495000
      K=1                                                               01496000
      PI=3.141593                                                       01497000
      DO 50   I=1,NUMSC                                                 01498000
      J1=I+1                                                            01499000
      IF(J1.GT.NUMSC) GO TO 50                                          01500000
      DO 60  J=J1,NUMSC                                                 01501000
      RX=LX(I)-LX(J)                                                    01502000
      RY=LY(I)-LY(J)                                                    01503000
      RZ=LZ(I)-LZ(J)                                                    01504000
      R=SQRT(RX*RX+RY*RY+RZ*RZ)                                         01505000
      IF (RX) 1010,1040,1080                                            01506000
 1010 IF (RY) 1020,1020,1030                                            01507000
 1020 FI=ATAN(RY/RX)-PI                                                 01508000
      GOTO 1090                                                         01509000
 1030 FI=ATAN(RY/RX)+PI                                                 01510000
      GOTO 1090                                                         01511000
 1040 IF (RY) 1050,1060,1070                                            01512000
 1050 FI=-0.5*PI                                                        01513000
      GOTO 1090                                                         01514000
 1060 FI=0.0                                                            01515000
      GOTO 1090                                                         01516000
 1070 FI=0.5*PI                                                         01517000
      GOTO 1090                                                         01518000
 1080 FI=ATAN(RY/RX)                                                    01519000
 1090 CONTINUE                                                          01520000
      THETA=RZ/R                                                        01521000
      R12(K)=R                                                          01522000
      COSTHE(K)=THETA                                                   01523000
      APHI(K)=FI                                                        01524000
      K=K+1                                                             01525000
   60 CONTINUE                                                          01526000
   50 CONTINUE                                                          01527000
      RETURN                                                            01528000
      END                                                               01529000
      REAL FUNCTION NL(L,R)                                             01530000
C**** TO EVALUATE SPHERICAL NEUMANN FUNCTIONS                           01531000
      NL=-1.0E60                                                        01532000
      IF(R)20,10,20                                                     01533000
   10 WRITE(6,1)L                                                       01534000
    1 FORMAT(//' ERROR IN SPHERICAL NEUMANN FUNCTION R=0    L=',I4)     01535000
      GOTO 100                                                          01536000
   20 IF(L)40,30,40                                                     01537000
   30 NL=-COS(R)/R                                                      01538000
      GOTO 100                                                          01539000
C**** COMPUTATION OF SUM                                                01540000
   40 A=1.0                                                             01541000
      SUM=1.0                                                           01542000
      NT=1                                                              01543000
   50 A=-(R*R/(2*NT*(2*NT-1-2*L)))*A                                    01544000
      SUM=SUM+A                                                         01545000
      NT=NT+1                                                           01546000
      RI=ABS(A/SUM)                                                     01547000
      IF(RI.LT.1.0E-6) GOTO 80                                          01548000
      IF(NT-150)70,70,60                                                01549000
   60 WRITE(6,2)L,R                                                     01550000
    2 FORMAT(//' SERIES IN NEUMANN FUNCTION DID NOT CONVERGE AFTER 150  01551000
     1TERMS L=',I4,' R= ',F12.6)                                        01552000
      GOTO 80                                                           01553000
   70 CONTINUE                                                          01554000
      GOTO 50                                                           01555000
   80 L1=2*L-1                                                          01556000
      NL=-DF(L1)*SUM/(R**(L+1))                                         01557000
  100 CONTINUE                                                          01558000
      RETURN                                                            01559000
      END                                                               01560000
      REAL FUNCTION JL(L,R)                                             01561000
C**** CALCULATES BESSEL FUNCTIONS OF ORDER L AND ARGUMENT R             01562000
