

Electric field enhances the electronic and diffusion properties of penta-graphene nanoribbon anodes in lithium-ion batteries

Thi Nhan Tran,¹ Nguyen Vo Anh Duy,² Nguyen Hoang Hieu,³ Truc Anh Nguyen,⁴ Nguyen To Van,⁵ Thi Viet Bac Phung,⁶ Yohandys A. Zulueta,⁷ Minh Tho Nguyen^{8,9} Peter Schall,¹⁰ and Minh Triet Dang^{3,*}

¹ Faculty of Fundamental Sciences, Hanoi University of Industry, 298 Cau Dien, Bac Tu Liem, Hanoi, Vietnam.

² FPT University, 600 Nguyen Van Cu, Ninh Kieu, Can Tho, Vietnam.

³ Department of Physics, Can Tho University, 3/2 Street, Ninh Kieu, Can Tho, Vietnam.

⁴ Faculty of Mechanics, Can Tho University of Technology, 256 Nguyen Van Cu Street, Ninh Kieu, Can Tho, Vietnam

⁵ Faculty of Chemico-Physical Engineering, Le Quy Don Technical University, Ha Noi, Vietnam

⁶ Center for Environmental Intelligence and College of Engineering & Computer Science, VinUniversity, Hanoi, Vietnam

⁷ Departamento de Física, Facultad de Ciencias Naturales y Exactas, Universidad de Oriente, CP 90500, Santiago de Cuba, Cuba

⁸ Laboratory for Chemical Computation and Modeling, Institute for Computational Science and Artificial Intelligence, Van Lang University, Ho Chi Minh City, Vietnam

⁹ Faculty of Applied Technology, School of Technology, Van Lang University, Ho Chi Minh City, Vietnam

¹⁰ Van der Waals-Zeeman Institute, University of Amsterdam, Science Park 904, Amsterdam, The Netherlands

* Email: dmtriet@ctu.edu.vn

Contents

1. Part 1: Structural stability of (pristine) penta-graphene nanoribbons upon lithium adsorption
2. Part 2: The electronic properties of (pristine) penta-graphene nanoribbons upon lithium adsorption
3. Part 3: Examples of simulation inputs performed in the Amsterdam Modeling Suite and VASP packages for calculating the density of states of pristine penta-graphene nanoribbons are included for readers to reproduce the calculations.

Part 1: Structural stability of (pristine) penta-graphene nanoribbons upon lithium adsorption

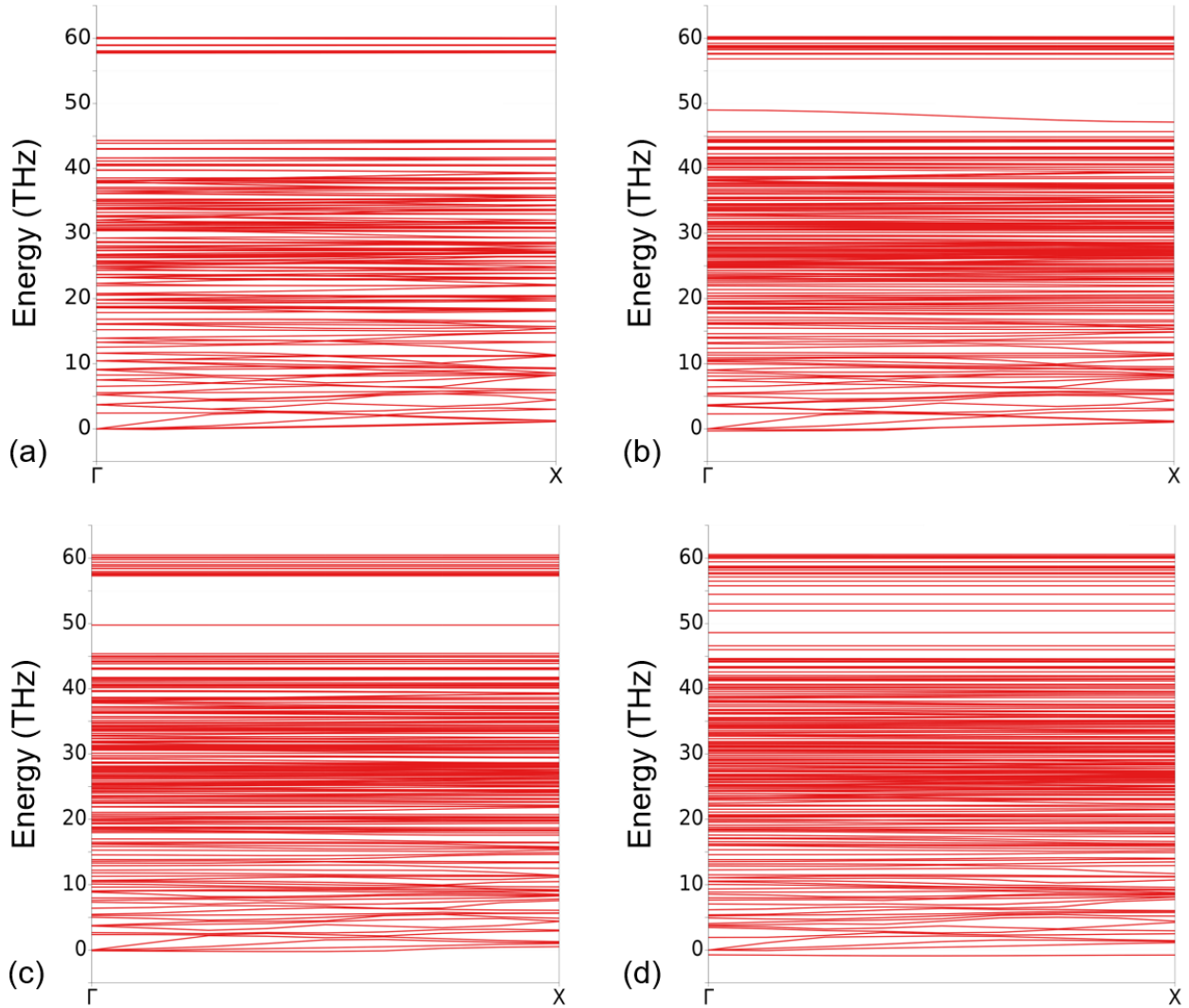


Figure S1. Phonon spectra of a pristine penta-graphene nanoribbon (a) and a penta-graphene nanoribbon upon lithium adsorption in a non-zero electric field (b), in a -2 V/nm (c) and 2 V/nm (d) electric field. The phonon spectra are calculated using the BP86-D3 exchange-correlation potential implemented in the AMS package.

Part 2: The electronic properties of (pristine) penta-graphene nanoribbons upon lithium adsorption

To explore the optoelectronic properties of penta-graphene nanoribbons upon lithium adsorption, beside the DFT approach presented in the main text, we also perform density functional theory (DFT) simulations using the Projector Augmented Wave (PAW) method implemented in the Vienna Ab initio Simulation Package (VASP) using the hybrid exchange-correlation functional (HSE06). The integration in the Brillouin zone was employed using the Monkhorst–Pack scheme ($7 \times 1 \times 1$). Lattice parameters and internal coordinates were fully relaxed until the atomic force on each atom was less than 0.01 eV/Å, and the convergence threshold for the self-consistent field calculations was set to 10^{-4}

eV per cell. A plane-wave energy cut-off of 500 eV is enough to get sufficient convergence. To avoid atomic interactions between the imaged periodic systems, a vacuum of 20 Å thickness was employed between the neighboring nanoribbons. To stabilize PGNR samples, their dangling bonds at the edges are passivated by hydrogen atoms.

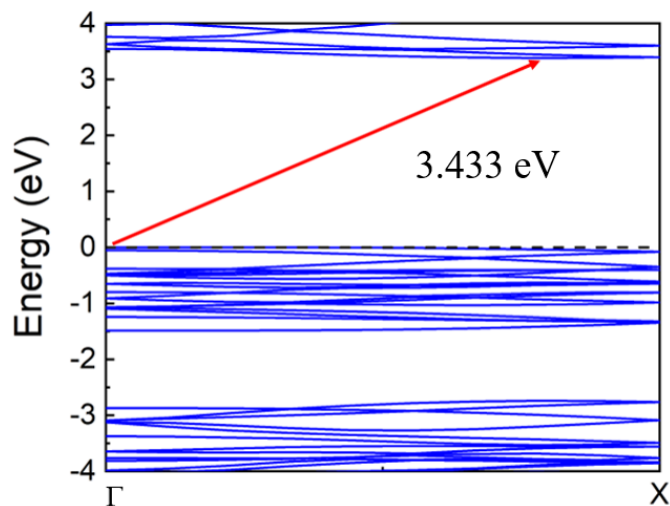


Figure S2. Band structure of a pristine penta-graphene nanoribbon calculated in the VASP package. The Fermi level is indicated by a dashed line.

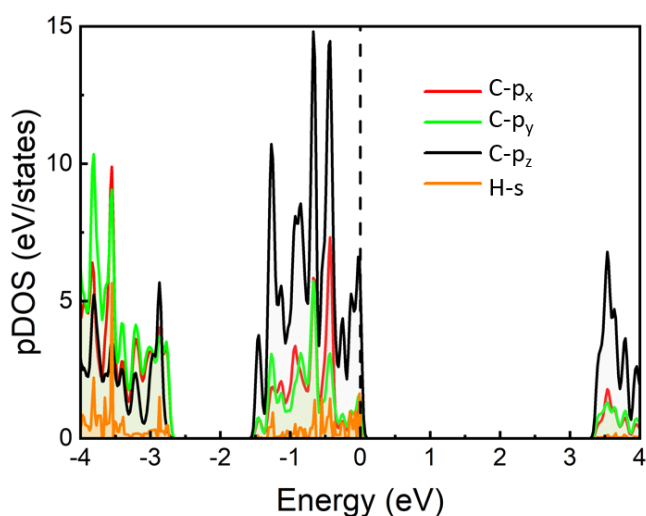


Figure S3. Partial density of states (pDOS) of a pristine penta-graphene nanoribbon calculated in the VASP package. The red, green, black, and orange curves demonstrate the C- p_x , C- p_y , C- p_z , and H-s orbitals, respectively. The Fermi level is indicated by a dashed line.

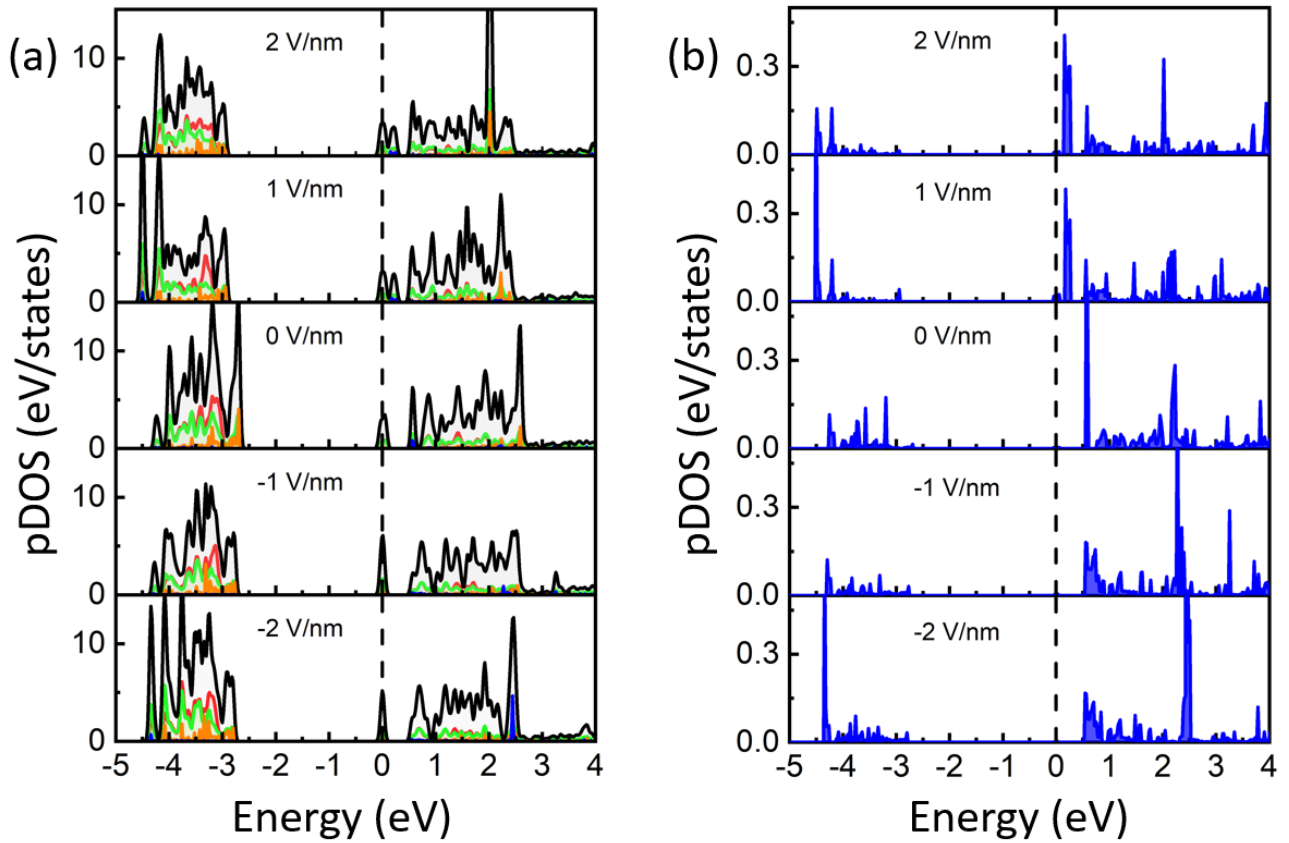


Figure S4. Partial density of states (pDOS) of all atoms in a penta-graphene nanoribbon (a) and of the *s* orbital of the lithium-ion adsorbed on the nanoribbon (b) calculated in the VASP package under an external electric field. In figure (a), the red, green, black, and orange curves demonstrate the C- p_x , C- p_y , C- p_z , and H-*s* orbitals, respectively. The Fermi level is indicated by a dashed line.

Part 3: Examples of simulation inputs performed in the Amsterdam Modeling Suite and VASP packages for calculating the density of states of pristine penta-graphene nanoribbons are included for readers to reproduce the calculations.

1. Input files performed in the Amsterdam Modeling Suite package (version 2023.104)

```
#!/bin/sh
```

```
"$AMSBIN/ams" << eor
```

```
Task SinglePoint
```

```
System
```

```
Atoms
```

```
C 0.5412706912883621 13.98229815319913 4.571629502421934  
C 1.561679797845947 14.82545176619118 4.357554133174196  
C 2.330426069746323 13.00974944512177 5.674562632438038  
C 2.783784970051826 14.32801860967339 5.080077934812825  
C 0.5029836238826506 10.31212583101279 4.407517070772294  
C 1.45079746565912 11.25945193408243 4.433724023799442  
C 3.283832786715102 12.07218078450307 5.69707039096658  
C 2.322871508238264 9.385625791280152 5.57459128836972  
C 0.9827746800573934 12.58686879466244 5.126772812288674  
C 2.797625280279821 10.75366796864177 5.030574062438204  
C 0.5109754877865634 6.687885932441226 4.30778964907207  
C 1.46432120793486 7.625504619491638 4.285385225910834  
C 3.270754409200095 8.4383522674852 5.548446616767916  
C 2.361511458848069 5.715083403808778 5.410506532717639  
C 0.977956811369266 8.944084639206974 4.951661341680608  
C 2.802931182620159 7.110739627505394 4.855727144314693  
C 3.38184225959829 4.871615635331824 5.623872042950689  
C 0.9644603063821362 5.369417913766706 4.901739134614558  
C 4.180872896120095 13.98229380467915 4.571621440416992  
C 5.20127901676747 14.82544287313597 4.35754755794592  
C 5.970024473580364 13.00974963668551 5.674561882101274  
C 6.423382644066922 14.32802067290248 5.080082495175692  
C 4.142585092007 10.31212729694928 4.407515038350637  
C 5.09039945414147 11.25945321899948 4.433723999082034  
C 6.923433021230329 12.07218193141531 5.697068844521872  
C 5.962470821295604 9.385625151509874 5.574590584198958  
C 4.622374562133984 12.58686698937718 5.126769687532759  
C 6.437226696570639 10.75366850711297 5.030575341603706  
C 4.150573736406983 6.687885522357137 4.30778810321718  
C 5.103922659871101 7.625505894261913 4.285379402119014  
C 6.910354332891719 8.438351059741704 5.548445483275892  
C 6.001110228929656 5.715082207328254 5.410496764370356  
C 4.617557335396574 8.944084272734539 4.951656850237168  
C 6.442530994714841 7.110739171018528 4.855720559679201  
C 7.021438828751565 4.87161583243765 5.623864639826726  
C 4.604058442109225 5.369420419262396 4.901735278340686  
C 7.820471178082318 13.98229965086547 4.571633362082332  
C 8.840879370481955 14.82545778439094 4.357571833789236  
C 9.6096273719201 13.0097475326408 5.674568395301308  
C 10.06298681641205 14.32802290356469 5.080092982073286
```

C 7.782186784517863 10.31212664390403 4.407516414676136
C 8.729999596274807 11.25945187214318 4.433727346607816
C 10.5630324228476 12.07218158314827 5.697069187243188
C 9.602070978882772 9.385625763016257 5.574592085347668
C 8.261975845993044 12.58686881804837 5.126774077596858
C 10.07682599975516 10.75366734159703 5.030576624197418
C 7.790176974153872 6.687887033483704 4.307786967428139
C 8.743522821804941 7.625504927499152 4.285384733874174
C 10.54995510518296 8.438351514130252 5.548449891770206
C 9.64071049088712 5.715084515963902 5.410505381826391
C 8.257158665363091 8.944084386512738 4.951658419707214
C 10.08213194073898 7.110741178656784 4.855728162252122
C 10.66104095715395 4.871614386957249 5.623873288049211
C 8.243661223735225 5.36942027599432 4.901736134730846
H 2.955875824165382 15.11498304175604 5.843162980531268
H 1.455973896999942 15.87498696573331 4.080937281301019
H 3.275794331588746 3.821724943709208 5.899289679250942
H 1.137034272388432 4.582443499141466 4.138805863751482
H 6.59545721117881 15.11498564563938 5.843169348926543
H 5.095568795928034 15.87497949747111 4.080923815973114
H 6.915391745290886 3.821726415588584 5.899286476047338
H 4.776634934006249 4.582445830681731 4.138801869066402
H 10.23507965782144 15.11498306532898 5.843182843395138
H 8.735165301410431 15.87499520821821 4.080962902267006
H 10.55498977812679 3.821726044943468 5.899286943523144
H 8.416237292897597 4.582446769955822 4.138799815906302

End

Lattice

10.918800354 0.0 0.0

End

BondOrders

1 2 2.0
1 9 1.0
1 40 1.0 -1
2 4 1.0
2 56 1.0
3 4 1.0
3 7 2.0
3 9 1.0
4 19 1.0
4 55 1.0
5 6 2.0
5 15 1.0
5 46 1.0 -1
6 9 1.0
6 10 1.0
7 10 1.0
7 27 1.0
8 10 1.0
8 13 2.0
8 15 1.0
9 43 1.0 -1

10 23 1.0
11 12 2.0
11 18 1.0
11 52 1.0 -1
12 15 1.0
12 16 1.0
13 16 1.0
13 33 1.0
14 16 1.0
14 17 2.0
14 18 1.0
15 49 1.0 -1
16 29 1.0
17 36 1.0
17 57 1.0
18 53 1.0 -1
18 58 1.0
19 20 2.0
19 27 1.0
20 22 1.0
20 60 1.0
21 22 1.0
21 25 2.0
21 27 1.0
22 37 1.0
22 59 1.0
23 24 2.0
23 33 1.0
24 27 1.0
24 28 1.0
25 28 1.0
25 45 1.0
26 28 1.0
26 31 2.0
26 33 1.0
28 41 1.0
29 30 2.0
29 36 1.0
30 33 1.0
30 34 1.0
31 34 1.0
31 51 1.0
32 34 1.0
32 35 2.0
32 36 1.0
34 47 1.0
35 54 1.0
35 61 1.0
36 62 1.0
37 38 2.0
37 45 1.0
38 40 1.0

38 64 1.0
39 40 1.0
39 43 2.0
39 45 1.0
40 63 1.0
41 42 2.0
41 51 1.0
42 45 1.0
42 46 1.0
43 46 1.0
44 46 1.0
44 49 2.0
44 51 1.0
47 48 2.0
47 54 1.0
48 51 1.0
48 52 1.0
49 52 1.0
50 52 1.0
50 53 2.0
50 54 1.0
53 65 1.0
54 66 1.0

End

End

Engine BAND

Basis

Type TZP

Core None

End

BandStructure

Enabled Yes

DeltaK 0.01

EnergyAboveFermi 8 [eV]

EnergyBelowFermi 8 [eV]

End

DOS

DeltaE 0.01 [eV]

CalcPDOS Yes

End

KSpace

Type Symmetric

Symmetric

KInteg 5

End

End

XC

libxc hse06

End

EndEngine

Eor

2. Input files performed in the VASP package (version vasp.5.4.4.pl2)

a. INCAR-----

```
SYSTEM = PGNR
ISTART = 1
ICHARG = 1
LWAVE = .TRUE.
LCHARG = .TRUE.
LVTOT = .FALSE.
LELF = .FALSE.
LMAXMIX= 4
LORBIT = 11
EMIN = -10
EMAX = 10
NEDOS = 1000
```

```
##### SCF #####
ENCUT = 500
ISMEAR = -5
SIGMA = 0.05
EDIFF = 1E-4
NELMIN = 5
NELM = 300
GGA = PE
LREAL = .FALSE.
```

```
### GEO OPT ###
EDIFFG = -0.01
IBRION = 2
POTIM = 0.2
NSW = 0
ISIF = 3
```

```
##### HSE06 #####
LHFCALC = .TRUE.
AEXX = 0.25
HFSCREEN = 0.2
ALGO = ALL
TIME = 0.4
```

b. K-point -----

```
Automatic generation
0
Monkhorst-pack
7 1 1
0 0 0
```

c. POSCAR -----

POSCAR

1.0000000000000000

10.9188003540000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C H

54 12

Direct

0.0495723590266098 0.6991149076599565 0.2285814751210967

0.1430266830800547 0.7412725883095588 0.2178777066587098

0.2134324279399974 0.6504874722560887 0.2837281316219019

0.2549533721469696 0.7164009304836694 0.2540038967406412

0.0460658321038343 0.5156062915506393 0.2203758535386147

0.1328715077318576 0.5629725967041217 0.2216862011899721

0.3007503278977072 0.6036090392251536 0.2848535195483290

0.2127405422691241 0.4692812895640076 0.2787295644184860

0.0900075693477959 0.6293434397331219 0.2563386406144337

0.2562209390755036 0.5376833984320888 0.2515287031219102

0.0467977681814992 0.3343942966220613 0.2153894824536035

0.1341100817360782 0.3812752309745819 0.2142692612955417

0.2995525426931984 0.4219176133742600 0.2774223308383958

0.2162793880541054 0.2857541701904389 0.2705253266358819

0.0895663241073000 0.4472042319603487 0.2475830670840304

0.2567068809526617 0.3555369813752697 0.2427863572157347

0.3097265404582092 0.2435807817665912 0.2811936021475344

0.0883302446343215 0.2684708956883353 0.2450869567307279

0.3829058834827465 0.6991146902339576 0.2285810720208496

0.4763599340711482 0.7412721436567984 0.2178773778972960

0.5467656042811793 0.6504874818342756 0.2837280941050637

0.5882864816475718 0.7164010336451242 0.2540041247587846

0.3793992890885126 0.5156063648474641 0.2203757519175318

0.4662050123736029 0.5629726609499742 0.2216861999541017

0.6340836719021055 0.6036090965707656 0.2848534422260936

0.5460738018816608 0.4692812575754937 0.2787295292099479

0.4233408810740477 0.6293433494688588 0.2563384843766380

0.5895543913130000 0.5376834253556486 0.2515287670801853

0.3801309303074178 0.3343942761178568 0.2153894051608590

0.4674435372381662 0.3812752947130956 0.2142689701059507

0.6328858582307695 0.4219175529870852 0.2774222741637946

0.5496125979381248 0.2857541103664127 0.2705248382185178

0.4228996946267064 0.4472042136367269 0.2475828425118584

0.5900401862696097 0.3555369585509264 0.2427860279839600

0.6430595487698726 0.2435807916218825 0.2811932319913363

0.4216633964208872 0.2684710209631198 0.2450867639170343

0.7162390486622793 0.6991149825432734 0.2285816681041166

0.8096932889924288 0.7412728892195471 0.2178785916894618

0.8800991922523524 0.6504873766320399 0.2837284197650654

0.9216201862987238 0.7164011451782345 0.2540046491036643

0.7127327666236641 0.5156063321952017 0.2203758207338068

0.7995383479171916 0.5629725936071592 0.2216863673303908

0.9674169396254173 0.6036090791574135 0.2848534593621594

0.8794071388405910 0.4692812881508129 0.2787296042673834
0.7566743211827613 0.6293434409024183 0.2563387038798429
0.9228876500213334 0.5376833670798516 0.2515288312098709
0.7134645493632470 0.3343943516741852 0.2153893483714069
0.8007768745951870 0.3812752463749576 0.2142692366937087
0.9662192514874660 0.4219175757065126 0.2774224945885103
0.8829459444558244 0.2857542257981951 0.2705252690913195
0.7562331389581786 0.4472042193256369 0.2475829209853607
0.9233735954376600 0.3555370589328392 0.2427864081126061
0.9763930662262157 0.2435807193478625 0.2811936644024605
0.7549969737028150 0.2684710137997160 0.2450868067365423
0.2707143393351381 0.7557491520878018 0.2921581490265634
0.1333455919877278 0.7937493482866653 0.2040468640650510
0.3000141247558107 0.1910862471854604 0.2949644839625471
0.1041354576990585 0.2291221749570733 0.2069402931875741
0.6040459571882021 0.7557492822819688 0.2921584674463272
0.4666784473315624 0.7937489748735553 0.2040461907986557
0.6333472104156110 0.1910863207794292 0.2949643238023669
0.4374688408197127 0.2291222915340866 0.2069400934533201
0.9373813354936847 0.7557491532664491 0.2921591421697569
0.8000114498119186 0.7937497604109107 0.2040481451133503
0.9666803527788717 0.1910863022471734 0.2949643471761572
0.7708023793854228 0.2291223384977911 0.2069399907953151

0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00

d. POTCAR

PAW_PBE C 08Apr2002

4.0000000000000000

parameters from PSCTR are:

VRHFIN =C: s2p2

LEXCH = PE

EATOM = 147.1560 eV, 10.8157 Ry

TITEL = PAW_PBE C 08Apr2002

LULTRA = F use ultrasoft PP ?

IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no

RPACOR = 1.200 partial core radius

POMASS = 12.011; ZVAL = 4.000 mass and valenz

RCORE = 1.500 outmost cutoff radius

RWIGS = 1.630; RWIGS = 0.863 wigner-seitz radius (au A)

ENMAX = 400.000; ENMIN = 300.000 eV

ICORE = 2 local potential

LCOR = T correct aug charges

LPAW = T paw PP

EAUG = 644.873

DEXC = 0.000

RMAX = 1.529 core radius for proj-oper

RAUG = 1.300 factor for augmentation sphere

RDEP = 1.501 radius for radial grids

RDEPT = 1.300 core radius for aug-charge

Atomic configuration

4 entries

n	l	j	E	occ.
1	0	0.50	-273.3789	2.0000
2	0	0.50	-13.7508	2.0000
2	1	0.50	-5.2854	2.0000
3	2	1.50	-5.4423	0.0000

Description

l	E	TYP	RCUT	TYP	RCUT
0	-13.7508458	23	1.200		
0	-8.2022199	23	1.200		
1	-5.2854383	23	1.500		
1	34.0145650	23	1.500		
2	-5.4423304	7	1.500		

Error from kinetic energy argument (eV)

NDATA = 100

STEP = 20.000 1.050

51.3	49.5	48.6	46.8	45.9	44.1	42.4	41.6
39.9	38.2	37.4	35.8	34.3	32.8	31.4	30.0
28.6	27.3	26.1	24.3	23.2	22.1	20.5	19.6
18.6	17.3	16.0	15.2	14.1	13.1	12.1	11.1
10.3	9.47	8.72	8.02	7.15	6.55	5.82	5.31
4.69	4.13	3.63	3.17	2.76	2.40	2.07	1.72
1.47	1.20	0.971	0.815	0.650	0.512	0.380	0.292
0.222	0.158	0.110	0.748E-01	0.504E-01	0.337E-01	0.227E-01	0.149E-01

0.111E-01 0.869E-02 0.756E-02 0.700E-02 0.657E-02 0.614E-02 0.551E-02 0.474E-02
0.392E-02 0.314E-02 0.237E-02 0.184E-02 0.143E-02 0.118E-02 0.104E-02 0.993E-03
0.959E-03 0.910E-03 0.829E-03 0.707E-03 0.570E-03 0.442E-03 0.343E-03 0.275E-03
0.245E-03 0.238E-03 0.236E-03 0.227E-03 0.202E-03 0.169E-03 0.131E-03 0.102E-03
0.851E-04 0.796E-04 0.787E-04 0.761E-04

END of PSCTR-controll parameters

local part

124.721915246209

0.20536679E+02 0.20533657E+02 0.20529589E+02 0.20522813E+02 0.20513330E+02
0.20501145E+02 0.20486261E+02 0.20468683E+02 0.20448412E+02 0.20425452E+02
0.20399802E+02 0.20371460E+02 0.20340424E+02 0.20306688E+02 0.20270245E+02
0.20231085E+02 0.20189197E+02 0.20144567E+02 0.20097181E+02 0.20047020E+02
0.19994064E+02 0.19938291E+02 0.19879675E+02 0.19818187E+02 0.19753797E+02
0.19686468E+02 0.19616163E+02 0.19542839E+02 0.19466452E+02 0.19386953E+02
0.19304291E+02 0.19218411E+02 0.19129256E+02 0.19036766E+02 0.18940879E+02
0.18841532E+02 0.18738659E+02 0.18632194E+02 0.18522069E+02 0.18408216E+02
0.18290567E+02 0.18169055E+02 0.18043614E+02 0.17914181E+02 0.17780693E+02
0.17643093E+02 0.17501325E+02 0.17355339E+02 0.17205092E+02 0.17050542E+02
0.16891658E+02 0.16728413E+02 0.16560791E+02 0.16388780E+02 0.16212381E+02
0.16031603E+02 0.15846465E+02 0.15656997E+02 0.15463240E+02 0.15265248E+02
0.15063085E+02 0.14856829E+02 0.14646569E+02 0.14432410E+02 0.14214467E+02
0.13992870E+02 0.13767760E+02 0.13539295E+02 0.13307641E+02 0.13072982E+02
0.12835510E+02 0.12595433E+02 0.12352969E+02 0.12108348E+02 0.11861810E+02
0.11613607E+02 0.11363998E+02 0.11113253E+02 0.10861649E+02 0.10609471E+02
0.10357008E+02 0.10104557E+02 0.98524172E+01 0.96008926E+01 0.93502881E+01
0.91009101E+01 0.88530648E+01 0.86070573E+01 0.83631900E+01 0.81217619E+01
0.78830672E+01 0.76473942E+01 0.74150243E+01 0.71862308E+01 0.69612776E+01
0.67404187E+01 0.65238968E+01 0.63119422E+01 0.61047727E+01 0.59025917E+01
0.57055883E+01 0.55139361E+01 0.53277925E+01 0.51472988E+01 0.49725787E+01
0.48037390E+01 0.46408683E+01 0.44840374E+01 0.43332989E+01 0.41886874E+01
0.40502189E+01 0.39178918E+01 0.37916864E+01 0.36715655E+01 0.35574745E+01
0.34493423E+01 0.33470813E+01 0.32505886E+01 0.31597459E+01 0.30744209E+01
0.29944678E+01 0.29197283E+01 0.28500323E+01 0.27851991E+01 0.27250381E+01
0.26693502E+01 0.26179285E+01 0.25705596E+01 0.25270244E+01 0.24870999E+01
0.24505592E+01 0.24171738E+01 0.23867139E+01 0.23589496E+01 0.23336521E+01
0.23105951E+01 0.22895548E+01 0.22703120E+01 0.22526521E+01 0.22363666E+01
0.22212536E+01 0.22071186E+01 0.21937754E+01 0.21810463E+01 0.21687632E+01
0.21567679E+01 0.21449124E+01 0.21330595E+01 0.21210829E+01 0.21088678E+01
0.20963104E+01 0.20833187E+01 0.20698122E+01 0.20557216E+01 0.20409891E+01
0.20255681E+01 0.20094230E+01 0.19925285E+01 0.19748698E+01 0.19564420E+01
0.19372495E+01 0.19173056E+01 0.18966322E+01 0.18752586E+01 0.18532215E+01
0.18305644E+01 0.18073362E+01 0.17835915E+01 0.17593892E+01 0.17347923E+01
0.17098666E+01 0.16846809E+01 0.16593056E+01 0.16338121E+01 0.16082728E+01
0.15827594E+01 0.15573435E+01 0.15320949E+01 0.15070820E+01 0.14823704E+01
0.14580234E+01 0.14341006E+01 0.14106582E+01 0.13877482E+01 0.13654185E+01
0.13437123E+01 0.13226680E+01 0.13023191E+01 0.12826937E+01 0.12638151E+01
0.12457010E+01 0.12283641E+01 0.12118119E+01 0.11960465E+01 0.11810654E+01
0.11668609E+01 0.11534209E+01 0.11407288E+01 0.11287638E+01 0.11175012E+01
0.11069129E+01 0.10969673E+01 0.10876300E+01 0.10788640E+01 0.10706301E+01
0.10628873E+01 0.10555931E+01 0.10487039E+01 0.10421755E+01 0.10359631E+01
0.10300222E+01 0.10243085E+01 0.10187787E+01 0.10133901E+01 0.10081016E+01
0.10028739E+01 0.99766914E+00 0.99245199E+00 0.98718929E+00 0.98185044E+00

0.97640757E+00 0.97083565E+00 0.96511259E+00 0.95921935E+00 0.95313999E+00
0.94686170E+00 0.94037476E+00 0.93367258E+00 0.92675161E+00 0.91961125E+00
0.91225380E+00 0.90468429E+00 0.89691039E+00 0.88894221E+00 0.88079215E+00
0.87247470E+00 0.86400626E+00 0.85540490E+00 0.84669017E+00 0.83788285E+00
0.82900471E+00 0.82007832E+00 0.81112676E+00 0.80217342E+00 0.79324179E+00
0.78435519E+00 0.77553658E+00 0.76680836E+00 0.75819218E+00 0.74970874E+00
0.74137760E+00 0.73321709E+00 0.72524409E+00 0.71747397E+00 0.70992043E+00
0.70259545E+00 0.69550921E+00 0.68867000E+00 0.68208424E+00 0.67575641E+00
0.66968909E+00 0.66388297E+00 0.65833684E+00 0.65304770E+00 0.64801081E+00
0.64321973E+00 0.63866645E+00 0.63434148E+00 0.63023398E+00 0.62633184E+00
0.62262188E+00 0.61908994E+00 0.61572103E+00 0.61249952E+00 0.60940923E+00
0.60643364E+00 0.60355603E+00 0.60075958E+00 0.59802761E+00 0.59534364E+00
0.59269159E+00 0.59005587E+00 0.58742152E+00 0.58477436E+00 0.58210102E+00
0.57938914E+00 0.57662737E+00 0.57380549E+00 0.57091446E+00 0.56794649E+00
0.56489504E+00 0.56175490E+00 0.55852216E+00 0.55519422E+00 0.55176980E+00
0.54824889E+00 0.54463277E+00 0.54092389E+00 0.53712588E+00 0.53324346E+00
0.52928237E+00 0.52524931E+00 0.52115182E+00 0.51699821E+00 0.51279747E+00
0.50855913E+00 0.50429321E+00 0.50001005E+00 0.49572026E+00 0.49143459E+00
0.48716380E+00 0.48291861E+00 0.47870953E+00 0.47454683E+00 0.47044040E+00
0.46639965E+00 0.46243349E+00 0.45855020E+00 0.45475737E+00 0.45106184E+00
0.44746968E+00 0.44398609E+00 0.44061541E+00 0.43736105E+00 0.43422553E+00
0.43121043E+00 0.42831638E+00 0.42554312E+00 0.42288946E+00 0.42035335E+00
0.41793186E+00 0.41562129E+00 0.41341716E+00 0.41131429E+00 0.40930684E+00
0.40738840E+00 0.40555205E+00 0.40379040E+00 0.40209574E+00 0.40046001E+00
0.39887500E+00 0.39733232E+00 0.39582354E+00 0.39434027E+00 0.39287418E+00
0.39141716E+00 0.38996131E+00 0.38849906E+00 0.38702322E+00 0.38552701E+00
0.38400417E+00 0.38244898E+00 0.38085627E+00 0.37922153E+00 0.37754088E+00
0.37581110E+00 0.37402968E+00 0.37219479E+00 0.37030533E+00 0.36836086E+00
0.36636167E+00 0.36430869E+00 0.36220354E+00 0.36004844E+00 0.35784621E+00
0.35560022E+00 0.35331437E+00 0.35099299E+00 0.34864087E+00 0.34626312E+00
0.34386519E+00 0.34145274E+00 0.33903165E+00 0.33660792E+00 0.33418762E+00
0.33177682E+00 0.32938154E+00 0.32700771E+00 0.32466108E+00 0.32234719E+00
0.32007131E+00 0.31783840E+00 0.31565306E+00 0.31351949E+00 0.31144146E+00
0.30942227E+00 0.30746476E+00 0.30557121E+00 0.30374344E+00 0.30198268E+00
0.30028967E+00 0.29866456E+00 0.29710702E+00 0.29561616E+00 0.29419059E+00
0.29282844E+00 0.29152735E+00 0.29028456E+00 0.28909688E+00 0.28796075E+00
0.28687228E+00 0.28582730E+00 0.28482136E+00 0.28384986E+00 0.28290798E+00
0.28199084E+00 0.28109345E+00 0.28021084E+00 0.27933805E+00 0.27847019E+00
0.27760249E+00 0.27673035E+00 0.27584937E+00 0.27495537E+00 0.27404447E+00
0.27311308E+00 0.27215795E+00 0.27117620E+00 0.27016532E+00 0.26912320E+00
0.26804815E+00 0.26693889E+00 0.26579457E+00 0.26461477E+00 0.26339951E+00
0.26214922E+00 0.26086472E+00 0.25954725E+00 0.25819841E+00 0.25682018E+00
0.25541485E+00 0.25398500E+00 0.25253353E+00 0.25106354E+00 0.24957836E+00
0.24808148E+00 0.24657655E+00 0.24506730E+00 0.24355753E+00 0.24205108E+00
0.24055176E+00 0.23906335E+00 0.23758952E+00 0.23613386E+00 0.23469978E+00
0.23329051E+00 0.23190908E+00 0.23055828E+00 0.22924064E+00 0.22795840E+00
0.22671351E+00 0.22550759E+00 0.22434194E+00 0.22321755E+00 0.22213502E+00
0.22109464E+00 0.22009637E+00 0.21913978E+00 0.21822417E+00 0.21734849E+00
0.21651138E+00 0.21571120E+00 0.21494604E+00 0.21421374E+00 0.21351191E+00
0.21283797E+00 0.21218915E+00 0.21156255E+00 0.21095513E+00 0.21036380E+00
0.20978537E+00 0.20921666E+00 0.20865446E+00 0.20809562E+00 0.20753703E+00
0.20697569E+00 0.20640871E+00 0.20583334E+00 0.20524699E+00 0.20464728E+00

