

T I O N

S T R U C T U R A L I N F O R M A

SUBSTANCE: cein3

LATTICE = P
:POT : POTENTIAL OPTION EX_PBE EC_PBE VX_PBE VC_PBE
:LAT : LATTICE CONSTANTS= 8.86282 8.86282 8.86282 1.571
1.571 1.571
:NATO : 2 INDEPENDENT AND 4 TOTAL ATOMS IN UNITCELL
MODE OF CALCULATION IS = RELA
SELFCONSISTENT CYCLE-NUMBER = 1

NOT EQUIV ATOM Ce LOCAL ROTATION MATRIX
1.00000 0.00000 0.00000
0.00000 1.00000 0.00000
0.00000 0.00000 1.00000
EQUIV ATOM 1 POSITION: 0.000 0.000 0.000
-1.00000 0.00000 0.00000
0.00000 -1.00000 0.00000
0.00000 0.00000 -1.00000

NOT EQUIV ATOM In LOCAL ROTATION MATRIX
1.00000 0.00000 0.00000
0.00000 1.00000 0.00000
0.00000 0.00000 1.00000
EQUIV ATOM 1 POSITION: 0.500 0.500 0.000
-1.00000 0.00000 0.00000
0.00000 -1.00000 0.00000
0.00000 0.00000 -1.00000
EQUIV ATOM 2 POSITION: 0.000 0.500 0.500
0.00000 0.00000 -1.00000
-1.00000 0.00000 0.00000
0.00000 -1.00000 0.00000
EQUIV ATOM 3 POSITION: 0.500 0.000 0.500
-1.00000 0.00000 0.00000
0.00000 0.00000 -1.00000
0.00000 -1.00000 0.00000

NON-SPINPOLARIZED CALCULATION
allocation of V,clm,clmsp,exc,vxc: 29 MB

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allocation of X(nkk) arrays:      0 MB
:FFT    global FFT-parameters:   72    72    72 Factor: 2.00
:FFT    local  FFT-parameters:   72    72    72
:FFT    allocation of cfft,cfft1,ust,fft: 35 MB
1

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M U L T I P O L M O M E N T S

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ATOM= 1    Ce            Z=58.00    LM= 5        POSITION= 0.000
0.000  0.000

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L= 0    M= 0    SPHERE MM =    0.848150717  0.0000000000
L= 4    M= 0    SPHERE MM =    0.033336942  0.0000000000
L= 4    M= 4    SPHERE MM =    0.019922634  0.0000000000
L= 6    M= 0    SPHERE MM =    0.062970423  0.0000000000
L= 6    M= 4    SPHERE MM =   -0.117806875  0.0000000000

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ATOM= 2    In            Z=49.00    LM= 6        POSITION= 0.500
0.500  0.000

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L= 0    M= 0    SPHERE MM =    0.472665292  0.0000000000
L= 2    M= 0    SPHERE MM =    0.023933822  0.0000000000
L= 4    M= 0    SPHERE MM =    0.036934215  0.0000000000
L= 4    M= 4    SPHERE MM =    0.024039525  0.0000000000
L= 6    M= 0    SPHERE MM =    0.050341861  0.0000000000
L= 6    M= 4    SPHERE MM =   -0.103432483  0.0000000000
L= 4    M=-4    SPHERE MM =    0.024039525  0.0000000000
L= 6    M=-4    SPHERE MM =   -0.103432483  0.0000000000

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ATOM= 1    Ce            Z=58.00    LM= 5        POSITION= 0.000
0.000  0.000

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L= 0    M= 0    PLANE WAVE MULTIPOLMOMENT =    2.030138100
0.0000000000
L= 4    M= 0    PLANE WAVE MULTIPOLMOMENT =   -0.033457272
0.0000000000
L= 4    M= 4    PLANE WAVE MULTIPOLMOMENT =   -0.019994544 -
0.0000000000
L= 6    M= 0    PLANE WAVE MULTIPOLMOMENT =   -0.063450752 -
0.0000000000
L= 6    M= 4    PLANE WAVE MULTIPOLMOMENT =    0.118705487
0.0000000000

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ATOM= 2    In            Z=49.00    LM= 6        POSITION= 0.500
0.500  0.000

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L= 0	M= 0	PLANE WAVE MULTIPOLMOMENT =	1.349131235 -
0.0000000000			
L= 2	M= 0	PLANE WAVE MULTIPOLMOMENT =	-0.023943404 -
0.0000000000			
L= 4	M= 0	PLANE WAVE MULTIPOLMOMENT =	-0.036249935
0.0000000000			
L= 4	M= 4	PLANE WAVE MULTIPOLMOMENT =	-0.023957733 -
0.0000000000			
L= 6	M= 0	PLANE WAVE MULTIPOLMOMENT =	-0.051348662 -
0.0000000000			
L= 6	M= 4	PLANE WAVE MULTIPOLMOMENT =	0.102607034
0.0000000000			
L= 4	M=-4	PLANE WAVE MULTIPOLMOMENT =	-0.023957733
0.0000000000			
L= 6	M=-4	PLANE WAVE MULTIPOLMOMENT =	0.102607034 -
0.0000000000			