      IF(R)20,10,20                                                     01563000
   10 IF(L.EQ.0) JL=1.0                                                 01564000
      IF(L.GT.0) JL=0.0                                                 01565000
      GOTO 100                                                          01566000
   20 L1=2*L+1                                                          01567000
      A=(R**L)/DF(L1)                                                   01568000
      K=1                                                               01569000
      SUM=A                                                             01570000
   30 A=-R*R/(2.0*(2.0*K+2.0*L+1.0)*K)*A                                01571000
      SUM=SUM+A                                                         01572000
      IF(ABS(A/SUM).LT.1.0E-6) GOTO 40                                  01573000
      K=K+1                                                             01574000
                                                                        01575000
                                                                        01576000
```

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      IF(K.LE.150) GOTO 30                                              01577000
      WRITE(6,1) L,R                                                    01578000
    1 FORMAT(//' SERIES FOR SPHERICAL BESSEL FUNCTION DID NOT CONVERGE  01579000
     1AFTER 150 TERMS L= ',I4,'   R= ',F12.6)                           01580000
      GOTO 40                                                           01581000
   30 JL=SUM                                                            01582000
  100 CONTINUE                                                          01583000
      RETURN                                                            01584000
      END                                                               01585000
      FUNCTION P(N,M,X)                                                 01586000
C**** THIS FUNCTION EVALUATES ASSOCIATED LEGENDRE POLYNOMIALS OF        01587000
C**** ORDER(N,M) ARGUMENT X                                             01588000
C**** TREAT SPECIAL CASES                                               01589000
      IF(M)20,10,20                                                     01590000
   10 P=1.0                                                             01591000
      GOTO 100                                                          01592000
   20 IF(X)50,22,50                                                     01593000
   22 RI=(N-M)/2                                                        01594000
      RII=(N-M)/2                                                       01595000
      RI=ABS(RI-RII)                                                    01596000
      IF(RI.GT.0.002) GOTO 30                                           01597000
      GOTO 40                                                           01598000
   30 P=0.0                                                             01599000
      GOTO 100                                                          01600000
   40 T=(-1)**((N-M)/2)                                                 01601000
      P=T*DF(N+M-1)/DF(N-M)                                             01602000
      GOTO 100                                                          01603000
   50 IF((1-ABS(X)).GT.0.001) GOTO 70                                   01604000
   60 IF(M.EQ.0) P=X**N                                                 01605000
      IF(M.NE.0) P=0.0                                                  01606000
      GOTO 100                                                          01607000
   70 CONTINUE                                                          01608000
C**** NOW TO COMPUTE GENERAL CASE                                       01609000
      N1=2*N-1                                                          01610000
      NM=N-M                                                            01611000
      IF(NM)90,80,90                                                    01612000
   80 SUM=DF(N1)                                                        01613000
      GOTO 1000                                                         01614000
   90 B=DF(N1)*(X**(N-M))/F(NM)                                         01615000
      SUM=B                                                             01616000
      IF(NM.EQ.1) GOTO 1000                                             01617000
                                                                        01618000
      KM=NM/2                                                           01619000
      DO 110 K=1,KM                                                     01620000
      T1=2.0*N-2.0*K+1.0                                                01621000
      T2=NM-2.0*K+1.0                                                   01622000
      T3=NM-2.0*K+2.0                                                   01623000
      B=-((T2*T3)/(2.0*X*X*T1*K))*B                                     01624000
  110 SUM=SUM+B                                                         01625000
 1000 T=1.0                                                             01626000
      X1=1.0-X*X                                                        01627000
      R2=(FLOAT(M)/2.0)*ALOG(X1)                                        01628000