0.20403203E+00 0.20339927E+00 0.20274730E+00 0.20207466E+00 0.20138014E+00
0.20066282E+00 0.19992206E+00 0.19915750E+00 0.19836904E+00 0.19755686E+00
0.19672144E+00 0.19586349E+00 0.19498399E+00 0.19408415E+00 0.19316540E+00
0.19222939E+00 0.19127796E+00 0.19031309E+00 0.18933694E+00 0.18835178E+00
0.18735999E+00 0.18636399E+00 0.18536631E+00 0.18436946E+00 0.18337598E+00
0.18238837E+00 0.18140910E+00 0.18044056E+00 0.17948505E+00 0.17854475E+00
0.17762172E+00 0.17671787E+00 0.17583493E+00 0.17497445E+00 0.17413779E+00
0.17332610E+00 0.17254032E+00 0.17178116E+00 0.17104912E+00 0.17034445E+00
0.16966719E+00 0.16901714E+00 0.16839388E+00 0.16779679E+00 0.16722502E+00
0.16667754E+00 0.16615313E+00 0.16565038E+00 0.16516776E+00 0.16470358E+00
0.16425602E+00 0.16382318E+00 0.16340305E+00 0.16299357E+00 0.16259264E+00
0.16219812E+00 0.16180789E+00 0.16141982E+00 0.16103185E+00 0.16064193E+00
0.16024813E+00 0.15984859E+00 0.15944157E+00 0.15902544E+00 0.15859872E+00
0.15816007E+00 0.15770834E+00 0.15724250E+00 0.15676175E+00 0.15626543E+00
0.15575311E+00 0.15522450E+00 0.15467954E+00 0.15411835E+00 0.15354122E+00
0.15294862E+00 0.15234122E+00 0.15171981E+00 0.15108538E+00 0.15043903E+00
0.14978200E+00 0.14911565E+00 0.14844143E+00 0.14776089E+00 0.14707565E+00
0.14638738E+00 0.14569777E+00 0.14500857E+00 0.14432149E+00 0.14363826E+00
0.14296055E+00 0.14229002E+00 0.14162822E+00 0.14097667E+00 0.14033677E+00
0.13970982E+00 0.13909702E+00 0.13849942E+00 0.13791795E+00 0.13735341E+00
0.13680643E+00 0.13627749E+00 0.13576693E+00 0.13527491E+00 0.13480145E+00
0.13434640E+00 0.13390946E+00 0.13349018E+00 0.13308797E+00 0.13270210E+00
0.13233171E+00 0.13197582E+00 0.13163335E+00 0.13130312E+00 0.13098386E+00
0.13067424E+00 0.13037286E+00 0.13007827E+00 0.12978902E+00 0.12950362E+00
0.12922058E+00 0.12893844E+00 0.12865574E+00 0.12837108E+00 0.12808312E+00
0.12779058E+00 0.12749225E+00 0.12718701E+00 0.12687386E+00 0.12655188E+00
0.12622028E+00 0.12587838E+00 0.12552565E+00 0.12516167E+00 0.12478615E+00
0.12439895E+00 0.12400005E+00 0.12358958E+00 0.12316778E+00 0.12273504E+00
0.12229185E+00 0.12183882E+00 0.12137669E+00 0.12090626E+00 0.12042847E+00
0.11994429E+00 0.11945481E+00 0.11896113E+00 0.11846444E+00 0.11796594E+00
0.11746686E+00 0.11696845E+00 0.11647196E+00 0.11597861E+00 0.11548961E+00
0.11500612E+00 0.11452927E+00 0.11406013E+00 0.11359967E+00 0.11314883E+00
0.11270842E+00 0.11227920E+00 0.11186179E+00 0.11145673E+00 0.11106444E+00
0.11068525E+00 0.11031934E+00 0.10996680E+00 0.10962759E+00 0.10930157E+00
0.10898848E+00 0.10868795E+00 0.10839950E+00 0.10812256E+00 0.10785648E+00
0.10760050E+00 0.10735380E+00 0.10711549E+00 0.10688461E+00 0.10666016E+00
0.10644111E+00 0.10622637E+00 0.10601486E+00 0.10580548E+00 0.10559714E+00
0.10538875E+00 0.10517926E+00 0.10496764E+00 0.10475291E+00 0.10453414E+00
0.10431046E+00 0.10408108E+00 0.10384526E+00 0.10360238E+00 0.10335187E+00
0.10309326E+00 0.10282620E+00 0.10255042E+00 0.10226574E+00 0.10197210E+00
0.10166952E+00 0.10135814E+00 0.10103820E+00 0.10071001E+00 0.10037398E+00
0.10003061E+00 0.99680492E-01 0.99324263E-01 0.98962643E-01 0.98596409E-01
0.98226387E-01 0.97853446E-01 0.97478487E-01 0.97102437E-01 0.96726239E-01
0.96350840E-01 0.95977184E-01 0.95606203E-01 0.95238808E-01 0.94875876E-01
0.94518248E-01 0.94166719E-01 0.93822027E-01 0.93484851E-01 0.93155803E-01
0.92835421E-01 0.92524169E-01 0.92222427E-01 0.91930492E-01 0.91648576E-01
0.91376800E-01 0.91115200E-01 0.90863721E-01 0.90622220E-01 0.90390473E-01
0.90168170E-01 0.89954922E-01 0.89750269E-01 0.89553678E-01 0.89364557E-01
0.89182251E-01 0.89006058E-01 0.88835233E-01 0.88668991E-01 0.88506523E-01
0.88346995E-01 0.88189565E-01 0.88033383E-01 0.87877605E-01 0.87721401E-01
0.87563957E-01 0.87404492E-01 0.87242255E-01 0.87076542E-01 0.86906693E-01
0.86732107E-01 0.86552238E-01 0.86366609E-01 0.86174807E-01 0.85976493E-01

0.85771402E-01 0.85559347E-01 0.85340216E-01 0.85113977E-01 0.84880676E-01
0.84640435E-01 0.84393450E-01 0.84139993E-01 0.83880402E-01 0.83615080E-01
0.83344492E-01 0.83069158E-01 0.82789649E-01 0.82506580E-01 0.82220603E-01
0.81932403E-01 0.81642689E-01 0.81352188E-01 0.81061636E-01 0.80771774E-01
0.80483339E-01 0.80197054E-01 0.79913627E-01 0.79633738E-01 0.79358037E-01
0.79087137E-01 0.78821607E-01 0.78561967E-01 0.78308685E-01 0.78062171E-01
0.77822775E-01 0.77590783E-01 0.77366416E-01 0.77149827E-01 0.76941098E-01
0.76740244E-01 0.76547211E-01 0.76361877E-01 0.76184053E-01 0.76013487E-01
0.75849867E-01 0.75692822E-01 0.75541928E-01 0.75396714E-01 0.75256663E-01
0.75121221E-01 0.74989799E-01 0.74861783E-01 0.74736536E-01 0.74613407E-01
0.74491737E-01 0.74370864E-01 0.74250130E-01 0.74128889E-01 0.74006513E-01
0.73882393E-01 0.73755953E-01 0.73626647E-01 0.73493971E-01 0.73357463E-01
0.73216707E-01 0.73071340E-01 0.72921051E-01 0.72765588E-01 0.72604755E-01
0.72438417E-01 0.72266501E-01 0.72088993E-01 0.71905941E-01 0.71717454E-01
0.71523696E-01 0.71324891E-01 0.71121313E-01 0.70913288E-01 0.70701188E-01
0.70485429E-01 0.70266464E-01 0.70044779E-01 0.69820891E-01 0.69595339E-01
0.69368679E-01 0.69141483E-01 0.68914327E-01 0.68687789E-01 0.68462442E-01
0.68238850E-01 0.68017560E-01 0.67799100E-01 0.67583969E-01 0.67372640E-01
0.67165547E-01 0.66963087E-01 0.66765615E-01 0.66573439E-01 0.66386821E-01
0.66205971E-01 0.66031047E-01 0.65862154E-01 0.65699344E-01 0.65542611E-01
0.65391901E-01 0.65247101E-01 0.65108051E-01 0.64974539E-01 0.64846309E-01
0.64723057E-01 0.64604441E-01 0.64490081E-01 0.64379564E-01 0.64272448E-01
0.64168266E-01 0.64066531E-01 0.63966741E-01 0.63868385E-01 0.63770944E-01
0.63673904E-01 0.63576750E-01 0.63478983E-01 0.63380115E-01 0.63279679E-01
0.63177232E-01 0.63072359E-01 0.62964677E-01 0.62853837E-01 0.62739529E-01
0.62621485E-01 0.62499480E-01 0.62373332E-01 0.62242909E-01 0.62108124E-01
0.61968939E-01 0.61825365E-01 0.61677460E-01 0.61525329E-01 0.61369122E-01
0.61209034E-01 0.61045298E-01 0.60878190E-01 0.60708018E-01 0.60535124E-01
0.60359879E-01 0.60182678E-01 0.60003939E-01 0.59824094E-01 0.59643590E-01
0.59462880E-01 0.59282423E-01 0.59102675E-01 0.58924086E-01 0.58747098E-01
0.58572136E-01 0.58399609E-01 0.58229903E-01 0.58063376E-01 0.57900360E-01
0.57741152E-01 0.57586016E-01 0.57435178E-01 0.57288823E-01 0.57147096E-01
0.57010103E-01 0.56877901E-01 0.56750509E-01 0.56627899E-01 0.56510002E-01
0.56396706E-01 0.56287861E-01 0.56183276E-01 0.56082724E-01 0.55985943E-01
0.55892643E-01 0.55802501E-01 0.55715173E-01 0.55630292E-01 0.55547472E-01
0.55466316E-01 0.55386413E-01 0.55307350E-01 0.55228710E-01 0.55150077E-01
0.55071045E-01 0.54991215E-01 0.54910204E-01 0.54827645E-01 0.54743195E-01
0.54656534E-01 0.54567368E-01 0.54475435E-01 0.54380505E-01 0.54282381E-01
0.54180903E-01 0.54075949E-01 0.53967436E-01 0.53855316E-01 0.53739586E-01
0.53620279E-01 0.53497466E-01 0.53371257E-01 0.53241797E-01 0.53109269E-01
0.52973883E-01 0.52835884E-01 0.52695542E-01 0.52553154E-01 0.52409036E-01
0.52263526E-01 0.52116975E-01 0.51969746E-01 0.51822212E-01 0.51674748E-01
0.51527733E-01 0.51381539E-01 0.51236536E-01 0.51093078E-01 0.50951511E-01
0.50812160E-01 0.50675332E-01 0.50541309E-01 0.50410349E-01 0.50282683E-01
0.50158508E-01 0.50037993E-01 0.49921273E-01 0.49808446E-01 0.49699577E-01
0.49594694E-01 0.49493790E-01 0.49396820E-01 0.49303707E-01 0.49214336E-01
0.49128563E-01 0.49046210E-01 0.48967070E-01 0.48890910E-01 0.48817472E-01
0.48746474E-01 0.48677618E-01 0.48610585E-01 0.48545048E-01 0.48480667E-01
0.48417094E-01 0.48353982E-01 0.48290980E-01 0.48227743E-01 0.48163933E-01
0.48099221E-01 0.48033292E-01 0.47965849E-01 0.47896611E-01 0.47825321E-01
0.47751746E-01 0.47675678E-01 0.47596937E-01 0.47515375E-01 0.47430872E-01
0.47343340E-01 0.47252727E-01 0.47159009E-01 0.47062200E-01 0.46962343E-01

gradient corrections used for XC

5

core charge-density (partial)

0.46291985E-01 0.46276698E-01 0.46230865E-01 0.46154570E-01 0.46047953E-01
0.45911209E-01 0.45744589E-01 0.45548396E-01 0.45322989E-01 0.45068776E-01
0.44786219E-01 0.44475828E-01 0.44138161E-01 0.43773822E-01 0.43383463E-01
0.42967775E-01 0.42527492E-01 0.42063388E-01 0.41576271E-01 0.41066985E-01
0.40536407E-01 0.39985443E-01 0.39415025E-01 0.38826113E-01 0.38219686E-01
0.37596745E-01 0.36958307E-01 0.36305403E-01 0.35639076E-01 0.34960380E-01
0.34270373E-01 0.33570118E-01 0.32860680E-01 0.32143122E-01 0.31418503E-01
0.30687878E-01 0.29952291E-01 0.29212777E-01 0.28470357E-01 0.27726038E-01
0.26980808E-01 0.26235640E-01 0.25491480E-01 0.24749257E-01 0.24009871E-01
0.23274199E-01 0.22543089E-01 0.21817361E-01 0.21097805E-01 0.20385180E-01
0.19680211E-01 0.18983592E-01 0.18295983E-01 0.17618009E-01 0.16950260E-01
0.16293291E-01 0.15647620E-01 0.15013732E-01 0.14392072E-01 0.13783052E-01
0.13187046E-01 0.12604395E-01 0.12035401E-01 0.11480334E-01 0.10939428E-01
0.10412882E-01 0.99008641E-02 0.94035074E-02 0.89209139E-02 0.84531546E-02
0.80002701E-02 0.75622716E-02 0.71391423E-02 0.67308379E-02 0.63372878E-02
0.59583968E-02 0.55940452E-02 0.52440911E-02 0.49083705E-02 0.45866994E-02
0.42788744E-02 0.39846745E-02 0.37038616E-02 0.34361824E-02 0.31813693E-02
0.29391416E-02 0.27092067E-02 0.24912616E-02 0.22849935E-02 0.20900816E-02
0.19061977E-02 0.17330074E-02 0.15701717E-02 0.14173471E-02 0.12741874E-02
0.11403443E-02 0.10154686E-02 0.89921078E-03 0.79122198E-03 0.69115496E-03
0.59866471E-03 0.51340931E-03 0.43505053E-03 0.36325455E-03 0.29769256E-03
0.23804132E-03 0.18398367E-03 0.13520908E-03 0.91414029E-04 0.52302440E-04
0.17586039E-04 -0.13015323E-04 -0.39773390E-04 -0.62951250E-04 -0.82803131E-04
-0.99574225E-04 -0.11350055E-03 -0.12480886E-03 -0.13371655E-03 -0.14043163E-03
-0.14515273E-03 -0.14806908E-03 -0.14936058E-03 -0.14919790E-03 -0.14774249E-03
-0.14514679E-03 -0.14155432E-03 -0.13709983E-03 -0.13190950E-03 -0.12610113E-03
-0.11978434E-03 -0.11306077E-03 -0.10602436E-03 -0.98761548E-04 -0.91351557E-04
-0.83866636E-04 -0.76372331E-04 -0.68927767E-04 -0.61585915E-04 -0.54393883E-04
-0.47393191E-04 -0.40620059E-04 -0.34105691E-04 -0.27876557E-04 -0.21954673E-04
-0.16357880E-04 -0.11100120E-04 -0.61917050E-05 -0.16395800E-05 0.25524141E-05
0.63832892E-05 0.98546635E-05 0.12970522E-04 0.15736987E-04 0.18162093E-04
0.20255572E-04 0.22028649E-04 0.23493847E-04 0.24664794E-04 0.25556049E-04
0.26182930E-04 0.26561358E-04 0.26707705E-04 0.26638653E-04 0.26371063E-04
0.25921855E-04 0.25307895E-04 0.24545889E-04 0.23652293E-04 0.22643224E-04
0.21534385E-04 0.20340994E-04 0.19077725E-04 0.17758654E-04 0.16397214E-04
0.15006155E-04 0.13597515E-04 0.12182592E-04 0.10771928E-04 0.93752921E-05
0.80016776E-05 0.66592955E-05 0.53555785E-05 0.40971881E-05 0.28900248E-05
0.17392431E-05 0.64926975E-06 -0.37617522E-06 -0.13340545E-05 -0.22219869E-05
-0.30382189E-05 -0.37815942E-05 -0.44515215E-05 -0.50479414E-05 -0.55712921E-05
-0.60224743E-05 -0.64028158E-05 -0.67140353E-05 -0.69582068E-05 -0.71377240E-05
-0.72552646E-05 -0.73137554E-05 -0.73163384E-05 -0.72663372E-05 -0.71672248E-05
-0.70225919E-05 -0.68361175E-05 -0.66115394E-05 -0.63526270E-05 -0.60631559E-05
-0.57468826E-05 -0.54075224E-05 -0.50487278E-05 -0.46740689E-05 -0.42870157E-05
-0.38909214E-05 -0.34890082E-05 -0.30843542E-05 -0.26798819E-05 -0.22783484E-05
-0.18823376E-05 -0.14942529E-05 -0.11163127E-05 -0.75054611E-06 -0.39879060E-06
-0.62691160E-07 0.25629983E-06 0.55692119E-06 0.83810059E-06 0.10989511E-05
0.13387669E-05 0.15570180E-05 0.17533441E-05 0.19275481E-05 0.20795886E-05
0.22095717E-05 0.23177432E-05 0.24044790E-05 0.24702766E-05 0.25157452E-05
0.25415965E-05 0.25486343E-05 0.25377455E-05 0.25098894E-05 0.24660888E-05

0.24074195E-05 0.23350016E-05 0.22499893E-05 0.21535628E-05 0.20469189E-05
0.19312628E-05 0.18078000E-05 0.16777288E-05 0.15422329E-05 0.14024746E-05
0.12595884E-05 0.11146754E-05 0.96879788E-06 0.82297404E-06 0.67817409E-06
0.53531618E-06 0.39526307E-06 0.25881922E-06 0.12672850E-06 -0.32778477E-09
-0.12173224E-06 -0.23693239E-06 -0.34544115E-06 -0.44683694E-06 -0.54076337E-06
-0.62692850E-06 -0.70510383E-06 -0.77512281E-06 -0.83687918E-06 -0.89032491E-06
-0.93546791E-06 -0.97236951E-06 -0.10011417E-05 -0.10219443E-05 -0.10349815E-05
-0.10404992E-05 -0.10387810E-05 -0.10301454E-05 -0.10149418E-05 -0.99354711E-06
-0.96636230E-06 -0.93380872E-06 -0.89632463E-06 -0.85436165E-06 -0.80838144E-06
-0.75885227E-06 -0.70624584E-06 -0.65103414E-06 -0.59368647E-06 -0.53466660E-06
-0.47443003E-06 -0.41342150E-06 -0.35207261E-06 -0.29079964E-06 -0.23000155E-06
-0.17005815E-06 -0.11132852E-06 -0.54149536E-07 0.11653316E-08 0.54327060E-07
0.10507192E-06 0.15316214E-06 0.19838637E-06 0.24055994E-06 0.27952504E-06
0.31515057E-06 0.34733201E-06 0.37599097E-06 0.40107472E-06 0.42255547E-06
0.44042965E-06 0.45471694E-06 0.46545930E-06 0.47271980E-06 0.47658149E-06
0.47714605E-06 0.47453247E-06 0.46887566E-06 0.46032499E-06 0.44904280E-06
0.43520290E-06 0.41898905E-06 0.40059344E-06 0.38021515E-06 0.35805865E-06
0.33433234E-06 0.30924704E-06 0.28301465E-06 0.25584669E-06 0.22795306E-06
0.19954073E-06 0.17081259E-06 0.14196625E-06 0.11319306E-06 0.84677100E-07
0.56594264E-07 0.29111477E-07 0.23859478E-08 -0.23435473E-07 -0.48216851E-07
-0.71833638E-07 -0.94173057E-07 -0.11513440E-06 -0.13462923E-06 -0.15258154E-06
-0.16892775E-06 -0.18361673E-06 -0.19660967E-06 -0.20787988E-06 -0.21741258E-06
-0.22520457E-06 -0.23126383E-06 -0.23560915E-06 -0.23826959E-06 -0.23928398E-06
-0.23870033E-06 -0.23657523E-06 -0.23297323E-06 -0.22796612E-06 -0.22163227E-06
-0.21405592E-06 -0.20532645E-06 -0.19553765E-06 -0.18478698E-06 -0.17317486E-06
-0.16080391E-06 -0.14777825E-06 -0.13420281E-06 -0.12018263E-06 -0.10582220E-06
-0.91224820E-07 -0.76491991E-07 -0.61722843E-07 -0.47013579E-07 -0.32456970E-07
-0.18141881E-07 -0.41528373E-08 0.94303688E-08 0.22533029E-07 0.35085825E-07
0.47025101E-07 0.58293076E-07 0.68838031E-07 0.78614441E-07 0.87583066E-07
0.95711007E-07 0.10297171E-06 0.10934495E-06 0.11481675E-06 0.11937926E-06
0.12303068E-06 0.12577502E-06 0.12762192E-06 0.12858643E-06 0.12868876E-06
0.12795396E-06 0.12641165E-06 0.12409569E-06 0.12104381E-06 0.11729733E-06
0.11290071E-06 0.10790124E-06 0.10234861E-06 0.96294584E-07 0.89792562E-07
0.82897228E-07 0.75664158E-07 0.68149447E-07 0.60409345E-07 0.52499898E-07
0.44476600E-07 0.36394067E-07 0.28305717E-07 0.20263468E-07 0.12317460E-07
0.45157886E-08 -0.30957348E-08 -0.10473808E-07 -0.17577835E-07 -0.24370106E-07
-0.30815947E-07 -0.36883858E-07 -0.42545612E-07 -0.47776350E-07 -0.52554631E-07
-0.56862479E-07 -0.60685393E-07 -0.64012346E-07 -0.66835752E-07 -0.69151420E-07
-0.70958489E-07 -0.72259336E-07 -0.73059475E-07 -0.73367436E-07 -0.73194627E-07
-0.72555188E-07 -0.71465820E-07 -0.69945619E-07 -0.68015885E-07 -0.65699932E-07
-0.63022887E-07 -0.60011483E-07 -0.56693848E-07 -0.53099292E-07 -0.49258092E-07
-0.45201276E-07 -0.40960409E-07 -0.36567381E-07 -0.32054198E-07 -0.27452780E-07
-0.22794762E-07 -0.18111304E-07 -0.13432909E-07 -0.87892490E-08 -0.42090006E-08
0.28030765E-09 0.46524382E-08 0.88825748E-08 0.12947440E-07 0.16825404E-07
0.20496572E-07 0.23942868E-07 0.27148101E-07 0.30098016E-07 0.32780334E-07
0.35184778E-07 0.37303087E-07 0.39129016E-07 0.40658323E-07 0.41888746E-07
0.42819964E-07 0.43453555E-07 0.43792932E-07 0.43843281E-07 0.43611480E-07
0.43106016E-07 0.42336890E-07 0.41315518E-07 0.40054622E-07 0.38568122E-07
0.36871014E-07 0.34979253E-07 0.32909630E-07 0.30679643E-07 0.28307373E-07
0.25811356E-07 0.23210455E-07 0.20523733E-07 0.17770334E-07 0.14969354E-07
0.12139729E-07 0.93001160E-08 0.64687854E-08 0.36635158E-08 0.90149391E-09
-0.18007779E-08 -0.44275690E-08 -0.69639999E-08 -0.93961156E-08 -0.11710950E-07

-0.13896584E-07 -0.15942194E-07 -0.17838098E-07 -0.19575780E-07 -0.21147926E-07
-0.22548436E-07 -0.23772432E-07 -0.24816265E-07 -0.25677504E-07 -0.26354925E-07
-0.26848492E-07 -0.27159325E-07 -0.27289671E-07 -0.27242862E-07 -0.27023266E-07
-0.26636241E-07 -0.26088075E-07 -0.25385925E-07 -0.24537756E-07 -0.23552268E-07
-0.22438828E-07 -0.21207395E-07 -0.19868444E-07 -0.18432889E-07 -0.16912005E-07
-0.15317349E-07 -0.13660682E-07 -0.11953889E-07 -0.10208906E-07 -0.84376371E-08
-0.66518894E-08 -0.48632949E-08 -0.30832442E-08 -0.13228207E-08 0.40726238E-09
0.20967205E-08 0.37357524E-08 0.53150911E-08 0.68260495E-08 0.82605621E-08
0.96112220E-08 0.10871312E-07 0.12034832E-07 0.13096521E-07 0.14051873E-07
0.14897149E-07 0.15629384E-07 0.16246388E-07 0.16746744E-07 0.17129798E-07
0.17395649E-07 0.17545131E-07 0.17579791E-07 0.17501867E-07 0.17314253E-07
0.17020475E-07 0.16624649E-07 0.16131445E-07 0.15546048E-07 0.14874109E-07
0.14121707E-07 0.13295295E-07 0.12401656E-07 0.11447855E-07 0.10441182E-07
0.93891101E-08 0.82992385E-08 0.71792460E-08 0.60368398E-08 0.48797071E-08
0.37154677E-08 0.25516274E-08 0.13955336E-08 0.25433284E-09 -0.86506996E-09
-0.19560494E-08 -0.30122955E-08 -0.40278462E-08 -0.49971179E-08 -0.59149323E-08
-0.67765406E-08 -0.75776442E-08 -0.83144124E-08 -0.89834969E-08 -0.95820427E-08
-0.10107696E-07 -0.10558609E-07 -0.10933440E-07 -0.11231353E-07 -0.11452013E-07
-0.11595576E-07 -0.11662678E-07 -0.11654426E-07 -0.11572375E-07 -0.11418514E-07
-0.11195242E-07 -0.10905349E-07 -0.10551985E-07 -0.10138638E-07 -0.96691022E-08
-0.91474505E-08 -0.85780025E-08 -0.79652925E-08 -0.73140373E-08 -0.66291030E-08
-0.59154716E-08 -0.51782077E-08 -0.44224252E-08 -0.36532543E-08 -0.28758092E-08
-0.20951565E-08 -0.13162843E-08 -0.54407278E-09 0.21673428E-09 0.96155659E-09
0.16860027E-08 0.23858937E-08 0.30572855E-08 0.36964886E-08 0.43000866E-08
0.48649520E-08 0.53882602E-08 0.58675018E-08 0.63004915E-08 0.66853762E-08
0.70206400E-08 0.73051073E-08 0.75379435E-08 0.77186541E-08 0.78470809E-08
0.79233971E-08 0.79480996E-08 0.79220000E-08 0.78462133E-08 0.77221459E-08
0.75514805E-08 0.73361610E-08 0.70783753E-08 0.67805369E-08 0.64452661E-08
0.60753692E-08 0.56738179E-08 0.52437273E-08 0.47883344E-08 0.43109750E-08
0.38150613E-08 0.33040592E-08 0.27814656E-08 0.22507861E-08 0.17155125E-08
0.11791020E-08 0.64495563E-09 0.11639813E-09 -0.40334123E-09 -0.91114721E-09
-0.14040360E-08 -0.18791714E-08 -0.23338800E-08 -0.27656647E-08 -0.31722174E-08
-0.35514298E-08 -0.39014030E-08 -0.42204557E-08 -0.45071307E-08 -0.47601999E-08
-0.49786680E-08 -0.51617748E-08 -0.53089950E-08 -0.54200381E-08 -0.54948457E-08
-0.55335874E-08 -0.55366564E-08 -0.55046625E-08 -0.54384248E-08 -0.53389624E-08
-0.52074854E-08 -0.50453828E-08 -0.48542119E-08 -0.46356845E-08 -0.43916542E-08
-0.41241023E-08 -0.38351229E-08 -0.35269078E-08 -0.32017316E-08 -0.28619355E-08
-0.25099119E-08 -0.21480883E-08 -0.17789118E-08 -0.14048332E-08 -0.10282917E-08
-0.65170011E-09 -0.27742985E-09 0.92202860E-10 0.45495065E-09 0.80864782E-09
0.11512225E-08 0.14807078E-08 0.17952528E-08 0.20931313E-08 0.23727515E-08
0.26326627E-08 0.28715626E-08 0.30883026E-08 0.32818925E-08 0.34515039E-08
0.35964729E-08 0.37163011E-08 0.38106562E-08 0.38793711E-08 0.39224422E-08
0.39400270E-08 0.39324398E-08 0.39001477E-08 0.38437648E-08 0.37640460E-08
0.36618799E-08 0.35382810E-08 0.33943816E-08 0.32314223E-08 0.30507426E-08
0.28537710E-08 0.26420148E-08 0.24170487E-08 0.21805047E-08 0.19340605E-08
0.16794280E-08 0.14183429E-08 0.11525525E-08 0.88380526E-09 0.61383969E-09
0.34437350E-09 0.77093382E-10 -0.18635510E-09 -0.44437710E-09 -0.69543760E-09
-0.93807007E-09 -0.11708845E-08 -0.13925749E-08 -0.16019259E-08 -0.17978191E-08
-0.19792386E-08 -0.21452751E-08 -0.22951307E-08 -0.24281215E-08 -0.25436801E-08
-0.26413577E-08 -0.27208244E-08 -0.27818698E-08 -0.28244025E-08 -0.28484481E-08
-0.28541481E-08 -0.28417565E-08 -0.28116366E-08 -0.27642571E-08 -0.27001876E-08
-0.26200932E-08 -0.25247288E-08 -0.24149334E-08 -0.22916230E-08 -0.21557842E-08

-0.20084664E-08 -0.18507746E-08 -0.16838617E-08 -0.15089201E-08 -0.13271743E-08
-0.11398722E-08 -0.94827697E-09 -0.75365940E-09 -0.55728934E-09 -0.36042803E-09
-0.16432030E-09 0.29812970E-10 0.22078206E-09 0.40743540E-09 0.58866615E-09
0.76341845E-09 0.93069319E-09 0.10895534E-08 0.12391293E-08 0.13786222E-08
0.15073092E-08 0.16245458E-08 0.17297692E-08 0.18225002E-08 0.19023455E-08
0.19689981E-08 0.20222385E-08 0.20619346E-08 0.20880409E-08 0.21005978E-08
0.20997302E-08 0.20856449E-08 0.20586286E-08 0.20190446E-08 0.19673295E-08
0.19039893E-08 0.18295954E-08 0.17447798E-08 0.16502304E-08 0.15466857E-08
0.14349298E-08 0.13157864E-08 0.11901132E-08 0.10587963E-08 0.92274390E-09
0.78288043E-09 0.64014060E-09 0.49546330E-09 0.34978576E-09 0.20403768E-09
0.59135536E-10 -0.84022935E-10 -0.22456408E-09 -0.36164342E-09 -0.49445050E-09
-0.62221348E-09 -0.74420335E-09 -0.85973786E-09 -0.96818516E-09 -0.10689669E-08
-0.11615612E-08 -0.12455051E-08 -0.13203962E-08 -0.13858950E-08 -0.14417254E-08
-0.14876762E-08 -0.15236007E-08 -0.15494174E-08 -0.15651091E-08 -0.15707224E-08
-0.15663663E-08 -0.15522105E-08 -0.15284840E-08 -0.14954720E-08 -0.14535143E-08
-0.14030013E-08 -0.13443720E-08 -0.12781095E-08 -0.12047381E-08 -0.11248192E-08
-0.10389471E-08 -0.94774500E-09 -0.85186073E-09 -0.75196226E-09 -0.64873326E-09
-0.54286865E-09 -0.43507007E-09 -0.32604139E-09 -0.21648433E-09 -0.10709405E-09
0.14450301E-11 0.10846343E-09 0.21331054E-09 0.31535840E-09 0.41400536E-09
0.50867943E-09 0.59884144E-09 0.68398797E-09 0.76365400E-09 0.83741526E-09
0.90489031E-09 0.96574237E-09 0.10196808E-08 0.10664621E-08 0.11058912E-08
0.11378215E-08 0.11621555E-08 0.11788447E-08 0.11878888E-08 0.11893357E-08
0.11832800E-08 0.11698622E-08 0.11492667E-08 0.11217204E-08 0.10874909E-08
0.10468837E-08 0.10002400E-08 0.94793458E-09 0.89037218E-09 0.82798514E-09
0.76123015E-09 0.69058504E-09 0.61654558E-09 0.53962208E-09 0.46033604E-09
0.37921673E-09 0.29679780E-09 0.21361385E-09 0.13019711E-09 0.47074146E-10
-0.35237363E-10 -0.11623174E-09 -0.19541830E-09 -0.27232422E-09 -0.34649726E-09
-0.41750828E-09 -0.48495367E-09 -0.54845747E-09 -0.60767340E-09 -0.66228660E-09
-0.71201519E-09 -0.75661159E-09 -0.79586363E-09 -0.82959537E-09 -0.85766776E-09
-0.87997900E-09 -0.89646470E-09 -0.90709778E-09 -0.91188813E-09 -0.91088211E-09
-0.90416176E-09 -0.89184379E-09 -0.87407845E-09 -0.85104812E-09 -0.82296576E-09
-0.79007318E-09 -0.75263916E-09 -0.71095741E-09 -0.66534443E-09 -0.61613722E-09
-0.56369091E-09 -0.50837633E-09 -0.45057744E-09 -0.39068883E-09 -0.32911307E-09
-0.26625811E-09 -0.20253465E-09 -0.13835357E-09 -0.74123327E-10 -0.10247448E-10
0.52877922E-10 0.11486640E-09 0.17534367E-09 0.23394963E-09 0.29034050E-09
0.34419074E-09 0.39519486E-09 0.44306905E-09 0.48755272E-09 0.52840978E-09
0.56542984E-09 0.59842920E-09 0.62725163E-09 0.65176903E-09 0.67188186E-09
0.68751939E-09 0.69863979E-09 0.70523006E-09 0.70730567E-09 0.70491018E-09
0.69811459E-09 0.68701653E-09 0.67173936E-09 0.65243102E-09 0.62926288E-09
0.60242828E-09 0.57214113E-09 0.53863428E-09 0.50215782E-09 0.46297734E-09
0.42137204E-09 0.37763285E-09 0.33206044E-09 0.28496323E-09 0.23665539E-09
0.18745478E-09 0.13768092E-09 0.87652982E-10 0.37687813E-10 -0.11902041E-10
-0.60810216E-10 -0.10873837E-09 -0.15539796E-09 -0.20051191E-09 -0.24381620E-09
-0.28506137E-09 -0.32401389E-09 -0.36045742E-09 -0.39419396E-09 -0.42504486E-09
-0.45285171E-09 -0.47747705E-09 -0.49880502E-09 -0.51674180E-09 -0.53121590E-09
-0.54217840E-09 -0.54960293E-09 -0.55348557E-09 -0.55384463E-09 -0.55072023E-09
-0.54417383E-09 -0.53428755E-09 -0.52116343E-09 -0.50492253E-09 -0.48570400E-09
kinetic energy density (partial)
0.16448022E+02 0.16442614E+02 0.16426398E+02 0.16399405E+02 0.16361683E+02
0.16313302E+02 0.16254349E+02 0.16184932E+02 0.16105175E+02 0.16015225E+02
0.15915241E+02 0.15805404E+02 0.15685911E+02 0.15556974E+02 0.15418822E+02
0.15271699E+02 0.15115864E+02 0.14951587E+02 0.14779155E+02 0.14598864E+02