ATOM= 1	Ce	Z=58.00	LM= 5	POSITION= 0.000
0.000	0.000			

L= 0	M= 0	PSEUDO MULTIPOLMOMENT =	2.878288817
0.0000000000			
L= 4	M= 0	PSEUDO MULTIPOLMOMENT =	-0.000120330
0.0000000000			
L= 4	M= 4	PSEUDO MULTIPOLMOMENT =	-0.000071911 -
0.0000000000			
L= 6	M= 0	PSEUDO MULTIPOLMOMENT =	-0.000480328 -
0.0000000000			
L= 6	M= 4	PSEUDO MULTIPOLMOMENT =	0.000898612
0.0000000000			
L= 4	M=-4	PSEUDO MULTIPOLMOMENT =	-0.000071911
0.0000000000			
L= 6	M=-4	PSEUDO MULTIPOLMOMENT =	0.000898612 -
0.0000000000			

ATOM= 2	In	Z=49.00	LM= 6	POSITION= 0.500
0.500	0.000			

L= 0	M= 0	PSEUDO MULTIPOLMOMENT =	1.821796527 -
0.0000000000			
L= 2	M= 0	PSEUDO MULTIPOLMOMENT =	-0.000009582 -
0.0000000000			
L= 4	M= 0	PSEUDO MULTIPOLMOMENT =	0.000684280
0.0000000000			
L= 4	M= 4	PSEUDO MULTIPOLMOMENT =	0.000081793 -
0.0000000000			
L= 6	M= 0	PSEUDO MULTIPOLMOMENT =	-0.001006800 -
0.0000000000			
L= 6	M= 4	PSEUDO MULTIPOLMOMENT =	-0.000825449
0.0000000000			

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      L= 4   M=-4   PSEUDO MULTIPOLMOMENT   =   0.000081793
0.0000000000
      L= 6   M=-4   PSEUDO MULTIPOLMOMENT   =  -0.000825449 -
0.0000000000
1

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                        C O N V E R G E N C E   PARAMETERS
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CONVERGENCE PARAMETER FOR PSEUDOCHARGE: NCON= 9
MAXIMAL VALUE OF RMT(JATOM)*ABSK(NKK) : RK =29.97306

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amass, r0:   140.100006103516           1.177782195447225E-004
nuc:         156
TEST of density continuity (clm,rhopw) for atom           1
  1   0.27057E+01   0.27064E+01
  2  -0.68507E-02  -0.34552E-02
  3   0.00000E+00  -0.40882E-02
  4  -0.12784E-01  -0.64465E-02
  5   0.00000E+00   0.24365E-02
:VCOUL001 ATOMNUMBER= 1 Ce      VCOUL-ZERO = 0.13454E+00
amass, r0:   114.800003051758           1.102130192550634E-004
nuc:         152
TEST of density continuity (clm,rhopw) for atom           2
  1   0.22231E+01   0.22252E+01
  2  -0.97078E-02  -0.97643E-02
  3  -0.45860E-02  -0.45113E-02
  4  -0.37022E-02  -0.37369E-02
  5  -0.12903E-02  -0.13341E-02
  6   0.37367E-02   0.38039E-02
:VCOUL002 ATOMNUMBER= 2 In      VCOUL-ZERO = 0.47731E+00
:EFG002:      EFG              =  -0.07456   *10**21
V / m**2

      V20 TOT/SRF=  -0.06457   -0.08317
      V22 TOT/SRF=   0.00000   0.00000
      V22M TOT/SRF=  0.00000   0.00000
      V21 TOT/SRF=  0.00000   0.00000
      V21M TOT/SRF=  0.00000   0.00000

      0.03728   0.00000   0.00000   0.03728
0.00000   0.00000
      0.00000   0.03728   0.00000   0.00000
0.03728   0.00000
      0.00000   0.00000   -0.07456   0.00000
0.00000  -0.07456

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MAIN DIRECTIONS OF THE EFG	1.0000	0.0000	0.0000
	0.0000	1.0000	0.0000
	0.0000	0.0000	1.0000

:ANG002: ANGLE WITH OLD X-AXIS = 0.0

:ETA002: ASYMM. ETA = 0.00000

XC-potentials inside spheres (XCPOT1)
 Lebedev grid of 350
 Condition Number of XCPOT1 1.05364E+00