      P=T*EXP(R2)*SUM                                                   01629000
  100 CONTINUE                                                          01630000
      RETURN                                                            01631000
      END                                                               01632000
      COMPLEX FUNCTION DETC(A,N)                                        01633000
      COMPLEX A(140,140)                                                01634000
C**** EVALUATES THE DETERMINANT OF A COMPLEX MATRIX WITH ROW PIVOTING   01635000
      COMPLEX T,W                                                       01636000
C**** BEGIN COMPUTATION OF DET                                          01637000
    4 DETC=CMPLX(1.0,0.0)                                               01638000
      DO 10 I=1,N                                                       01639000
    1 PIVOT=CABS(A(I,I))*(CABS(A(I,1)))                                 01640000
      K=I                                                               01641000
C**** LOOK FOR PIVOT ELEMENT                                            01642000
      I1=I+1                                                            01643000
      IF(I1.GT.N) GO TO 50                                              01644000
      DO 20 J=I1,N                                                      01645000
    2 RK=REAL(A(J,I))                                                   01646000
    3 RI=AIMAG(A(J,I))                                                  01647000
      AV=RK*RK+RI*RI                                                    01648000
      IF(PIVOT-AV) 30,20,20                                             01649000
   30 PIVOT=AV                                                          01650000
      K=J                                                               01651000
   20 CONTINUE                                                          01652000
C**** K IS THE ROW WITH THE LARGEST ELEMENT                             01653000
C**** INTERCHANGE ROWS                                                  01654000
      IF(K-I) 40,50,40                                                  01655000
   40 DO 60 J=I,N                                                       01656000
    5 T=A(I,J)                                                          01657000
    6 A(I,J)=A(K,J)                                                     01658000
   60 A(K,J)=T                                                          01659000
```

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      7 DETC=-DETC                                                      01660000
C**** END INTERCHANGE ROWS                                              01661000
     50 CONTINUE                                                        01662000
      8 RK=REAL(A(I,I))                                                 01663000
      9 RI=AIMAG(A(I,I))                                                01664000
        IF(RK)80,70,80                                                  01665000
     70 IF(RI)80,1000,80                                                01666000
   1001 DETC=CMPLX(0.0,0.0)                                             01667000
        GOTO 1000                                                       01668000
     80 CONTINUE                                                        01669000
C**** MULTIPLY ROW I  BY -A(I,J)/A(I,I) AND ADD IT TO ROW J             01670000
        I1=I+1                                                          01671000
        IF(I1.GT.N) GO TO 10                                            01672000
        DO 90 J=I1,N                                                    01673000
    199 W=-A(J,I)/A(I,I)                                                01674000
        DO 100 L=I,N                                                    01675000
    100 A(J,L)=A(J,L)+W*A(I,L)                                          01676000
     90 CONTINUE                                                        01677000
                                                                        01678000
     10 CONTINUE                                                        01679000
        DO 110 I=1,N                                                    01680000
    110 DETC=DETC*A(I,I)/CABS(A(I,I))                                   01681000
   1000 CONTINUE                                                        01682000
        RETURN                                                          01683000
        END                                                             01684000
        FUNCTION C(LT1,MT1,LT2,MT2,LT3,MT3)                             01685000
C**** COMPUTES THE GAUNT NUMBERS                                        01686000
        INTEGER S                                                       01687000
C**** CHECK GENERAL CONDITIONS                                          01688000
        L1=LT3                                                          01689000
        M1=MT3                                                          01690000
        L2=LT2                                                          01691000
        M2=MT2                                                          01692000
        L3=LT1                                                          01693000
        M3=MT1                                                          01694000