0.14411024E+02 0.14215952E+02 0.14013979E+02 0.13805442E+02 0.13590686E+02
0.13370063E+02 0.13143934E+02 0.12912660E+02 0.12676610E+02 0.12436157E+02
0.12191672E+02 0.11943532E+02 0.11692112E+02 0.11437787E+02 0.11180933E+02
0.10921921E+02 0.10661120E+02 0.10398897E+02 0.10135613E+02 0.98716225E+01
0.96072771E+01 0.93429197E+01 0.90788865E+01 0.88155057E+01 0.85530969E+01
0.82919706E+01 0.80324279E+01 0.77747597E+01 0.75192463E+01 0.72661572E+01
0.70157505E+01 0.67682729E+01 0.65239590E+01 0.62830316E+01 0.60457008E+01
0.58121646E+01 0.55826081E+01 0.53572040E+01 0.51361121E+01 0.49194797E+01
0.47074412E+01 0.45001184E+01 0.42976208E+01 0.41000453E+01 0.39074764E+01
0.37199870E+01 0.35376379E+01 0.33604781E+01 0.31885457E+01 0.30218674E+01
0.28604594E+01 0.27043274E+01 0.25534670E+01 0.24078642E+01 0.22674956E+01
0.21323289E+01 0.20023232E+01 0.18774296E+01 0.17575915E+01 0.16427448E+01
0.15328189E+01 0.14277364E+01 0.13274141E+01 0.12317633E+01 0.11406900E+01
0.10540958E+01 0.97187759E+00 0.89392878E+00 0.82013918E+00 0.75039560E+00
0.68458223E+00 0.62258101E+00 0.56427202E+00 0.50953386E+00 0.45824401E+00
0.41027915E+00 0.36551551E+00 0.32382922E+00 0.28509657E+00 0.24919433E+00
0.21600004E+00 0.18539223E+00 0.15725073E+00 0.13145687E+00 0.10789370E+00
0.86446206E-01 0.67001503E-01 0.49449000E-01 0.33680571E-01 0.19590693E-01
0.70765857E-02 -0.39616767E-02 -0.13621058E-01 -0.21995472E-01 -0.29175704E-01
-0.35249347E-01 -0.40300751E-01 -0.44410983E-01 -0.47657797E-01 -0.50115622E-01
-0.51855551E-01 -0.52945348E-01 -0.53449461E-01 -0.53429046E-01 -0.52941994E-01
-0.52042978E-01 -0.50783496E-01 -0.49211923E-01 -0.47373578E-01 -0.45310787E-01
-0.43062955E-01 -0.40666644E-01 -0.38155658E-01 -0.35561122E-01 -0.32911577E-01
-0.30233071E-01 -0.27549252E-01 -0.24881464E-01 -0.22248851E-01 -0.19668449E-01
-0.17155293E-01 -0.14722513E-01 -0.12381439E-01 -0.10141698E-01 -0.80113170E-02
-0.59968215E-02 -0.41033322E-02 -0.23346625E-02 -0.69341288E-03 0.81893600E-03
0.22019332E-02 0.34560691E-02 0.45826899E-02 0.55839148E-02 0.64625557E-02
0.72220408E-02 0.78663398E-02 0.83998943E-02 0.88275491E-02 0.91544892E-02
0.93861780E-02 0.95283005E-02 0.95867089E-02 0.95673723E-02 0.94763290E-02
0.93196427E-02 0.91033620E-02 0.88334829E-02 0.85159146E-02 0.81564485E-02
0.77607301E-02 0.73342342E-02 0.68822425E-02 0.64098246E-02 0.59218209E-02
0.54228287E-02 0.49171907E-02 0.44089857E-02 0.39020211E-02 0.33998286E-02
0.29056608E-02 0.24224902E-02 0.19530100E-02 0.14996361E-02 0.10645110E-02
0.64950889E-03 0.25624196E-03 -0.11393202E-03 -0.45990129E-03 -0.78079063E-03
-0.10759513E-02 -0.13449499E-02 -0.15875574E-02 -0.18037367E-02 -0.19936309E-02
-0.21575503E-02 -0.22959598E-02 -0.24094662E-02 -0.24988050E-02 -0.25648279E-02
-0.26084897E-02 -0.26308361E-02 -0.26329911E-02 -0.26161452E-02 -0.25815435E-02
-0.25304745E-02 -0.24642595E-02 -0.23842416E-02 -0.22917765E-02 -0.21882226E-02
-0.20749322E-02 -0.19532437E-02 -0.18244733E-02 -0.16899082E-02 -0.15508003E-02
-0.14083596E-02 -0.12637498E-02 -0.11180827E-02 -0.97241463E-03 -0.82774263E-03
-0.68500155E-03 -0.54506155E-03 -0.40872617E-03 -0.27673098E-03 -0.14974261E-03
-0.28358330E-04 0.86893937E-04 0.19555519E-03 0.29723453E-03 0.39160796E-03
0.47841681E-03 0.55746594E-03 0.62862155E-03 0.69180876E-03 0.74700903E-03
0.79425724E-03 0.83363873E-03 0.86528608E-03 0.88937585E-03 0.90612518E-03
0.91578829E-03 0.91865303E-03 0.91503725E-03 0.90528535E-03 0.88976468E-03
0.86886209E-03 0.84298051E-03 0.81253553E-03 0.77795219E-03 0.73966181E-03
0.69809892E-03 0.65369836E-03 0.60689250E-03 0.55810863E-03 0.50776648E-03
0.45627593E-03 0.40403490E-03 0.35142736E-03 0.29882161E-03 0.24656864E-03
0.19500076E-03 0.14443036E-03 0.95148853E-04 0.47425817E-04 0.15083070E-05
-0.42379674E-04 -0.84037530E-04 -0.12328827E-03 -0.15997854E-03 -0.19397854E-03
-0.22518174E-03 -0.25350454E-03 -0.27888575E-03 -0.30128595E-03 -0.32068682E-03
-0.33709028E-03 -0.35051757E-03 -0.36100830E-03 -0.36861937E-03 -0.37342383E-03

-0.37550977E-03 -0.37497905E-03 -0.37194610E-03 -0.36653663E-03 -0.35888636E-03
-0.34913975E-03 -0.33744867E-03 -0.32397116E-03 -0.30887017E-03 -0.29231230E-03
-0.27446663E-03 -0.25550350E-03 -0.23559342E-03 -0.21490599E-03 -0.19360883E-03
-0.17186662E-03 -0.14984021E-03 -0.12768572E-03 -0.10555376E-03 -0.83588731E-04
-0.61928129E-04 -0.40701975E-04 -0.20032296E-04 -0.32669813E-07 0.19192146E-04
0.37546526E-04 0.54944220E-04 0.71308517E-04 0.86572361E-04 0.10067839E-03
0.11357891E-03 0.12523583E-03 0.13562053E-03 0.14471365E-03 0.15250487E-03
0.15899264E-03 0.16418382E-03 0.16809335E-03 0.17074381E-03 0.17216501E-03
0.17239352E-03 0.17147221E-03 0.16944968E-03 0.16637981E-03 0.16232116E-03
0.15733648E-03 0.15149213E-03 0.14485753E-03 0.13750459E-03 0.12950722E-03
0.12094075E-03 0.11188139E-03 0.10240577E-03 0.92590394E-04 0.82511186E-04
0.72243027E-04 0.61859324E-04 0.51431599E-04 0.41029108E-04 0.30718485E-04
0.20563416E-04 0.10624345E-04 0.95820813E-06 -0.83818034E-05 -0.17346442E-04
-0.25890576E-04 -0.33973333E-04 -0.41558201E-04 -0.48613113E-04 -0.55110490E-04
-0.61027263E-04 -0.66344858E-04 -0.71049160E-04 -0.75130451E-04 -0.78583315E-04
-0.81406533E-04 -0.83602941E-04 -0.85179277E-04 -0.86146008E-04 -0.86517137E-04
-0.86309997E-04 -0.85545028E-04 -0.84245550E-04 -0.82437513E-04 -0.80149253E-04
-0.77411230E-04 -0.74255771E-04 -0.70716802E-04 -0.66829581E-04 -0.62630439E-04
-0.58156510E-04 -0.53445474E-04 -0.48535304E-04 -0.43464017E-04 -0.38269432E-04
-0.32988942E-04 -0.27659291E-04 -0.22316363E-04 -0.16994987E-04 -0.11728750E-04
-0.65498264E-05 -0.14888195E-05 0.34253789E-05 0.81657173E-05 0.12707096E-04
0.17026464E-04 0.21102898E-04 0.24917668E-04 0.28454288E-04 0.31698549E-04
0.34638536E-04 0.37264634E-04 0.39569514E-04 0.41548116E-04 0.43197603E-04
0.44517316E-04 0.45508708E-04 0.46175275E-04 0.46522469E-04 0.46557605E-04
0.46289759E-04 0.45729659E-04 0.44889567E-04 0.43783155E-04 0.42425381E-04
0.40832352E-04 0.39021193E-04 0.37009906E-04 0.34817234E-04 0.32462519E-04
0.29965565E-04 0.27346499E-04 0.24625637E-04 0.21823349E-04 0.18959929E-04
0.16055475E-04 0.13129762E-04 0.10202132E-04 0.72913833E-05 0.44156696E-05
0.15924027E-05 -0.11618339E-05 -0.38313657E-05 -0.64014994E-05 -0.88585875E-05
-0.11190084E-04 -0.13384591E-04 -0.15431899E-04 -0.17323018E-04 -0.19050197E-04
-0.20606939E-04 -0.21988009E-04 -0.23189428E-04 -0.24208464E-04 -0.25043617E-04
-0.25694590E-04 -0.26162262E-04 -0.26448646E-04 -0.26556848E-04 -0.26491016E-04
-0.26256288E-04 -0.25858728E-04 -0.25305267E-04 -0.24603635E-04 -0.23762289E-04
-0.22790343E-04 -0.21697491E-04 -0.20493932E-04 -0.19190292E-04 -0.17797546E-04
-0.16326940E-04 -0.14789912E-04 -0.13198018E-04 -0.11562854E-04 -0.98959837E-05
-0.82088660E-05 -0.65127864E-05 -0.48187911E-05 -0.31376237E-05 -0.14796662E-05
0.14511689E-06 0.17272298E-05 0.32576930E-05 0.47280856E-05 0.61305841E-05
0.74579954E-05 0.87037861E-05 0.98621059E-05 0.10927807E-04 0.11896458E-04
0.12764354E-04 0.13528519E-04 0.14186711E-04 0.14737410E-04 0.15179817E-04
0.15513833E-04 0.15740049E-04 0.15859720E-04 0.15874743E-04 0.15787628E-04
0.15601466E-04 0.15319897E-04 0.14947072E-04 0.14487617E-04 0.13946587E-04
0.13329428E-04 0.12641934E-04 0.11890198E-04 0.11080568E-04 0.10219604E-04
0.93140287E-05 0.83706808E-05 0.73964718E-05 0.63983395E-05 0.53832045E-05
0.43579269E-05 0.33292648E-05 0.23038350E-05 0.12880746E-05 0.28820476E-06
-0.68980225E-06 -0.16402551E-05 -0.25577722E-05 -0.34373075E-05 -0.42741748E-05
-0.50640680E-05 -0.58030789E-05 -0.64877128E-05 -0.71149000E-05 -0.76820053E-05
-0.81868340E-05 -0.86276356E-05 -0.90031040E-05 -0.93123753E-05 -0.95550231E-05
-0.97310506E-05 -0.98408808E-05 -0.98853443E-05 -0.98656639E-05 -0.97834386E-05
-0.96406248E-05 -0.94395152E-05 -0.91827174E-05 -0.88731302E-05 -0.85139185E-05
-0.81084875E-05 -0.76604562E-05 -0.71736294E-05 -0.66519702E-05 -0.60995711E-05
-0.55206258E-05 -0.49194004E-05 -0.43002056E-05 -0.36673678E-05 -0.30252028E-05
-0.23779882E-05 -0.17299378E-05 -0.10851766E-05 -0.44771711E-06 0.17856329E-06

0.78994370E-06 0.13828794E-05 0.19540202E-05 0.25002270E-05 0.30185867E-05
0.35064258E-05 0.39613212E-05 0.43811105E-05 0.47638996E-05 0.51080683E-05
0.54122751E-05 0.56754590E-05 0.58968403E-05 0.60759190E-05 0.62124726E-05
0.63065505E-05 0.63584687E-05 0.63688015E-05 0.63383726E-05 0.62682446E-05
0.61597069E-05 0.60142633E-05 0.58336176E-05 0.56196588E-05 0.53744456E-05
0.51001893E-05 0.47992374E-05 0.44740556E-05 0.41272099E-05 0.37613489E-05
0.33791849E-05 0.29834757E-05 0.25770069E-05 0.21625734E-05 0.17429617E-05
0.13209330E-05 0.89920636E-06 0.48044223E-06 0.67227490E-07 -0.33793944E-06
-0.73266233E-06 -0.11146601E-05 -0.14817784E-05 -0.18320010E-05 -0.21634592E-05
-0.24744402E-05 -0.27633955E-05 -0.30289462E-05 -0.32698889E-05 -0.34851992E-05
-0.36740348E-05 -0.38357369E-05 -0.39698304E-05 -0.40760236E-05 -0.41542058E-05
-0.42044449E-05 -0.42269828E-05 -0.42222309E-05 -0.41907636E-05 -0.41333121E-05
-0.40507560E-05 -0.39441152E-05 -0.38145409E-05 -0.36633054E-05 -0.34917918E-05
-0.33014834E-05 -0.30939523E-05 -0.28708478E-05 -0.26338845E-05 -0.23848304E-05
-0.21254948E-05 -0.18577161E-05 -0.15833498E-05 -0.13042566E-05 -0.10222905E-05
-0.73928749E-06 -0.45705438E-06 -0.17735807E-06 0.98084700E-07 0.36761714E-06
0.62965158E-06 0.88267808E-06 0.11252724E-05 0.13561030E-05 0.15739382E-05
0.17776511E-05 0.19662255E-05 0.21387592E-05 0.22944684E-05 0.24326897E-05
0.25528821E-05 0.26546283E-05 0.27376346E-05 0.28017306E-05 0.28468678E-05
0.28731179E-05 0.28806696E-05 0.28698257E-05 0.28409987E-05 0.27947063E-05
0.27315663E-05 0.26522907E-05 0.25576796E-05 0.24486142E-05 0.23260505E-05
0.21910113E-05 0.20445788E-05 0.18878866E-05 0.17221120E-05 0.15484674E-05
0.13681923E-05 0.11825452E-05 0.99279501E-06 0.80021327E-06 0.60606594E-06
0.41160570E-06 0.21806430E-06 0.26645311E-07 -0.16148295E-06 -0.34519405E-06
-0.52340971E-06 -0.69510569E-06 -0.85931720E-06 -0.10151438E-05 -0.11617541E-05
-0.12983893E-05 -0.14243670E-05 -0.15390838E-05 -0.16420180E-05 -0.17327311E-05
-0.18108692E-05 -0.18761633E-05 -0.19284304E-05 -0.19675719E-05 -0.19935738E-05
-0.20065046E-05 -0.20065137E-05 -0.19938287E-05 -0.19687533E-05 -0.19316631E-05
-0.18830029E-05 -0.18232821E-05 -0.17530705E-05 -0.16729939E-05 -0.15837289E-05
-0.14859980E-05 -0.13805642E-05 -0.12682257E-05 -0.11498098E-05 -0.10261678E-05
-0.89816904E-06 -0.76669493E-06 -0.63263361E-06 -0.49687403E-06 -0.36030051E-06
-0.22378719E-06 -0.88192832E-07 0.45644338E-07 0.17691149E-06 0.30482585E-06
0.42863905E-06 0.54764124E-06 0.66116487E-06 0.76858812E-06 0.86933801E-06
0.96289316E-06 0.10487862E-05 0.11266056E-05 0.11959976E-05 0.12566673E-05
0.13083793E-05 0.13509585E-05 0.13842899E-05 0.14083187E-05 0.14230490E-05
0.14285435E-05 0.14249216E-05 0.14123579E-05 0.13910801E-05 0.13613670E-05
0.13235455E-05 0.12779879E-05 0.12251090E-05 0.11653624E-05 0.10992375E-05
0.10272555E-05 0.94996587E-06 0.86794215E-06 0.78177822E-06 0.69208417E-06
0.59948222E-06 0.50460263E-06 0.40807963E-06 0.31054740E-06 0.21263612E-06
0.11496805E-06 0.18153840E-07 -0.77211168E-07 -0.17055036E-06 -0.26130917E-06
-0.34895818E-06 -0.43299604E-06 -0.51295212E-06 -0.58838898E-06 -0.65890453E-06
-0.72413404E-06 -0.78375174E-06 -0.83747228E-06 -0.88505188E-06 -0.92628911E-06
-0.96102556E-06 -0.98914609E-06 -0.10105789E-05 -0.10252952E-05 -0.10333088E-05
-0.10346753E-05 -0.10294912E-05 -0.10178924E-05 -0.10000529E-05 -0.97618320E-06
-0.94652808E-06 -0.91136490E-06 -0.87100113E-06 -0.82577206E-06 -0.77603817E-06
-0.72218259E-06 -0.66460827E-06 -0.60373520E-06 -0.53999748E-06 -0.47384043E-06
-0.40571761E-06 -0.33608784E-06 -0.26541229E-06 -0.19415154E-06 -0.12276271E-06
-0.51696669E-07 0.18604710E-07 0.87711141E-07 0.15520646E-06 0.22069098E-06
0.28378377E-06 0.34412473E-06 0.40137651E-06 0.45522629E-06 0.50538735E-06
0.55160045E-06 0.59363507E-06 0.63129035E-06 0.66439597E-06 0.69281268E-06
0.71643273E-06 0.73518009E-06 0.74901039E-06 0.75791076E-06 0.76189942E-06
0.76102509E-06 0.75536626E-06 0.74503019E-06 0.73015187E-06 0.71089272E-06

0.68743922E-06 0.66000132E-06 0.62881083E-06 0.59411960E-06 0.55619768E-06
0.51533136E-06 0.47182111E-06 0.42597951E-06 0.37812914E-06 0.32860037E-06
0.27772922E-06 0.22585517E-06 0.17331894E-06 0.12046043E-06 0.67616530E-07
0.15119098E-07 -0.36707047E-07 -0.87546055E-07 -0.13709288E-06 -0.18505504E-06
-0.23115424E-06 -0.27512793E-06 -0.31673069E-06 -0.35573555E-06 -0.39193508E-06
-0.42514247E-06 -0.45519235E-06 -0.48194153E-06 -0.50526957E-06 -0.52507921E-06
-0.54129663E-06 -0.55387160E-06 -0.56277741E-06 -0.56801074E-06 -0.56959132E-06
-0.56756149E-06 -0.56198559E-06 -0.55294926E-06 -0.54055862E-06 -0.52493927E-06
-0.50623525E-06 -0.48460787E-06 -0.46023448E-06 -0.43330710E-06 -0.40403103E-06
-0.37262338E-06 -0.33931154E-06 -0.30433161E-06 -0.26792682E-06 -0.23034587E-06
-0.19184136E-06 -0.15266811E-06 -0.11308152E-06 -0.73336039E-07 -0.33683517E-07
0.56282985E-08 0.44357258E-07 0.82268248E-07 0.11913456E-06 0.15473919E-06
0.18887605E-06 0.22135113E-06 0.25198351E-06 0.28060632E-06 0.30706762E-06
0.33123107E-06 0.35297665E-06 0.37220111E-06 0.38881843E-06 0.40276012E-06
0.41397538E-06 0.42243117E-06 0.42811222E-06 0.43102083E-06 0.43117665E-06
0.42861629E-06 0.42339287E-06 0.41557549E-06 0.40524853E-06 0.39251095E-06
0.37747547E-06 0.36026766E-06 0.34102500E-06 0.31989584E-06 0.29703835E-06
0.27261938E-06 0.24681330E-06 0.21980084E-06 0.19176781E-06 0.16290394E-06
0.13340160E-06 0.10345457E-06 0.73256824E-07 0.43001304E-07 0.12878723E-07
-0.16923584E-07 -0.46222793E-07 -0.74841672E-07 -0.10260961E-06 -0.12936361E-06
-0.15494917E-06 -0.17922117E-06 -0.20204467E-06 -0.22329554E-06 -0.24286118E-06
-0.26064103E-06 -0.27654704E-06 -0.29050404E-06 -0.30245008E-06 -0.31233662E-06
-0.32012864E-06 -0.32580471E-06 -0.32935694E-06 -0.33079082E-06 -0.33012506E-06
-0.32739126E-06 -0.32263356E-06 -0.31590821E-06 -0.30728303E-06 -0.29683686E-06
-0.28465893E-06 -0.27084814E-06 -0.25551235E-06 -0.23876754E-06 -0.22073704E-06
-0.20155063E-06 -0.18134364E-06 -0.16025604E-06 -0.13843153E-06 -0.11601656E-06
-0.93159377E-07 -0.70009120E-07 -0.46714828E-07 -0.23424536E-07 -0.28435297E-09
0.22562421E-07 0.44976157E-07 0.66821721E-07 0.87969264E-07 0.10829496E-06
0.12768171E-06 0.14601979E-06 0.16320742E-06 0.17915134E-06 0.19376723E-06
0.20698019E-06 0.21872503E-06 0.22894657E-06 0.23759990E-06 0.24465045E-06
0.25007417E-06 0.25385746E-06 0.25599718E-06 0.25650052E-06 0.25538483E-06
0.25267737E-06 0.24841504E-06 0.24264399E-06 0.23541927E-06 0.22680433E-06
0.21687052E-06 0.20569658E-06 0.19336804E-06 0.17997656E-06 0.16561936E-06
0.15039847E-06 0.13442007E-06 0.11779379E-06 0.10063193E-06 0.83048777E-07
0.65159827E-07 0.47081080E-07 0.28928292E-07 0.10816258E-07 -0.71418951E-08
-0.24835391E-07 -0.42156471E-07 -0.59001028E-07 -0.75269214E-07 -0.90866009E-07
-0.10570176E-06 -0.11969267E-06 -0.13276126E-06 -0.14483676E-06 -0.15585548E-06
-0.16576113E-06 -0.17450507E-06 -0.18204652E-06 -0.18835272E-06 -0.19339903E-06
-0.19716903E-06 -0.19965447E-06 -0.20085522E-06 -0.20077923E-06 -0.19944233E-06
-0.19686805E-06 -0.19308740E-06 -0.18813856E-06 -0.18206656E-06 -0.17492293E-06

atomic pseudo charge-density

0.40000000E+01 0.39894900E+01 0.39582020E+01 0.39068475E+01 0.38365676E+01
0.37488701E+01 0.36455522E+01 0.35286148E+01 0.34001764E+01 0.32623924E+01
0.31173852E+01 0.29671861E+01 0.28136923E+01 0.26586361E+01 0.25035670E+01
0.23498438E+01 0.21986345E+01 0.20509225E+01 0.19075176E+01 0.17690689E+01
0.16360799E+01 0.15089238E+01 0.13878591E+01 0.12730444E+01 0.11645520E+01
0.10623816E+01 0.96647127E+00 0.87670876E+00 0.79294050E+00 0.71498025E+00
0.64261635E+00 0.57561818E+00 0.51374165E+00 0.45673396E+00 0.40433763E+00
0.35629386E+00 0.31234537E+00 0.27223873E+00 0.23572619E+00 0.20256723E+00
0.17252965E+00 0.14539051E+00 0.12093668E+00 0.98965284E-01 0.79283927E-01
0.61710762E-01 0.46074455E-01 0.32214035E-01 0.19978673E-01 0.92273854E-02
-0.17129956E-03 -0.83397205E-02 -0.15391484E-01 -0.21431884E-01 -0.26558327E-01

-0.30860766E-01 -0.34422125E-01 -0.37318725E-01 -0.39620690E-01 -0.41392352E-01
-0.42692633E-01 -0.43575414E-01 -0.44089892E-01 -0.44280910E-01 -0.44189276E-01
-0.43852065E-01 -0.43302904E-01 -0.42572230E-01 -0.41687546E-01 -0.40673653E-01
-0.39552863E-01 -0.38345209E-01 -0.37068626E-01 -0.35739132E-01 -0.34370988E-01
-0.32976850E-01 -0.31567909E-01 -0.30154016E-01 -0.28743808E-01 -0.27344814E-01
-0.25963555E-01 -0.24605642E-01 -0.23275860E-01 -0.21978245E-01 -0.20716161E-01
-0.19492364E-01 -0.18309064E-01 -0.17167982E-01 -0.16070401E-01 -0.15017212E-01
-0.14008961E-01 -0.13045883E-01 -0.12127944E-01 -0.11254869E-01 -0.10426176E-01
-0.96411988E-02 -0.88991164E-02 -0.81989731E-02 -0.75396994E-02 -0.69201311E-02
-0.63390254E-02 -0.57950769E-02 -0.52869307E-02 -0.48131950E-02 -0.43724521E-02
-0.39632686E-02 -0.35842040E-02 -0.32338186E-02 -0.29106808E-02 -0.26133730E-02
-0.23404976E-02 -0.20906808E-02 -0.18625780E-02 -0.16548763E-02 -0.14662983E-02
-0.12956043E-02 -0.11415948E-02 -0.10031117E-02 -0.87904040E-03 -0.76831032E-03
-0.66989595E-03 -0.58281726E-03 -0.50613997E-03 -0.43897557E-03 -0.38048116E-03
-0.32985908E-03 -0.28635641E-03 -0.24926428E-03 -0.21791713E-03 -0.19169172E-03
-0.17000618E-03 -0.15231889E-03 -0.13812728E-03 -0.12696662E-03 -0.11840867E-03
-0.11206037E-03 -0.10756242E-03 -0.10458787E-03 -0.10284067E-03 -0.10205420E-03
-0.10198982E-03 -0.10243540E-03 -0.10320381E-03 -0.10413150E-03 -0.10507701E-03
-0.10591958E-03 -0.10655770E-03 -0.10690776E-03 -0.10690264E-03 -0.10649045E-03
-0.10563321E-03 -0.10430558E-03 -0.10249369E-03 -0.10019394E-03 -0.97411911E-04
-0.94161248E-04 -0.90462667E-04 -0.86342961E-04 -0.81834072E-04 -0.76972211E-04
-0.71797037E-04 -0.66350872E-04 -0.60677984E-04 -0.54823910E-04 -0.48834832E-04
-0.42757009E-04 -0.36636254E-04 -0.30517460E-04 -0.24444174E-04 -0.18458223E-04
-0.12599380E-04 -0.69050721E-05 -0.14101426E-05 0.38533586E-05 0.88563377E-05
0.13572784E-04 0.17979862E-04 0.22057967E-04 0.25790753E-04 0.29165127E-04
0.32171219E-04 0.34802322E-04 0.37054812E-04 0.38928050E-04 0.40424254E-04
0.41548366E-04 0.42307895E-04 0.42712754E-04 0.42775079E-04 0.42509045E-04
0.41930673E-04 0.41057630E-04 0.39909026E-04 0.38505213E-04 0.36867577E-04
0.35018338E-04 0.32980351E-04 0.30776904E-04 0.28431535E-04 0.25967843E-04
0.23409313E-04 0.20779146E-04 0.18100103E-04 0.15394356E-04 0.12683347E-04
0.99876640E-05 0.73269233E-05 0.47196682E-05 0.21832762E-05 -0.26611907E-06
-0.26136953E-05 -0.48459956E-05 -0.69509705E-05 -0.89180088E-05 -0.10737956E-04
-0.12403122E-04 -0.13907277E-04 -0.15245638E-04 -0.16414845E-04 -0.17412928E-04
-0.18239265E-04 -0.18894534E-04 -0.19380651E-04 -0.19700711E-04 -0.19858916E-04
-0.19860500E-04 -0.19711651E-04 -0.19419425E-04 -0.18991663E-04 -0.18436898E-04
-0.17764271E-04 -0.16983436E-04 -0.16104469E-04 -0.15137778E-04 -0.14094017E-04
-0.12983993E-04 -0.11818582E-04 -0.10608652E-04 -0.93649739E-05 -0.80981549E-05
-0.68185622E-05 -0.55362575E-05 -0.42609349E-05 -0.30018635E-05 -0.17678359E-05
-0.56712184E-06 0.59257268E-06 0.17041405E-05 0.27611027E-05 0.37576322E-05
0.46885720E-05 0.55494475E-05 0.63364736E-05 0.70465565E-05 0.76772901E-05
0.82269481E-05 0.86944707E-05 0.90794475E-05 0.93820958E-05 0.96032358E-05
0.97442615E-05 0.98071090E-05 0.97942222E-05 0.97085152E-05 0.95533338E-05
0.93324139E-05 0.90498402E-05 0.87100024E-05 0.83175518E-05 0.78773569E-05
0.73944594E-05 0.68740306E-05 0.63213285E-05 0.57416551E-05 0.51403164E-05
0.45225824E-05 0.38936495E-05 0.32586051E-05 0.26223937E-05 0.19897858E-05
0.13653488E-05 0.75342093E-06 0.15808744E-06 -0.41684024E-06 -0.96784258E-06
-0.14917073E-05 -0.19855417E-05 -0.24467825E-05 -0.28732025E-05 -0.32629145E-05
-0.36143732E-05 -0.39263737E-05 -0.41980477E-05 -0.44288581E-05 -0.46185900E-05
-0.47673410E-05 -0.48755085E-05 -0.49437760E-05 -0.49730972E-05 -0.49646791E-05
-0.49199634E-05 -0.48406076E-05 -0.47284643E-05 -0.45855603E-05 -0.44140752E-05
-0.42163194E-05 -0.39947125E-05 -0.37517607E-05 -0.34900354E-05 -0.32121516E-05
-0.29207469E-05 -0.26184610E-05 -0.23079159E-05 -0.19916977E-05 -0.16723379E-05

-0.13522973E-05 -0.10339502E-05 -0.71956995E-06 -0.41131587E-06 -0.11122164E-06
0.17881514E-06 0.45704193E-06 0.72185874E-06 0.97182426E-06 0.12056605E-05
0.14222563E-05 0.16206688E-05 0.18001246E-05 0.19600187E-05 0.20999125E-05
0.22195310E-05 0.23187585E-05 0.23976331E-05 0.24563411E-05 0.24952091E-05
0.25146972E-05 0.25153893E-05 0.24979852E-05 0.24632899E-05 0.24122043E-05
0.23457144E-05 0.22648808E-05 0.21708280E-05 0.20647338E-05 0.19478179E-05
0.18213320E-05 0.16865486E-05 0.15447514E-05 0.13972251E-05 0.12452456E-05
0.10900716E-05 0.93293555E-06 0.77503563E-06 0.61752849E-06 0.46152234E-06
0.30807068E-06 0.15816686E-06 0.12739167E-07 -0.12735334E-06 -0.26132429E-06
-0.38846284E-06 -0.50813574E-06 -0.61978881E-06 -0.72294774E-06 -0.81721822E-06
-0.90228552E-06 -0.97791349E-06 -0.10439430E-05 -0.11002897E-05 -0.11469420E-05
-0.11839572E-05 -0.12114591E-05 -0.12296337E-05 -0.12387253E-05 -0.12390322E-05
-0.12309023E-05 -0.12147287E-05 -0.11909441E-05 -0.11600169E-05 -0.11224455E-05
-0.10787540E-05 -0.10294868E-05 -0.97520407E-06 -0.91647693E-06 -0.85388294E-06
-0.78800162E-06 -0.71941025E-06 -0.64867984E-06 -0.57637137E-06 -0.50303225E-06
-0.42919310E-06 -0.35536471E-06 -0.28203540E-06 -0.20966861E-06 -0.13870082E-06
-0.69539753E-07 -0.25628666E-08 0.61883812E-07 0.12348661E-06 0.18196481E-06
0.23707103E-06 0.28859129E-06 0.33634484E-06 0.38018381E-06 0.41999255E-06
0.45568682E-06 0.48721284E-06 0.51454607E-06 0.53768993E-06 0.55667434E-06
0.57155419E-06 0.58240765E-06 0.58933453E-06 0.59245441E-06 0.59190490E-06
0.58783976E-06 0.58042708E-06 0.56984743E-06 0.55629204E-06 0.53996103E-06
0.52106168E-06 0.49980673E-06 0.47641281E-06 0.45109886E-06 0.42408468E-06
0.39558958E-06 0.36583111E-06 0.33502384E-06 0.30337829E-06 0.27109999E-06
0.23838851E-06 0.20543674E-06 0.17243016E-06 0.13954628E-06 0.10695408E-06
0.74813643E-07 0.43275801E-07 0.12481876E-07 -0.17436491E-07 -0.46357461E-07
-0.74169037E-07 -0.10076906E-06 -0.12606516E-06 -0.14997463E-06 -0.17242430E-06
-0.19335033E-06 -0.21269803E-06 -0.23042162E-06 -0.24648397E-06 -0.26085633E-06
-0.27351806E-06 -0.28445634E-06 -0.29366587E-06 -0.30114861E-06 -0.30691344E-06
-0.31097592E-06 -0.31335800E-06 -0.31408770E-06 -0.31319890E-06 -0.31073103E-06
-0.30672883E-06 -0.30124210E-06 -0.29432543E-06 -0.28603799E-06 -0.27644327E-06
-0.26560883E-06 -0.25360610E-06 -0.24051008E-06 -0.22639916E-06 -0.21135482E-06
-0.19546140E-06 -0.17880584E-06 -0.16147739E-06 -0.14356734E-06 -0.12516871E-06
-0.10637597E-06 -0.87284706E-07 -0.67991261E-07 -0.48592428E-07 -0.29185064E-07
-0.98657277E-08 0.92697130E-08 0.28126473E-07 0.46611256E-07 0.64632668E-07
0.82101638E-07 0.98931835E-07 0.11504010E-06 0.13034685E-06 0.14477652E-06
0.15825794E-06 0.17072478E-06 0.18211587E-06 0.19237561E-06 0.20145433E-06
0.20930856E-06 0.21590136E-06 0.22120257E-06 0.22518906E-06 0.22784490E-06
0.22916153E-06 0.22913787E-06 0.22778040E-06 0.22510318E-06 0.22112780E-06
0.21588339E-06 0.20940643E-06 0.20174063E-06 0.19293667E-06 0.18305201E-06
0.17215053E-06 0.16030220E-06 0.14758265E-06 0.13407280E-06 0.11985829E-06
0.10502906E-06 0.89678716E-07 0.73904010E-07 0.57804207E-07 0.41480468E-07
0.25035199E-07 0.85713988E-08 -0.78080133E-08 -0.24000865E-07 -0.39906403E-07
-0.55425954E-07 -0.70463581E-07 -0.84926717E-07 -0.98726783E-07 -0.11177978E-06
-0.12400685E-06 -0.13533479E-06 -0.14569657E-06 -0.15503174E-06 -0.16328689E-06
-0.17041591E-06 -0.17638040E-06 -0.18114982E-06 -0.18470175E-06 -0.18702198E-06
-0.18810460E-06 -0.18795202E-06 -0.18657494E-06 -0.18399219E-06 -0.18023066E-06
-0.17532499E-06 -0.16931734E-06 -0.16225709E-06 -0.15420042E-06 -0.14520987E-06
-0.13535395E-06 -0.12470653E-06 -0.11334637E-06 -0.10135649E-06 -0.88823604E-07
-0.75837439E-07 -0.62490119E-07 -0.48875489E-07 -0.35088437E-07 -0.21224221E-07
-0.73777912E-08 0.63568809E-08 0.19887461E-07 0.33123893E-07 0.45979023E-07
0.58369191E-07 0.70214800E-07 0.81440843E-07 0.91977404E-07 0.10176010E-06
0.11073051E-06 0.11883650E-06 0.12603257E-06 0.13228010E-06 0.13754756E-06