1	-0.697645826523054	-0.697835605404443
2	-0.697645826523054	-0.697835605404443
4	-0.697645826523054	-0.697835605404443
6	-0.699190503538423	-0.697835605404443
8	-0.697580866980724	-0.697603513024629
10	-0.697580866980724	-0.697603513024629
12	-0.697580866980724	-0.697603513024629
14	-0.697580866980724	-0.697603513024629
16	-0.694920260764563	-0.694947330348002
18	-0.694920260764563	-0.694947330348002
20	-0.694920260764563	-0.694947330348002
22	-0.694920260764563	-0.694947330348002
24	-0.694920260764563	-0.694947330348002
26	-0.694920260764563	-0.694947330348002
28	-0.694920260764563	-0.694947330348002
30	-0.694920260764563	-0.694947330348002
32	-0.694920260764563	-0.694947330348002
34	-0.694920260764563	-0.694947330348002
36	-0.694920260764563	-0.694947330348002
38	-0.694920260764563	-0.694947330348002
40	-0.697134317093302	-0.697143164593902
42	-0.697134317093302	-0.697143164593902
44	-0.697134317093302	-0.697143164593902
46	-0.697134317093302	-0.697143164593902
48	-0.697134317093302	-0.697143164593902
50	-0.697134317093302	-0.697143164593902
52	-0.697134317093302	-0.697143164593902
54	-0.697134317093302	-0.697143164593902
56	-0.697134317093302	-0.697143164593902
58	-0.697134317093302	-0.697143164593902
60	-0.697134317093302	-0.697143164593902
62	-0.697134317093302	-0.697143164593902
64	-0.697107067100073	-0.697147214431988
66	-0.697107067100073	-0.697147214431988
68	-0.697107067100073	-0.697147214431988
70	-0.697107067100073	-0.697147214431988
72	-0.697107067100073	-0.697147214431988
74	-0.697107067100073	-0.697147214431988
76	-0.697107067100073	-0.697147214431988

78	-0.697107067100073	-0.697147214431988
80	-0.697107067100073	-0.697147214431988
82	-0.697107067100073	-0.697147214431988
84	-0.697107067100073	-0.697147214431988
86	-0.697107067100073	-0.697147214431988
88	-0.695621391499026	-0.695613031688598
90	-0.695621391499026	-0.695613031688598
92	-0.695621391499026	-0.695613031688598
94	-0.695621391499026	-0.695613031688598
96	-0.695621391499026	-0.695613031688598
98	-0.695621391499026	-0.695613031688598
100	-0.695621391499026	-0.695613031688598
102	-0.695621391499026	-0.695613031688598
104	-0.695621391499026	-0.695613031688598
106	-0.695621391499026	-0.695613031688598
108	-0.695621391499026	-0.695613031688598
110	-0.695621391499026	-0.695613031688598
112	-0.696621796978569	-0.696635499030590
114	-0.696621796978569	-0.696635499030590
116	-0.696621796978569	-0.696635499030590
118	-0.696621796978569	-0.696635499030590
120	-0.696621796978569	-0.696635499030590
122	-0.696621796978569	-0.696635499030590
124	-0.696621796978569	-0.696635499030590
126	-0.696621796978569	-0.696635499030590
128	-0.696621796978569	-0.696635499030590
130	-0.696621796978569	-0.696635499030590
132	-0.696621796978569	-0.696635499030590
134	-0.696621796978569	-0.696635499030590
136	-0.696976453725844	-0.696964111265027
138	-0.696976453725844	-0.696964111265027
140	-0.696976453725844	-0.696964111265027
142	-0.696976453725844	-0.696964111265027
144	-0.696976453725844	-0.696964111265027
146	-0.696976453725844	-0.696964111265027
148	-0.696976453725844	-0.696964111265027
150	-0.696976453725844	-0.696964111265027
152	-0.696976453725844	-0.696964111265027
154	-0.696976453725844	-0.696964111265027
156	-0.696976453725844	-0.696964111265027
158	-0.696976453725844	-0.696964111265027
160	-0.697336258544291	-0.697418477540324
162	-0.697336258544291	-0.697418477540324
164	-0.697336258544291	-0.697418477540324
166	-0.697336258544291	-0.697418477540324
168	-0.697336258544291	-0.697418477540324
170	-0.697336258544291	-0.697418477540324
172	-0.697336258544291	-0.697418477540324
174	-0.697336258544291	-0.697418477540324
176	-0.697336258544291	-0.697418477540324
178	-0.697336258544291	-0.697418477540324
180	-0.697336258544291	-0.697418477540324