        LT=L1+L2+L3                                                     01695000
        RL=FLOAT(LT/2)*2.0                                              01696000
        RL1=L1+L2+L3                                                    01697000
        IF(RL-RL1)10,20,10                                              01698000
     10 C=0.0                                                           01699000
        GOTO 100                                                        01700000
     20 IF((IABS(M1).GT.L1).OR.(IABS(M2).GT.L2).OR.(IABS(M3).GT.L3))    01701000
       1 GO TO 10                                                       01702000
        L12=L1+L2                                                       01703000
        L11=IABS(L1-L2)                                                 01704000
        L23=L2+L3                                                       01705000
        L22=IABS(L3-L2)                                                 01706000
        M22=M2+M1                                                       01707000
        L13=L1+L3                                                       01708000
        L33=IABS(L1-L3)                                                 01709000
        IF((L3.GT.L12).OR.(L3.LT.L11)) GOTO 10                          01710000
        IF((L1.GT.L23).OR.(L1.LT.L22)) GOTO 10                          01711000
        IF((M3.NE.M22).OR.(L1.LT.0).OR.(L2.LT.0).OR.(L3.LT.0)) GOTO 10  01712000
        IF((L2.GT.L13).OR.(L2.LT.L33)) GOTO 10                          01713000
C**** REARRANGEMENT OF THE M                                            01714000
        LT=(L1+L2+L3)/2                                                 01715000
        COEF1=SQRT((2*L1+1)*(2*L2+1)/(4*3.1416*(2*L3+1)))*(-1)**(L1-L2  01716000
       1+LT)                                                            01717000
        COEF2=SQRT(F(2*LT-2*L1)*F(2*LT-2*L2)*F(2*LT-2*L3)/F(2*LT+1))*   01718000
       1(2*L3+1)*F(LT)/(F(LT-L1)*F(LT-L2)*F(LT-L3))                     01719000
        COEF3=SQRT(F(L1+L2-L3)*F(L1-M1)*F(L2-M2)*F(L3-M3)*F(L3+M3)/     01720000
       1(F(2*LT+1)*F(L1-L2+L3)*F(L2+L3-L1)*F(L1+M1)*F(L2+M2)))          01721000
        S=0                                                             01722000
        FF=0.0                                                          01723000
     30 F1=(-1)**(S+L1-M1)                                              01724000
        MT=L1-M1-S                                                      01725000
        IF(MT.LT.0) GOTO 40                                             01726000
        F2=F(MT)                                                        01727000
        MT=L3-M3-S                                                      01728000
        IF(MT.LT.0) GOTO 40                                             01729000
        IF(-(L2-L3+M1+S).LT.1) FF=FF+F(L1+M1+S)*F(L2+L3-M1-S)*F1/(F(S)* 01730000
       1F2*F(MT)*F(L2-L3+M1+S))                                         01731000
        S=S+1                                                           01732000
        GOTO 30                                                         01733000
     40 C=COEF1*COEF2*COEF3*FF                                          01734000
    100 CONTINUE                                                        01735000
        RETURN                                                          01736000
        END                                                             01737000
        FUNCTION F(N)                                                   01738000
C**** F=N FACTORIAL                                                     01739000
        IF(N)10,20,30                                                   01740000
     10 F=0.0                                                           01741000
        GOTO 100                                                        01742000
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      20 F=1.0                                                          01743000
         GOTO 100                                                       01744000
      30 RF=1.0                                                         01745000
         IF(N.LT.2) GOTO 50                                             01746000
         DO 40 L=3,N                                                    01747000
      40 DF=L*RF                                                        01748000
      50 F=RF                                                           01749000
     100 RETURN                                                         01750000
         END                                                            01751000
                                                                        01752000
         FUNCTION DF(N)                                                 01753000
C**** DF=DOUBLE FACTORIAL OF N                                          01754000
         IF(N)10,20,30                                                  01755000
      10 DF=0.0                                                         01756000
         GOTO 100                                                       01757000
      20 DF=1.0                                                         01758000
         GOTO 100                                                       01759000
      30 RN=N/2.0                                                       01760000