0.14181065E-06 0.14505242E-06 0.14726331E-06 0.14844111E-06 0.14859093E-06
0.14772507E-06 0.14586285E-06 0.14303037E-06 0.13926029E-06 0.13459145E-06
0.12906857E-06 0.12274182E-06 0.11566643E-06 0.10790217E-06 0.99512895E-07
0.90566036E-07 0.81132037E-07 0.71283824E-07 0.61096233E-07 0.50645444E-07
0.40008409E-07 0.29262279E-07 0.18483846E-07 0.77489827E-08 -0.28678905E-08
-0.13294329E-07 -0.23460361E-07 -0.33298961E-07 -0.42746490E-07 -0.51743114E-07
-0.60233174E-07 -0.68165529E-07 -0.75493860E-07 -0.82176926E-07 -0.88178787E-07
-0.93468977E-07 -0.98022636E-07 -0.10182060E-06 -0.10484943E-06 -0.10710146E-06
-0.10857468E-06 -0.10927271E-06 -0.10920466E-06 -0.10838495E-06 -0.10683314E-06
-0.10457366E-06 -0.10163556E-06 -0.98052212E-07 -0.93860993E-07 -0.89102915E-07
-0.83822274E-07 -0.78066253E-07 -0.71884526E-07 -0.65328843E-07 -0.58452612E-07
-0.51310471E-07 -0.43957866E-07 -0.36450626E-07 -0.28844547E-07 -0.21194983E-07
-0.13556449E-07 -0.59822376E-08 0.14759451E-08 0.87683264E-08 0.15847391E-07
0.22668179E-07 0.29188565E-07 0.35369499E-07 0.41175231E-07 0.46573494E-07
0.51535668E-07 0.56036902E-07 0.60056215E-07 0.63576554E-07 0.66584835E-07
0.69071940E-07 0.71032692E-07 0.72465798E-07 0.73373762E-07 0.73762781E-07
0.73642599E-07 0.73026354E-07 0.71930396E-07 0.70374081E-07 0.68379558E-07
0.65971530E-07 0.63177010E-07 0.60025060E-07 0.56546522E-07 0.52773748E-07
0.48740322E-07 0.44480775E-07 0.40030312E-07 0.35424531E-07 0.30699156E-07
0.25889764E-07 0.21031537E-07 0.16159009E-07 0.11305837E-07 0.65045755E-08
0.17864747E-08 -0.28187116E-08 -0.72828982E-08 -0.11579823E-07 -0.15685184E-07
-0.19576754E-07 -0.23234482E-07 -0.26640569E-07 -0.29779525E-07 -0.32638210E-07
-0.35205853E-07 -0.37474053E-07 -0.39436762E-07 -0.41090248E-07 -0.42433048E-07
-0.43465898E-07 -0.44191654E-07 -0.44615193E-07 -0.44743313E-07 -0.44584610E-07
-0.44149350E-07 -0.43449338E-07 -0.42497775E-07 -0.41309105E-07 -0.39898868E-07
-0.38283548E-07 -0.36480410E-07 -0.34507352E-07 -0.32382746E-07 -0.30125288E-07
-0.27753852E-07 -0.25287344E-07 -0.22744566E-07 -0.20144087E-07 -0.17504118E-07
-0.14842395E-07 -0.12176079E-07 -0.95216549E-08 -0.68948449E-08 -0.43105330E-08
-0.17826977E-08 0.67564447E-09 0.30524844E-08 0.53368566E-08 0.75188641E-08
0.95896949E-08 0.11541628E-07 0.13368031E-07 0.15063349E-07 0.16623084E-07
0.18043771E-07 0.19322942E-07 0.20459089E-07 0.21451615E-07 0.22300792E-07
0.23007700E-07 0.23574176E-07 0.24002749E-07 0.24296588E-07 0.24459433E-07
0.24495533E-07 0.24409591E-07 0.24206695E-07 0.23892262E-07 0.23471983E-07
0.22951762E-07 0.22337667E-07 0.21635884E-07 0.20852664E-07 0.19994287E-07
0.19067022E-07 0.18077093E-07 0.17030650E-07 0.15933740E-07 0.14792291E-07
0.13612090E-07 0.12398773E-07 0.11157809E-07 0.98945025E-08 0.86139808E-08
0.73212005E-08 0.60209467E-08 0.47178386E-08 0.34163358E-08 0.21207462E-08
0.83523555E-09 -0.43616260E-09 -0.16895364E-08 -0.29210851E-08 -0.41271087E-08
-0.53039984E-08 -0.64482281E-08 -0.75563465E-08 -0.86249715E-08 -0.96507858E-08
-0.10630535E-07 -0.11561025E-07 -0.12439130E-07 -0.13261788E-07 -0.14026016E-07
-0.14728912E-07 -0.15367671E-07 -0.15939596E-07 -0.16442113E-07 -0.16872790E-07
-0.17229354E-07 -0.17509713E-07 -0.17711979E-07 -0.17834487E-07 -0.17875819E-07
-0.17834832E-07 -0.17710675E-07 -0.17502818E-07 -0.17211070E-07 -0.16835604E-07
-0.16376972E-07 -0.15836130E-07 -0.15214447E-07 -0.14513725E-07 -0.13736202E-07
-0.12884569E-07 -0.11961967E-07 -0.10971991E-07 -0.99186893E-08 -0.88065540E-08
-0.76405118E-08 -0.64259101E-08 -0.51684985E-08 -0.38744064E-08 -0.25501169E-08
-0.12024370E-08 0.16153688E-09 0.15344557E-08 0.29087587E-08 0.42767170E-08
0.56304798E-08 0.69621237E-08 0.82637035E-08 0.95273052E-08 0.10745100E-07
0.11909398E-07 0.13012707E-07 0.14047782E-07 0.15007686E-07 0.15885841E-07
0.16676079E-07 0.17372696E-07 0.17970499E-07 0.18464847E-07 0.18851702E-07
0.19127658E-07 0.19289981E-07 0.19336640E-07 0.19266328E-07 0.19078485E-07
0.18773313E-07 0.18351784E-07 0.17815647E-07 0.17167424E-07 0.16410404E-07

0.15548628E-07 0.14586872E-07 0.13530621E-07 0.12386036E-07 0.11159926E-07
0.98596966E-08 0.84933135E-08 0.70692460E-08 0.55964140E-08 0.40841294E-08
0.25420335E-08 0.98003243E-09 -0.59177109E-09 -0.21631473E-08 -0.37238108E-08
-0.52634929E-08 -0.67720137E-08 -0.82393551E-08 -0.96557318E-08 -0.11011662E-07
-0.12298036E-07 -0.13506184E-07 -0.14627935E-07 -0.15655682E-07 -0.16582436E-07
-0.17401876E-07 -0.18108398E-07 -0.18697157E-07 -0.19164104E-07 -0.19506014E-07
-0.19720516E-07 -0.19806107E-07 -0.19762166E-07 -0.19588960E-07 -0.19287646E-07
-0.18860259E-07 -0.18309704E-07 -0.17639732E-07 -0.16854917E-07 -0.15960622E-07
-0.14962964E-07 -0.13868765E-07 -0.12685513E-07 -0.11421300E-07 -0.10084769E-07
-0.86850511E-08 -0.72317011E-08 -0.57346286E-08 -0.42040280E-08 -0.26503060E-08
-0.10840075E-08 0.48425928E-09 0.20438982E-08 0.35844000E-08 0.50954169E-08
0.65668346E-08 0.79888435E-08 0.93520070E-08 0.10647327E-07 0.11866307E-07
0.13001010E-07 0.14044112E-07 0.14988951E-07 0.15829574E-07 0.16560771E-07
0.17178115E-07 0.17677984E-07 0.18057587E-07 0.18314975E-07 0.18449058E-07
0.18459598E-07 0.18347214E-07 0.18113370E-07 0.17760360E-07 0.17291286E-07
0.16710033E-07 0.16021236E-07 0.15230242E-07 0.14343068E-07 0.13366354E-07
0.12307312E-07 0.11173672E-07 0.99736232E-08 0.87157545E-08 0.74089892E-08
0.60625206E-08 0.46857457E-08 0.32881972E-08 0.18794762E-08 0.46918430E-09
-0.93314355E-09 -0.23181056E-08 -0.36764979E-08 -0.49993772E-08 -0.62781212E-08
-0.75044852E-08 -0.86706566E-08 -0.97693052E-08 -0.10793630E-07 -0.11737403E-07
-0.12595003E-07 -0.13361457E-07 -0.14032458E-07 -0.14604397E-07 -0.15074376E-07
-0.15440222E-07 -0.15700496E-07 -0.15854493E-07 -0.15902242E-07 -0.15844495E-07
-0.15682716E-07 -0.15419062E-07 -0.15056359E-07 -0.14598075E-07 -0.14048292E-07
-0.13411668E-07 -0.12693396E-07 -0.11899166E-07 -0.11035117E-07 -0.10107790E-07
-0.91240747E-08 -0.80911627E-08 -0.70164909E-08 -0.59076884E-08 -0.47725214E-08
-0.36188374E-08 -0.24545102E-08 -0.12873853E-08 -0.12522678E-09 0.10243349E-08
0.21538530E-08 0.32561128E-08 0.43241777E-08 0.53514335E-08 0.63316286E-08
0.72589114E-08 0.81278647E-08 0.89335351E-08 0.96714604E-08 0.10337692E-07
0.10928815E-07 0.11441961E-07 0.11874825E-07 0.12225664E-07 0.12493308E-07
0.12677152E-07 0.12777157E-07 0.12793835E-07 0.12728243E-07 0.12581963E-07
0.12357085E-07 0.12056185E-07 0.11682297E-07 0.11238888E-07 0.10729825E-07
0.10159343E-07 0.95320149E-08 0.88527073E-08 0.81265507E-08 0.73588972E-08
0.65552820E-08 0.57213827E-08 0.48629795E-08 0.39859151E-08 0.30960556E-08
25.1333556480997 T

Non local Part

0 2 0.809018704071853

6.64147061569650 8.75060766577616 8.75060766577616

11.5256250087982

Reciprocal Space Part

0.35673024E+02 0.35300975E+02 0.34187891E+02 0.32342969E+02 0.29781539E+02
0.26525068E+02 0.22601151E+02 0.18043493E+02 0.12891857E+02 0.71919796E+01
0.99544169E+00 -0.56405267E+01 -0.12653309E+02 -0.19975249E+02 -0.27534082E+02
-0.35253471E+02 -0.43053640E+02 -0.50852104E+02 -0.58564504E+02 -0.66105539E+02
-0.73389971E+02 -0.80333712E+02 -0.86854960E+02 -0.92875371E+02 -0.98321250E+02
-0.10312473E+03 -0.10722490E+03 -0.11056890E+03 -0.11311292E+03 -0.11482305E+03
-0.11567603E+03 -0.11565984E+03 -0.11477409E+03 -0.11303021E+03 -0.11045146E+03
-0.10707271E+03 -0.10294000E+03 -0.98109876E+02 -0.92648565E+02 -0.86630907E+02
-0.80139141E+02 -0.73261533E+02 -0.66090881E+02 -0.58722929E+02 -0.51254709E+02
-0.43782871E+02 -0.36402011E+02 -0.29203050E+02 -0.22271689E+02 -0.15686982E+02
-0.95200463E+01 -0.38329536E+01 0.13221936E+01 0.59039664E+01 0.98820882E+01
0.13237678E+02 0.15963259E+02 0.18062524E+02 0.19549889E+02 0.20449822E+02
0.20795986E+02 0.20630211E+02 0.20001326E+02 0.18963872E+02 0.17576747E+02

0.15901789E+02 0.14002360E+02 0.11941941E+02 0.97827900E+01 0.75846703E+01
0.54037004E+01 0.32913316E+01 0.12934806E+01 -0.55016896E+00 -0.22066858E+01
-0.36502260E+01 -0.48621821E+01 -0.58311508E+01 -0.65527286E+01 -0.70291465E+01
-0.72687617E+01 -0.72854257E+01 -0.70977500E+01 -0.67282941E+01 -0.62027004E+01
-0.55488012E+01 -0.47957236E+01 -0.39730149E+01 -0.31098122E+01 -0.22340745E+01
-0.13718974E+01 -0.54692152E+00 0.22015167E+00 0.91193078E+00 0.15145877E+01
0.20179927E+01 0.24157349E+01 0.27050337E+01 0.28865508E+01 0.29641137E+01

Real Space Part

-0.17810705E+04 -0.17800710E+04 -0.17770736E+04 -0.17720814E+04 -0.17650997E+04
-0.17561358E+04 -0.17451993E+04 -0.17323017E+04 -0.17174568E+04 -0.17006804E+04
-0.16819906E+04 -0.16614075E+04 -0.16389537E+04 -0.16146537E+04 -0.15885347E+04
-0.15606261E+04 -0.15309597E+04 -0.14995701E+04 -0.14664944E+04 -0.14317725E+04
-0.13954473E+04 -0.13575649E+04 -0.13181745E+04 -0.12773289E+04 -0.12350842E+04
-0.11915007E+04 -0.11466425E+04 -0.11005781E+04 -0.10533803E+04 -0.10051266E+04
-0.95589940E+03 -0.90578602E+03 -0.85487908E+03 -0.80327656E+03 -0.75108191E+03
-0.69840422E+03 -0.64535824E+03 -0.59206446E+03 -0.53864905E+03 -0.48524386E+03
-0.43198628E+03 -0.37901906E+03 -0.32649010E+03 -0.27455215E+03 -0.22336243E+03
-0.17308219E+03 -0.12387615E+03 -0.75911935E+02 -0.29359341E+02 0.15610436E+02
0.58825684E+02 0.10011513E+03 0.13930898E+03 0.17624007E+03 0.21074507E+03
0.24266574E+03 0.27185034E+03 0.29815495E+03 0.32144502E+03 0.34159674E+03
0.35849866E+03 0.37205307E+03 0.38217756E+03 0.38880644E+03 0.39189209E+03
0.39140630E+03 0.38734139E+03 0.37971132E+03 0.36855255E+03 0.35392475E+03
0.33591128E+03 0.31461949E+03 0.29018073E+03 0.26275008E+03 0.23250596E+03
0.19964986E+03 0.16439876E+03 0.12690104E+03 0.87156862E+02 0.59182296E+02
0.44271643E+02 0.29005121E+02 0.13897646E+02 -0.68913937E+00 -0.14500503E+02
-0.27287699E+02 -0.38803943E+02 -0.48809637E+02 -0.57074430E+02 -0.63379750E+02
-0.67521095E+02 -0.69309996E+02 -0.68575851E+02 -0.65167610E+02 -0.58957620E+02
-0.49826941E+02 -0.37681807E+02 -0.22859048E+02 -0.29432209E+01 0.00000000E+00

Reciprocal Space Part

-0.22652168E+02 -0.22380564E+02 -0.21567988E+02 -0.20221161E+02 -0.18351283E+02
-0.15974044E+02 -0.13109624E+02 -0.97826757E+01 -0.60223016E+01 -0.18619951E+01
0.26604494E+01 0.75030719E+01 0.12619934E+02 0.17961368E+02 0.23474290E+02
0.29102590E+02 0.34787596E+02 0.40468608E+02 0.46083518E+02 0.51569487E+02
0.56863703E+02 0.61904172E+02 0.66630568E+02 0.70985103E+02 0.74913408E+02
0.78365410E+02 0.81296182E+02 0.83666748E+02 0.85444820E+02 0.86605458E+02
0.87131614E+02 0.87014575E+02 0.86254250E+02 0.84859334E+02 0.82847299E+02
0.80244236E+02 0.77084531E+02 0.73410386E+02 0.69271179E+02 0.64722691E+02
0.59826194E+02 0.54647432E+02 0.49255506E+02 0.43721694E+02 0.38118214E+02
0.32516981E+02 0.26988360E+02 0.21599955E+02 0.16415466E+02 0.11493616E+02
0.68871940E+01 0.26422303E+01 -0.12026934E+01 -0.46169667E+01 -0.75783065E+01
-0.10072937E+02 -0.12095591E+02 -0.13649339E+02 -0.14745245E+02 -0.15401872E+02
-0.15644632E+02 -0.15505023E+02 -0.15019749E+02 -0.14229764E+02 -0.13179249E+02
-0.11914561E+02 -0.10483170E+02 -0.89326126E+01 -0.73094828E+01 -0.56584886E+01
-0.40215898E+01 -0.24372354E+01 -0.93971757E+00 0.44134967E+00 0.16814163E+01
0.27612448E+01 0.36670190E+01 0.43903182E+01 0.49279614E+01 0.52817321E+01
0.54579957E+01 0.54672251E+01 0.53234490E+01 0.50436429E+01 0.46470809E+01
0.41546657E+01 0.35882586E+01 0.29700241E+01 0.23218081E+01 0.16645637E+01
0.10178381E+01 0.39933054E+00 -0.17546938E+00 -0.69355860E+00 -0.11446090E+01
-0.15210674E+01 -0.18181697E+01 -0.20338733E+01 -0.21687153E+01 -0.22256039E+01

Real Space Part

0.13380756E+04 0.13373358E+04 0.13351170E+04 0.13314215E+04 0.13262528E+04
0.13196160E+04 0.13115176E+04 0.13019656E+04 0.12909693E+04 0.12785397E+04

0.12646894E+04 0.12494321E+04 0.12327837E+04 0.12147611E+04 0.11953834E+04
0.11746711E+04 0.11526467E+04 0.11293345E+04 0.11047609E+04 0.10789541E+04
0.10519448E+04 0.10237661E+04 0.99445313E+03 0.96404408E+03 0.93257968E+03
0.90010360E+03 0.86666259E+03 0.83230666E+03 0.79708918E+03 0.76106712E+03
0.72430114E+03 0.68685577E+03 0.64879953E+03 0.61020508E+03 0.57114928E+03
0.53171333E+03 0.49198276E+03 0.45204751E+03 0.41200190E+03 0.37194462E+03
0.33197859E+03 0.29221089E+03 0.25275257E+03 0.21371841E+03 0.17522664E+03
0.13739862E+03 0.10035844E+03 0.64232440E+02 0.29148680E+02 -0.47636269E+01
-0.37374797E+02 -0.68555391E+02 -0.98177011E+02 -0.12611315E+03 -0.15224012E+03
-0.17643798E+03 -0.19859161E+03 -0.21859175E+03 -0.23633607E+03 -0.25173032E+03
-0.26468946E+03 -0.27513878E+03 -0.28301504E+03 -0.28826751E+03 -0.29085910E+03
-0.29076724E+03 -0.28798485E+03 -0.28252111E+03 -0.27440213E+03 -0.26367152E+03
-0.25039071E+03 -0.23463925E+03 -0.21651476E+03 -0.19613277E+03 -0.17362643E+03
-0.14914631E+03 -0.12285473E+03 -0.94862862E+02 -0.65171132E+02 -0.44263828E+02
-0.33119072E+02 -0.21702925E+02 -0.10400939E+02 0.51584918E+00 0.10856251E+02
0.20433452E+02 0.29062017E+02 0.36561812E+02 0.42759562E+02 0.47490760E+02
0.50601400E+02 0.51949458E+02 0.51406278E+02 0.48857853E+02 0.44207716E+02
0.37365937E+02 0.28261481E+02 0.17146376E+02 0.22078540E+01 0.00000000E+00

Non local Part

1 2 0.809018704071853
-1.25459431793475 2.49934797684719 2.49934797684719
-6.92024382817034

Reciprocal Space Part

0.00000000E+00 0.58012143E+00 0.11501102E+01 0.17000290E+01 0.22203268E+01
0.27020214E+01 0.31368709E+01 0.35175277E+01 0.38376752E+01 0.40921416E+01
0.42769903E+01 0.43895839E+01 0.44286217E+01 0.43941491E+01 0.42875405E+01
0.41114539E+01 0.38697615E+01 0.35674552E+01 0.32105320E+01 0.28058598E+01
0.23610281E+01 0.18841869E+01 0.13838772E+01 0.86885653E+00 0.34792451E+00
-0.17024888E+00 -0.67728829E+00 -0.11652677E+01 -0.16268519E+01 -0.20554220E+01
-0.24451824E+01 -0.27912476E+01 -0.30897079E+01 -0.33376718E+01 -0.35332864E+01
-0.36757355E+01 -0.37652149E+01 -0.38028888E+01 -0.37908257E+01 -0.37319189E+01
-0.36297914E+01 -0.34886898E+01 -0.33133689E+01 -0.31089700E+01 -0.28808962E+01
-0.26346881E+01 -0.23759012E+01 -0.21099893E+01 -0.18421958E+01 -0.15774544E+01
-0.13203019E+01 -0.10748047E+01 -0.84449921E+00 -0.63234735E+00 -0.44070810E+00
-0.27132386E+00 -0.12532214E+00 -0.32312103E-02 0.94991000E-01 0.16991640E+00
0.22259609E+00 0.25450133E+00 0.26745814E+00 0.26357737E+00 0.24518230E+00
0.21473567E+00 0.17476809E+00 0.12780942E+00 0.76324852E-01 0.22656906E-01
-0.31025405E-01 -0.82769423E-01 -0.13087304E+00 -0.17390992E+00 -0.21074552E+00
-0.24054426E+00 -0.26276801E+00 -0.27716654E+00 -0.28376085E+00 -0.28282004E+00
-0.27483302E+00 -0.26047599E+00 -0.24057705E+00 -0.21607892E+00 -0.18800118E+00
-0.15740294E+00 -0.12534711E+00 -0.92867149E-01 -0.60937076E-01 -0.30445471E-01
-0.21739016E-02 0.23219840E-01 0.45213529E-01 0.63427285E-01 0.77625482E-01
0.87714030E-01 0.93733442E-01 0.95848151E-01 0.94332667E-01 0.89555201E-01

Real Space Part

0.00000000E+00 -0.27845427E+01 -0.55507472E+01 -0.82804813E+01 -0.10956021E+02
-0.13560245E+02 -0.16076823E+02 -0.18490386E+02 -0.20786682E+02 -0.22952719E+02
-0.24976879E+02 -0.26849017E+02 -0.28560536E+02 -0.30104437E+02 -0.31475347E+02
-0.32669524E+02 -0.33684836E+02 -0.34520725E+02 -0.35178145E+02 -0.35659482E+02
-0.35968467E+02 -0.36110057E+02 -0.36090324E+02 -0.35916323E+02 -0.35595954E+02
-0.35137823E+02 -0.34551101E+02 -0.33845383E+02 -0.33030547E+02 -0.32116621E+02
-0.31113661E+02 -0.30031624E+02 -0.28880267E+02 -0.27669046E+02 -0.26407031E+02
-0.25102834E+02 -0.23764547E+02 -0.22399701E+02 -0.21015228E+02 -0.19617447E+02

-0.18212054E+02 -0.16804128E+02 -0.15398151E+02 -0.13998037E+02 -0.12607166E+02
-0.11228434E+02 -0.98643076E+01 -0.85168792E+01 -0.71879367E+01 -0.58790277E+01
-0.45915304E+01 -0.33267220E+01 -0.20858476E+01 -0.87018546E+00 0.31889190E+00
0.14798612E+01 0.26109992E+01 0.37103415E+01 0.47756496E+01 0.58043885E+01
0.67937141E+01 0.77404725E+01 0.86412110E+01 0.94922002E+01 0.10289469E+02
0.11028852E+02 0.11706045E+02 0.12316678E+02 0.12856388E+02 0.13320913E+02
0.13706185E+02 0.14008430E+02 0.14224277E+02 0.14350866E+02 0.14385958E+02
0.14328043E+02 0.14176445E+02 0.13931423E+02 0.13594262E+02 0.13167350E+02
0.12654257E+02 0.12059786E+02 0.11390009E+02 0.10652304E+02 0.98553494E+01
0.90091221E+01 0.81248560E+01 0.72150055E+01 0.62931637E+01 0.53739861E+01
0.44730813E+01 0.36068889E+01 0.27925530E+01 0.20477631E+01 0.13905980E+01
0.83938824E+00 0.41250510E+00 0.12734221E+00 0.68991025E-02 0.00000000E+00

Reciprocal Space Part

0.00000000E+00 0.17585757E+00 0.34749514E+00 0.51077994E+00 0.66175174E+00
0.79670440E+00 0.91226180E+00 0.10054466E+01 0.10737404E+01 0.11151335E+01
0.11281643E+01 0.11119464E+01 0.10661834E+01 0.99117138E+00 0.88778850E+00
0.75747289E+00 0.60218852E+00 0.42438063E+00 0.22692143E+00 0.13047569E-01
-0.21370930E+00 -0.44959706E+00 -0.69072129E+00 -0.93312507E+00 -0.11728688E+01
-0.14061082E+01 -0.16291688E+01 -0.18386157E+01 -0.20313163E+01 -0.22044959E+01
-0.23557842E+01 -0.24832521E+01 -0.25854390E+01 -0.26613687E+01 -0.27105553E+01
-0.27329985E+01 -0.27291684E+01 -0.26999817E+01 -0.26467685E+01 -0.25712319E+01
-0.24754005E+01 -0.23615764E+01 -0.22322791E+01 -0.20901862E+01 -0.19380738E+01
-0.17787568E+01 -0.16150309E+01 -0.14496175E+01 -0.12851123E+01 -0.11239395E+01
-0.96831116E+00 -0.82019361E+00 -0.68128066E+00 -0.55297424E+00 -0.43637243E+00
-0.33226491E+00 -0.24113561E+00 -0.16317208E+00 -0.98281031E-01 -0.46109462E-01
-0.60704908E-02 0.22626925E-01 0.40945312E-01 0.49983992E-01 0.50943348E-01
0.45088963E-01 0.33716537E-01 0.18118398E-01 -0.44763576E-03 -0.20786416E-01
-0.41790091E-01 -0.62458795E-01 -0.81917111E-01 -0.99426136E-01 -0.11439111E+00
-0.12636471E+00 -0.13504612E+00 -0.14027634E+00 -0.14202989E+00 -0.14040350E+00
-0.13560237E+00 -0.12792426E+00 -0.11774235E+00 -0.10548715E+00 -0.91628142E-01
-0.76655762E-01 -0.61064058E-01 -0.45334607E-01 -0.29922013E-01 -0.15241310E-01
-0.16575205E-02 0.10522474E-01 0.21055670E-01 0.29766264E-01 0.36546633E-01
0.41356100E-01 0.44217666E-01 0.45212951E-01 0.44475619E-01 0.42183586E-01

Real Space Part

0.00000000E+00 -0.22584117E+01 -0.45030118E+01 -0.67201336E+01 -0.88963977E+01
-0.11018850E+02 -0.13075093E+02 -0.15053408E+02 -0.16942868E+02 -0.18733439E+02
-0.20416064E+02 -0.21982736E+02 -0.23426558E+02 -0.24741781E+02 -0.25923832E+02
-0.26969320E+02 -0.27876037E+02 -0.28642931E+02 -0.29270076E+02 -0.29758622E+02
-0.30110742E+02 -0.30329555E+02 -0.30419058E+02 -0.30384034E+02 -0.30229968E+02
-0.29962950E+02 -0.29589578E+02 -0.29116867E+02 -0.28552148E+02 -0.27902974E+02
-0.27177033E+02 -0.26382059E+02 -0.25525752E+02 -0.24615704E+02 -0.23659331E+02
-0.22663813E+02 -0.21636042E+02 -0.20582577E+02 -0.19509611E+02 -0.18422940E+02
-0.17327947E+02 -0.16229588E+02 -0.15132390E+02 -0.14040455E+02 -0.12957466E+02
-0.11886709E+02 -0.10831087E+02 -0.97931530E+01 -0.87751357E+01 -0.77789730E+01
-0.68063480E+01 -0.58587253E+01 -0.49373887E+01 -0.40434784E+01 -0.31780271E+01
-0.23419956E+01 -0.15363043E+01 -0.76186313E+00 -0.19596962E-01 0.68953306E+00
0.13645128E+01 0.20042638E+01 0.26076373E+01 0.31734138E+01 0.37003094E+01
0.41869867E+01 0.46320724E+01 0.50341809E+01 0.53919419E+01 0.57040341E+01
0.59692232E+01 0.61864026E+01 0.63546383E+01 0.64732152E+01 0.65416849E+01
0.65599141E+01 0.65281312E+01 0.64469719E+01 0.63175229E+01 0.61413588E+01
0.59205774E+01 0.56578277E+01 0.53563295E+01 0.50198915E+01 0.46529116E+01
0.42603812E+01 0.38478674E+01 0.34214996E+01 0.29879345E+01 0.25543235E+01

0.21282640E+01 0.17177450E+01 0.13310897E+01 0.97688277E+00 0.66389818E+00
0.40103575E+00 0.19722203E+00 0.60924737E-01 0.32993883E-02 0.00000000E+00

PAW radial sets

387 0.699084555240741

(5E20.12)

augmentation charges (non spherical)

-0.610085078461E-01 -0.825288497502E-01 -0.286321348804E-01 0.837941172581E-01 -
0.825288497502E-01
-0.111642379860E+00 -0.379980343121E-01 0.111528043221E+00 -0.286321348804E-01 -
0.379980343121E-01
0.535065847904E-01 -0.104336069865E+00 0.837941172581E-01 0.111528043221E+00 -
0.104336069865E+00
0.206747784148E+00

occupancies in atom

0.199999999999E+01 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00
0.666666666191E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00
0.000000000000E+00

grid

0.266163843696E-04 0.274818827895E-04 0.283755250589E-04 0.292982263456E-04
0.302509315762E-04
0.312346164042E-04 0.322502882088E-04 0.332989871268E-04 0.343817871173E-04
0.354997970623E-04
0.366541619016E-04 0.378460638057E-04 0.390767233863E-04 0.403474009463E-04
0.416593977706E-04
0.430140574586E-04 0.444127673002E-04 0.458569596965E-04 0.473481136267E-04
0.488877561628E-04
0.504774640331E-04 0.521188652376E-04 0.538136407145E-04 0.555635260619E-04
0.573703133154E-04
0.592358527830E-04 0.611620549401E-04 0.631508923861E-04 0.652044018643E-04
0.673246863478E-04
0.695139171933E-04 0.717743363644E-04 0.741082587279E-04 0.765180744243E-04
0.790062513153E-04
0.815753375116E-04 0.842279639819E-04 0.869668472475E-04 0.897947921642E-04
0.927146947948E-04
0.957295453747E-04 0.988424313742E-04 0.102056540661E-03 0.105375164763E-03
0.108801702242E-03
0.112339662172E-03 0.115992667733E-03 0.119764459921E-03 0.123658901382E-03
0.127679980364E-03
0.131831814803E-03 0.136118656540E-03 0.140544895676E-03 0.145115065067E-03
0.149833844965E-03
0.154706067814E-03 0.159736723194E-03 0.164930962938E-03 0.170294106401E-03
0.175831645909E-03
0.181549252388E-03 0.187452781165E-03 0.193548277971E-03 0.199841985127E-03
0.206340347939E-03
0.213050021297E-03 0.219977876495E-03 0.227131008261E-03 0.234516742027E-03
0.242142641430E-03
0.250016516057E-03 0.258146429445E-03 0.266540707334E-03 0.275207946198E-03
0.284157022049E-03

0.293397099521E-03	0.302937641261E-03	0.312788417618E-03	0.322959516647E-03
0.333461354443E-03			
0.344304685805E-03	0.355500615252E-03	0.367060608395E-03	0.378996503676E-03
0.391320524495E-03			
0.404045291726E-03	0.417183836643E-03	0.430749614264E-03	0.444756517131E-03
0.459218889537E-03			
0.474151542213E-03	0.489569767503E-03	0.505489355015E-03	0.521926607798E-03
0.538898359036E-03			
0.556421989285E-03	0.574515444273E-03	0.593197253280E-03	0.612486548111E-03
0.632403082688E-03			
0.652967253285E-03	0.674200119407E-03	0.696123425367E-03	0.718759622544E-03
0.742131892384E-03			
0.766264170131E-03	0.791181169349E-03	0.816908407220E-03	0.843472230686E-03
0.870899843422E-03			
0.899219333701E-03	0.928459703155E-03	0.958650896478E-03	0.989823832089E-03
0.102201043380E-02			
0.105524366350E-02	0.108955755493E-02	0.112498724850E-02	0.116156902732E-02
0.119934035433E-02			
0.123833991067E-02	0.127860763528E-02	0.132018476584E-02	0.136311388097E-02
0.140743894383E-02			
0.145320534715E-02	0.150045995974E-02	0.154925117444E-02	0.159962895772E-02
0.165164490084E-02			
0.170535227266E-02	0.176080607424E-02	0.181806309510E-02	0.187718197144E-02
0.193822324615E-02			
0.200124943084E-02	0.206632506983E-02	0.213351680625E-02	0.220289345031E-02
0.227452604977E-02			
0.234848796266E-02	0.242485493244E-02	0.250370516557E-02	0.258511941158E-02
0.266918104576E-02			
0.275597615457E-02	0.284559362380E-02	0.293812522956E-02	0.303366573230E-02
0.313231297384E-02			
0.323416797759E-02	0.333933505196E-02	0.344792189722E-02	0.356003971581E-02
0.367580332615E-02			
0.379533128031E-02	0.391874598535E-02	0.404617382872E-02	0.417774530766E-02
0.431359516287E-02			
0.445386251646E-02	0.459869101447E-02	0.474822897393E-02	0.490262953478E-02
0.506205081668E-02			
0.522665608097E-02	0.539661389781E-02	0.557209831886E-02	0.575328905551E-02
0.594037166289E-02			
0.613353772995E-02	0.633298507563E-02	0.653891795142E-02	0.675154725060E-02
0.697109072414E-02			
0.719777320374E-02	0.743182683208E-02	0.767349130052E-02	0.792301409459E-02
0.818065074744E-02			
0.844666510152E-02	0.872132957877E-02	0.900492545962E-02	0.929774317102E-02
0.960008258391E-02			
0.991225332026E-02	0.102345750702E-01	0.105673779193E-01	0.109110026869E-01
0.112658012746E-01			
0.116321370274E-01	0.120103851049E-01	0.124009328662E-01	0.128041802665E-01
0.132205402662E-01			
0.136504392545E-01	0.140943174853E-01	0.145526295289E-01	0.150258447369E-01
0.155144477228E-01			
0.160189388589E-01	0.165398347883E-01	0.170776689537E-01	0.176329921445E-01
0.182063730601E-01			

0.187983988927E-01	0.194096759284E-01	0.200408301684E-01	0.206925079697E-01
0.213653767074E-01			
0.220601254578E-01	0.227774657044E-01	0.235181320663E-01	0.242828830506E-01
0.250725018290E-01			
0.258877970402E-01	0.267296036178E-01	0.275987836452E-01	0.284962272388E-01
0.294228534593E-01			
0.303796112527E-01	0.313674804228E-01	0.323874726339E-01	0.334406324470E-01
0.345280383900E-01			
0.356508040616E-01	0.368100792718E-01	0.380070512198E-01	0.392429457094E-01
0.405190284047E-01			
0.418366061258E-01	0.431970281875E-01	0.446016877807E-01	0.460520233998E-01
0.475495203150E-01			
0.490957120941E-01	0.506921821726E-01	0.523405654753E-01	0.540425500908E-01
0.557998790001E-01			
0.576143518615E-01	0.594878268538E-01	0.614222225791E-01	0.634195200277E-01
0.654817646066E-01			
0.676110682346E-01	0.698096115046E-01	0.720796459171E-01	0.744234961856E-01
0.768435626176E-01			
0.793423235727E-01	0.819223380004E-01	0.845862480609E-01	0.873367818310E-01
0.901767560975E-01			
0.931090792423E-01	0.961367542205E-01	0.992628816359E-01	0.102490662916E+00
0.105823403591E+00			
0.109264516679E+00	0.112817526180E+00	0.116486070686E+00	0.120273907107E+00
0.124184914520E+00			
0.128223098136E+00	0.132392593410E+00	0.136697670269E+00	0.141142737487E+00
0.145732347202E+00			
0.150471199575E+00	0.155364147606E+00	0.160416202100E+00	0.165632536802E+00
0.171018493697E+00			
0.176579588473E+00	0.182321516178E+00	0.188250157047E+00	0.194371582528E+00
0.200692061494E+00			
0.207218066668E+00	0.213956281250E+00	0.220913605761E+00	0.228097165108E+00
0.235514315885E+00			
0.243172653901E+00	0.251080021964E+00	0.259244517910E+00	0.267674502897E+00
0.276378609965E+00			
0.285365752880E+00	0.294645135264E+00	0.304226260013E+00	0.314118939037E+00
0.324333303303E+00			
0.334879813214E+00	0.345769269317E+00	0.357012823366E+00	0.368621989744E+00
0.380608657251E+00			
0.392985101282E+00	0.405763996398E+00	0.418958429304E+00	0.432581912251E+00
0.446648396878E+00			
0.461172288493E+00	0.476168460830E+00	0.491652271281E+00	0.507639576621E+00
0.524146749247E+00			
0.541190693946E+00	0.558788865208E+00	0.576959285097E+00	0.595720561711E+00
0.615091908236E+00			
0.635093162626E+00	0.655744807911E+00	0.677067993181E+00	0.699084555241E+00
0.721817040975E+00			
0.745288730434E+00	0.769523660679E+00	0.794546650398E+00	0.820383325317E+00
0.847060144451E+00			
0.874604427192E+00	0.903044381293E+00	0.932409131752E+00	0.962728750640E+00
0.994034287897E+00			
0.102635780313E+01	0.105973239844E+01	0.109419225232E+01	0.112977265469E+01
0.116651004299E+01			

0.120444203950E+01	0.124360748991E+01	0.128404650306E+01	0.132580049203E+01
0.136891221656E+01			
0.141342582683E+01	0.145938690865E+01	0.150684253020E+01	0.155584129017E+01
0.160643336757E+01			
0.165867057312E+01	0.171260640229E+01	0.176829609006E+01	0.182579666755E+01
0.188516702037E+01			
0.194646794896E+01	0.200976223081E+01	0.207511468481E+01	0.214259223759E+01
0.221226399204E+01			
0.228420129814E+01	0.235847782597E+01	0.243516964118E+01	0.251435528291E+01
0.259611584416E+01			
0.268053505490E+01	0.276769936777E+01	0.285769804664E+01	0.295062325803E+01
0.304657016548E+01			
0.314563702700E+01	0.324792529571E+01	0.335353972374E+01	0.346258846950E+01
0.357518320843E+01			
0.369143924737E+01	0.381147564268E+01	0.393541532212E+01	0.406338521073E+01
0.419551636088E+01			
0.433194408640E+01	0.447280810121E+01	0.461825266237E+01	0.476842671782E+01
0.492348405891E+01			
0.508358347792E+01	0.524888893063E+01	0.541956970428E+01	0.559580059089E+01
0.577776206629E+01			
0.596564047493E+01	0.615962822072E+01		
aepotential			
0.383328804076E+05	0.370762948344E+05	0.358217095976E+05	0.345726252882E+05
0.333330009801E+05			
0.321073100859E+05	0.308990027475E+05	0.297112579734E+05	0.285470185480E+05
0.274086534757E+05			
0.262983217747E+05	0.252177255157E+05	0.241682639899E+05	0.231510336720E+05
0.221668206654E+05			
0.212161523450E+05	0.202993089195E+05	0.194163512706E+05	0.185671453571E+05
0.177513823771E+05			
0.169686112716E+05	0.162182385991E+05	0.154995933650E+05	0.148118476947E+05
0.141542106924E+05			
0.135257328829E+05	0.129254549012E+05	0.123524491628E+05	0.118056441197E+05
0.112840588384E+05			
0.107867322799E+05	0.103126055590E+05	0.986067799936E+04	0.943003808334E+04
0.901968771335E+04			
0.862866725594E+04	0.825619406765E+04	0.790128698326E+04	0.756316280024E+04
0.724098179375E+04			
0.693401931363E+04	0.664146376933E+04	0.636265689571E+04	0.609691269687E+04
0.584355585206E+04			
0.560201130594E+04	0.537162896015E+04	0.515192505606E+04	0.494229805610E+04
0.474228363281E+04			
0.455140325769E+04	0.436917315736E+04	0.419518650353E+04	0.402901920288E+04
0.387029444363E+04			
0.371861679843E+04	0.357369980447E+04	0.343515531604E+04	0.330264392012E+04
0.317595847826E+04			
0.305476231086E+04	0.293879848658E+04	0.282781727187E+04	0.272155582268E+04
0.261982242199E+04			
0.252237467965E+04	0.242905308330E+04	0.233960505836E+04	0.225387269463E+04
0.217170272589E+04			
0.209290416947E+04	0.201733557851E+04	0.194484567833E+04	0.187528387113E+04
0.180853248493E+04			