182	-0.697336258544291	-0.697418477540324
184	-0.696429439835485	-0.696402429361060
186	-0.696429439835485	-0.696402429361060
188	-0.696429439835485	-0.696402429361060
190	-0.696429439835485	-0.696402429361060
192	-0.696429439835485	-0.696402429361060
194	-0.696429439835485	-0.696402429361060
196	-0.696429439835485	-0.696402429361060
198	-0.696429439835485	-0.696402429361060
200	-0.696429439835485	-0.696402429361060
202	-0.696429439835485	-0.696402429361060
204	-0.696429439835485	-0.696402429361060
206	-0.696429439835485	-0.696402429361060
208	-0.696347343292686	-0.696338779834161
210	-0.696347343292686	-0.696338779834161
212	-0.696347343292686	-0.696338779834161
214	-0.696347343292686	-0.696338779834161
216	-0.696347343292686	-0.696338779834161
218	-0.696347343292686	-0.696338779834161
220	-0.696347343292686	-0.696338779834161
222	-0.696347343292686	-0.696338779834161
224	-0.696347343292686	-0.696338779834161
226	-0.696347343292686	-0.696338779834161
228	-0.696347343292686	-0.696338779834161
230	-0.696347343292686	-0.696338779834161
232	-0.696347343292686	-0.696338779834161
234	-0.696347343292686	-0.696338779834161
236	-0.696347343292686	-0.696338779834161
238	-0.696347343292686	-0.696338779834161
240	-0.696347343292686	-0.696338779834161
242	-0.696347343292686	-0.696338779834161
244	-0.696347343292686	-0.696338779834161
246	-0.696347343292686	-0.696338779834161
248	-0.696347343292686	-0.696338779834161
250	-0.696347343292686	-0.696338779834161
252	-0.696347343292686	-0.696338779834161
254	-0.696347343292686	-0.696338779834161
256	-0.695498850610886	-0.695495431255377
258	-0.695498850610886	-0.695495431255377
260	-0.695498850610886	-0.695495431255377
262	-0.695498850610886	-0.695495431255377
264	-0.695498850610886	-0.695495431255377
266	-0.695498850610886	-0.695495431255377
268	-0.695498850610886	-0.695495431255377
270	-0.695498850610886	-0.695495431255377
272	-0.695498850610886	-0.695495431255377
274	-0.695498850610886	-0.695495431255377
276	-0.695498850610886	-0.695495431255377
278	-0.695498850610886	-0.695495431255377
280	-0.695498850610886	-0.695495431255377
282	-0.695498850610886	-0.695495431255377
284	-0.695498850610886	-0.695495431255377

286	-0.695498850610886	-0.695495431255377
288	-0.695498850610886	-0.695495431255377
290	-0.695498850610886	-0.695495431255377
292	-0.695498850610886	-0.695495431255377
294	-0.695498850610886	-0.695495431255377
296	-0.695498850610886	-0.695495431255377
298	-0.695498850610886	-0.695495431255377
300	-0.695498850610886	-0.695495431255377
302	-0.695498850610886	-0.695495431255377
304	-0.696489691404277	-0.696482249524337
306	-0.696489691404277	-0.696482249524337
308	-0.696489691404277	-0.696482249524337
310	-0.696489691404277	-0.696482249524337
312	-0.696489691404277	-0.696482249524337
314	-0.696489691404277	-0.696482249524337
316	-0.696489691404277	-0.696482249524337
318	-0.696489691404277	-0.696482249524337
320	-0.696489691404277	-0.696482249524337
322	-0.696489691404277	-0.696482249524337
324	-0.696489691404277	-0.696482249524337
326	-0.696489691404277	-0.696482249524337
328	-0.696489691404277	-0.696482249524337
330	-0.696489691404277	-0.696482249524337
332	-0.696489691404277	-0.696482249524337
334	-0.696489691404277	-0.696482249524337
336	-0.696489691404277	-0.696482249524337
338	-0.696489691404277	-0.696482249524337
340	-0.696489691404277	-0.696482249524337
342	-0.696489691404277	-0.696482249524337
344	-0.696489691404277	-0.696482249524337
346	-0.696489691404277	-0.696482249524337
348	-0.696489691404277	-0.696482249524337
350	-0.696489691404277	-0.696482249524337

ATOM 1 AT RMT: SIGMA OF V-XC FIT: 0.11055E-03
 ATOM 1 LARGEST SIGMA AT R(781)= 2.500 and MAX DIFF: 0.11055E-03
 0.13549E-02

Lebedev grid of 350
 Condition Number of XCPOT1 1.05364E+00

INDEX	V-XC	FIT	DIFFERENCE
1	-0.66890	-0.66858	-0.00032
2	-0.66890	-0.66858	-0.00032
4	-0.66890	-0.66858	-0.00032
6	-0.66481	-0.66255	-0.00226
8	-0.66753	-0.66744	-0.00009
10	-0.66753	-0.66744	-0.00009
12	-0.66753	-0.66744	-0.00009
14	-0.66753	-0.66744	-0.00009
16	-0.67163	-0.67138	-0.00025
18	-0.67163	-0.67138	-0.00025
20	-0.67163	-0.67138	-0.00025
22	-0.67163	-0.67138	-0.00025
24	-0.65917	-0.65887	-0.00030