         RI=N/2                                                         01761000
         IF(RN.EQ.RI) GOTO 50                                           01762000
         T=1.0                                                          01763000
         DO 40 K=1,N,2                                                  01764000
      40 T=T*K                                                          01765000
         DF=T                                                           01766000
         GOTO 100                                                       01767000
      50 T=1.0                                                          01768000
         IF(N.LT.2) GOTO 70                                             01769000
         DO 60 K=2,N,2                                                  01770000
      60 T=T*K                                                          01771000
      70 DF=T                                                           01772000
     100 RETURN                                                         01773000
         END                                                            01774000
         COMPLEX FUNCTION HL(L,R)                                       01775000
         REAL HL, JL                                                    01776000
         AH=JL(L,R)                                                     01777000
         BH=NL(L,R)                                                     01778000
         HL=CMPLX(AH,BH)                                                01779000
         RETURN                                                         01780000
         END                                                            01781000
         SUBROUTINE REGIS(OMEGA,EFERMI,Z,DELELE,N)                      01782000
C***     OMEGA = VOLUMEN ATOMICO; SIGMA = DIAMETRO DE ESFERAS.          01783000
C***     DELELE = CORRIMIENTOS DE FASE; KFERMI = VECTOR DE FERMI.       01784000
C***     EFERMI = ENERGIA DEL NIVEL DE FERMI; VFERMI = VELOCIDAD DE FERMI. 01785000
C***     AQUP,XAQUP = TABLA DEL FACTOR DE ESTRUCTURA; POT = POTENCIAL.  01786000
C***     PACFRN = EMPAQUETAMIENTO; TSQ = MATRIZ DE TRANSICION.          01787000
C***     VINTEG = VALOR DE LA INTEGRAL; RHO(I) = RESISTIVIDAD.          01788000
C***     KFERMI VALE SQRT EFERMI EN 1/METRO                             01789000
         DIMENSION C(9), AQUP(40), DELELE(4), XAQUP(40),                01790000
        %SIGM(9),RHO(9),VECFER(9),PACFRN(9)                             01791000
         REAL INTER                                                     01792000
         REAL KFERMI,KFERMO, M                                          01793000
         CE=2.                                                          01794000
         PI=3.14159265                                                  01795000
         LSIGMA=1                                                       01796000
         SIGMA=(((3./4.)*((0.5+OMEGA)/PI))**(1./3.))*2                  01797000
         CONTRA=21.744443D                                              01798000
      53 READ(5,130) (AQUP(J), J=1,40)                                  01799000
         DO 1 KL=1,40                                                   01800000
       1 XAQUP(KL)=(1./2.)*KL                                           01801000
      60 WRITE(6,200)                                                   01802000
      61 WRITE(6,210)                                                   01803000
      70 WRITE(6,200)                                                   01804000
      71 WRITE(6,310)                                                   01805000
      62 WRITE(6,320)          EFERMI,OMEGA                             01806000
      63 WRITE(6,230) (DELELE(K),K=1,4)                                 01807000
         I=0                                                            01808000
         KFERMI=SQRT(EFERMI)                                            01809000
         KFERMO=KFERMI                                                  01810000
      64 WRITE(6,240)                                                   01811000
       2 I=I+1                                                          01812000
         M=6.0                                                          01813000
         SUMA1=0.0                                                      01814000
         SUMA2=0.0                                                      01815000
         QOLD=0.0                                                       01816000
         VINTEG=0.0                                                     01817000
         TETHA=0.0                                                      01818000
         SIGM(I)=SIGMA                                                  01819000
         VFERMI=CE*KFERMI                                               01820000
         C(I)=3.*(PI**3)/(OMEGA*KFERMI**3)                              01821000
         PACFRN(I)=4.*PI*(SIGMA    **3)/(24.*OMEGA)                     01822000
       3 TETHA=TETHA+M*PI/180.                                          01823000
         X=COS(TETHA)                                                   01824000
         P1=1.                                                          01825000
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      P2=X
      P3=0.5*(5.*X**3-3.*X)
      P4=0.125*(35.*X**4-30.*X**2+3.)