0.174445352079E+04	0.168292896943E+04	0.162385135846E+04	0.156710537427E+04
0.151258783624E+04			
0.146020339252E+04	0.140985792646E+04	0.136146299958E+04	0.131493418458E+04
0.127019101775E+04			
0.122715672443E+04	0.118575962480E+04	0.114593099862E+04	0.110760396171E+04
0.107070651667E+04			
0.103520451183E+04	0.100101088459E+04	0.968091802877E+03	0.936381867802E+03
0.905845183464E+03			
0.876421028969E+03	0.848073384973E+03	0.820755931088E+03	0.794426431624E+03
0.769046414655E+03			
0.744579446659E+03	0.720989524679E+03	0.698240135630E+03	0.676301958222E+03
0.655139332074E+03			
0.634726249551E+03	0.615030754835E+03	0.596027584404E+03	0.577689131883E+03
0.559990127135E+03			
0.542906895649E+03	0.526416244883E+03	0.510495661724E+03	0.495123583751E+03
0.480280223531E+03			
0.465945613541E+03	0.452100833559E+03	0.438728114109E+03	0.425809982475E+03
0.413329790354E+03			
0.401271728896E+03	0.389620237479E+03	0.378360801376E+03	0.367478907923E+03
0.356961416298E+03			
0.346794990453E+03	0.336967464448E+03	0.327465172449E+03	0.318279061795E+03
0.309395547322E+03			
0.300805595705E+03	0.292497550174E+03	0.284462130405E+03	0.276689924398E+03
0.269170828502E+03			
0.261896959957E+03	0.254858820273E+03	0.248048717086E+03	0.241458664403E+03
0.235080585995E+03			
0.228907443808E+03	0.222931945973E+03	0.217147278061E+03	0.211546657772E+03
0.206123890067E+03			
0.200872609013E+03	0.195786939906E+03	0.190861088430E+03	0.186089538866E+03
0.181466841308E+03			
0.176987908270E+03	0.172647655838E+03	0.168441295856E+03	0.164364122488E+03
0.160411626224E+03			
0.156579452144E+03	0.152863354393E+03	0.149259278236E+03	0.145763250400E+03
0.142371469496E+03			
0.139080232904E+03	0.135885937598E+03	0.132785169440E+03	0.129774593464E+03
0.126850839457E+03			
0.124010930009E+03	0.121251702096E+03	0.118570267127E+03	0.115963708692E+03
0.113429322567E+03			
0.110964391233E+03	0.108566288318E+03	0.106232519107E+03	0.103960611342E+03
0.101748181283E+03			
0.995929544000E+02	0.974926385374E+02	0.954450836786E+02	0.934481682153E+02
0.914998227731E+02			
0.895980661822E+02	0.877409460661E+02	0.859265662312E+02	0.841530966237E+02
0.824187431453E+02			
0.807217668397E+02	0.790604709806E+02	0.774332032093E+02	0.758383570515E+02
0.742743659073E+02			
0.727397031261E+02	0.712328774177E+02	0.697524425804E+02	0.682969771870E+02
0.668651058824E+02			
0.654554792603E+02	0.640667833792E+02	0.626977361811E+02	0.613470840671E+02
0.600136053606E+02			
0.586961078333E+02	0.573934195701E+02	0.561044158555E+02	0.548279681501E+02
0.535630013651E+02			

0.523084550664E+02	0.510632893537E+02	0.498265006258E+02	0.485970926303E+02
0.473741113791E+02			
0.461566141511E+02	0.449436834936E+02	0.437344274477E+02	0.425279746080E+02
0.413234757930E+02			
0.401201100510E+02	0.389170674315E+02	0.377135731765E+02	0.365088662094E+02
0.353022121371E+02			
0.340928978788E+02	0.328802340596E+02	0.316635541436E+02	0.304422146074E+02
0.292155955188E+02			
0.279831025433E+02	0.267441625748E+02	0.254982293340E+02	0.242447812557E+02
0.229833209882E+02			
0.217133780960E+02	0.204345078153E+02	0.191462919597E+02	0.178483392299E+02
0.165402865084E+02			
0.152217979003E+02	0.138925669163E+02	0.125523146984E+02	0.112007935790E+02
0.983778478330E+01			
0.846310060664E+01	0.707658465253E+01	0.567811249650E+01	0.426759239333E+01
0.284496588089E+01			
0.141020946990E+01	-0.366652636038E-01	-0.149560960598E+01	-0.296653640043E+01 -
0.444931861799E+01			
-0.594378617581E+01	-0.744972422562E+01	-0.896686921767E+01	-0.104949048103E+02 -
0.120334571378E+02			
-0.135820885573E+02	-0.151402898688E+02	-0.167074716821E+02	-0.182829529802E+02 -
0.198659478184E+02			
-0.214555494532E+02	-0.230507112270E+02	-0.246502241160E+02	-0.262526907866E+02 -
0.278564955907E+02			
-0.294597710374E+02	-0.310603607581E+02	-0.326557801964E+02	-0.342431765206E+02 -
0.358192903254E+02			
-0.373804228940E+02	-0.389224139660E+02	-0.404406364483E+02	-0.419300157762E+02 -
0.433850825586E+02			
-0.448000675559E+02	-0.461690475413E+02	-0.474861492314E+02	-0.487458172385E+02 -
0.499431493679E+02			
-0.510743076105E+02	-0.521370166218E+02	-0.531311805536E+02	-0.540596712709E+02 -
0.549293631741E+02			
-0.557524765683E+02	-0.565481669054E+02	-0.573439201877E+02	-0.581754999681E+02 -
0.590828863845E+02			
-0.600984576118E+02	-0.612246895190E+02	-0.624054074814E+02	-0.635079323312E+02 -
0.643429504949E+02			
-0.647341329964E+02	-0.646074104177E+02	-0.640374463782E+02	-0.632091678036E+02 -
0.623198219118E+02			
-0.614972752054E+02	-0.607833039597E+02	-0.601643930087E+02	-0.596083078232E+02 -
0.590852923916E+02			
-0.585747946239E+02	-0.580649269373E+02	-0.575497821005E+02	-0.570268365480E+02 -
0.564950807490E+02			
-0.559539031478E+02	-0.554025554700E+02	-0.548399926931E+02	-0.542649354782E+02 -
0.536760012662E+02			
-0.530718627590E+02	-0.524513698152E+02	-0.518136366584E+02	-0.511580884872E+02 -
0.504844864280E+02			
-0.497929153596E+02	-0.490837725865E+02	-0.483577386859E+02	-0.476157420048E+02 -
0.468589260287E+02			
-0.460886089348E+02	-0.453062468303E+02	-0.445133911429E+02	-0.437116507593E+02 -
0.429026500773E+02			
-0.420879861315E+02	-0.412691919596E+02	-0.404476909331E+02	-0.396247719317E+02 -
0.388015521266E+02			

-0.379789658056E+02	-0.371577579970E+02	-0.363384972642E+02	-0.355216049809E+02	-
0.347074009332E+02				
-0.338961613729E+02	-0.330881837015E+02	-0.322838503173E+02	-0.314836839549E+02	-
0.306883864908E+02				
-0.298988653613E+02	-0.291162209872E+02	-0.283417366413E+02	-0.275768340325E+02	-
0.268230227561E+02				
-0.260818408398E+02	-0.253547924009E+02	-0.246432867362E+02	-0.239485824283E+02	-
0.232717393566E+02				
-0.226135808533E+02	-0.219746677937E+02	-0.213552858717E+02	-0.207554467100E+02	-
0.201749026405E+02				
-0.196131739946E+02	-0.190695866871E+02	-0.185433169571E+02	-0.180334395474E+02	-
0.175389754993E+02				
-0.170589361410E+02	-0.165923606379E+02	-0.161383454990E+02	-0.156960654681E+02	-
0.152647861295E+02				
-0.148438692120E+02	-0.144327719526E+02	-0.140310420185E+02	-0.136383094263E+02	-
0.132542767148E+02				
-0.128787083902E+02	-0.125114204025E+02	-0.121522701780E+02	-0.118011475320E+02	-
0.114579666292E+02				
-0.111226590432E+02	-0.107951678898E+02	-0.104754429619E+02	-0.101634367651E+02	-
0.985910134803E+01				
-0.956238582002E+01	-0.927323445724E+01			
core charge-density				
0.210201468504E-05	0.224075660865E-05	0.238865454703E-05	0.254631257969E-05	
0.271437462578E-05				
0.289352706997E-05	0.308450156137E-05	0.328807799655E-05	0.350508769917E-05	
0.373641680884E-05				
0.398300989302E-05	0.424587379676E-05	0.452608174576E-05	0.482477771943E-05	
0.514318111173E-05				
0.548259169866E-05	0.584439493255E-05	0.623006758455E-05	0.664118375830E-05	
0.707942129902E-05				
0.754656862406E-05	0.804453200246E-05	0.857534331313E-05	0.914116831281E-05	
0.974431544755E-05				
0.103872452429E-04	0.110725803114E-04	0.118031160169E-04	0.125818318394E-04	
0.134119034870E-04				
0.142967158011E-04	0.152398765106E-04	0.162452308880E-04	0.173168773664E-04	
0.184591841821E-04				
0.196768071083E-04	0.209747083513E-04	0.223581766855E-04	0.238328489087E-04	
0.254047327025E-04				
0.270802309904E-04	0.288661678914E-04	0.307698163727E-04	0.327989277127E-04	
0.349617628907E-04				
0.372671260325E-04	0.397244000403E-04	0.423435845547E-04	0.451353363953E-04	
0.481110126455E-04				
0.512827165500E-04	0.546633464086E-04	0.582666476625E-04	0.621072683763E-04	
0.662008183409E-04				
0.705639320258E-04	0.752143356366E-04	0.801709185365E-04	0.854538093201E-04	
0.910844568382E-04				
0.970857164856E-04	0.103481942106E-03	0.110299083866E-03	0.117564792478E-03	
0.125308530201E-03				
0.133561689026E-03	0.142357716535E-03	0.151732249904E-03	0.161723258590E-03	
0.172371196249E-03				
0.183719162469E-03	0.195813074966E-03	0.208701852883E-03	0.222437611932E-03	
0.237075872101E-03				

0.252675778750E-03	0.269300337936E-03	0.287016666869E-03	0.305896260460E-03
0.326015274982E-03			
0.347454829922E-03	0.370301329168E-03	0.394646802758E-03	0.420589270471E-03
0.448233128653E-03			
0.477689561701E-03	0.509076979780E-03	0.542521484393E-03	0.578157363538E-03
0.616127618296E-03			
0.656584522829E-03	0.699690219758E-03	0.745617353275E-03	0.794549742109E-03
0.846683095013E-03			
0.902225771137E-03	0.961399588301E-03	0.102444068184E-02	0.109160041724E-02
0.116314635984E-02			
0.123936330490E-02	0.132055437184E-02	0.140704216640E-02	0.149917001484E-02
0.159730327436E-02			
0.170183072449E-02	0.181316604393E-02	0.193174937813E-02	0.205804900283E-02
0.219256308907E-02			
0.233582157576E-02	0.248838815581E-02	0.265086238248E-02	0.282388190278E-02
0.300812482511E-02			
0.320431222877E-02	0.341321082327E-02	0.363563576573E-02	0.387245364528E-02
0.412458564339E-02			
0.439301088000E-02	0.467876995521E-02	0.498296869724E-02	0.530678212746E-02
0.565145865399E-02			
0.601832450569E-02	0.640878841904E-02	0.682434659052E-02	0.726658790853E-02
0.773719947716E-02			
0.823797244864E-02	0.877080817630E-02	0.933772470611E-02	0.994086362061E-02
0.105824972520E-01			
0.112650362817E-01	0.119910377420E-01	0.127632134386E-01	0.135844388099E-01
0.144577622428E-01			
0.153864148621E-01	0.163738208108E-01	0.174236080418E-01	0.185396196362E-01
0.197259256691E-01			
0.209868356375E-01	0.223269114704E-01	0.237509811352E-01	0.252641528577E-01
0.268718299690E-01			
0.285797263952E-01	0.303938827986E-01	0.323206833829E-01	0.343668733704E-01
0.365395771561E-01			
0.388463171409E-01	0.412950332459E-01	0.438941031012E-01	0.466523629020E-01
0.495791289190E-01			
0.526842196442E-01	0.559779785470E-01	0.594712974124E-01	0.631756402168E-01
0.671030674994E-01			
0.712662611744E-01	0.756785497050E-01	0.803539335818E-01	0.853071109950E-01
0.905535036121E-01			
0.961092823309E-01	0.101991392883E+00	0.108217581132E+00	0.114806417888E+00
0.121777323063E+00			
0.129150588940E+00	0.136947402321E+00	0.145189865298E+00	0.153901014348E+00
0.163104837441E+00			
0.172826288801E+00	0.183091300956E+00	0.193926793631E+00	0.205360679068E+00
0.217421863244E+00			
0.230140242488E+00	0.243546694909E+00	0.257673066023E+00	0.272552147930E+00
0.288217651333E+00			
0.304704169661E+00	0.322047134501E+00	0.340282761509E+00	0.359447985920E+00
0.379580386758E+00			
0.400718098756E+00	0.422899711031E+00	0.446164151468E+00	0.470550555770E+00
0.496098120115E+00			
0.522845936321E+00	0.550832808457E+00	0.580097049822E+00	0.610676259199E+00
0.642607075470E+00			

0.675924909478E+00	0.710663652386E+00	0.746855359644E+00	0.784529909866E+00
0.823714638197E+00			
0.864433943583E+00	0.906708869968E+00	0.950556661364E+00	0.995990291126E+00
0.104301796610E+01			
0.109164260663E+01	0.114186130363E+01	0.119366475489E+01	0.124703668237E+01
0.130195323381E+01			
0.135838237157E+01	0.141628325300E+01	0.147560560673E+01	0.153628911031E+01
0.159826277524E+01			
0.166144434603E+01	0.172573972094E+01	0.179104240282E+01	0.185723298888E+01
0.192417870954E+01			
0.199173302681E+01	0.205973530356E+01	0.212801055565E+01	0.219636929929E+01
0.226460750673E+01			
0.233250668331E+01	0.239983407943E+01	0.246634305055E+01	0.253177357859E+01
0.259585296687E+01			
0.265829672079E+01	0.271880962466E+01	0.277708702402E+01	0.283281632102E+01
0.288567868816E+01			
0.293535100328E+01	0.298150800569E+01	0.302382467012E+01	0.306197879142E+01
0.309565376873E+01			
0.312454157399E+01	0.314834588406E+01	0.316678535175E+01	0.317959698546E+01
0.318653960182E+01			
0.318739731118E+01	0.318198299014E+01	0.317014169094E+01	0.315175393310E+01
0.312673881894E+01			
0.309505691139E+01	0.305671281059E+01	0.301175736450E+01	0.296028944882E+01
0.290245725317E+01			
0.283845901348E+01	0.276854313525E+01	0.269300765895E+01	0.261219902737E+01
0.252651012486E+01			
0.243637757120E+01	0.234227826665E+01	0.224472520121E+01	0.214426255840E+01
0.204146016301E+01			
0.193690734182E+01	0.183120628627E+01	0.172496502410E+01	0.161879013108E+01
0.151327931464E+01			
0.140901403128E+01	0.130655229510E+01	0.120642184097E+01	0.110911380351E+01
0.101507706531E+01			
0.924713415194E+00	0.838373638610E+00	0.756354633044E+00	0.678897593873E+00
0.606187236204E+00			
0.538351896201E+00	0.475464205711E+00	0.417541937039E+00	0.364548734625E+00
0.316394937835E+00			
0.272939426163E+00	0.233993808891E+00	0.199329712126E+00	0.168688507801E+00
0.141791603050E+00			
0.118349382675E+00	0.980680112101E-01	0.806544732036E-01	0.658206201563E-01
0.532867335828E-01			
0.427847430624E-01	0.340610365053E-01	0.268787587444E-01	0.210195270580E-01
0.162845404237E-01			
0.124951006491E-01	0.949259332511E-02	0.713799597409E-02	0.531099207142E-02
0.390877476465E-02			
0.284462447136E-02	0.204634105555E-02	0.145460472883E-02	0.102133087181E-02
0.708073371823E-03			
0.484519558958E-03	0.327108147341E-03	0.217790418137E-03	0.142944771955E-03
0.924461358421E-04			
0.588847724706E-04	0.369238866702E-04	0.227819974745E-04	0.138241719848E-04
0.824565667318E-05			
0.483190804996E-05	0.278022714905E-05	0.156986819816E-05	0.869385578152E-06
0.471916061192E-06			

0.250927600539E-06	0.130611975426E-06	0.665087883488E-07	0.331083796014E-07
0.161009521940E-07			
0.764367183337E-08	0.353965782606E-08	0.159768325477E-08	0.702329008374E-09
0.300434573515E-09			
0.124952631311E-09	0.504825516273E-10	0.197942287197E-10	0.752531117071E-11
0.277122464384E-11			
0.987502501209E-12	0.340146596908E-12	0.113131008036E-12	0.362906131860E-13
0.112149279727E-13			
0.333474817006E-14	0.952907632269E-15	0.261335374456E-15	0.686949545635E-16
0.172834778617E-16			
0.415621394002E-17	0.953862737148E-18	0.208610125967E-18	0.434075915325E-19
0.857974812426E-20			
0.160819058566E-20	0.285369383433E-21	0.478534578100E-22	0.756937854171E-23
0.112726955183E-23			
0.157750098174E-24	0.207020098419E-25	0.254246621267E-26	0.291586617747E-27
0.311594459329E-28			
0.309549927396E-29	0.285211910372E-30	0.243133423243E-31	0.191280930878E-32
0.138523480089E-33			
0.920954428784E-35	0.560553051251E-36	0.311473608922E-37	0.157533893086E-38
0.723029790652E-40			
0.300197305477E-41	0.112388359667E-42		
kinetic energy-density			
0.187150680411E-01	0.190026985814E-01	0.193019283134E-01	0.196129173070E-01
0.199362223466E-01			
0.202724419468E-01	0.206221543328E-01	0.209860257628E-01	0.213647226431E-01
0.217589775679E-01			
0.221695415277E-01	0.225972126098E-01	0.230428378309E-01	0.235073034297E-01
0.239915471047E-01			
0.244965558870E-01	0.250233707629E-01	0.255730888854E-01	0.261468664952E-01
0.267459235750E-01			
0.273715465014E-01	0.280250895166E-01	0.287079913502E-01	0.294217584179E-01
0.301679710924E-01			
0.309483397777E-01	0.317646148821E-01	0.326186941670E-01	0.335125544355E-01
0.344482822830E-01			
0.354280835526E-01	0.364543418389E-01	0.375294924859E-01	0.386561676031E-01
0.398371591378E-01			
0.410753556967E-01	0.423738802306E-01	0.437360347427E-01	0.451652704063E-01
0.466652725530E-01			
0.482399624092E-01	0.498934420309E-01	0.516300997537E-01	0.534545677412E-01
0.553717643623E-01			
0.573869038141E-01	0.595054977624E-01	0.617333975662E-01	0.640768238205E-01
0.665423375565E-01			
0.691369324164E-01	0.718680440951E-01	0.747434678602E-01	0.777715799423E-01
0.809612451375E-01			
0.843218068714E-01	0.878632235574E-01	0.915961919098E-01	0.955317657996E-01
0.996819738419E-01			
0.104059410495E+00	0.108677558667E+00	0.113550751509E+00	0.118694009125E+00
0.124123562101E+00			
0.129856352963E+00	0.135910725070E+00	0.142305909177E+00	0.149062372919E+00
0.156201887226E+00			
0.163747683412E+00	0.171724270648E+00	0.180157855663E+00	0.189076184814E+00
0.198508756288E+00			

0.208487008025E+00	0.219044218093E+00	0.230215862622E+00	0.242039644974E+00
0.254555573574E+00			
0.267806271633E+00	0.281836963724E+00	0.296695778960E+00	0.312433876512E+00
0.329105665113E+00			
0.346768934502E+00	0.365485178087E+00	0.385319738759E+00	0.406342299553E+00
0.428626319638E+00			
0.452250811218E+00	0.477299133274E+00	0.503860065302E+00	0.532028116709E+00
0.561903690270E+00			
0.593593578349E+00	0.627211198034E+00	0.662877454503E+00	0.700720535203E+00
0.740876913977E+00			
0.783491674899E+00	0.828719021384E+00	0.876723053688E+00	0.927677946205E+00
0.981769171581E+00			
0.103919370898E+01	0.110016096119E+01	0.116489360136E+01	0.123362833680E+01
0.130661661966E+01			
0.138412586602E+01	0.146644018669E+01	0.155386160506E+01	0.164671104314E+01
0.174532941130E+01			
0.185007923747E+01	0.196134535531E+01	0.207953691172E+01	0.220508839009E+01
0.233846140011E+01			
0.248014627968E+01	0.263066369200E+01	0.279056681584E+01	0.296044277199E+01
0.314091518937E+01			
0.333264611749E+01	0.353633838721E+01	0.375273804219E+01	0.398263660637E+01
0.422687458666E+01			
0.448634348549E+01	0.476198914713E+01	0.505481485628E+01	0.536588521073E+01
0.569632846347E+01			
0.604734168350E+01	0.642019328426E+01	0.681622831347E+01	0.723687181489E+01
0.768363431181E+01			
0.815811524083E+01	0.866200956136E+01	0.919711174825E+01	0.976532184364E+01
0.103686508668E+02			
0.110092276427E+02	0.116893036632E+02	0.124112613988E+02	0.131776195862E+02
0.139910413414E+02			
0.148543415690E+02	0.157704940605E+02	0.167426403621E+02	0.177740977546E+02
0.188683678238E+02			
0.200291458399E+02	0.212603296720E+02	0.225660297404E+02	0.239505785547E+02
0.254185412760E+02			
0.269747259644E+02	0.286241940618E+02	0.303722720010E+02	0.322245613189E+02
0.341869521407E+02			
0.362656310230E+02	0.384670962459E+02	0.407981680571E+02	0.432659994877E+02
0.458780892017E+02			
0.486422929258E+02	0.515668348377E+02	0.546603175459E+02	0.579317349340E+02
0.613904801615E+02			
0.650463580181E+02	0.689095912942E+02	0.729908305915E+02	0.773011621109E+02
0.818521105386E+02			
0.866556486375E+02	0.917241956191E+02	0.970706219281E+02	0.102708246459E+03
0.108650834969E+03			
0.114912594297E+03	0.121508163679E+03	0.128452604363E+03	0.135761383144E+03
0.143450355641E+03			
0.151535742131E+03	0.160034099930E+03	0.168962291836E+03	0.178337447425E+03
0.188176919071E+03			
0.198498232491E+03	0.209319028881E+03	0.220657000669E+03	0.232529819785E+03
0.244955056061E+03			
0.257950088896E+03	0.271532008273E+03	0.285717504386E+03	0.300522754903E+03
0.315963285134E+03			

0.332053838257E+03	0.348808220954E+03	0.366239132464E+03	0.384358000459E+03
0.403174789793E+03			
0.422697798265E+03	0.442933458751E+03	0.463886103536E+03	0.485557742440E+03
0.507947812996E+03			
0.531052932116E+03	0.554866632342E+03	0.579379095189E+03	0.604576875584E+03
0.630442628426E+03			
0.656954821546E+03	0.684087465758E+03	0.711809833678E+03	0.740086192341E+03
0.768875546863E+03			
0.798131392336E+03	0.827801489661E+03	0.857827658044E+03	0.888145600146E+03
0.918684755398E+03			
0.949368191402E+03	0.980112541578E+03	0.101082798537E+04	0.104141828954E+04
0.107178090505E+04			
0.110180713074E+04	0.113138235160E+04	0.116038634783E+04	0.118869368921E+04
0.121617421709E+04			
0.124269360739E+04	0.126811403533E+04	0.129229492606E+04	0.131509380150E+04
0.133636722257E+04			
0.135597181755E+04	0.137376540057E+04	0.138960817150E+04	0.140336398576E+04
0.141490169432E+04			
0.142409653034E+04	0.143083154366E+04	0.143499905050E+04	0.143650210136E+04
0.143525592873E+04			
0.143118937160E+04	0.142424624166E+04	0.141438661835E+04	0.140158804204E+04
0.138584658853E+04			
0.136717779395E+04	0.134561741249E+04	0.132122198211E+04	0.129406917573E+04
0.126425792178E+04			
0.123190827482E+04	0.119716102057E+04	0.116017700834E+04	0.112113619678E+04
0.108023641419E+04			
0.103769182805E+04	0.993731131746E+03	0.948595453821E+03	0.902536005198E+03
0.855811483068E+03			
0.808685257261E+03	0.761422372854E+03	0.714286418421E+03	0.667536262912E+03
0.621422839948E+03			
0.576185893651E+03	0.532050870231E+03	0.489225992918E+03	0.447899597545E+03
0.408237796197E+03			
0.370382528656E+03	0.334450064146E+03	0.300530043929E+03	0.268685226036E+03
0.238952207605E+03			
0.211343498969E+03	0.185851228999E+03	0.162452188108E+03	0.141112750315E+03
0.121791110847E+03			
0.104434777425E+03	0.889742185534E+02	0.753170557654E+02	0.633476452322E+02
0.529332849457E+02			
0.439337166013E+02	0.362092956134E+02	0.296256559048E+02	0.240555383003E+02
0.193793213930E+02			
0.154852579438E+02	0.122697443411E+02	0.963761240902E+01	0.750235296064E+01
0.578620179852E+01			
0.442005835664E+01	0.334323785953E+01	0.250307632968E+01	0.185441692241E+01
0.135900892802E+01			
0.984850381857E+00	0.705502792228E+00	0.499403133335E+00	0.349194330804E+00
0.241091269916E+00			
0.164295078647E+00	0.110464301123E+00	0.732477230045E-01	0.478802256025E-01
0.308402279439E-01			
0.195650888517E-01	0.122192971365E-01	0.750933655477E-02	0.453870368119E-02
0.269658352619E-02			
0.157404513698E-02	0.902201484903E-03	0.507489172708E-03	0.279983567033E-03
0.151411198640E-03			

0.802105783757E-04	0.415980630557E-04	0.211053671140E-04	0.104686890169E-04
0.507297848390E-05			
0.239986650930E-05	0.110748150676E-05	0.498164580656E-06	0.218246379238E-06
0.930462196847E-07			
0.385705455035E-07	0.155322268676E-07	0.607064880761E-08	0.230064087530E-08
0.844596878183E-09			
0.300052065756E-09	0.103046733453E-09	0.341735409287E-10	0.109313728196E-10
0.336885124397E-11			
0.999049233363E-12	0.284739053522E-12	0.778933982620E-13	0.204252292154E-13
0.512679043400E-14			
0.123003166906E-14	0.281668714654E-15	0.614683195298E-16	0.127635706458E-16
0.251766102280E-17			
0.470977863823E-18	0.834128701543E-19	0.139611967675E-19	0.220431009579E-20
0.327688784500E-21			
0.457764137294E-22	0.599706635674E-23	0.735276399386E-24	0.841871972901E-25
0.898181817836E-26			
0.890868262820E-27	0.819539719856E-28	0.697552702429E-29	0.547953332399E-30
0.396226358746E-31			
0.263035065187E-32	0.159865238670E-33	0.887003495144E-35	0.447969335314E-36
0.205306373339E-37			
0.851186687055E-39	0.318206326318E-40		
mkinetic energy-density pseudized			
0.242933787425E-06	0.258989864073E-06	0.276107125328E-06	0.294355707424E-06
0.313810382066E-06			
0.334550862801E-06	0.356662131637E-06	0.380234787243E-06	0.405365416173E-06
0.432156988617E-06			
0.460719280311E-06	0.491169322334E-06	0.523631880625E-06	0.558239967207E-06
0.595135385182E-06			
0.634469309760E-06	0.676402907683E-06	0.721107997585E-06	0.768767754007E-06
0.819577457932E-06			
0.873745296929E-06	0.931493218182E-06	0.993057837892E-06	0.105869141079E-05
0.112866286373E-05			
0.120325889757E-05	0.128278516192E-05	0.136756750751E-05	0.145795332130E-05
0.155431294989E-05			
0.165704121697E-05	0.176655904107E-05	0.188331516022E-05	0.200778797061E-05
0.214048748678E-05			
0.228195743133E-05	0.243277746278E-05	0.259356555066E-05	0.276498050754E-05
0.294772468852E-05			
0.314254686896E-05	0.335024531257E-05	0.357167104219E-05	0.380773132677E-05
0.405939339878E-05			
0.432768841736E-05	0.461371569338E-05	0.491864719373E-05	0.524373234334E-05
0.559030314455E-05			
0.595977963482E-05	0.635367570519E-05	0.677360530328E-05	0.722128904623E-05
0.769856127075E-05			
0.820737754905E-05	0.874982270164E-05	0.932811933957E-05	0.994463697130E-05
0.106019017115E-04			
0.113026066316E-04	0.120496227939E-04	0.128460110160E-04	0.136950344115E-04
0.146001717606E-04			
0.155651317639E-04	0.165938682378E-04	0.176905963154E-04	0.188598097170E-04
0.201062991627E-04			
0.214351720014E-04	0.228518731377E-04	0.243622073412E-04	0.259723630312E-04
0.276889376321E-04			

0.295189646058E-04	0.314699422699E-04	0.335498645208E-04	0.357672535872E-04
0.381311949487E-04			
0.406513745615E-04	0.433381185448E-04	0.462024354903E-04	0.492560615674E-04
0.525115086099E-04			
0.559821153802E-04	0.596821022222E-04	0.636266293256E-04	0.678318588411E-04
0.723150211012E-04			
0.770944852161E-04	0.821898343371E-04	0.876219458924E-04	0.934130771262E-04
0.995869562912E-04			
0.106168879867E-03	0.113185816205E-03	0.120666516021E-03	0.128641630188E-03
0.137143835323E-03			
0.146207967660E-03	0.155871165778E-03	0.166173022762E-03	0.177155748415E-03
0.188864342192E-03			
0.201346777564E-03	0.214654198560E-03	0.228841129302E-03	0.243965697383E-03
0.260089872011E-03			
0.277279717881E-03	0.295605665831E-03	0.315142801379E-03	0.335971172326E-03
0.358176116681E-03			
0.381848612262E-03	0.407085649390E-03	0.433990628207E-03	0.462673782250E-03
0.493252630012E-03			
0.525852456329E-03	0.560606825577E-03	0.597658128777E-03	0.637158166835E-03
0.679268772317E-03			
0.724162472303E-03	0.772023195015E-03	0.823047023139E-03	0.877442996890E-03
0.935433970130E-03			
0.997257523028E-03	0.106316693500E-02	0.113343222188E-02	0.120834124164E-02
0.128820087308E-02			
0.137333827231E-02	0.146410221232E-02	0.156086451086E-02	0.166402155266E-02
0.177399591212E-02			
0.189123808310E-02	0.201622832289E-02	0.214947861787E-02	0.229153477889E-02
0.244297867491E-02			
0.260443061400E-02	0.277655188143E-02	0.296004744513E-02	0.315566883962E-02
0.336421724010E-02			
0.358654673923E-02	0.382356783990E-02	0.407625117820E-02	0.434563149178E-02
0.463281184963E-02			
0.493896816045E-02	0.526535397800E-02	0.561330562278E-02	0.598424764087E-02
0.637969862201E-02			
0.680127740039E-02	0.725070966332E-02	0.772983499435E-02	0.824061437927E-02
0.878513820531E-02			
0.936563478561E-02	0.998447944331E-02	0.106442041916E-01	0.113475080490E-01
0.120972680298E-01			
0.128965508562E-01	0.137486254355E-01	0.146569761547E-01	0.156253170447E-01
0.166576068690E-01			
0.177580651986E-01	0.189311895349E-01	0.201817735492E-01	0.215149265097E-01
0.229360939724E-01			
0.244510798168E-01	0.260660697120E-01	0.277876561036E-01	0.296228648198E-01
0.315791833964E-01			
0.336645912317E-01	0.358875916844E-01	0.382572462377E-01	0.407832108570E-01
0.434757746795E-01			
0.463459011780E-01	0.494052719525E-01	0.526663333102E-01	0.561423458042E-01
0.598474369091E-01			
0.637966570233E-01	0.680060389966E-01	0.724926613914E-01	0.772747156982E-01
0.823715777346E-01			
0.878038834706E-01	0.935936095317E-01	0.997641586447E-01	0.106340450301E+00
0.113349016925E+00			

0.120818105843E+00	0.128777787364E+00	0.137260069290E+00	0.146299018181E+00
0.155930887723E+00			
0.166194254523E+00	0.177130161708E+00	0.188782270658E+00	0.201197021250E+00
0.214423800957E+00			
0.228515123159E+00	0.243526815015E+00	0.259518215224E+00	0.276552381985E+00
0.294696311464E+00			
0.314021167009E+00	0.334602519343E+00	0.356520597904E+00	0.379860553436E+00
0.404712731863E+00			
0.431172959396E+00	0.459342838694E+00	0.489330055791E+00	0.521248697343E+00
0.555219577559E+00			
0.591370573996E+00	0.629836971117E+00	0.670761810277E+00	0.714296244428E+00
0.760599895486E+00			
0.809841211871E+00	0.862197823212E+00	0.917856888672E+00	0.977015434687E+00
0.103988067716E+01			
0.110667032240E+01	0.117761283994E+01	0.125294769975E+01	0.133292556447E+01
0.141780842672E+01			
0.150786967948E+01	0.160339410601E+01	0.170467777408E+01	0.181202781699E+01
0.192576208168E+01			
0.204620862165E+01	0.217370500983E+01	0.230859744316E+01	0.245123960790E+01
0.260199127059E+01			
0.276121655632E+01	0.292928187163E+01	0.310655342528E+01	0.329339429574E+01
0.349016098973E+01			
0.369719943168E+01	0.391484031937E+01	0.414339377710E+01	0.438314323338E+01
0.463433844763E+01			
0.489718760727E+01	0.517184841625E+01	0.545841809623E+01	0.575692222455E+01
0.606730233906E+01			
0.638940224870E+01	0.672295300265E+01	0.706755648999E+01	0.742266766740E+01
0.778757544628E+01			
0.816138231364E+01	0.854298281570E+01	0.893104109990E+01	0.932396779333E+01
0.971989659434E+01			
0.101166610716E+02	0.105117723029E+02	0.109023981461E+02	0.112853451175E+02
0.116570440592E+02			
0.120135410044E+02	0.123504948958E+02	0.126631840740E+02	0.129465237164E+02
0.131950966656E+02			
0.134032003222E+02	0.135649124562E+02	0.136741789025E+02	0.137249260851E+02
0.137112011302E+02			
0.136273419110E+02	0.134681786353E+02	0.132292674761E+02	0.129071551298E+02
0.124996709957E+02			
0.120062407678E+02	0.114282115459E+02	0.107691740143E+02	0.100352617809E+02
0.923540165197E+01			
0.838148158224E+01	0.748839557384E+01	0.657391741102E+01	0.565834855831E+01
0.476388092557E+01			
0.391361399582E+01	0.313016995527E+01	0.243386234317E+01	0.184039615305E+01
0.135811333861E+01			
0.984850381857E+00	0.705502792228E+00	0.499403133335E+00	0.349194330804E+00
0.241091269916E+00			
0.164295078647E+00	0.110464301123E+00	0.732477230045E-01	0.478802256025E-01
0.308402279439E-01			
0.195650888517E-01	0.122192971365E-01	0.750933655477E-02	0.453870368119E-02
0.269658352619E-02			
0.157404513698E-02	0.902201484903E-03	0.507489172708E-03	0.279983567033E-03
0.151411198640E-03			

0.802105783757E-04	0.415980630557E-04	0.211053671140E-04	0.104686890169E-04
0.507297848390E-05			
0.239986650930E-05	0.110748150676E-05	0.498164580656E-06	0.218246379238E-06
0.930462196847E-07			
0.385705455035E-07	0.155322268676E-07	0.607064880761E-08	0.230064087530E-08
0.844596878183E-09			
0.300052065756E-09	0.103046733453E-09	0.341735409287E-10	0.109313728196E-10
0.336885124397E-11			
0.999049233363E-12	0.284739053522E-12	0.778933982620E-13	0.204252292154E-13
0.512679043400E-14			
0.123003166906E-14	0.281668714654E-15	0.614683195298E-16	0.127635706458E-16
0.251766102280E-17			
0.470977863823E-18	0.834128701543E-19	0.139611967675E-19	0.220431009579E-20
0.327688784500E-21			
0.457764137294E-22	0.599706635674E-23	0.735276399386E-24	0.841871972901E-25
0.898181817836E-26			
0.890868262820E-27	0.819539719856E-28	0.697552702429E-29	0.547953332399E-30
0.396226358746E-31			
0.263035065187E-32	0.159865238670E-33	0.887003495144E-35	0.447969335314E-36
0.205306373339E-37			
0.851186687055E-39	0.318206326318E-40		
local pseudopotential core			
-0.882847027633E+02	-0.882817457667E+02	-0.882788819000E+02	-0.882761082305E+02 -
0.882734219178E+02			
-0.882708202114E+02	-0.882683004468E+02	-0.882658600438E+02	-0.882634965037E+02 -
0.882612074058E+02			
-0.882589904062E+02	-0.882568432348E+02	-0.882547636928E+02	-0.882527496510E+02 -
0.882507990470E+02			
-0.882489098837E+02	-0.882470802265E+02	-0.882453082020E+02	-0.882435919962E+02 -
0.882419298517E+02			
-0.882403200667E+02	-0.882387609930E+02	-0.882372510348E+02	-0.882357886459E+02 -
0.882343723294E+02			
-0.882330006352E+02	-0.882316721594E+02	-0.882303855422E+02	-0.882291394664E+02 -
0.882279326568E+02			
-0.882267638784E+02	-0.882256319348E+02	-0.882245356678E+02	-0.882234739558E+02 -
0.882224457124E+02			
-0.882214498857E+02	-0.882204854570E+02	-0.882195514398E+02	-0.882186468789E+02 -
0.882177708494E+02			
-0.882169224556E+02	-0.882161008300E+02	-0.882153051332E+02	-0.882145345520E+02 -
0.882137882990E+02			
-0.882130656122E+02	-0.882123657534E+02	-0.882116880085E+02	-0.882110316856E+02 -
0.882103961153E+02			
-0.882097806494E+02	-0.882091846607E+02	-0.882086075420E+02	-0.882080487056E+02 -
0.882075075827E+02			
-0.882069836232E+02	-0.882064762944E+02	-0.882059850811E+02	-0.882055094850E+02 -
0.882050490238E+02			
-0.882046032315E+02	-0.882041716570E+02	-0.882037538643E+02	-0.882033494320E+02 -
0.882029579527E+02			
-0.882025790328E+02	-0.882022122919E+02	-0.882018573627E+02	-0.882015138905E+02 -
0.882011815330E+02			
-0.882008599597E+02	-0.882005488520E+02	-0.882002479027E+02	-0.881999568156E+02 -
0.881996753056E+02			