26	-0.65917	-0.65887	-0.00030
28	-0.65917	-0.65887	-0.00030
30	-0.65917	-0.65887	-0.00030
32	-0.65917	-0.65887	-0.00030
34	-0.65917	-0.65887	-0.00030
36	-0.65917	-0.65887	-0.00030
38	-0.65917	-0.65887	-0.00030
40	-0.66296	-0.66280	-0.00016
42	-0.66296	-0.66280	-0.00016
44	-0.66296	-0.66280	-0.00016
46	-0.66296	-0.66280	-0.00016
48	-0.66845	-0.66852	0.00007
50	-0.66845	-0.66852	0.00007
52	-0.66845	-0.66852	0.00007
54	-0.66845	-0.66852	0.00007
56	-0.66845	-0.66852	0.00007
58	-0.66845	-0.66852	0.00007
60	-0.66845	-0.66852	0.00007
62	-0.66845	-0.66852	0.00007
64	-0.66059	-0.66076	0.00017
66	-0.66059	-0.66076	0.00017
68	-0.66059	-0.66076	0.00017
70	-0.66059	-0.66076	0.00017
72	-0.66827	-0.66827	-0.00000
74	-0.66827	-0.66827	-0.00000
76	-0.66827	-0.66827	-0.00000
78	-0.66827	-0.66827	-0.00000
80	-0.66827	-0.66827	-0.00000
82	-0.66827	-0.66827	-0.00000
84	-0.66827	-0.66827	-0.00000
86	-0.66827	-0.66827	-0.00000
88	-0.67151	-0.67145	-0.00007
90	-0.67151	-0.67145	-0.00007
92	-0.67151	-0.67145	-0.00007
94	-0.67151	-0.67145	-0.00007
96	-0.66065	-0.66048	-0.00018
98	-0.66065	-0.66048	-0.00018
100	-0.66065	-0.66048	-0.00018
102	-0.66065	-0.66048	-0.00018
104	-0.66065	-0.66048	-0.00018
106	-0.66065	-0.66048	-0.00018
108	-0.66065	-0.66048	-0.00018
110	-0.66065	-0.66048	-0.00018
112	-0.65980	-0.65988	0.00008
114	-0.65980	-0.65988	0.00008
116	-0.65980	-0.65988	0.00008
118	-0.65980	-0.65988	0.00008
120	-0.66811	-0.66830	0.00018
122	-0.66811	-0.66830	0.00018
124	-0.66811	-0.66830	0.00018
126	-0.66811	-0.66830	0.00018
128	-0.66811	-0.66830	0.00018

130	-0.66811	-0.66830	0.00018
132	-0.66811	-0.66830	0.00018
134	-0.66811	-0.66830	0.00018
136	-0.67058	-0.67065	0.00007
138	-0.67058	-0.67065	0.00007
140	-0.67058	-0.67065	0.00007
142	-0.67058	-0.67065	0.00007
144	-0.66433	-0.66423	-0.00011
146	-0.66433	-0.66423	-0.00011
148	-0.66433	-0.66423	-0.00011
150	-0.66433	-0.66423	-0.00011
152	-0.66433	-0.66423	-0.00011
154	-0.66433	-0.66423	-0.00011
156	-0.66433	-0.66423	-0.00011
158	-0.66433	-0.66423	-0.00011
160	-0.66916	-0.66898	-0.00018
162	-0.66916	-0.66898	-0.00018
164	-0.66916	-0.66898	-0.00018
166	-0.66916	-0.66898	-0.00018
168	-0.66140	-0.66149	0.00008
170	-0.66140	-0.66149	0.00008
172	-0.66779	-0.66771	-0.00008
174	-0.66779	-0.66771	-0.00008
176	-0.66140	-0.66149	0.00008
178	-0.66140	-0.66149	0.00008
180	-0.66779	-0.66771	-0.00008
182	-0.66779	-0.66771	-0.00008
184	-0.66998	-0.66996	-0.00001
186	-0.66998	-0.66996	-0.00001
188	-0.66998	-0.66996	-0.00001
190	-0.66998	-0.66996	-0.00001
192	-0.65893	-0.65924	0.00031
194	-0.65893	-0.65924	0.00031
196	-0.66507	-0.66524	0.00018
198	-0.66507	-0.66524	0.00018
200	-0.65893	-0.65924	0.00031
202	-0.65893	-0.65924	0.00031
204	-0.66507	-0.66524	0.00018
206	-0.66507	-0.66524	0.00018
208	-0.66474	-0.66480	0.00006
210	-0.66474	-0.66480	0.00006
212	-0.66474	-0.66480	0.00006
214	-0.66474	-0.66480	0.00006
216	-0.66023	-0.66019	-0.00005
218	-0.66023	-0.66019	-0.00005
220	-0.66023	-0.66019	-0.00005
222	-0.66023	-0.66019	-0.00005
224	-0.66474	-0.66480	0.00006
226	-0.66474	-0.66480	0.00006
228	-0.66474	-0.66480	0.00006
230	-0.66474	-0.66480	0.00006
232	-0.67055	-0.67065	0.00009