      SUMA1=      SIN(DELELE(1))*COS(DELELE(1))+3.*P2*SIN(DELELE(2))*COS
     %(DELELE(2))+5.*P3*SIN(DELELE(3))*COS(DELELE(3))+7.*P4*SIN(DELELE(4
     %))*COS(DELELE(4))
      SUMA2=      P1*(SIN(DELELE(1)))**2)+3.*P2*(SIN(DELELE(2))**2)+5.*P3
     %*(SIN(DELELE(3)))**2)+7.*P4*(SIN(DELELE(4))**2)
      OOLD=0
      TSQ=SUMA1**2+SUMA2**2
      POT=SQRT(TSQ)
      Q=KFERMI*SQRT(2.*(1-X))
      AQ=INTER(AQUP,XAQUP,40,Q*SIGMA    ,10)
      COSA=AQ*Q**3/EFERMI
      VINTEG=VINTEG+COSA*TSQ*(Q-OOLD)
      IF(ETHA.LT.0.999*PI) GO TO 3
      RHO(I)=C(I)*VINTEG
      RHO(I)= CONTRA*RHO(I)
      SIGMA=SIGMA-0.05*STO(I)
      LSIGMA=LSIGMA+1
      VECFER(I)=KFERMI
      IF (LSIGMA.LT.40)GO TO 2
   65 WRITE(6,251) VECFER(I),C(I)
      SIGMA=SIGM(I)
      KFERMI=KFERMI-0.05*KFERMI
      LSIGMA=1
      IF(I.LT.9) GO TO 2
   74 WRITE(6,254) (PACFER(M),M=1,3)
   66 WRITE(6,290) TEMP
   67 WRITE(6,270)
   68 WRITE(6,280) (AQUP(L),XAQUP(L),L=1,40)
   69 WRITE(6,801)
   72 WRITE(6,800) (SIG1(M),VECFER(M),RHO(M),M=1,9)
   73 WRITE(6,330)

C
C     FORMATOS DE LECTURA E IMPRESION
C
  100 FORMAT(8F10.5)
  200 FORMAT(/31X,57("*"))
  210 FORMAT(1H1,7,31X,"*                CALCULO DE LA RESISTIVIDAD DE METALE
     %S          *")
  310 FORMAT(////,40X,                "ENERGIA DEL NIVEL DE FERMI",20X,"V
     %OLUMEN ATOMICO",/)
  220 FORMAT(21X,F12.5,32X,F12.5)
  230 FORMAT(//5X,"CORRECCIONES DE FASE",5X,"DELTA(S)=",F9.6,2X,"DELTA(P
     %)=",F9.6,2X,"DELTA(D)=",F9.6,2X,"DELTA(F)=",F9.6,2X)
  240 FORMAT(//40X,"VELOCIDAD DE FERMI",15X,"CONSTANTE")
  250 FORMAT(/42X,F12.8,16X,F12.6)
  254 FORMAT(//20X,"EMPAQUETAMIENTOS",10X,"I =",F10.8,8X,"II =",F10.8,8X
     %,"III =",F10.8)
  260 FORMAT(//25X,"TABLA DE VALORES DEL FACTOR DE ESTRUCTURA A T = ",I4
     %," GRADOS CENT.",/)
  270 FORMAT(10X,5("AQUP",5X,"XAQUP",7X))
  280 FORMAT (10(8X,F8.3,4X,F8.3,5X),/)
  290 FORMAT(//,"MATRIZ DE TRANSICION",3X,"POTENCIAL",3X,"DIAMETRO DE
     %LA ESFERA",3X,"VECTOR DE FERMI",5X,"INTEGRAL",8X,"RESISTIVIDADES
     %ESPECIFICAS"/)
  320 FORMAT(3X,"*",2X,F15.10,3X,"*",1X,F9.5,1X,"*",5X,F12.10,5X,"*",4X,
     %F9.6,6X,"*",1X,F10.5,5X,"*",2X,F15.10,3X,"MM-OHM-CM *")
  330 FORMAT(1H1)
  801 FORMAT(//,25X,"DIAMETRO DE LA ESFERA",10X,"VECTOR DE FERMI",13X,"R
     %ESISTIVIDADES ESPECIFICAS",/)
  800 FORMAT(21X,"*",3X,F15.10,10X,"*",3X,F15.10,6X,"*",6X,F15.10,3X,"MM
     %-OHM-CM *")
      RETURN
      END
      SUBROUTINE PUNCH(PARA,IAL)
      DIMENSION A(20)
      INTEGER PARA
      REWIND IAL
    1 READ(IAL,2,END=3)A
    2 FORMAT(20A4)
      PUNCH 2,A
    3 IF(PARA.GT.0) CALL EXIT
      RETURN
      END
```