-0.881994030981E+02 -0.881991399291E+02 -0.881988855446E+02 -0.881986397008E+02 -
0.881984021638E+02
-0.881981727091E+02 -0.881979511221E+02 -0.881977371973E+02 -0.881975307385E+02 -
0.881973315590E+02
-0.881971394807E+02 -0.881969543347E+02 -0.881967759612E+02 -0.881966042090E+02 -
0.881964389359E+02
-0.881962800088E+02 -0.881961273030E+02 -0.881959807030E+02 -0.881958401022E+02 -
0.881957054031E+02
-0.881955765172E+02 -0.881954533653E+02 -0.881953358774E+02 -0.881952239932E+02 -
0.881951176620E+02
-0.881950168431E+02 -0.881949215059E+02 -0.881948316301E+02 -0.881947472063E+02 -
0.881946682361E+02
-0.881945947323E+02 -0.881945267198E+02 -0.881944642355E+02 -0.881944073292E+02 -
0.881943560637E+02
-0.881943105158E+02 -0.881942707767E+02 -0.881942369523E+02 -0.881942091647E+02 -
0.881941875524E+02
-0.881941722710E+02 -0.881941634948E+02 -0.881941614169E+02 -0.881941662507E+02 -
0.881941782312E+02
-0.881941976155E+02 -0.881942246848E+02 -0.881942597452E+02 -0.881943031297E+02 -
0.881943551990E+02
-0.881944163440E+02 -0.881944869871E+02 -0.881945675839E+02 -0.881946586260E+02 -
0.881947606423E+02
-0.881948742021E+02 -0.881949999169E+02 -0.881951384436E+02 -0.881952904870E+02 -
0.881954568029E+02
-0.881956382015E+02 -0.881958355507E+02 -0.881960497797E+02 -0.881962818830E+02 -
0.881965329248E+02
-0.881968040431E+02 -0.881970964547E+02 -0.881974114604E+02 -0.881977504500E+02 -
0.881981149086E+02
-0.881985064223E+02 -0.881989266853E+02 -0.881993775065E+02 -0.881998608170E+02 -
0.882003786784E+02
-0.882009332911E+02 -0.882015270032E+02 -0.882021623207E+02 -0.882028419172E+02 -
0.882035686455E+02
-0.882043455487E+02 -0.882051758732E+02 -0.882060630817E+02 -0.882070108679E+02 -
0.882080231709E+02
-0.882091041919E+02 -0.882102584111E+02 -0.882114906064E+02 -0.882128058724E+02 -
0.882142096417E+02
-0.882157077068E+02 -0.882173062440E+02 -0.882190118381E+02 -0.882208315100E+02 -
0.882227727445E+02
-0.882248435215E+02 -0.882270523479E+02 -0.882294082926E+02 -0.882319210231E+02 -
0.882346008449E+02
-0.882374587431E+02 -0.882405064274E+02 -0.882437563790E+02 -0.882472219016E+02 -
0.882509171748E+02
-0.882548573117E+02 -0.882590584197E+02 -0.882635376655E+02 -0.882683133445E+02 -
0.882734049540E+02
-0.882788332715E+02 -0.882846204387E+02 -0.882907900493E+02 -0.882973672442E+02 -
0.883043788115E+02
-0.883118532931E+02 -0.883198210989E+02 -0.883283146269E+02 -0.883373683921E+02 -
0.883470191628E+02
-0.883573061058E+02 -0.883682709401E+02 -0.883799581011E+02 -0.883924149145E+02 -
0.884056917807E+02
-0.884198423708E+02 -0.884349238348E+02 -0.884509970222E+02 -0.884681267159E+02 -
0.884863818804E+02

-0.885058359250E+02 -0.885265669818E+02 -0.885486582012E+02 -0.885721980636E+02 -
0.885972807105E+02
-0.886240062928E+02 -0.886524813407E+02 -0.886828191532E+02 -0.887151402099E+02 -
0.887495726048E+02
-0.887862525044E+02 -0.888253246295E+02 -0.888669427628E+02 -0.889112702822E+02 -
0.889584807217E+02
-0.890087583595E+02 -0.890622988355E+02 -0.891193097968E+02 -0.891800115741E+02 -
0.892446378876E+02
-0.893134365838E+02 -0.893866704025E+02 -0.894646177750E+02 -0.895475736523E+02 -
0.896358503637E+02
-0.897297785034E+02 -0.898297078466E+02 -0.899360082908E+02 -0.900490708225E+02 -
0.901693085058E+02
-0.902971574900E+02 -0.904330780329E+02 -0.905775555360E+02 -0.907311015845E+02 -
0.908942549890E+02
-0.910675828188E+02 -0.912516814209E+02 -0.914471774136E+02 -0.916547286435E+02 -
0.918750250939E+02
-0.921087897285E+02 -0.923567792526E+02 -0.926197847731E+02 -0.928986323317E+02 -
0.931941832864E+02
-0.935073345075E+02 -0.938390183546E+02 -0.941902023900E+02 -0.945618887824E+02 -
0.949551133443E+02
-0.953709441385E+02 -0.958104795825E+02 -0.962748459639E+02 -0.967651942732E+02 -
0.972826962441E+02
-0.978285394781E+02 -0.984039215140E+02 -0.990100426869E+02 -0.996480976023E+02 -
0.100319265032E+03
-0.101024696022E+03 -0.101765499973E+03 -0.102542728449E+03 -0.103357356444E+03 -
0.104210260799E+03
-0.105102195492E+03 -0.106033763458E+03 -0.107005384626E+03 -0.108017259839E+03 -
0.109069330339E+03
-0.110161232496E+03 -0.111292247523E+03 -0.112461245937E+03 -0.113666626597E+03 -
0.114906250278E+03
-0.116177367829E+03 -0.117476543170E+03 -0.118799571597E+03 -0.120141394124E+03 -
0.121496008972E+03
-0.122856381684E+03 -0.124214355841E+03 -0.125560566852E+03 -0.126884361879E+03 -
0.128173729476E+03
-0.129415243065E+03 -0.130594022793E+03 -0.131693720607E+03 -0.132696533549E+03 -
0.133583250220E+03
-0.134333335320E+03 -0.134925057119E+03 -0.135335662944E+03 -0.135541608607E+03 -
0.135518849269E+03
-0.135243201915E+03 -0.134690793297E+03 -0.133838611620E+03 -0.132665184906E+03 -
0.131151412645E+03
-0.129281578797E+03 -0.127044571543E+03 -0.124435326368E+03 -0.121456491762E+03 -
0.118120288562E+03
-0.114450492543E+03 -0.110484413869E+03 -0.106274677134E+03 -0.101890526345E+03 -
0.974179250314E+02
-0.929875171973E+02 -0.886941197618E+02 -0.846923560113E+02 -0.810793738948E+02 -
0.779624469981E+02
-0.754501521950E+02 -0.736154702789E+02 -0.724996876586E+02 -0.702099271430E+02 -
0.679987731649E+02
-0.658572612018E+02 -0.637831941547E+02 -0.617744484196E+02 -0.598289643009E+02 -
0.579447518677E+02
-0.561198790771E+02 -0.543524753374E+02 -0.526407356178E+02 -0.509829028983E+02 -
0.493772807736E+02

-0.478222247219E+02	-0.463161425369E+02	-0.448574917176E+02	-0.434447785525E+02	-
0.420765563375E+02				
-0.407514239174E+02	-0.394680242603E+02	-0.382250430676E+02	-0.370212075492E+02	-
0.358552759099E+02				
-0.347260802381E+02	-0.336324383714E+02	-0.325732388825E+02	-0.315473970684E+02	-
0.305538623964E+02				
-0.295916173995E+02	-0.286596767291E+02	-0.277570859810E+02	-0.268829208191E+02	-
0.260362860999E+02				
-0.252163147669E+02	-0.244221671166E+02	-0.236530298768E+02	-0.229081153855E+02	-
0.221866607865E+02				
-0.214879272448E+02	-0.208111991946E+02	-0.201557836057E+02	-0.195210092745E+02	-
0.189062261365E+02				
-0.183108046008E+02	-0.177341349052E+02	-0.171756264918E+02	-0.166347074013E+02	-
0.161108236876E+02				
-0.156034388505E+02	-0.151120332858E+02	-0.146361037532E+02	-0.141751628611E+02	-
0.137287385672E+02				
-0.132963736952E+02	-0.128776254668E+02	-0.124720650482E+02	-0.120792771105E+02	-
0.116988594053E+02				
-0.113304223519E+02	-0.109735886390E+02	-0.106279928380E+02	-0.102932810287E+02	-
0.996911043712E+01				
-0.965514908449E+01	-0.935107544702E+01			
pspotential valence only				
-0.677029363228E+02	-0.676999792830E+02	-0.676971153701E+02	-0.676943416514E+02	-
0.676916552862E+02				
-0.676890535239E+02	-0.676865336996E+02	-0.676840932331E+02	-0.676817296252E+02	-
0.676794404551E+02				
-0.676772233785E+02	-0.676750761250E+02	-0.676729964954E+02	-0.676709823603E+02	-
0.676690316568E+02				
-0.676671423875E+02	-0.676653126172E+02	-0.676635404721E+02	-0.676618241378E+02	-
0.676601618563E+02				
-0.676585519253E+02	-0.676569926958E+02	-0.676554825716E+02	-0.676540200057E+02	-
0.676526035005E+02				
-0.676512316052E+02	-0.676499029149E+02	-0.676486160691E+02	-0.676473697495E+02	-
0.676461626801E+02				
-0.676449936246E+02	-0.676438613857E+02	-0.676427648039E+02	-0.676417027563E+02	-
0.676406741551E+02				
-0.676396779468E+02	-0.676387131114E+02	-0.676377786607E+02	-0.676368736375E+02	-
0.676359971152E+02				
-0.676351481961E+02	-0.676343260105E+02	-0.676335297166E+02	-0.676327584988E+02	-
0.676320115671E+02				
-0.676312881568E+02	-0.676305875268E+02	-0.676299089596E+02	-0.676292517600E+02	-
0.676286152552E+02				
-0.676279987930E+02	-0.676274017421E+02	-0.676268234910E+02	-0.676262634474E+02	-
0.676257210375E+02				
-0.676251957059E+02	-0.676246869143E+02	-0.676241941416E+02	-0.676237168830E+02	-
0.676232546495E+02				
-0.676228069676E+02	-0.676223733787E+02	-0.676219534386E+02	-0.676215467167E+02	-
0.676211527967E+02				
-0.676207712747E+02	-0.676204017597E+02	-0.676200438731E+02	-0.676196972480E+02	-
0.676193615292E+02				
-0.676190363725E+02	-0.676187214446E+02	-0.676184164225E+02	-0.676181209935E+02	-
0.676178348546E+02				

-0.676175577123E+02 -0.676172892822E+02 -0.676170292890E+02 -0.676167774659E+02 -
0.676165335542E+02
-0.676162973037E+02 -0.676160684716E+02 -0.676158468229E+02 -0.676156321298E+02 -
0.676154241716E+02
-0.676152227345E+02 -0.676150276112E+02 -0.676148386009E+02 -0.676146555089E+02 -
0.676144781466E+02
-0.676143063312E+02 -0.676141398853E+02 -0.676139786371E+02 -0.676138224201E+02 -
0.676136710725E+02
-0.676135244379E+02 -0.676133823641E+02 -0.676132447038E+02 -0.676131113140E+02 -
0.676129820559E+02
-0.676128567947E+02 -0.676127353997E+02 -0.676126177440E+02 -0.676125037043E+02 -
0.676123931607E+02
-0.676122859968E+02 -0.676121820996E+02 -0.676120813589E+02 -0.676119836677E+02 -
0.676118889219E+02
-0.676117970199E+02 -0.676117078630E+02 -0.676116213548E+02 -0.676115374015E+02 -
0.676114559113E+02
-0.676113767947E+02 -0.676112999642E+02 -0.676112253343E+02 -0.676111528211E+02 -
0.676110823425E+02
-0.676110138179E+02 -0.676109471684E+02 -0.676108823160E+02 -0.676108191844E+02 -
0.676107576979E+02
-0.676106977820E+02 -0.676106393633E+02 -0.676105823685E+02 -0.676105267256E+02 -
0.676104723625E+02
-0.676104192076E+02 -0.676103671898E+02 -0.676103162374E+02 -0.676102662792E+02 -
0.676102172435E+02
-0.676101690580E+02 -0.676101216501E+02 -0.676100749463E+02 -0.676100288723E+02 -
0.676099833526E+02
-0.676099383102E+02 -0.676098936669E+02 -0.676098493426E+02 -0.676098052553E+02 -
0.676097613207E+02
-0.676097174522E+02 -0.676096735604E+02 -0.676096295529E+02 -0.676095853342E+02 -
0.676095408051E+02
-0.676094958622E+02 -0.676094503984E+02 -0.676094043015E+02 -0.676093574546E+02 -
0.676093097350E+02
-0.676092610146E+02 -0.676092111585E+02 -0.676091600252E+02 -0.676091074659E+02 -
0.676090533235E+02
-0.676089974327E+02 -0.676089396189E+02 -0.676088796976E+02 -0.676088174737E+02 -
0.676087527408E+02
-0.676086852801E+02 -0.676086148599E+02 -0.676085412342E+02 -0.676084641422E+02 -
0.676083833066E+02
-0.676082984331E+02 -0.676082092086E+02 -0.676081153002E+02 -0.676080163534E+02 -
0.676079119911E+02
-0.676078018115E+02 -0.676076853864E+02 -0.676075622595E+02 -0.676074319443E+02 -
0.676072939218E+02
-0.676071476379E+02 -0.676069925014E+02 -0.676068278810E+02 -0.676066531024E+02 -
0.676064674448E+02
-0.676062701380E+02 -0.676060603583E+02 -0.676058372247E+02 -0.676055997945E+02 -
0.676053470589E+02
-0.676050779374E+02 -0.676047912728E+02 -0.676044858252E+02 -0.676041602655E+02 -
0.676038131684E+02
-0.676034430051E+02 -0.676030481348E+02 -0.676026267958E+02 -0.676021770962E+02 -
0.676016970028E+02
-0.676011843301E+02 -0.676006367272E+02 -0.676000516650E+02 -0.675994264203E+02 -
0.675987580603E+02

-0.675980434246E+02 -0.675972791059E+02 -0.675964614282E+02 -0.675955864247E+02 -
0.675946498113E+02
-0.675936469596E+02 -0.675925728663E+02 -0.675914221196E+02 -0.675901888632E+02 -
0.675888667563E+02
-0.675874489296E+02 -0.675859279381E+02 -0.675842957081E+02 -0.675825434805E+02 -
0.675806617478E+02
-0.675786401861E+02 -0.675764675798E+02 -0.675741317408E+02 -0.675716194189E+02 -
0.675689162058E+02
-0.675660064292E+02 -0.675628730391E+02 -0.675594974837E+02 -0.675558595757E+02 -
0.675519373480E+02
-0.675477068978E+02 -0.675431422201E+02 -0.675382150288E+02 -0.675328945665E+02 -
0.675271474021E+02
-0.675209372171E+02 -0.675142245808E+02 -0.675069667152E+02 -0.674991172503E+02 -
0.674906259726E+02
-0.674814385676E+02 -0.674714963593E+02 -0.674607360496E+02 -0.674490894629E+02 -
0.674364832975E+02
-0.674228388926E+02 -0.674080720140E+02 -0.673920926679E+02 -0.673748049480E+02 -
0.673561069266E+02
-0.673358905977E+02 -0.673140418811E+02 -0.672904406985E+02 -0.672649611314E+02 -
0.672374716689E+02
-0.672078355565E+02 -0.671759112523E+02 -0.671415529964E+02 -0.671046114981E+02 -
0.670649347404E+02
-0.670223688986E+02 -0.669767593642E+02 -0.669279518613E+02 -0.668757936324E+02 -
0.668201346675E+02
-0.667608289374E+02 -0.666977355866E+02 -0.666307200262E+02 -0.665596548614E+02 -
0.664844205716E+02
-0.664049058520E+02 -0.663210075134E+02 -0.662326298231E+02 -0.661396831633E+02 -
0.660420818717E+02
-0.659397411276E+02 -0.658325727459E+02 -0.657204797519E+02 -0.656033496314E+02 -
0.654810461818E+02
-0.653533999520E+02 -0.652201973321E+02 -0.650811684692E+02 -0.649359743260E+02 -
0.647841933800E+02
-0.646253086764E+02 -0.644586961856E+02 -0.642836156687E+02 -0.640992054826E+02 -
0.639044829298E+02
-0.636983518079E+02 -0.634796186944E+02 -0.632470191307E+02 -0.629992542045E+02 -
0.627350370545E+02
-0.624531475609E+02 -0.621524920643E+02 -0.618321635480E+02 -0.614914965947E+02 -
0.611301108549E+02
-0.607479369979E+02 -0.603452202783E+02 -0.599224989073E+02 -0.594805571213E+02 -
0.590203557841E+02
-0.585429460523E+02 -0.580493736305E+02 -0.575405821488E+02 -0.570173241578E+02 -
0.564800873173E+02
-0.559290419140E+02 -0.553640142810E+02 -0.547844894175E+02 -0.541896454493E+02 -
0.535780467204E+02
-0.529764775147E+02 -0.523620166995E+02 -0.517623261271E+02 -0.511452816143E+02 -
0.504956221092E+02
-0.498167682175E+02 -0.491051419461E+02 -0.483644386275E+02 -0.476157420048E+02 -
0.468589260287E+02
-0.460886089348E+02 -0.453062468303E+02 -0.445133911429E+02 -0.437116507593E+02 -
0.429026500773E+02
-0.420879861315E+02 -0.412691919596E+02 -0.404476909331E+02 -0.396247719317E+02 -
0.388015521266E+02

-0.379789658056E+02	-0.371577579970E+02	-0.363384972642E+02	-0.355216049809E+02	-
0.347074009332E+02				
-0.338961613729E+02	-0.330881837015E+02	-0.322838503173E+02	-0.314836839549E+02	-
0.306883864908E+02				
-0.298988653613E+02	-0.291162209872E+02	-0.283417366413E+02	-0.275768340325E+02	-
0.268230227561E+02				
-0.260818408398E+02	-0.253547924009E+02	-0.246432867362E+02	-0.239485824283E+02	-
0.232717393566E+02				
-0.226135808533E+02	-0.219746677937E+02	-0.213552858717E+02	-0.207554467100E+02	-
0.201749026405E+02				
-0.196131739946E+02	-0.190695866871E+02	-0.185433169571E+02	-0.180334395474E+02	-
0.175389754993E+02				
-0.170589361410E+02	-0.165923606379E+02	-0.161383454990E+02	-0.156960654681E+02	-
0.152647861295E+02				
-0.148438692120E+02	-0.144327719526E+02	-0.140310420185E+02	-0.136383094263E+02	-
0.132542767148E+02				
-0.128787083902E+02	-0.125114204025E+02	-0.121522701780E+02	-0.118011475320E+02	-
0.114579666292E+02				
-0.111226590432E+02	-0.107951678898E+02	-0.104754429619E+02	-0.101634367651E+02	-
0.985910134803E+01				
-0.956238582002E+01	-0.927323445724E+01			
core charge-density (pseudized)				
0.680655423365E-09	0.725641572739E-09	0.773600964596E-09	0.824730107660E-09	
0.879238498384E-09				
0.937349479347E-09	0.999301154371E-09	0.106534736413E-08	0.113575872624E-08	
0.121082374407E-08				
0.129084998888E-08	0.137616536006E-08	0.146711942862E-08	0.156408486960E-08	
0.166745898898E-08				
0.177766535168E-08	0.189515551701E-08	0.202041088893E-08	0.215394468853E-08	
0.229630405692E-08				
0.244807229706E-08	0.260987126380E-08	0.278236391187E-08	0.296625701223E-08	
0.316230404807E-08				
0.337130830202E-08	0.359412614763E-08	0.383167055817E-08	0.408491484753E-08	
0.435489665820E-08				
0.464272221296E-08	0.494957084744E-08	0.527669984241E-08	0.562544957529E-08	
0.599724901223E-08				
0.639362156314E-08	0.681619132370E-08	0.726668972992E-08	0.774696265252E-08	
0.825897796016E-08				
0.880483358261E-08	0.938676610676E-08	0.100071599408E-07	0.106685570840E-07	
0.113736675425E-07				
0.121253804330E-07	0.129267758206E-07	0.137811373394E-07	0.146919656461E-07	
0.156629927645E-07				
0.166981973761E-07	0.178018211230E-07	0.189783859870E-07	0.202327128184E-07	
0.215699410884E-07				
0.229955499479E-07	0.245153806772E-07	0.261356606205E-07	0.278630287010E-07	
0.297045626236E-07				
0.316678078750E-07	0.337608086398E-07	0.359921407609E-07	0.383709468778E-07	
0.409069738877E-07				
0.436106128814E-07	0.464929417201E-07	0.495657704248E-07	0.528416895668E-07	
0.563341218552E-07				
0.600573771349E-07	0.640267110188E-07	0.682583873954E-07	0.727697450678E-07	
0.775792687963E-07				

0.827066650370E-07	0.881729426855E-07	0.940004991575E-07	0.100213212158E-06
0.106836537516E-06			
0.113897613485E-06	0.121425371938E-06	0.129450656906E-06	0.138006350962E-06
0.147127509944E-06			
0.156851506590E-06	0.167218183670E-06	0.178270017224E-06	0.190052290604E-06
0.202613280005E-06			
0.216004452271E-06	0.230280675763E-06	0.245500445163E-06	0.261726121146E-06
0.279024185878E-06			
0.297465515407E-06	0.317125670056E-06	0.338085204001E-06	0.360429995314E-06
0.384251597816E-06			
0.409647616182E-06	0.436722105830E-06	0.465585999250E-06	0.496357560490E-06
0.529162869689E-06			
0.564136339626E-06	0.601421266397E-06	0.641170416497E-06	0.683546652678E-06
0.728723601185E-06			
0.776886363065E-06	0.828232272488E-06	0.882971705178E-06	0.941328940256E-06
0.100354307904E-05			
0.106986902453E-05	0.114057852567E-05	0.121596129054E-05	0.129632617312E-05
0.138200243849E-05			
0.147334111161E-05	0.157071641518E-05	0.167452730252E-05	0.178519909173E-05
0.190318520777E-05			
0.202896903965E-05	0.216306592032E-05	0.230602523727E-05	0.245843268262E-05
0.262091265180E-05			
0.279413080063E-05	0.297879677137E-05	0.317566709868E-05	0.338554830757E-05
0.360930021594E-05			
0.384783945510E-05	0.410214322280E-05	0.437325328409E-05	0.466228023621E-05
0.497040805507E-05			
0.529889894187E-05	0.564909848953E-05	0.602244119016E-05	0.642045630594E-05
0.684477412734E-05			
0.729713264433E-05	0.777938465760E-05	0.829350535885E-05	0.884160041108E-05
0.942591456159E-05			
0.100488408230E-04	0.107129302593E-04	0.114209024173E-04	0.121756564448E-04
0.129802829424E-04			
0.138380765944E-04	0.147525496332E-04	0.157274461895E-04	0.167667575864E-04
0.178747386415E-04			
0.190559250400E-04	0.203151518517E-04	0.216575732639E-04	0.230886836131E-04
0.246143397969E-04			
0.262407851583E-04	0.279746749383E-04	0.298231033983E-04	0.317936327207E-04
0.338943238050E-04			
0.361337690812E-04	0.385211274706E-04	0.410661616363E-04	0.437792776673E-04
0.466715673579E-04			
0.497548532456E-04	0.530417365892E-04	0.565456484733E-04	0.602809042408E-04
0.642627614675E-04			
0.685074817037E-04	0.730323962245E-04	0.778559760424E-04	0.829979064541E-04
0.884791664075E-04			
0.943221129929E-04	0.100550571381E-03	0.107189930551E-03	0.114267245161E-03
0.121811343960E-03			
0.129852945127E-03	0.138424778976E-03	0.147561718479E-03	0.157300918069E-03
0.167681961246E-03			
0.178747017500E-03	0.190541009111E-03	0.203111788417E-03	0.216510326162E-03
0.230790911566E-03			
0.246011364805E-03	0.262233262597E-03	0.279522177644E-03	0.297947932694E-03
0.317584870034E-03			

0.338512137249E-03	0.360813990100E-03	0.384580113432E-03	0.409905961023E-03
0.436893115323E-03			
0.465649668047E-03	0.496290622615E-03	0.528938319422E-03	0.563722884960E-03
0.600782705767E-03			
0.640264928227E-03	0.682325985165E-03	0.727132150179E-03	0.774860120604E-03
0.825697629925E-03			
0.879844090362E-03	0.937511266261E-03	0.998923978765E-03	0.106432084208E-02
0.113395503140E-02			
0.120809508246E-02	0.128702572199E-02	0.137104872867E-02	0.146048382286E-02
0.155566958380E-02			
0.165696439167E-02	0.176474739161E-02	0.187941947594E-02	0.200140427978E-02
0.213114918441E-02			
0.226912632133E-02	0.241583356873E-02	0.257179553038E-02	0.273756448524E-02
0.291372129399E-02			
0.310087624632E-02	0.329966983032E-02	0.351077340217E-02	0.373488973100E-02
0.397275339029E-02			
0.422513096256E-02	0.449282101976E-02	0.477665383641E-02	0.507749078661E-02
0.539622337006E-02			
0.573377180461E-02	0.609108311565E-02	0.646912864392E-02	0.686890088431E-02
0.729140955832E-02			
0.773767681229E-02	0.820873142232E-02	0.870560187496E-02	0.922930818049E-02
0.978085226298E-02			
0.103612067587E-01	0.109713020417E-01	0.116120112844E-01	0.122841333480E-01
0.129883732919E-01			
0.137253202817E-01	0.144954226725E-01	0.152989600493E-01	0.161360120087E-01
0.170064234864E-01			
0.179097664579E-01	0.188452978780E-01	0.198119137802E-01	0.208080995245E-01
0.218318762803E-01			
0.228807439482E-01	0.239516208771E-01	0.250407809209E-01	0.261437886059E-01
0.272554334580E-01			
0.283696648654E-01	0.294795292383E-01	0.305771116751E-01	0.316534848547E-01
0.326986684502E-01			
0.337016029989E-01	0.346501428490E-01	0.355310735372E-01	0.363301596914E-01
0.370322302804E-01			
0.376213086872E-01	0.380807956058E-01	0.383937130609E-01	0.385430178178E-01
0.385119919395E-01			
0.382847170908E-01	0.378466371795E-01	0.371852108168E-01	0.362906506140E-01
0.351567402099E-01			
0.337817118604E-01	0.321691571353E-01	0.303289305618E-01	0.282779908182E-01
0.260411064303E-01			
0.236513332426E-01	0.211501500302E-01	0.185871178814E-01	0.160189105124E-01
0.135075495444E-01			
0.111176750989E-01	0.891269325872E-02	0.694967463079E-02	0.527294027830E-02
0.390637125059E-02			
0.284462447136E-02	0.204634105555E-02	0.145460472883E-02	0.102133087181E-02
0.708073371823E-03			
0.484519558958E-03	0.327108147341E-03	0.217790418137E-03	0.142944771955E-03
0.924461358421E-04			
0.588847724706E-04	0.369238866702E-04	0.227819974745E-04	0.138241719848E-04
0.824565667318E-05			
0.483190804996E-05	0.278022714905E-05	0.156986819816E-05	0.869385578152E-06
0.471916061192E-06			

0.250927600539E-06	0.130611975426E-06	0.665087883488E-07	0.331083796014E-07
0.161009521940E-07			
0.764367183337E-08	0.353965782606E-08	0.159768325477E-08	0.702329008374E-09
0.300434573515E-09			
0.124952631311E-09	0.504825516273E-10	0.197942287197E-10	0.752531117071E-11
0.277122464384E-11			
0.987502501209E-12	0.340146596908E-12	0.113131008036E-12	0.362906131860E-13
0.112149279727E-13			
0.333474817006E-14	0.952907632269E-15	0.261335374456E-15	0.686949545635E-16
0.172834778617E-16			
0.415621394002E-17	0.953862737148E-18	0.208610125967E-18	0.434075915325E-19
0.857974812426E-20			
0.160819058566E-20	0.285369383433E-21	0.478534578100E-22	0.756937854171E-23
0.112726955183E-23			
0.157750098174E-24	0.207020098419E-25	0.254246621267E-26	0.291586617747E-27
0.311594459329E-28			
0.309549927396E-29	0.285211910372E-30	0.243133423243E-31	0.191280930878E-32
0.138523480089E-33			
0.920954428784E-35	0.560553051251E-36	0.311473608922E-37	0.157533893086E-38
0.723029790652E-40			
0.300197305477E-41	0.112388359667E-42		
pseudo wavefunction			
0.717870221570E-04	0.741213570279E-04	0.765315986450E-04	0.790202153064E-04
0.815897555729E-04			
0.842428508782E-04	0.869822182238E-04	0.898106629610E-04	0.927310816645E-04
0.957464650981E-04			
0.988599012779E-04	0.102074578634E-03	0.105393789278E-03	0.108820932371E-03
0.112359517606E-03			
0.116013168805E-03	0.119785627624E-03	0.123680757392E-03	0.127702547062E-03
0.131855115297E-03			
0.136142714689E-03	0.140569736116E-03	0.145140713234E-03	0.149860327122E-03
0.154733411077E-03			
0.159764955563E-03	0.164960113321E-03	0.170324204645E-03	0.175862722833E-03
0.181581339813E-03			
0.187485911945E-03	0.193582486029E-03	0.199877305487E-03	0.206376816765E-03
0.213087675929E-03			
0.220016755484E-03	0.227171151412E-03	0.234558190439E-03	0.242185437538E-03
0.250060703674E-03			
0.258192053808E-03	0.266587815149E-03	0.275256585691E-03	0.284207243009E-03
0.293448953358E-03			
0.302991181053E-03	0.312843698168E-03	0.323016594538E-03	0.333520288095E-03
0.344365535535E-03			
0.355563443337E-03	0.367125479132E-03	0.379063483451E-03	0.391389681850E-03
0.404116697426E-03			
0.417257563750E-03	0.430825738211E-03	0.444835115799E-03	0.459300043332E-03
0.474235334152E-03			
0.489656283293E-03	0.505578683143E-03	0.522018839620E-03	0.538993588868E-03
0.556520314500E-03			
0.574616965399E-03	0.593302074102E-03	0.612594775772E-03	0.632514827803E-03
0.653082630046E-03			
0.674319245704E-03	0.696246422899E-03	0.718886616948E-03	0.742263013355E-03
0.766399551556E-03			

0.791320949436E-03	0.817052728641E-03	0.843621240714E-03	0.871053694078E-03
0.899378181907E-03			
0.928623710885E-03	0.958820230921E-03	0.989998665811E-03	0.102219094491E-02
0.105543003584E-02			
0.108974997822E-02	0.112518591856E-02	0.116177414623E-02	0.119955213064E-02
0.123855855960E-02			
0.127883337892E-02	0.132041783337E-02	0.136335450884E-02	0.140768737603E-02
0.145346183542E-02			
0.150072476379E-02	0.154952456220E-02	0.159991120560E-02	0.165193629393E-02
0.170565310505E-02			
0.176111664923E-02	0.181838372549E-02	0.187751297980E-02	0.193856496511E-02
0.200160220334E-02			
0.206668924941E-02	0.213389275739E-02	0.220328154868E-02	0.227492668251E-02
0.234890152874E-02			
0.242528184293E-02	0.250414584394E-02	0.258557429402E-02	0.266965058149E-02
0.275646080614E-02			
0.284609386739E-02	0.293864155529E-02	0.303419864454E-02	0.313286299147E-02
0.323473563430E-02			
0.333992089653E-02	0.344852649379E-02	0.356066364408E-02	0.367644718168E-02
0.379599567467E-02			
0.391943154634E-02	0.404688120051E-02	0.417847515092E-02	0.431434815486E-02
0.445463935109E-02			
0.459949240227E-02	0.474905564202E-02	0.490348222673E-02	0.506293029235E-02
0.522756311621E-02			
0.539754928412E-02	0.557306286293E-02	0.575428357865E-02	0.594139700035E-02
0.613459473007E-02			
0.633407459884E-02	0.654004086911E-02	0.675270444371E-02	0.697228308162E-02
0.719900162071E-02			
0.743309220774E-02	0.767479453578E-02	0.792435608932E-02	0.818203239741E-02
0.844808729489E-02			
0.872279319213E-02	0.900643135356E-02	0.929929218513E-02	0.960167553113E-02
0.991389098060E-02			
0.102362581837E-01	0.105691071781E-01	0.109127787264E-01	0.112676246639E-01
0.116340082579E-01			
0.120123045786E-01	0.124029008818E-01	0.128061970045E-01	0.132226057720E-01
0.136525534200E-01			
0.140964800283E-01	0.145548399699E-01	0.150281023741E-01	0.155167516042E-01
0.160212877506E-01			
0.165422271405E-01	0.170801028629E-01	0.176354653106E-01	0.182088827407E-01
0.188009418510E-01			
0.194122483768E-01	0.200434277053E-01	0.206951255102E-01	0.213680084068E-01
0.220627646270E-01			
0.227801047161E-01	0.235207622523E-01	0.242854945879E-01	0.250750836144E-01
0.258903365517E-01			
0.267320867619E-01	0.276011945887E-01	0.284985482228E-01	0.294250645945E-01
0.303816902938E-01			
0.313694025195E-01	0.323892100566E-01	0.334421542847E-01	0.345293102167E-01
0.356517875691E-01			
0.368107318657E-01	0.380073255731E-01	0.392427892716E-01	0.405183828602E-01
0.418354067981E-01			
0.431952033824E-01	0.445991580628E-01	0.460487007954E-01	0.475453074346E-01
0.490905011654E-01			

0.506858539757E-01	0.523329881700E-01	0.540335779250E-01	0.557893508874E-01
0.576020898148E-01			
0.594736342602E-01	0.614058823004E-01	0.634007923085E-01	0.654603847712E-01
0.675867441501E-01			
0.697820207884E-01	0.720484328616E-01	0.743882683718E-01	0.768038871870E-01
0.792977231217E-01			
0.818722860604E-01	0.845301641212E-01	0.872740258592E-01	0.901066225060E-01
0.930307902454E-01			
0.960494525206E-01	0.991656223704E-01	0.102382404791E+00	0.105702999121E+00
0.109130701435E+00			
0.112668906961E+00	0.116321112487E+00	0.120090918776E+00	0.123982032961E+00
0.127998270925E+00			
0.132143559645E+00	0.136421939489E+00	0.140837566466E+00	0.145394714392E+00
0.150097776967E+00			
0.154951269751E+00	0.159959831997E+00	0.165128228340E+00	0.170461350292E+00
0.175964217537E+00			
0.181641978973E+00	0.187499913472E+00	0.193543430319E+00	0.199778069280E+00
0.206209500243E+00			
0.212843522393E+00	0.219686062832E+00	0.226743174602E+00	0.234021034004E+00
0.241525937159E+00			
0.249264295685E+00	0.257242631406E+00	0.265467569968E+00	0.273945833231E+00
0.282684230297E+00			
0.291689647019E+00	0.300969033799E+00	0.310529391512E+00	0.320377755309E+00
0.330521176085E+00			
0.340966699343E+00	0.351721341170E+00	0.362792060995E+00	0.374185730802E+00
0.385909100393E+00			
0.397968758277E+00	0.410371087735E+00	0.423122217527E+00	0.436227966691E+00
0.449693782803E+00			
0.463524673038E+00	0.477725127263E+00	0.492299032385E+00	0.507249577030E+00
0.522579145630E+00			
0.538289200839E+00	0.554380153169E+00	0.570851216609E+00	0.587700248917E+00
0.604923575183E+00			
0.622515793152E+00	0.640469558713E+00	0.658775349906E+00	0.677421207663E+00
0.696392451526E+00			
0.715671368462E+00	0.735236872979E+00	0.755064136705E+00	0.775124185745E+00
0.795383464233E+00			
0.815803362772E+00	0.836339710771E+00	0.856942232158E+00	0.877553964559E+00
0.898110642833E+00			
0.918540048854E+00	0.938761330676E+00	0.958684295753E+00	0.978208684757E+00
0.997223434710E+00			
0.101560594277E+01	0.103322134497E+01	0.104992182775E+01	0.106554599372E+01
0.107991830756E+01			
0.109284865230E+01	0.110413203106E+01	0.111354845387E+01	0.112086305394E+01
0.112582648164E+01			
0.112815826106E+01	0.112766527052E+01	0.112429219447E+01	0.111806470733E+01
0.110902663595E+01			
0.109723971307E+01	0.108278314009E+01	0.106575297336E+01	0.104626134213E+01
0.102443550803E+01			
0.100041678212E+01	0.974359309855E+00	0.946428740503E+00	0.916800792167E+00
0.885659728694E+00			
0.853196759964E+00	0.819608376596E+00	0.785094634226E+00	0.749857393961E+00
0.714098533766E+00			