234	-0.67055	-0.67065	0.00009
236	-0.67055	-0.67065	0.00009
238	-0.67055	-0.67065	0.00009
240	-0.66023	-0.66019	-0.00005
242	-0.66023	-0.66019	-0.00005
244	-0.66023	-0.66019	-0.00005
246	-0.66023	-0.66019	-0.00005
248	-0.67055	-0.67065	0.00009
250	-0.67055	-0.67065	0.00009
252	-0.67055	-0.67065	0.00009
254	-0.67055	-0.67065	0.00009
256	-0.66223	-0.66218	-0.00005
258	-0.66223	-0.66218	-0.00005
260	-0.66223	-0.66218	-0.00005
262	-0.66223	-0.66218	-0.00005
264	-0.65811	-0.65816	0.00005
266	-0.65811	-0.65816	0.00005
268	-0.65811	-0.65816	0.00005
270	-0.65811	-0.65816	0.00005
272	-0.66223	-0.66218	-0.00005
274	-0.66223	-0.66218	-0.00005
276	-0.66223	-0.66218	-0.00005
278	-0.66223	-0.66218	-0.00005
280	-0.67104	-0.67096	-0.00008
282	-0.67104	-0.67096	-0.00008
284	-0.67104	-0.67096	-0.00008
286	-0.67104	-0.67096	-0.00008
288	-0.65811	-0.65816	0.00005
290	-0.65811	-0.65816	0.00005
292	-0.65811	-0.65816	0.00005
294	-0.65811	-0.65816	0.00005
296	-0.67104	-0.67096	-0.00008
298	-0.67104	-0.67096	-0.00008
300	-0.67104	-0.67096	-0.00008
302	-0.67104	-0.67096	-0.00008
304	-0.66592	-0.66611	0.00019
306	-0.66592	-0.66611	0.00019
308	-0.66592	-0.66611	0.00019
310	-0.66592	-0.66611	0.00019
312	-0.65912	-0.65936	0.00024
314	-0.65912	-0.65936	0.00024
316	-0.65912	-0.65936	0.00024
318	-0.65912	-0.65936	0.00024
320	-0.66592	-0.66611	0.00019
322	-0.66592	-0.66611	0.00019
324	-0.66592	-0.66611	0.00019
326	-0.66592	-0.66611	0.00019
328	-0.66956	-0.66964	0.00008
330	-0.66956	-0.66964	0.00008
332	-0.66956	-0.66964	0.00008
334	-0.66956	-0.66964	0.00008
336	-0.65912	-0.65936	0.00024

338	-0.65912	-0.65936	0.00024
340	-0.65912	-0.65936	0.00024
342	-0.65912	-0.65936	0.00024
344	-0.66956	-0.66964	0.00008
346	-0.66956	-0.66964	0.00008
348	-0.66956	-0.66964	0.00008
350	-0.66956	-0.66964	0.00008

ATOM 2 AT RMT: SIGMA OF V-XC FIT: 0.22510E-03
 ATOM 2 LARGEST SIGMA AT R(781)= 2.500 and MAX DIFF: 0.22510E-03
 0.22596E-02

XC Quadrature in Interstitial, 19 points

H=-1 K=-1 L= 0	H= 0 K=-1 L=-1	H= 0 K=-1 L= 0
H= 0 K=-1 L= 1	H= 1 K=-1 L= 0	H=-1 K= 0 L=-1
H=-1 K= 0 L= 0	H=-1 K= 0 L= 1	H= 0 K= 0 L=-1
H= 0 K= 0 L= 0	H= 0 K= 0 L= 1	H= 1 K= 0 L=-1
H= 1 K= 0 L= 0	H= 1 K= 0 L= 1	H=-1 K= 1 L= 0
H= 0 K= 1 L=-1	H= 0 K= 1 L= 0	H= 0 K= 1 L= 1
H= 1 K= 1 L= 0	H=	

SELECTED FOURIERCOEFF. OF V-XC

0 0 0	-0.72499E+00	0.00000E+00	-0.72499E+00	
0.00000E+00				
0 0 1	-0.97766E-02	0.18004E-17	-0.97766E-02	
0.18004E-17				
0 0 2	-0.39203E-01	-0.84188E-19	-0.39203E-01	-
0.84188E-19				
0 0 3	0.56878E-03	0.22232E-17	0.56878E-03	
0.22232E-17				
0 0 4	0.30140E-02	-0.24184E-17	0.30140E-02	-
0.24184E-17				
0 0 5	-0.18214E-03	-0.23290E-17	-0.18214E-03	-
0.23290E-17				
0 0 6	-0.48633E-03	-0.98490E-17	-0.48633E-03	-
0.98490E-17				
0 0 7	0.85262E-04	-0.11345E-17	0.85262E-04	-
0.11345E-17				
0 0 8	-0.41242E-04	0.17288E-17	-0.41242E-04	
0.17288E-17				
0 0 9	-0.13730E-04	0.00000E+00	-0.13730E-04	
0.00000E+00				
0 0 10	0.30761E-04	-0.78181E-17	0.30761E-04	-
0.78181E-17				
0 0 11	-0.10001E-04	0.30271E-17	-0.10001E-04	
0.30271E-17				
0 0 12	-0.68558E-05	0.21202E-17	-0.68558E-05	
0.21202E-17				
0 0 13	0.57687E-05	0.20457E-17	0.57687E-05	
0.20457E-17				
0 0 14	-0.19842E-05	-0.35529E-17	-0.19842E-05	-
0.35529E-17				

0 0 15	-0.55751E-06	-0.47071E-17	-0.55751E-06	-
0.47071E-17				
0 0 16	0.20549E-05	0.11276E-16	0.20549E-05	
0.11276E-16				
0 0 17	-0.86930E-06	-0.31202E-17	-0.86930E-06	-
0.31202E-17				
0 0 18	-0.46319E-06	0.00000E+00	-0.46319E-06	
0.00000E+00				
0 0 19	0.57773E-06	-0.16762E-17	0.57773E-06	-
0.16762E-17				
0 0 20	-0.15114E-06	-0.52955E-17	-0.15114E-06	-
0.52955E-17				
0 0 21	-0.11811E-06	-0.22267E-17	-0.11811E-06	-
0.22267E-17				
0 0 22	0.14487E-06	-0.87219E-17	0.14487E-06	-
0.87219E-17				
0 0 23	-0.42386E-07	-0.32047E-17	-0.42386E-07	-
0.32047E-17				
0 0 24	-0.34770E-07	-0.20725E-17	-0.34770E-07	-
0.20725E-17				
0 0 25	0.38557E-07	0.83887E-19	0.38557E-07	
0.83887E-19				
0 0 26	-0.10173E-07	-0.17003E-16	-0.10173E-07	-
0.17003E-16				
0 0 27	-0.92295E-08	0.00000E+00	-0.92295E-08	
0.00000E+00				
0 0 28	0.10020E-07	0.65025E-17	0.10020E-07	
0.65025E-17				
0 0 29	-0.23940E-08	-0.45048E-17	-0.23940E-08	-
0.45048E-17				
0 0 30	-0.26347E-08	0.19652E-16	-0.26347E-08	
0.19652E-16				
0 0 31	0.25607E-08	-0.24901E-17	0.25607E-08	-
0.24901E-17				
0 0 32	-0.48499E-09	-0.17862E-17	-0.48499E-09	-
0.17862E-17				
0 0 33	-0.75908E-09	0.46945E-17	-0.75908E-09	
0.46945E-17				
0 0 34	0.62428E-09	0.11700E-16	0.62428E-09	
0.11700E-16				
0 0 35	0.52135E-10	-0.48620E-17	0.52135E-10	-
0.48620E-17				
0 0 36	-0.38412E-09	0.00000E+00	-0.38412E-09	
0.00000E+00				
0 0 37	0.52135E-10	0.51271E-17	0.52135E-10	
0.51271E-17				
0 0 38	0.62428E-09	-0.10554E-16	0.62428E-09	-
0.10554E-16				
0 0 39	-0.75908E-09	-0.46967E-17	-0.75908E-09	-
0.46967E-17				
0 0 40	-0.48499E-09	0.18982E-17	-0.48499E-09	
0.18982E-17				