0.678018143175E+00	0.641812717436E+00	0.605673371275E+00	0.569784097583E+00
0.534320101530E+00			
0.499446245117E+00	0.465315639789E+00	0.432068424391E+00	0.399830761938E+00
0.368714080846E+00			
0.338814578409E+00	0.310212986327E+00	0.282974595666E+00	0.257149518103E+00
0.232773157866E+00			
0.209866860870E+00	0.188438705583E+00	0.168484400595E+00	0.149988256722E+00
0.132924206010E+00			
0.117256845498E+00	0.102942489298E+00	0.899302179309E-01	0.781629182481E-01
0.675783104418E-01			
0.581099602697E-01	0.496882747085E-01	0.422414779727E-01	0.356965625613E-01
0.299802072516E-01			
0.250196513184E-01	0.207435122674E-01	0.170825334309E-01	0.139702480956E-01
0.113435484336E-01			
0.914315019797E-02	0.731394763783E-02	0.580525701209E-02	0.457095106550E-02
0.356949055362E-02			
0.276386210284E-02	0.212143419578E-02	0.161374479048E-02	0.121623499533E-02
0.907943375789E-03			
0.671174951044E-03	0.491157868352E-03	0.355699254177E-03	0.254849973252E-03
0.180586112853E-03			
0.126513070001E-03	0.875962562766E-04		
ae wavefunction			
-0.435742514578E-03	-0.449893173649E-03	-0.464503222989E-03	-0.479587566674E-03 -
0.495161591687E-03			
-0.511241183499E-03	-0.527842742197E-03	-0.544983199085E-03	-0.562680033846E-03 -
0.580951292243E-03			
-0.599815604395E-03	-0.619292203629E-03	-0.639400945949E-03	-0.660162330117E-03 -
0.681597518387E-03			
-0.703728357893E-03	-0.726577402730E-03	-0.750167936736E-03	-0.774523997005E-03 -
0.799670398145E-03			
-0.825632757324E-03	-0.852437520094E-03	-0.880111987065E-03	-0.908684341398E-03 -
0.938183677211E-03			
-0.968640028848E-03	-0.100008440111E-02	-0.103254880045E-02	-0.106606626709E-02 -
0.110067090830E-02			
-0.113639793256E-02	-0.117328368495E-02	-0.121136568354E-02	-0.125068265706E-02 -
0.129127458362E-02			
-0.133318273078E-02	-0.137644969680E-02	-0.142111945320E-02	-0.146723738870E-02 -
0.151485035453E-02			
-0.156400671110E-02	-0.161475637625E-02	-0.166715087488E-02	-0.172124339025E-02 -
0.177708881681E-02			
-0.183474381472E-02	-0.189426686600E-02	-0.195571833256E-02	-0.201916051588E-02 -
0.208465771867E-02			
-0.215227630834E-02	-0.222208478250E-02	-0.229415383648E-02	-0.236855643288E-02 -
0.244536787331E-02			
-0.252466587232E-02	-0.260653063363E-02	-0.269104492853E-02	-0.277829417692E-02 -
0.286836653072E-02			
-0.296135295968E-02	-0.305734733997E-02	-0.315644654536E-02	-0.325875054120E-02 -
0.336436248121E-02			
-0.347338880713E-02	-0.358593935143E-02	-0.370212744297E-02	-0.382207001596E-02 -
0.394588772206E-02			
-0.407370504572E-02	-0.420565042307E-02	-0.434185636420E-02	-0.448245957901E-02 -
0.462760110681E-02			

-0.477742644954E-02	-0.493208570898E-02	-0.509173372782E-02	-0.525653023476E-02	-
0.542663999378E-02				
-0.560223295764E-02	-0.578348442568E-02	-0.597057520602E-02	-0.616369178236E-02	-
0.636302648532E-02				
-0.656877766855E-02	-0.678114988958E-02	-0.700035409569E-02	-0.722660781469E-02	-
0.746013535083E-02				
-0.770116798608E-02	-0.794994418617E-02	-0.820670981288E-02	-0.847171834084E-02	-
0.874523108078E-02				
-0.902751740759E-02	-0.931885499488E-02	-0.961953005468E-02	-0.992983758350E-02	-
0.102500816140E-01				
-0.105805754729E-01	-0.109216420446E-01	-0.112736140413E-01	-0.116368342794E-01	-
0.120116559606E-01				
-0.123984429619E-01	-0.127975701289E-01	-0.132094235773E-01	-0.136344009996E-01	-
0.140729119784E-01				
-0.145253783055E-01	-0.149922343075E-01	-0.154739271763E-01	-0.159709173069E-01	-
0.164836786401E-01				
-0.170126990107E-01	-0.175584805012E-01	-0.181215398015E-01	-0.187024085725E-01	-
0.193016338146E-01				
-0.199197782419E-01	-0.205574206586E-01	-0.212151563406E-01	-0.218935974198E-01	-
0.225933732713E-01				
-0.233151309034E-01	-0.240595353487E-01	-0.248272700566E-01	-0.256190372874E-01	-
0.264355585034E-01				
-0.272775747629E-01	-0.281458471081E-01	-0.290411569533E-01	-0.299643064675E-01	-
0.309161189519E-01				
-0.318974392124E-01	-0.329091339217E-01	-0.339520919759E-01	-0.350272248370E-01	-
0.361354668647E-01				
-0.372777756339E-01	-0.384551322354E-01	-0.396685415589E-01	-0.409190325545E-01	-
0.422076584723E-01				
-0.435354970752E-01	-0.449036508243E-01	-0.463132470317E-01	-0.477654379797E-01	-
0.492614010011E-01				
-0.508023385179E-01	-0.523894780347E-01	-0.540240720813E-01	-0.557073981023E-01	-
0.574407582862E-01				
-0.592254793313E-01	-0.610629121421E-01	-0.629544314502E-01	-0.649014353539E-01	-
0.669053447709E-01				
-0.689676027958E-01	-0.710896739566E-01	-0.732730433619E-01	-0.755192157306E-01	-
0.778297142958E-01				
-0.802060795758E-01	-0.826498679973E-01	-0.851626503688E-01	-0.877460101862E-01	-
0.904015417653E-01				
-0.931308481845E-01	-0.959355390311E-01	-0.988172279344E-01	-0.101777529872E+00	-
0.104818058242E+00				
-0.107940421673E+00	-0.111146220575E+00	-0.114437043397E+00	-0.117814462593E+00	-
0.121280030256E+00				
-0.124835273436E+00	-0.128481689081E+00	-0.132220738625E+00	-0.136053842174E+00	-
0.139982372278E+00				
-0.144007647276E+00	-0.148130924184E+00	-0.152353391106E+00	-0.156676159153E+00	-
0.161100253835E+00				
-0.165626605918E+00	-0.170256041712E+00	-0.174989272773E+00	-0.179826885000E+00	-
0.184769327090E+00				
-0.189816898348E+00	-0.194969735818E+00	-0.200227800717E+00	-0.205590864150E+00	-
0.211058492101E+00				
-0.216630029652E+00	-0.222304584450E+00	-0.228081009388E+00	-0.233957884480E+00	-
0.239933497948E+00				

-0.246005826490E+00	-0.252172514735E+00	-0.258430853893E+00	-0.264777759584E+00	-
0.271209748895E+00				
-0.277722916625E+00	-0.284312910796E+00	-0.290974907415E+00	-0.297703584545E+00	-
0.304493095718E+00				
-0.311337042745E+00	-0.318228447973E+00	-0.325159726084E+00	-0.332122655473E+00	-
0.339108349349E+00				
-0.346107226613E+00	-0.353108982667E+00	-0.360102560263E+00	-0.367076120546E+00	-
0.374017014443E+00				
-0.380911754590E+00	-0.387745987959E+00	-0.394504469434E+00	-0.401171036534E+00	-
0.407728585534E+00				
-0.414159049264E+00	-0.420443376855E+00	-0.426561515740E+00	-0.432492396241E+00	-
0.438213919077E+00				
-0.443702946157E+00	-0.448935295058E+00	-0.453885737559E+00	-0.458528002693E+00	-
0.462834784711E+00				
-0.466777756461E+00	-0.470327588609E+00	-0.473453975226E+00	-0.476125666209E+00	-
0.478310507061E+00				
-0.479975486546E+00	-0.481086792717E+00	-0.481609877879E+00	-0.481509532960E+00	-
0.480749971831E+00				
-0.479294926074E+00	-0.477107750666E+00	-0.474151541045E+00	-0.470389261998E+00	-
0.465783888731E+00				
-0.460298560491E+00	-0.453896747002E+00	-0.446542427922E+00	-0.438200285462E+00	-
0.428835910173E+00				
-0.418416019828E+00	-0.406908691171E+00	-0.394283604166E+00	-0.380512298197E+00	-
0.365568439513E+00				
-0.349428098971E+00	-0.332070038939E+00	-0.313476007975E+00	-0.293631041687E+00	-
0.272523767929E+00				
-0.250146714287E+00	-0.226496615652E+00	-0.201574719499E+00	-0.175387086471E+00	-
0.147944883809E+00				
-0.119264669293E+00	-0.893686634179E-01	-0.582850077441E-01	-0.260480074208E-01	
0.730164409990E-02				
0.417166604293E-01	0.771429806604E-01	0.113519615235E+00	0.150778526147E+00	
0.188844552594E+00				
0.227635400053E+00	0.267061721580E+00	0.307027335916E+00	0.347429646432E+00	
0.388160339643E+00				
0.429106427690E+00	0.470151610346E+00	0.511177717862E+00	0.552065673260E+00	
0.592695180898E+00				
0.632942589828E+00	0.672677321116E+00	0.711758452955E+00	0.750033483838E+00	
0.787340239577E+00				
0.823511019092E+00	0.858377022958E+00	0.891771647708E+00	0.923532424241E+00	
0.953502107831E+00				
0.981529484964E+00	0.100747023435E+01	0.103118796398E+01	0.105255542093E+01	
0.107145581585E+01				
0.108778418649E+01	0.110144872824E+01	0.111237203245E+01	0.112049218525E+01	
0.112576370005E+01				
0.112815826106E+01	0.112766527052E+01	0.112429219447E+01	0.111806470733E+01	
0.110902663595E+01				
0.109723971307E+01	0.108278314009E+01	0.106575297336E+01	0.104626134213E+01	
0.102443550803E+01				
0.100041678212E+01	0.974359309855E+00	0.946428740503E+00	0.916800792167E+00	
0.885659728694E+00				
0.853196759964E+00	0.819608376596E+00	0.785094634226E+00	0.749857393961E+00	
0.714098533766E+00				

0.678018143175E+00	0.641812717436E+00	0.605673371275E+00	0.569784097583E+00
0.534320101530E+00			
0.499446245117E+00	0.465315639789E+00	0.432068424391E+00	0.399830761938E+00
0.368714080846E+00			
0.338814578409E+00	0.310212986327E+00	0.282974595666E+00	0.257149518103E+00
0.232773157866E+00			
0.209866860870E+00	0.188438705583E+00	0.168484400595E+00	0.149988256722E+00
0.132924206010E+00			
0.117256845498E+00	0.102942489298E+00	0.899302179309E-01	0.781629182481E-01
0.675783104418E-01			
0.581099602697E-01	0.496882747085E-01	0.422414779727E-01	0.356965625613E-01
0.299802072516E-01			
0.250196513184E-01	0.207435122674E-01	0.170825334309E-01	0.139702480956E-01
0.113435484336E-01			
0.914315019797E-02	0.731394763783E-02	0.580525701209E-02	0.457095106550E-02
0.356949055362E-02			
0.276386210284E-02	0.212143419578E-02	0.161374479048E-02	0.121623499533E-02
0.907943375789E-03			
0.671174951044E-03	0.491157868352E-03	0.355699254177E-03	0.254849973252E-03
0.180586112853E-03			
0.126513070001E-03	0.875962562766E-04		
pseudo wavefunction			
0.981022797984E-04	0.101292321198E-03	0.104586094785E-03	0.107986973671E-03
0.111498440655E-03			
0.115124091784E-03	0.118867640042E-03	0.122732919149E-03	0.126723887490E-03
0.130844632164E-03			
0.135099373174E-03	0.139492467746E-03	0.144028414793E-03	0.148711859521E-03
0.153547598187E-03			
0.158540583008E-03	0.163695927238E-03	0.169018910400E-03	0.174514983693E-03
0.180189775576E-03			
0.186049097531E-03	0.192098950017E-03	0.198345528609E-03	0.204795230351E-03
0.211454660300E-03			
0.218330638293E-03	0.225430205933E-03	0.232760633796E-03	0.240329428880E-03
0.248144342293E-03			
0.256213377188E-03	0.264544796960E-03	0.273147133711E-03	0.282029196984E-03
0.291200082787E-03			
0.300669182907E-03	0.310446194528E-03	0.320541130164E-03	0.330964327908E-03
0.341726462025E-03			
0.352838553878E-03	0.364311983217E-03	0.376158499835E-03	0.388390235597E-03
0.401019716866E-03			
0.414059877331E-03	0.427524071252E-03	0.441426087137E-03	0.455780161860E-03
0.470600995242E-03			
0.485903765108E-03	0.501704142824E-03	0.518018309352E-03	0.534862971816E-03
0.552255380614E-03			
0.570213347085E-03	0.588755261745E-03	0.607900113126E-03	0.627667507215E-03
0.648077687539E-03			
0.669151555892E-03	0.690910693741E-03	0.713377384327E-03	0.736574635487E-03
0.760526203210E-03			
0.785256615974E-03	0.810791199855E-03	0.837156104472E-03	0.864378329761E-03
0.892485753625E-03			
0.921507160485E-03	0.951472270757E-03	0.982411771287E-03	0.101435734678E-02
0.104734171224E-02			

0.108139864648E-02	0.111656302671E-02	0.115287086426E-02	0.119035934145E-02
0.122906684965E-02			
0.126903302866E-02	0.131029880722E-02	0.135290644498E-02	0.139689957575E-02
0.144232325220E-02			
0.148922399198E-02	0.153764982540E-02	0.158765034452E-02	0.163927675406E-02
0.169258192374E-02			
0.174762044245E-02	0.180444867417E-02	0.186312481566E-02	0.192370895610E-02
0.198626313855E-02			
0.205085142357E-02	0.211753995475E-02	0.218639702647E-02	0.225749315386E-02
0.233090114495E-02			
0.240669617530E-02	0.248495586490E-02	0.256576035771E-02	0.264919240373E-02
0.273533744367E-02			
0.282428369654E-02	0.291612224989E-02	0.301094715312E-02	0.310885551381E-02
0.320994759711E-02			
0.331432692842E-02	0.342210039940E-02	0.353337837741E-02	0.364827481853E-02
0.376690738422E-02			
0.388939756181E-02	0.401587078889E-02	0.414645658171E-02	0.428128866782E-02
0.442050512297E-02			
0.456424851248E-02	0.471266603718E-02	0.486590968414E-02	0.502413638222E-02
0.518750816280E-02			
0.535619232558E-02	0.553036160987E-02	0.571019437143E-02	0.589587476501E-02
0.608759293289E-02			
0.628554519947E-02	0.648993427222E-02	0.670096944917E-02	0.691886683311E-02
0.714384955274E-02			
0.737614799102E-02	0.761600002094E-02	0.786365124893E-02	0.811935526613E-02
0.838337390793E-02			
0.865597752176E-02	0.893744524377E-02	0.922806528429E-02	0.952813522269E-02
0.983796231174E-02			
0.101578637918E-01	0.104881672154E-01	0.108292107819E-01	0.111813436836E-01
0.115449264625E-01			
0.119203313789E-01	0.123079427920E-01	0.127081575527E-01	0.131213854088E-01
0.135480494240E-01			
0.139885864101E-01	0.144434473727E-01	0.149130979722E-01	0.153980189990E-01
0.158987068643E-01			
0.164156741069E-01	0.169494499159E-01	0.175005806705E-01	0.180696304976E-01
0.186571818463E-01			
0.192638360822E-01	0.198902140996E-01	0.205369569543E-01	0.212047265160E-01
0.218942061423E-01			
0.226061013736E-01	0.233411406506E-01	0.241000760551E-01	0.248836840738E-01
0.256927663865E-01			
0.265281506805E-01	0.273906914891E-01	0.282812710583E-01	0.292008002406E-01
0.301502194162E-01			
0.311304994447E-01	0.321426426460E-01	0.331876838122E-01	0.342666912512E-01
0.353807678634E-01			
0.365310522517E-01	0.377187198664E-01	0.389449841853E-01	0.402110979305E-01
0.415183543233E-01			
0.428680883768E-01	0.442616782292E-01	0.457005465166E-01	0.471861617886E-01
0.487200399663E-01			
0.503037458439E-01	0.519388946358E-01	0.536271535693E-01	0.553702435245E-01
0.571699407226E-01			
0.590280784631E-01	0.609465489108E-01	0.629273049354E-01	0.649723620016E-01
0.670838001134E-01			

0.692637658118E-01	0.715144742280E-01	0.738382111914E-01	0.762373353942E-01
0.787142806128E-01			
0.812715579865E-01	0.839117583541E-01	0.866375546476E-01	0.894517043448E-01
0.923570519793E-01			
0.953565317073E-01	0.984531699327E-01	0.101650087986E+00	0.104950504863E+00
0.108357740007E+00			
0.111875216156E+00	0.115506462227E+00	0.119255116256E+00	0.123124928371E+00
0.127119763819E+00			
0.131243606010E+00	0.135500559607E+00	0.139894853625E+00	0.144430844562E+00
0.149113019517E+00			
0.153945999332E+00	0.158934541699E+00	0.164083544260E+00	0.169398047660E+00
0.174883238556E+00			
0.180544452548E+00	0.186387177027E+00	0.192417053911E+00	0.198639882247E+00
0.205061620648E+00			
0.211688389542E+00	0.218526473188E+00	0.225582321436E+00	0.232862551167E+00
0.240373947393E+00			
0.248123463935E+00	0.256118223644E+00	0.264365518086E+00	0.272872806618E+00
0.281647714785E+00			
0.290698031932E+00	0.300031707945E+00	0.309656848996E+00	0.319581712184E+00
0.329814698917E+00			
0.340364346893E+00	0.351239320514E+00	0.362448399533E+00	0.374000465729E+00
0.385904487393E+00			
0.398169501343E+00	0.410804592204E+00	0.423818868634E+00	0.437221436135E+00
0.451021366079E+00			
0.465227660508E+00	0.479849212240E+00	0.494894759755E+00	0.510372836282E+00
0.526291712443E+00			
0.542659331752E+00	0.559483238179E+00	0.576770494933E+00	0.594527593498E+00
0.612760351888E+00			
0.631473800980E+00	0.650672057654E+00	0.670358183380E+00	0.690534026738E+00
0.711200048236E+00			
0.732355125652E+00	0.753996337961E+00	0.776118725786E+00	0.798715026131E+00
0.821775379016E+00			
0.845287003488E+00	0.869233840362E+00	0.893596158905E+00	0.918350124624E+00
0.943467325264E+00			
0.968914252144E+00	0.994651734037E+00	0.102063432102E+01	0.104680961599E+01
0.107311755208E+01			
0.109948961475E+01	0.112584800844E+01	0.115210476858E+01	0.117816082162E+01
0.120390499732E+01			
0.122921300032E+01	0.125394635068E+01	0.127795130686E+01	0.130105778875E+01
0.132307832355E+01			
0.134380704281E+01	0.136301876597E+01	0.138046821280E+01	0.139588939545E+01
0.140899524948E+01			
0.141947757221E+01	0.142700734563E+01	0.143123552968E+01	0.143179441843E+01
0.142829965728E+01			
0.142035302034E+01	0.140760595896E+01	0.138995228327E+01	0.136736585757E+01
0.133984284992E+01			
0.130740125394E+01	0.127008010430E+01	0.122793839239E+01	0.118105368024E+01
0.112952040987E+01			
0.107344791071E+01	0.101295809801E+01	0.000000000000E+00	0.000000000000E+00
0.000000000000E+00			
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00
0.000000000000E+00			

-0.640363407451E-02	-0.661093841280E-02	-0.682492965274E-02	-0.704582189354E-02	-
0.727383598369E-02				
-0.750919972662E-02	-0.775214809228E-02	-0.800292343458E-02	-0.826177571486E-02	-
0.852896273163E-02				
-0.880475035659E-02	-0.908941277710E-02	-0.938323274523E-02	-0.968650183350E-02	-
0.999952069751E-02				
-0.103225993457E-01	-0.106560574156E-01	-0.110002244582E-01	-0.113554402286E-01	-
0.117220549856E-01				
-0.121004297966E-01	-0.124909368529E-01	-0.128939597904E-01	-0.133098940196E-01	-
0.137391470627E-01				
-0.141821388998E-01	-0.146393023217E-01	-0.151110832925E-01	-0.155979413191E-01	-
0.161003498295E-01				
-0.166187965598E-01	-0.171537839488E-01	-0.177058295410E-01	-0.182754663984E-01	-
0.188632435202E-01				
-0.194697262702E-01	-0.200954968134E-01	-0.207411545594E-01	-0.214073166146E-01	-
0.220946182415E-01				
-0.228037133258E-01	-0.235352748502E-01	-0.242899953765E-01	-0.250685875326E-01	-
0.258717845075E-01				
-0.267003405512E-01	-0.275550314803E-01	-0.284366551890E-01	-0.293460321645E-01	-
0.302840060054E-01				
-0.312514439444E-01	-0.322492373728E-01	-0.332783023663E-01	-0.343395802128E-01	-
0.354340379372E-01				
-0.365626688283E-01	-0.377264929597E-01	-0.389265577091E-01	-0.401639382713E-01	-
0.414397381639E-01				
-0.427550897260E-01	-0.441111546042E-01	-0.455091242290E-01	-0.469502202745E-01	-
0.484356951022E-01				
-0.499668321869E-01	-0.515449465181E-01	-0.531713849799E-01	-0.548475267004E-01	-
0.565747833726E-01				
-0.583545995386E-01	-0.601884528375E-01	-0.620778542097E-01	-0.640243480555E-01	-
0.660295123413E-01				
-0.680949586517E-01	-0.702223321782E-01	-0.724133116417E-01	-0.746696091428E-01	-
0.769929699313E-01				
-0.793851720911E-01	-0.818480261305E-01	-0.843833744727E-01	-0.869930908367E-01	-
0.896790795006E-01				
-0.924432744382E-01	-0.952876383193E-01	-0.982141613635E-01	-0.101224860036E+00	-
0.104321775575E+00				
-0.107506972340E+00	-0.110782535961E+00	-0.114150571288E+00	-0.117613200115E+00	-
0.121172558667E+00				
-0.124830794844E+00	-0.128590065184E+00	-0.132452531554E+00	-0.136420357527E+00	-
0.140495704453E+00				
-0.144680727169E+00	-0.148977569366E+00	-0.153388358561E+00	-0.157915200674E+00	-
0.162560174168E+00				
-0.167325323744E+00	-0.172212653561E+00	-0.177224119948E+00	-0.182361623593E+00	-
0.187627001180E+00				
-0.193022016437E+00	-0.198548350577E+00	-0.204207592103E+00	-0.210001225935E+00	-
0.215930621845E+00				
-0.221997022161E+00	-0.228201528712E+00	-0.234545088976E+00	-0.241028481419E+00	-
0.247652299971E+00				
-0.254416937628E+00	-0.261322569140E+00	-0.268369132764E+00	-0.275556311044E+00	-
0.282883510610E+00				
-0.290349840952E+00	-0.297954092161E+00	-0.305694711614E+00	-0.313569779581E+00	-
0.321576983758E+00				

-0.329713592689E+00	-0.337976428104E+00	-0.346361836153E+00	-0.354865657541E+00	-
0.363483196600E+00				
-0.372209189287E+00	-0.381037770155E+00	-0.389962438331E+00	-0.398976022543E+00	-
0.408070645252E+00				
-0.417237685960E+00	-0.426467743763E+00	-0.435750599269E+00	-0.445075175946E+00	-
0.454429501062E+00				
-0.463800666330E+00	-0.473174788428E+00	-0.482536969561E+00	-0.491871258255E+00	-
0.501160610617E+00				
-0.510386852273E+00	-0.519530641250E+00	-0.528571432100E+00	-0.537487441547E+00	-
0.546255616009E+00				
-0.554851601338E+00	-0.563249715179E+00	-0.571422922336E+00	-0.579342813606E+00	-
0.586979588535E+00				
-0.594302042587E+00	-0.601277559261E+00	-0.607872107677E+00	-0.614050246243E+00	-
0.619775132960E+00				
-0.625008543021E+00	-0.629710894329E+00	-0.633841281617E+00	-0.637357519832E+00	-
0.640216197506E+00				
-0.642372740817E+00	-0.643781489048E+00	-0.644395782202E+00	-0.644168061462E+00	-
0.643049983239E+00				
-0.640992547515E+00	-0.637946241147E+00	-0.633861196823E+00	-0.628687368265E+00	-
0.622374722263E+00				
-0.614873448055E+00	-0.606134184488E+00	-0.596108265298E+00	-0.584747982762E+00	-
0.572006869829E+00				
-0.557840000686E+00	-0.542204309549E+00	-0.525058927296E+00	-0.506365535278E+00	-
0.486088735474E+00				
-0.464196435820E+00	-0.440660249297E+00	-0.415455905044E+00	-0.388563669451E+00	-
0.359968774895E+00				
-0.329661853500E+00	-0.297639373059E+00	-0.263904072102E+00	-0.228465390951E+00	-
0.191339895644E+00				
-0.152551691668E+00	-0.112132824606E+00	-0.701236649737E-01	-0.265732747002E-01	
0.184602474066E-01				
0.649094442146E-01	0.112697206889E+00	0.161736515586E+00	0.211930223674E+00	
0.263170900712E+00				
0.315340758784E+00	0.368311701510E+00	0.421945556344E+00	0.476094577002E+00	
0.530602322111E+00				
0.585304995880E+00	0.640033214744E+00	0.694613873108E+00	0.748871346008E+00	
0.802626959138E+00				
0.855695993743E+00	0.907882772699E+00	0.958975996408E+00	0.100874705297E+01	
0.105695258255E+01				
0.110334004851E+01	0.114765366804E+01	0.118963880186E+01	0.122904451998E+01	
0.126562503679E+01				
0.129914077918E+01	0.132935953994E+01	0.135605787697E+01	0.137902275074E+01	
0.139805331884E+01				
0.141296278387E+01	0.142358019525E+01	0.142975212414E+01	0.143134414532E+01	
0.142824208777E+01				
0.142035302034E+01	0.140760595896E+01	0.138995228327E+01	0.136736585757E+01	
0.133984284992E+01				
0.130740125394E+01	0.127008010430E+01	0.122793839239E+01	0.118105368024E+01	
0.112952040987E+01				
0.107344791071E+01	0.101295809801E+01	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				

0.684760664837E-06	0.730018126104E-06	0.778266759685E-06	0.829704259077E-06
0.884541383783E-06			
0.943002822866E-06	0.100532811558E-05	0.107177263286E-05	0.114260862366E-05
0.121812633044E-05			
0.129863517842E-05	0.138446504339E-05	0.147596760331E-05	0.157351777930E-05
0.167751527175E-05			
0.178838619810E-05	0.190658483875E-05	0.203259549837E-05	0.216693449031E-05
0.231015225205E-05			
0.246283560054E-05	0.262561013657E-05	0.279914280804E-05	0.298414464262E-05
0.318137366109E-05			
0.339163798309E-05	0.361579913828E-05	0.385477559619E-05	0.410954652949E-05
0.438115582584E-05			
0.467071636499E-05	0.497941457846E-05	0.530851531063E-05	0.565936700107E-05
0.603340720932E-05			
0.643216850486E-05	0.685728474627E-05	0.731049777536E-05	0.779366455379E-05
0.830876477117E-05			
0.885790895608E-05	0.944334712303E-05	0.100674779909E-04	0.107328588104E-04
0.114422158416E-04			
0.121984555226E-04	0.130046763778E-04	0.138641817117E-04	0.147804931427E-04
0.157573650301E-04			
0.167987998555E-04	0.179090646197E-04	0.190927083236E-04	0.203545806044E-04
0.216998516021E-04			
0.231340331402E-04	0.246630013047E-04	0.262930205155E-04	0.280307691881E-04
0.298833670911E-04			
0.318584045101E-04	0.339639733402E-04	0.362087002306E-04	0.386017819205E-04
0.411530229082E-04			
0.438728756096E-04	0.467724831685E-04	0.498637250954E-04	0.531592659205E-04
0.566726070607E-04			
0.604181421117E-04	0.644112157922E-04	0.686681867807E-04	0.732064947021E-04
0.780447315371E-04			
0.832027177477E-04	0.887015834285E-04	0.945638548152E-04	0.100813546505E-03
0.107476259765E-03			
0.114579287327E-03	0.122151725104E-03	0.130224591274E-03	0.138830953222E-03
0.148006062867E-03			
0.157787500903E-03	0.168215330566E-03	0.179332261542E-03	0.191183824674E-03
0.203818558206E-03			
0.217288206294E-03	0.231647930605E-03	0.246956535863E-03	0.263276710261E-03
0.280675281707E-03			
0.299223490945E-03	0.318997282676E-03	0.340077615830E-03	0.362550794268E-03
0.386508819249E-03			
0.412049765072E-03	0.439278179435E-03	0.468305510103E-03	0.499250559624E-03
0.532239969909E-03			
0.567408738643E-03	0.604900769581E-03	0.644869458958E-03	0.687478320344E-03
0.732901650466E-03			
0.781325238632E-03	0.832947122605E-03	0.887978393930E-03	0.946644055911E-03
0.100918393764E-02			
0.107585366772E-02	0.114692571143E-02	0.122269047560E-02	0.130345748531E-02
0.138955663718E-02			
0.148133953409E-02	0.157918090654E-02	0.168348012603E-02	0.179466281658E-02
0.191318257027E-02			
0.203952277360E-02	0.217419855148E-02	0.231775883631E-02	0.247078856992E-02
0.263391104659E-02			

0.280779040588E-02	0.299313428461E-02	0.319069663749E-02	0.340128073689E-02
0.362574236248E-02			
0.386499319220E-02	0.412000440650E-02	0.439181051857E-02	0.468151344377E-02
0.499028682227E-02			
0.531938060933E-02	0.567012594866E-02	0.604394034467E-02	0.644233315037E-02
0.686691138804E-02			
0.731938592082E-02	0.780157799379E-02	0.831542616366E-02	0.886299363705E-02
0.944647603760E-02			
0.100682096227E-01	0.107306799709E-01	0.114365311621E-01	0.121885754702E-01
0.129898035926E-01			
0.138433954350E-01	0.147527314741E-01	0.157214047174E-01	0.167532332798E-01
0.178522735939E-01			
0.190228342703E-01	0.202694906209E-01	0.215970998561E-01	0.230108169619E-01
0.245161112602E-01			
0.261187836481E-01	0.278249845082E-01	0.296412322723E-01	0.315744326123E-01
0.336318982232E-01			
0.358213691494E-01	0.381510335918E-01	0.406295491177E-01	0.432660641750E-01
0.460702397936E-01			
0.490522713293E-01	0.522229100787E-01	0.555934845620E-01	0.591759212344E-01
0.629827643447E-01			
0.670271946152E-01	0.713230463635E-01	0.758848226312E-01	0.807277078176E-01
0.858675772448E-01			
0.913210030033E-01	0.971052553355E-01	0.103238298722E+00	0.109738781726E+00
0.116626019541E+00			
0.123919968059E+00	0.131641188140E+00	0.139810798645E+00	0.148450416593E+00
0.157582082726E+00			
0.167228170510E+00	0.177411276533E+00	0.188154090025E+00	0.199479239105E+00
0.211409111223E+00			
0.223965645116E+00	0.237170091524E+00	0.251042739846E+00	0.265602607917E+00
0.280867092151E+00			
0.296851575468E+00	0.313568990675E+00	0.331029337379E+00	0.349239151123E+00
0.368200924169E+00			
0.387912478423E+00	0.408366292286E+00	0.429548784860E+00	0.451439562966E+00
0.474010638877E+00			
0.497225629559E+00	0.521038951669E+00	0.545395030484E+00	0.570227545438E+00
0.595458739961E+00			
0.620998828800E+00	0.646745541851E+00	0.672583849544E+00	0.698385920832E+00
0.724011370291E+00			
0.749307855498E+00	0.774112088776E+00	0.798251327980E+00	0.821545408035E+00
0.843809367222E+00			
0.864856708241E+00	0.884503312055E+00	0.902571990708E+00	0.918897621556E+00
0.933332747883E+00			
0.945753457994E+00	0.956065265592E+00	0.964208608575E+00	0.970163462979E+00
0.973952437607E+00			
0.975641580220E+00	0.975337999364E+00	0.973183303801E+00	0.969341807032E+00
0.963982467720E+00			
0.957253675218E+00	0.949250286897E+00	0.939967138602E+00	0.929324947191E+00
0.917314312958E+00			
0.903972446061E+00	0.889343025994E+00	0.873475959863E+00	0.856427110339E+00
0.838257996483E+00			
0.819035465466E+00	0.798831331209E+00	0.777721981635E+00	0.755787934675E+00
0.733113356044E+00			

0.709785512647E+00	0.685894167526E+00	0.661530910292E+00	0.636788426821E+00
0.611759717633E+00			
0.586537281953E+00	0.561212291287E+00	0.535873781638E+00	0.510607896146E+00
0.485497205586E+00			
0.460620154111E+00	0.436050597673E+00	0.411857513539E+00	0.388104828742E+00
0.364851377592E+00			
0.342150965540E+00	0.320052513938E+00	0.298600256424E+00	0.277833956542E+00
0.257789117684E+00			
0.238497160225E+00	0.219985546498E+00	0.202277841546E+00	0.185393705814E+00
0.169348824436E+00			
0.154154785745E+00	0.139818928254E+00	0.126344179934E+00	0.113728915592E+00
0.101966857495E+00			
0.910470410839E-01	0.809538624583E-01	0.716672177710E-01	0.631627377902E-01
0.554121142439E-01			
0.483835088475E-01	0.420420314569E-01	0.363502707625E-01	0.312688593333E-01
0.267570544913E-01			
0.227733172285E-01	0.192758729338E-01	0.162232398193E-01	0.135747134141E-01
0.112907981381E-01			
0.933357961775E-02	0.766703395852E-02	0.625727254179E-02	0.507272301874E-02
0.408424898420E-02			
0.326521231213E-02	0.259148331194E-02		
ae wavefunction			
0.345880402561E-07	0.368147465608E-07	0.391630883389E-07	0.416408751981E-07
0.442563682518E-07			
0.470183105872E-07	0.499359582279E-07	0.530191141352E-07	0.562781638537E-07
0.597241132906E-07			
0.633686291385E-07	0.672240815764E-07	0.713035898076E-07	0.756210705151E-07
0.801912892549E-07			
0.850299152447E-07	0.901535795818E-07	0.955799372181E-07	0.101327732868E-06
0.107416871239E-06			
0.113868491594E-06	0.120705047417E-06	0.127950390772E-06	0.135629862989E-06
0.143770389519E-06			
0.152400583275E-06	0.161550852750E-06	0.171253517581E-06	0.181542932826E-06
0.192455619674E-06			
0.204030404779E-06	0.216308571060E-06	0.229334015078E-06	0.243153416083E-06
0.257816417222E-06			
0.273375816871E-06	0.289887772138E-06	0.307412018887E-06	0.326012101534E-06
0.345755622003E-06			
0.366714501862E-06	0.388965263970E-06	0.412589330822E-06	0.437673343061E-06
0.464309499980E-06			
0.492595919541E-06	0.522637026049E-06	0.554543957425E-06	0.588435006848E-06
0.624436085467E-06			
0.662681220544E-06	0.703313086421E-06	0.746483564184E-06	0.792354348040E-06
0.841097582411E-06			
0.892896545310E-06	0.947946371298E-06	0.100645483659E-05	0.106864317568E-05
0.113474696323E-05			
0.120501705095E-05	0.127972056978E-05	0.135914199296E-05	0.144358426774E-05
0.153337002759E-05			
0.162884287619E-05	0.173036876258E-05	0.183833744506E-05	0.195316404593E-05
0.207529070949E-05			
0.220518838047E-05	0.234335867813E-05	0.249033591206E-05	0.264668922148E-05
0.281302485110E-05			