0 0 41	0.25607E-08	0.23921E-17	0.25607E-08	
0.23921E-17				
0 0 42	-0.26347E-08	-0.19653E-16	-0.26347E-08	-
0.19653E-16				
0 0 43	-0.23940E-08	0.37389E-17	-0.23940E-08	
0.37389E-17				
0 0 44	0.10020E-07	-0.67997E-17	0.10020E-07	-
0.67997E-17				
0 0 45	-0.92295E-08	0.00000E+00	-0.92295E-08	
0.00000E+00				
0 0 46	-0.10173E-07	0.16604E-16	-0.10173E-07	
0.16604E-16				
0 0 47	0.38557E-07	-0.84970E-18	0.38557E-07	-
0.84970E-18				
0 0 48	-0.34770E-07	0.21202E-17	-0.34770E-07	
0.21202E-17				
0 0 49	-0.42386E-07	0.33111E-17	-0.42386E-07	
0.33111E-17				
0 0 50	0.14487E-06	0.87235E-17	0.14487E-06	
0.87235E-17				
0 0 51	-0.11811E-06	0.22119E-17	-0.11811E-06	
0.22119E-17				
0 0 52	-0.15114E-06	0.61072E-17	-0.15114E-06	
0.61072E-17				
0 0 53	0.57773E-06	0.16181E-17	0.57773E-06	
0.16181E-17				
0 0 54	-0.46319E-06	0.00000E+00	-0.46319E-06	
0.00000E+00				
0 0 55	-0.86930E-06	0.31972E-17	-0.86930E-06	
0.31972E-17				
0 0 56	0.20549E-05	-0.10169E-16	0.20549E-05	-
0.10169E-16				
0 0 57	-0.55751E-06	0.46646E-17	-0.55751E-06	
0.46646E-17				
0 0 58	-0.19842E-05	0.34616E-17	-0.19842E-05	
0.34616E-17				
0 0 59	0.57687E-05	-0.19102E-17	0.57687E-05	-
0.19102E-17				
0 0 60	-0.68558E-05	-0.21106E-17	-0.68558E-05	-
0.21106E-17				
0 0 61	-0.10001E-04	-0.23528E-17	-0.10001E-04	-
0.23528E-17				
0 0 62	0.30761E-04	0.76683E-17	0.30761E-04	
0.76683E-17				
0 0 63	-0.13730E-04	0.00000E+00	-0.13730E-04	
0.00000E+00				
0 0 64	-0.41242E-04	-0.19813E-17	-0.41242E-04	-
0.19813E-17				
0 0 65	0.85262E-04	-0.62798E-18	0.85262E-04	-
0.62798E-18				
0 0 66	-0.48633E-03	0.99067E-17	-0.48633E-03	
0.99067E-17				

```

0 0 67 -0.18214E-03 0.20597E-17 -0.18214E-03
0.20597E-17
0 0 68 0.30140E-02 0.25213E-17 0.30140E-02
0.25213E-17
0 0 69 0.56878E-03 -0.22783E-17 0.56878E-03 -
0.22783E-17
0 0 70 -0.39203E-01 -0.36087E-18 -0.39203E-01 -
0.36087E-18
0 0 71 -0.97766E-02 -0.98524E-18 -0.97766E-02 -
0.98524E-18
v-mean, v0,u0 (4.430081715293580E-002,-2.734844767664168E-018)
(3.015556136784225E-003,-2.734844767664168E-018)
(434.371150565359,0.000000000000000E+000)
(-4.128526101615158E-002,0.000000000000000E+000)

```

1

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-----
T O T A L   E N E R G Y
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```

1. DENSITY-POTENTIAL INTEGRALS (H)

SPHERE= 1 Ce

```

L= 0 : -3354.879649 SPHERE CHARGE
L= 4 : 0.000004 SPHERE CHARGE
L= 6 : 0.000002 SPHERE CHARGE
TOTAL= -3354.879643

```

SPHERE= 2 In

```

L= 0 : -2324.776092 SPHERE CHARGE
L= 2 : 0.000096 SPHERE CHARGE
L= 4 : -0.000002 SPHERE CHARGE
L= 4 : 0.000010 SPHERE CHARGE
L= 6 : 0.000000 SPHERE CHARGE
L= 6 : 0.000002 SPHERE CHARGE
TOTAL= -6974.327956

```

PLANE WAVE CONTRIBUTION

TOTAL= -0.654935

2. CONSTANT TERMS (H)

```

SPHERE 1 Ce = -36.827512
SPHERE 2 In = -66.802395

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TOTAL VALUE = -10433.492442 (H)
 :DEN : DENSITY INTEGRAL = -20866.98488444 (Ry)
 ELS_POTENTIAL AT Z=0 and Z=0.5: 0.00000 0.00000
 ELS_POTENTIAL AT Y=0 and Y=0.5: 0.00000 0.00000
 :VZERO:v0,v0c,v0x -0.72499 0.00000 -0.72499 v5,v5c,v5x -0.72499
 0.00000 -0.72499
 :VZERY:v0,v0c,v0x -0.72499 0.00000 -0.72499 v5,v5c,v5x -0.72499
 0.00000 -0.72499
 :VZERX:v0,v0c,v0x -3.70603 -2.70494 -1.00109 v5,v5c,v5x -2.16916
 -1.27994 -0.88921

=====>>> CPU-TIME SUMMARY
 TOTAL CPU/WALL-TIME USED : 1.9 100. PERCENT
 1.9 100. PERCENT
 TIME MULTIPOLMOMENTS: 0.0 3. PERCENT
 0.0 3. PERCENT
 TIME COULOMB POT INT: 0.0 1. PERCENT
 0.0 1. PERCENT
 TIME COULOMB POT RMT: 0.0 2. PERCENT
 0.0 2. PERCENT
 TIME COULOMB POT SPH: 0.0 0. PERCENT
 0.0 0. PERCENT
 TIME XCPOT SPHERES : 0.8 43. PERCENT
 0.8 43. PERCENT
 TIME XCPOT INTERST : 0.8 40. PERCENT
 0.8 40. PERCENT
 TIME TOTAL ENERGY : 0.0 2. PERCENT
 0.0 2. PERCENT
 TIME REAN0, REAN3 : 0.0 0. PERCENT
 0.0 0. PERCENT
 TIME REANALYSE : 0.2 9. PERCENT
 0.2 9. PERCENT