0.298998858788E-05	0.317826834453E-05	0.337859691910E-05	0.359175493691E-05
0.381857397934E-05			
0.405993992289E-05	0.431679649136E-05	0.459014904569E-05	0.488106861913E-05
0.519069621763E-05			
0.552024739866E-05	0.587101715321E-05	0.624438510273E-05	0.664182104660E-05
0.706489084968E-05			
0.751526273639E-05	0.799471399674E-05	0.850513809953E-05	0.904855231761E-05
0.962710579933E-05			
0.102430882160E-04	0.108989389268E-04	0.115972567834E-04	0.123408105402E-04
0.131325499614E-04			
0.139756176439E-04	0.148733616103E-04	0.158293487324E-04	0.168473789988E-04
0.179315007513E-04			
0.190860268698E-04	0.203155520373E-04	0.216249711105E-04	0.230194986913E-04
0.245046899579E-04			
0.260864628524E-04	0.277711217013E-04	0.295653823693E-04	0.314763990370E-04
0.335117927027E-04			
0.356796815422E-04	0.379887132080E-04	0.404480992276E-04	0.430676516082E-04
0.458578218053E-04			
0.488297421946E-04	0.519952702102E-04	0.553670353231E-04	0.589584890256E-04
0.627839580276E-04			
0.668587008569E-04	0.711989680793E-04	0.758220663881E-04	0.807464267292E-04
0.859916768552E-04			
0.915787184231E-04	0.975298090504E-04	0.103868649552E-03	0.110620476738E-03
0.117812162077E-03			
0.125472316611E-03	0.133631402501E-03	0.142321851613E-03	0.151578191560E-03
0.161437179714E-03			
0.171937945579E-03	0.183122142140E-03	0.195034106650E-03	0.207721031489E-03
0.221233145642E-03			
0.235623907512E-03	0.250950209665E-03	0.267272596296E-03	0.284655494115E-03
0.303167457488E-03			
0.322881428668E-03	0.343875013988E-03	0.366230776968E-03	0.390036549335E-03
0.415385760960E-03			
0.442377789844E-03	0.471118333287E-03	0.501719801461E-03	0.534301734648E-03
0.568991245506E-03			
0.605923487748E-03	0.645242152725E-03	0.687099995454E-03	0.731659391711E-03
0.779092927929E-03			
0.829584025597E-03	0.883327602105E-03	0.940530769960E-03	0.100141357636E-02
0.106620978528E-02			
0.113516770433E-02	0.120855105852E-02	0.128663991354E-02	0.136973165085E-02
0.145814199728E-02			
0.155220611170E-02	0.165227973161E-02	0.175874038246E-02	0.187198865268E-02
0.199244953728E-02			
0.212057385340E-02	0.225683973077E-02	0.240175418038E-02	0.255585474482E-02
0.271971123347E-02			
0.289392754615E-02	0.307914358853E-02	0.327603728299E-02	0.348532667828E-02
0.370777216155E-02			
0.394417877621E-02	0.419539864910E-02	0.446233353024E-02	0.474593744862E-02
0.504721948688E-02			
0.536724667827E-02	0.570714702827E-02	0.606811266380E-02	0.645140311210E-02
0.685834871134E-02			
0.729035415445E-02	0.774890216752E-02	0.823555732329E-02	0.875196998966E-02
0.929988041327E-02			

0.988112293607E-02	0.104976303435E-01	0.111514383409E-01	0.118446901545E-01
0.125796412519E-01			
0.133586641748E-01	0.141842534790E-01	0.150590307689E-01	0.159857498193E-01
0.169673017698E-01			
0.180067203793E-01	0.191071873222E-01	0.202720375108E-01	0.215047644194E-01
0.228090253904E-01			
0.241886468940E-01	0.256476297127E-01	0.271901540198E-01	0.288205843152E-01
0.305434741809E-01			
0.323635708125E-01	0.342858192811E-01	0.363153664754E-01	0.384575646690E-01
0.407179746533E-01			
0.431023683736E-01	0.456167309988E-01	0.482672623522E-01	0.510603776234E-01
0.540027072802E-01			
0.571010960885E-01	0.603626011492E-01	0.637944888488E-01	0.674042306226E-01
0.711994974168E-01			
0.751881527367E-01	0.793782441592E-01	0.837779931847E-01	0.883957833004E-01
0.932401461192E-01			
0.983197454628E-01	0.103643359244E+00	0.109219859013E+00	0.115058187029E+00
0.121167330707E+00			
0.127556294321E+00	0.134234067811E+00	0.141209592586E+00	0.148491724195E+00
0.156089191765E+00			
0.164010554118E+00	0.172264152490E+00	0.180858059809E+00	0.189800026499E+00
0.199097422821E+00			
0.208757177785E+00	0.218785714709E+00	0.229188883527E+00	0.239971890013E+00
0.251139222087E+00			
0.262694573450E+00	0.274640764784E+00	0.286979662805E+00	0.299712097432E+00
0.312837777352E+00			
0.326355204220E+00	0.340261585645E+00	0.354552747090E+00	0.369223042673E+00
0.384265264768E+00			
0.399670552251E+00	0.415428297180E+00	0.431526049827E+00	0.447949422205E+00
0.464681990771E+00			
0.481705199905E+00	0.498998269173E+00	0.516538109636E+00	0.534299257914E+00
0.552253841987E+00			
0.570371600836E+00	0.588619991828E+00	0.606964435228E+00	0.625368760465E+00
0.643795920443E+00			
0.662208998417E+00	0.680572399977E+00	0.698852866948E+00	0.717019635240E+00
0.735042946127E+00			
0.752890590704E+00	0.770523297677E+00	0.787890910568E+00	0.804931356845E+00
0.821572954344E+00			
0.837738647728E+00	0.853350001890E+00	0.868329657323E+00	0.882602265301E+00
0.896094574592E+00			
0.908735290203E+00	0.920455037628E+00	0.931186537640E+00	0.940864978815E+00
0.949428531581E+00			
0.956818939118E+00	0.962982128823E+00	0.967868802858E+00	0.971434977327E+00
0.973642457381E+00			
0.974459237649E+00	0.973859829103E+00	0.971825513245E+00	0.968344527516E+00
0.963412184303E+00			
0.957030932139E+00	0.949210357842E+00	0.939967138602E+00	0.929324947191E+00
0.917314312958E+00			
0.903972446061E+00	0.889343025994E+00	0.873475959863E+00	0.856427110339E+00
0.838257996483E+00			
0.819035465466E+00	0.798831331209E+00	0.777721981635E+00	0.755787934675E+00
0.733113356044E+00			

0.709785512647E+00	0.685894167526E+00	0.661530910292E+00	0.636788426821E+00	
0.611759717633E+00				
0.586537281953E+00	0.561212291287E+00	0.535873781638E+00	0.510607896146E+00	
0.485497205586E+00				
0.460620154111E+00	0.436050597673E+00	0.411857513539E+00	0.388104828742E+00	
0.364851377592E+00				
0.342150965540E+00	0.320052513938E+00	0.298600256424E+00	0.277833956542E+00	
0.257789117684E+00				
0.238497160225E+00	0.219985546498E+00	0.202277841546E+00	0.185393705814E+00	
0.169348824436E+00				
0.154154785745E+00	0.139818928254E+00	0.126344179934E+00	0.113728915592E+00	
0.101966857495E+00				
0.910470410839E-01	0.809538624583E-01	0.716672177710E-01	0.631627377902E-01	
0.554121142439E-01				
0.483835088475E-01	0.420420314569E-01	0.363502707625E-01	0.312688593333E-01	
0.267570544913E-01				
0.227733172285E-01	0.192758729338E-01	0.162232398193E-01	0.135747134141E-01	
0.112907981381E-01				
0.933357961775E-02	0.766703395852E-02	0.625727254179E-02	0.507272301874E-02	
0.408424898420E-02				
0.326521231213E-02	0.259148331194E-02			
pseudo wavefunction				
-0.157019150967E-07	-0.167396923265E-07	-0.178460587423E-07	-0.190255475677E-07	-
0.202829916383E-07				
-0.216235432029E-07	-0.230526950352E-07	-0.245763029393E-07	-0.262006097433E-07	-
0.279322708789E-07				
-0.297783816513E-07	-0.317465063112E-07	-0.338447090490E-07	-0.360815870366E-07	-
0.384663056535E-07				
-0.410086360412E-07	-0.437189951394E-07	-0.466084883681E-07	-0.496889551312E-07	-
0.529730173270E-07				
-0.564741310656E-07	-0.602066418031E-07	-0.641858431215E-07	-0.684280393920E-07	-
0.729506125808E-07				
-0.777720934696E-07	-0.829122375840E-07	-0.883921061393E-07	-0.942341523368E-07	-
0.100462313364E-06				
-0.107102108473E-06	-0.114180743545E-06	-0.121727222563E-06	-0.129772466453E-06	-
0.138349439776E-06				
-0.147493285803E-06	-0.157241470504E-06	-0.167633936067E-06	-0.178713264552E-06	-
0.190524852370E-06				
-0.203117096289E-06	-0.216541591732E-06	-0.230853344188E-06	-0.246110994589E-06	-
0.262377059585E-06				
-0.279718187698E-06	-0.298205432410E-06	-0.317914543296E-06	-0.338926276397E-06	-
0.361326725114E-06				
-0.385207672962E-06	-0.410666969643E-06	-0.437808931979E-06	-0.466744771332E-06	-
0.497593049288E-06				
-0.530480163441E-06	-0.565540865299E-06	-0.602918812412E-06	-0.642767156991E-06	-
0.685249173430E-06				
-0.730538927311E-06	-0.778821988608E-06	-0.830296192045E-06	-0.885172447695E-06	-
0.943675605164E-06				
-0.100604537488E-05	-0.107253731029E-05	-0.114342385492E-05	-0.121899545874E-05	-
0.129956176819E-05				
-0.138545289495E-05	-0.147702076851E-05	-0.157464057816E-05	-0.167871231028E-05	-
0.178966238724E-05				

-0.190794541459E-05	-0.203404604374E-05	-0.216848095776E-05	-0.231180098841E-05	-
0.246459337309E-05				
-0.262748416096E-05	-0.280114077806E-05	-0.298627476201E-05	-0.318364467738E-05	-
0.339405922383E-05				
-0.361838054958E-05	-0.385752778390E-05	-0.411248080313E-05	-0.438428424547E-05	-
0.467405179124E-05				
-0.498297072592E-05	-0.531230680484E-05	-0.566340943932E-05	-0.603771722560E-05	-
0.643676383915E-05				
-0.686218431855E-05	-0.731572176465E-05	-0.779923448249E-05	-0.831470359521E-05	-
0.886424116115E-05				
-0.945009882741E-05	-0.100746770553E-04	-0.107405349554E-04	-0.114504007730E-04	-
0.122071830655E-04				
-0.130139826199E-04	-0.138741051568E-04	-0.147910748742E-04	-0.157686488864E-04	-
0.168108326176E-04				
-0.179218962118E-04	-0.191063920280E-04	-0.203691732910E-04	-0.217154139750E-04	-
0.231506300012E-04				
-0.246807018358E-04	-0.263118985817E-04	-0.280509036623E-04	-0.299048422017E-04	-
0.318813102150E-04				
-0.339884057274E-04	-0.362347619486E-04	-0.386295826404E-04	-0.411826798209E-04	-
0.439045139592E-04				
-0.468062368270E-04	-0.498997371805E-04	-0.531976894613E-04	-0.567136057143E-04	-
0.604618909358E-04				
-0.644579020786E-04	-0.687180109542E-04	-0.732596712917E-04	-0.781014902255E-04	-
0.832633045056E-04				
-0.887662617425E-04	-0.946329070173E-04	-0.100887275214E-03	-0.107554989448E-03	-
0.114663365999E-03				
-0.122241526167E-03	-0.130320515522E-03	-0.138933431026E-03	-0.148115556545E-03	-
0.157904507314E-03				
-0.168340383937E-03	-0.179465936550E-03	-0.191326739832E-03	-0.203971379551E-03	-
0.217451651437E-03				
-0.231822773174E-03	-0.247143610376E-03	-0.263476917482E-03	-0.280889594538E-03	-
0.299452960918E-03				
-0.319243047102E-03	-0.340340905692E-03	-0.362832942940E-03	-0.386811272131E-03	-
0.412374090262E-03				
-0.439626079542E-03	-0.468678835353E-03	-0.499651322406E-03	-0.532670360936E-03	-
0.567871144923E-03				
-0.605397794420E-03	-0.645403944247E-03	-0.688053371407E-03	-0.733520663787E-03	-
0.781991932825E-03				
-0.833665573031E-03	-0.888753071417E-03	-0.947479870104E-03	-0.101008628556E-02	-
0.107682848818E-02				
-0.114797954614E-02	-0.122383053767E-02	-0.130469173625E-02	-0.139089387344E-02	-
0.148278948434E-02				
-0.158075434109E-02	-0.168518898013E-02	-0.179652032911E-02	-0.191520344017E-02	-
0.204172333608E-02				
-0.217659697680E-02	-0.232037535407E-02	-0.247364572210E-02	-0.263703397335E-02	-
0.281120716828E-02				
-0.299687622922E-02	-0.319479880842E-02	-0.340578234163E-02	-0.363068729861E-02	-
0.387043064303E-02				
-0.412598951505E-02	-0.439840515010E-02	-0.468878704881E-02	-0.499831741354E-02	-
0.532825586780E-02				
-0.567994447597E-02	-0.605481308154E-02	-0.645438498314E-02	-0.688028296866E-02	-
0.733423572867E-02				

-0.781808467183E-02	-0.833379116563E-02	-0.888344422727E-02	-0.946926869063E-02	-
0.100936338763E-01				
-0.107590627931E-01	-0.114682419003E-01	-0.122240314618E-01	-0.130294765233E-01	-
0.138878185460E-01				
-0.148025077311E-01	-0.157772160689E-01	-0.168158511504E-01	-0.179225707760E-01	-
0.191017984004E-01				
-0.203582394500E-01	-0.216968985517E-01	-0.231230977102E-01	-0.246424954714E-01	-
0.262611071077E-01				
-0.279853258608E-01	-0.298219452744E-01	-0.317781826467E-01	-0.338617036306E-01	-
0.360806480019E-01				
-0.384436566140E-01	-0.409598995477E-01	-0.436391054584E-01	-0.464915921120E-01	-
0.495282980900E-01				
-0.527608156283E-01	-0.562014245405E-01	-0.598631271552E-01	-0.637596841742E-01	-
0.679056513333E-01				
-0.723164167161E-01	-0.770082385375E-01	-0.819982831711E-01	-0.873046631510E-01	-
0.929464748238E-01				
-0.989438352683E-01	-0.105317918029E+00	-0.112090987138E+00	-0.119286428802E+00	-
0.126928780047E+00				
-0.135043753487E+00	-0.143658257270E+00	-0.152800409110E+00	-0.162499543158E+00	-
0.172786208302E+00				
-0.183692156283E+00	-0.195250317809E+00	-0.207494764630E+00	-0.220460655265E+00	-
0.234184161818E+00				
-0.248702375012E+00	-0.264053184261E+00	-0.280275129255E+00	-0.297407219188E+00	-
0.315488715366E+00				
-0.334558872574E+00	-0.354656634163E+00	-0.375820275439E+00	-0.398086989569E+00	-
0.421492409835E+00				
-0.446070061785E+00	-0.471850738539E+00	-0.498861792378E+00	-0.527126335656E+00	-
0.556662344175E+00				
-0.587481656479E+00	-0.619588862995E+00	-0.652980079836E+00	-0.687641603231E+00	-
0.723548442186E+00				
-0.760662729134E+00	-0.798932011073E+00	-0.838287427144E+00	-0.878641782861E+00	-
0.919887536327E+00				
-0.961894717908E+00	-0.100450881199E+01	-0.104754863774E+01	-0.109080427517E+01	-
0.113403509328E+01				
-0.117696794846E+01	-0.121929563350E+01	-0.126067567017E+01	-0.130072955078E+01	-
0.133904254586E+01				
-0.137516420519E+01	-0.140860968652E+01	-0.143886204957E+01	-0.146537564950E+01	-
0.148758075362E+01				
-0.150488948363E+01	-0.151670315271E+01	-0.152242101848E+01	-0.152145040848E+01	-
0.151321809284E+01				
-0.149718267898E+01	-0.147284768789E+01	-0.143977484538E+01	-0.139759699227E+01	-
0.134602989886E+01				
-0.128488217795E+01	-0.121406245379E+01	-0.113358299114E+01	-0.104355915767E+01	-
0.944204424555E+00				
-0.835821145497E+00	-0.718788127660E+00	-0.593547034806E+00	-0.460590929166E+00	-
0.320459697907E+00				
-0.173748585434E+00	-0.211373313850E-01	0.136551852224E+00	0.298274239761E+00	
0.462762923588E+00				
0.628552373797E+00	0.793969481873E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				

-0.754308290552E-05	-0.801807177011E-05	-0.852345720061E-05	-0.906120854629E-05	-
0.963342370744E-05				
-0.102423375591E-04	-0.108903309125E-04	-0.115799400758E-04	-0.123138670339E-04	-
0.130949902979E-04				
-0.139263764554E-04	-0.148112924878E-04	-0.157532188801E-04	-0.167558636165E-04	-
0.178231770330E-04				
-0.189593676959E-04	-0.201689193198E-04	-0.214566087124E-04	-0.228275250111E-04	-
0.242870900456E-04				
-0.258410801533E-04	-0.274956493000E-04	-0.292573538147E-04	-0.311331786525E-04	-
0.331305654142E-04				
-0.352574421733E-04	-0.375222552445E-04	-0.399340030479E-04	-0.425022721029E-04	-
0.452372754654E-04				
-0.481498935580E-04	-0.512517177247E-04	-0.545550965765E-04	-0.580731853632E-04	-
0.618199985254E-04				
-0.658104656683E-04	-0.700604911484E-04	-0.745870175293E-04	-0.794080931354E-04	-
0.845429439522E-04				
-0.900120502155E-04	-0.958372278923E-04	-0.102041715456E-03	-0.108650266231E-03	-
0.115689246694E-03				
-0.123186741097E-03	-0.131172662810E-03	-0.139678872834E-03	-0.148739305892E-03	-
0.158390104624E-03				
-0.168669762367E-03	-0.179619275070E-03	-0.191282302962E-03	-0.203705342405E-03	-
0.216937908918E-03				
-0.231032731659E-03	-0.246045960414E-03	-0.262037385658E-03	-0.279070672632E-03	-
0.297213610229E-03				
-0.316538375629E-03	-0.337121815676E-03	-0.359045745989E-03	-0.382397268915E-03	-
0.407269111528E-03				
-0.433759984766E-03	-0.461974965167E-03	-0.492025900435E-03	-0.524031840371E-03	-
0.558119494618E-03				
-0.594423718960E-03	-0.633088031720E-03	-0.674265162227E-03	-0.718117633126E-03	-
0.764818378624E-03				
-0.814551400771E-03	-0.867512465988E-03	-0.923909844246E-03	-0.983965093359E-03	-
0.104791389100E-02				
-0.111600691723E-02	-0.118851079039E-02	-0.126570905951E-02	-0.134790325628E-02	-
0.143541401012E-02				
-0.152858222980E-02	-0.162777035532E-02	-0.173336368400E-02	-0.184577177477E-02	-
0.196542993506E-02				
-0.209280079464E-02	-0.222837597111E-02	-0.237267783205E-02	-0.252626135865E-02	-
0.268971611650E-02				
-0.286366833866E-02	-0.304878312719E-02	-0.324576677871E-02	-0.345536924057E-02	-
0.367838670373E-02				
-0.391566433930E-02	-0.416809918538E-02	-0.443664319149E-02	-0.472230642777E-02	-
0.502616046652E-02				
-0.534934194381E-02	-0.569305630895E-02	-0.605858177008E-02	-0.644727344383E-02	-
0.686056771752E-02				
-0.729998683241E-02	-0.776714369618E-02	-0.826374693357E-02	-0.879160618337E-02	-
0.935263765030E-02				
-0.994886992028E-02	-0.105824500471E-01	-0.112556499183E-01	-0.119708729087E-01	-
0.127306608272E-01				
-0.135377011660E-01	-0.143948346557E-01	-0.153050631342E-01	-0.162715577323E-01	-
0.172976673812E-01				
-0.183869276427E-01	-0.195430698654E-01	-0.207700306652E-01	-0.220719617292E-01	-
0.234532399389E-01				

-0.249184778076E-01	-0.264725342224E-01	-0.281205254830E-01	-0.298678366194E-01	-
0.317201329767E-01				
-0.336833720422E-01	-0.357638154937E-01	-0.379680414380E-01	-0.403029568089E-01	-
0.427758098836E-01				
-0.453942028761E-01	-0.481661045545E-01	-0.510998628303E-01	-0.542042172492E-01	-
0.574883113190E-01				
-0.609617045894E-01	-0.646343843976E-01	-0.685167771810E-01	-0.726197592476E-01	-
0.769546668856E-01				
-0.815333056803E-01	-0.863679588940E-01	-0.914713947539E-01	-0.968568724745E-01	-
0.102538146830E+00				
-0.108529471078E+00	-0.114845598007E+00	-0.121501778887E+00	-0.128513760057E+00	-
0.135897776886E+00				
-0.143670544806E+00	-0.151849247117E+00	-0.160451519221E+00	-0.169495428932E+00	-
0.178999452487E+00				
-0.188982445854E+00	-0.199463610918E+00	-0.210462456091E+00	-0.221998750892E+00	-
0.234092473977E+00				
-0.246763754141E+00	-0.260032803719E+00	-0.273919843854E+00	-0.288445021056E+00	-
0.303628314449E+00				
-0.319489433116E+00	-0.336047702923E+00	-0.353321942209E+00	-0.371330325732E+00	-
0.390090236237E+00				
-0.409618103087E+00	-0.429929227350E+00	-0.451037592813E+00	-0.472955662420E+00	-
0.495694159663E+00				
-0.519261834543E+00	-0.543665213767E+00	-0.568908334909E+00	-0.594992464383E+00	-
0.621915799107E+00				
-0.649673151856E+00	-0.678255620342E+00	-0.707650240122E+00	-0.737839621451E+00	-
0.768801570202E+00				
-0.800508692896E+00	-0.832927985833E+00	-0.866020408148E+00	-0.899740438518E+00	-
0.934035615100E+00				
-0.968846058283E+00	-0.100410397597E+01	-0.103973315159E+01	-0.107564841601E+01	-
0.111175510602E+01				
-0.114794851474E+01	-0.118411334314E+01	-0.122012316749E+01	-0.125583994595E+01	-
0.129111360028E+01				
-0.132578172690E+01	-0.135966951774E+01	-0.139259000463E+01	-0.142434477036E+01	-
0.145472526595E+01				
-0.148351476841E+01	-0.151049071038E+01	-0.153542655224E+01	-0.155809172023E+01	-
0.157824799120E+01				
-0.159564185954E+01	-0.160999492151E+01	-0.162099661185E+01	-0.162830342717E+01	-
0.163154540440E+01				
-0.163033653297E+01	-0.162428448774E+01	-0.161299720195E+01	-0.159608659381E+01	-
0.157317100783E+01				
-0.154387770884E+01	-0.150784611799E+01	-0.146473200095E+01	-0.141421258852E+01	-
0.135599253630E+01				
-0.128981062766E+01	-0.121544715143E+01	-0.113273191968E+01	-0.104155291443E+01	-
0.941865577176E+00				
-0.833702751470E+00	-0.717185290542E+00	-0.592533320193E+00	-0.460078122778E+00	-
0.320274569992E+00				
-0.173713991262E+00	-0.211373011036E-01	0.136551852224E+00	0.298274239761E+00	
0.462762923588E+00				
0.628552373797E+00	0.793969481873E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				

```

0.000000000000E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00
0.000000000000E+00 0.000000000000E+00

```

End of Dataset

PAW_PBE H 15Jun2001

1.0000000000000000

parameters from PSCTR are:

VRHFIN =H: ultrasoft test

LEXCH = PE

EATOM = 12.4884 eV, 0.9179 Ry

TITEL = PAW_PBE H 15Jun2001

LULTRA = F use ultrasoft PP ?

IUNSCR = 0 unscreen: 0-lin 1-nonlin 2-no

RPACOR = 0.000 partial core radius

POMASS = 1.000; ZVAL = 1.000 mass and valenz

RCORE = 1.100 outmost cutoff radius

RWIGS = 0.700; RWIGS = 0.370 wigner-seitz radius (au A)

ENMAX = 250.000; ENMIN = 200.000 eV

RCLOC = 0.701 cutoff for local pot

LCOR = T correct aug charges

LPAW = T paw PP

EAUG = 400.000

RMAX = 1.123 core radius for proj-oper

RAUG = 1.200 factor for augmentation sphere

RDEP = 1.112 radius for radial grids

RDEPT = 0.926 core radius for aug-charge

Atomic configuration

2 entries

n	l	j	E	occ.
1	0	0.50	-6.4927	1.0000
2	1	0.50	-3.4015	0.0000

Description

```

1  E      TYP RCUT  TYP RCUT
0  -6.4927494  23 1.100
0  6.8029130  23 1.100
1  -4.0817478  23 1.100
Error from kinetic energy argument (eV)
NDATA = 100
STEP = 20.000 1.050
5.77  5.50  5.37  5.11  4.99  4.75  4.52  4.40
4.19  3.98  3.88  3.68  3.49  3.31  3.14  2.98
2.83  2.68  2.54  2.35  2.22  2.11  1.94  1.84
1.74  1.61  1.48  1.40  1.29  1.19  1.09  1.01
0.925 0.851 0.782 0.719 0.642 0.590 0.526 0.482
0.430 0.382 0.339 0.301 0.267 0.236 0.209 0.178
0.157 0.133 0.113 0.988E-01 0.832E-01 0.697E-01 0.562E-01 0.467E-01
0.386E-01 0.305E-01 0.239E-01 0.186E-01 0.143E-01 0.109E-01 0.820E-02 0.580E-02
0.425E-02 0.291E-02 0.195E-02 0.130E-02 0.808E-03 0.544E-03 0.368E-03 0.278E-03
0.239E-03 0.227E-03 0.225E-03 0.224E-03 0.218E-03 0.204E-03 0.181E-03 0.156E-03
0.127E-03 0.983E-04 0.735E-04 0.520E-04 0.369E-04 0.274E-04 0.225E-04 0.204E-04
0.201E-04 0.200E-04 0.193E-04 0.178E-04 0.151E-04 0.121E-04 0.914E-05 0.676E-05
0.512E-05 0.437E-05 0.412E-05 0.410E-05
END of PSCTR-controll parameters
local part
170.075338972103
0.24361675E+01 0.24358438E+01 0.24348697E+01 0.24332467E+01 0.24309759E+01
0.24280585E+01 0.24244962E+01 0.24202910E+01 0.24154452E+01 0.24099615E+01
0.24038429E+01 0.23970925E+01 0.23897140E+01 0.23817112E+01 0.23730884E+01
0.23638500E+01 0.23540009E+01 0.23435463E+01 0.23324918E+01 0.23208434E+01
0.23086076E+01 0.22957912E+01 0.22824016E+01 0.22684466E+01 0.22539345E+01
0.22388742E+01 0.22232749E+01 0.22071466E+01 0.21904995E+01 0.21733446E+01
0.21556932E+01 0.21375571E+01 0.21189488E+01 0.20998810E+01 0.20803670E+01
0.20604206E+01 0.20400561E+01 0.20192881E+01 0.19981317E+01 0.19766025E+01
0.19547164E+01 0.19324900E+01 0.19099398E+01 0.18870833E+01 0.18639378E+01
0.18405213E+01 0.18168520E+01 0.17929483E+01 0.17688290E+01 0.17445131E+01
0.17200197E+01 0.16953681E+01 0.16705779E+01 0.16456684E+01 0.16206593E+01
0.15955702E+01 0.15704206E+01 0.15452301E+01 0.15200181E+01 0.14948040E+01
0.14696067E+01 0.14444455E+01 0.14193389E+01 0.13943054E+01 0.13693634E+01
0.13445305E+01 0.13198243E+01 0.12952620E+01 0.12708602E+01 0.12466351E+01
0.12226024E+01 0.11987774E+01 0.11751747E+01 0.11518084E+01 0.11286919E+01
0.11058381E+01 0.10832593E+01 0.10609670E+01 0.10389722E+01 0.10172850E+01
0.99591506E+00 0.97487120E+00 0.95416158E+00 0.93379367E+00 0.91377423E+00
0.89410930E+00 0.87480424E+00 0.85586371E+00 0.83729166E+00 0.81909138E+00
0.80126545E+00 0.78381581E+00 0.76674374E+00 0.75004987E+00 0.73373423E+00
0.71779623E+00 0.70223469E+00 0.68704790E+00 0.67223359E+00 0.65778899E+00
0.64371083E+00 0.62999539E+00 0.61663851E+00 0.60363564E+00 0.59098183E+00
0.57867178E+00 0.56669988E+00 0.55506021E+00 0.54374657E+00 0.53275254E+00
0.52207146E+00 0.51169647E+00 0.50162059E+00 0.49183665E+00 0.48233738E+00
0.47311545E+00 0.46416343E+00 0.45547387E+00 0.44703928E+00 0.43885221E+00
0.43090520E+00 0.42319086E+00 0.41570186E+00 0.40843093E+00 0.40137093E+00
0.39451480E+00 0.38785563E+00 0.38138662E+00 0.37510113E+00 0.36899267E+00
0.36305492E+00 0.35728172E+00 0.35166708E+00 0.34620521E+00 0.34089048E+00
0.33571746E+00 0.33068091E+00 0.32577576E+00 0.32099717E+00 0.31634046E+00
0.31180113E+00 0.30737491E+00 0.30305766E+00 0.29884547E+00 0.29473457E+00

```

0.29072138E+00 0.28680248E+00 0.28297461E+00 0.27923465E+00 0.27557964E+00
0.27200675E+00 0.26851329E+00 0.26509669E+00 0.26175448E+00 0.25848433E+00
0.25528399E+00 0.25215132E+00 0.24908428E+00 0.24608088E+00 0.24313924E+00
0.24025756E+00 0.23743407E+00 0.23466710E+00 0.23195502E+00 0.22929625E+00
0.22668928E+00 0.22413261E+00 0.22162480E+00 0.21916444E+00 0.21675016E+00
0.21438060E+00 0.21205445E+00 0.20977041E+00 0.20752719E+00 0.20532354E+00
0.20315824E+00 0.20103005E+00 0.19893780E+00 0.19688029E+00 0.19485638E+00
0.19286493E+00 0.19090482E+00 0.18897497E+00 0.18707430E+00 0.18520178E+00
0.18335637E+00 0.18153710E+00 0.17974299E+00 0.17797310E+00 0.17622652E+00
0.17450237E+00 0.17279980E+00 0.17111800E+00 0.16945618E+00 0.16781359E+00
0.16618952E+00 0.16458329E+00 0.16299427E+00 0.16142185E+00 0.15986548E+00
0.15832464E+00 0.15679885E+00 0.15528768E+00 0.15379074E+00 0.15230767E+00
0.15083817E+00 0.14938195E+00 0.14793880E+00 0.14650851E+00 0.14509094E+00
0.14368594E+00 0.14229345E+00 0.14091340E+00 0.13954576E+00 0.13819055E+00
0.13684780E+00 0.13551756E+00 0.13419992E+00 0.13289498E+00 0.13160287E+00
0.13032374E+00 0.12905775E+00 0.12780507E+00 0.12656590E+00 0.12534042E+00
0.12412885E+00 0.12293139E+00 0.12174826E+00 0.12057967E+00 0.11942583E+00
0.11828694E+00 0.11716320E+00 0.11605479E+00 0.11496190E+00 0.11388469E+00
0.11282332E+00 0.11177791E+00 0.11074859E+00 0.10973545E+00 0.10873859E+00
0.10775806E+00 0.10679390E+00 0.10584613E+00 0.10491475E+00 0.10399974E+00
0.10310104E+00 0.10221858E+00 0.10135227E+00 0.10050197E+00 0.99667555E-01
0.98848839E-01 0.98045629E-01 0.97257704E-01 0.96484823E-01 0.95726718E-01
0.94983104E-01 0.94253671E-01 0.93538094E-01 0.92836028E-01 0.92147111E-01
0.91470966E-01 0.90807204E-01 0.90155420E-01 0.89515201E-01 0.88886123E-01
0.88267755E-01 0.87659657E-01 0.87061387E-01 0.86472496E-01 0.85892535E-01
0.85321052E-01 0.84757597E-01 0.84201723E-01 0.83652985E-01 0.83110946E-01
0.82575173E-01 0.82045245E-01 0.81520750E-01 0.81001287E-01 0.80486470E-01
0.79975928E-01 0.79469303E-01 0.78966256E-01 0.78466466E-01 0.77969631E-01
0.77475467E-01 0.76983711E-01 0.76494120E-01 0.76006474E-01 0.75520571E-01
0.75036232E-01 0.74553301E-01 0.74071641E-01 0.73591139E-01 0.73111703E-01
0.72633262E-01 0.72155768E-01 0.71679192E-01 0.71203528E-01 0.70728790E-01
0.70255010E-01 0.69782241E-01 0.69310552E-01 0.68840032E-01 0.68370783E-01
0.67902925E-01 0.67436589E-01 0.66971920E-01 0.66509072E-01 0.66048211E-01
0.65589511E-01 0.65133151E-01 0.64679316E-01 0.64228197E-01 0.63779986E-01
0.63334877E-01 0.62893064E-01 0.62454743E-01 0.62020103E-01 0.61589333E-01
0.61162617E-01 0.60740132E-01 0.60322051E-01 0.59908537E-01 0.59499744E-01
0.59095815E-01 0.58696886E-01 0.58303075E-01 0.57914494E-01 0.57531235E-01
0.57153381E-01 0.56780996E-01 0.56414134E-01 0.56052829E-01 0.55697104E-01
0.55346962E-01 0.55002395E-01 0.54663378E-01 0.54329872E-01 0.54001822E-01
0.53679163E-01 0.53361812E-01 0.53049677E-01 0.52742651E-01 0.52440616E-01
0.52143444E-01 0.51850995E-01 0.51563123E-01 0.51279668E-01 0.51000467E-01
0.50725348E-01 0.50454134E-01 0.50186641E-01 0.49922684E-01 0.49662075E-01
0.49404623E-01 0.49150137E-01 0.48898429E-01 0.48649311E-01 0.48402597E-01
0.48158108E-01 0.47915668E-01 0.47675106E-01 0.47436260E-01 0.47198973E-01
0.46963097E-01 0.46728493E-01 0.46495030E-01 0.46262587E-01 0.46031053E-01
0.45800326E-01 0.45570316E-01 0.45340942E-01 0.45112135E-01 0.44883837E-01
0.44655999E-01 0.44428587E-01 0.44201573E-01 0.43974943E-01 0.43748692E-01
0.43522826E-01 0.43297360E-01 0.43072319E-01 0.42847735E-01 0.42623650E-01
0.42400112E-01 0.42177175E-01 0.41954901E-01 0.41733354E-01 0.41512605E-01
0.41292727E-01 0.41073795E-01 0.40855886E-01 0.40639080E-01 0.40423455E-01
0.40209090E-01 0.39996062E-01 0.39784448E-01 0.39574321E-01 0.39365753E-01
0.39158811E-01 0.38953560E-01 0.38750058E-01 0.38548361E-01 0.38348518E-01

0.38150573E-01 0.37954562E-01 0.37760516E-01 0.37568461E-01 0.37378413E-01
0.37190382E-01 0.37004372E-01 0.36820380E-01 0.36638396E-01 0.36458402E-01
0.36280375E-01 0.36104287E-01 0.35930102E-01 0.35757781E-01 0.35587280E-01
0.35418549E-01 0.35251536E-01 0.35086184E-01 0.34922435E-01 0.34760227E-01
0.34599497E-01 0.34440179E-01 0.34282209E-01 0.34125520E-01 0.33970045E-01
0.33815720E-01 0.33662478E-01 0.33510257E-01 0.33358995E-01 0.33208634E-01
0.33059119E-01 0.32910397E-01 0.32762419E-01 0.32615143E-01 0.32468527E-01
0.32322539E-01 0.32177147E-01 0.32032328E-01 0.31888062E-01 0.31744334E-01
0.31601137E-01 0.31458466E-01 0.31316321E-01 0.31174710E-01 0.31033641E-01
0.30893129E-01 0.30753194E-01 0.30613857E-01 0.30475145E-01 0.30337085E-01
0.30199711E-01 0.30063056E-01 0.29927157E-01 0.29792053E-01 0.29657782E-01
0.29524387E-01 0.29391908E-01 0.29260386E-01 0.29129862E-01 0.29000376E-01
0.28871967E-01 0.28744670E-01 0.28618520E-01 0.28493549E-01 0.28369784E-01
0.28247251E-01 0.28125971E-01 0.28005961E-01 0.27887233E-01 0.27769796E-01
0.27653654E-01 0.27538806E-01 0.27425247E-01 0.27312967E-01 0.27201953E-01
0.27092184E-01 0.26983638E-01 0.26876288E-01 0.26770101E-01 0.26665042E-01
0.26561073E-01 0.26458148E-01 0.26356223E-01 0.26255247E-01 0.26155169E-01
0.26055933E-01 0.25957483E-01 0.25859760E-01 0.25762705E-01 0.25666256E-01
0.25570355E-01 0.25474940E-01 0.25379951E-01 0.25285330E-01 0.25191021E-01
0.25096967E-01 0.25003117E-01 0.24909420E-01 0.24815831E-01 0.24722305E-01
0.24628804E-01 0.24535291E-01 0.24441734E-01 0.24348107E-01 0.24254385E-01
0.24160552E-01 0.24066592E-01 0.23972497E-01 0.23878263E-01 0.23783890E-01
0.23689383E-01 0.23594754E-01 0.23500017E-01 0.23405193E-01 0.23310304E-01
0.23215381E-01 0.23120455E-01 0.23025564E-01 0.22930746E-01 0.22836046E-01
0.22741509E-01 0.22647184E-01 0.22553120E-01 0.22459369E-01 0.22365983E-01
0.22273017E-01 0.22180524E-01 0.22088556E-01 0.21997168E-01 0.21906411E-01
0.21816337E-01 0.21726993E-01 0.21638428E-01 0.21550687E-01 0.21463813E-01
0.21377844E-01 0.21292817E-01 0.21208765E-01 0.21125718E-01 0.21043701E-01
0.20962735E-01 0.20882837E-01 0.20804018E-01 0.20726288E-01 0.20649647E-01
0.20574096E-01 0.20499626E-01 0.20426227E-01 0.20353883E-01 0.20282575E-01
0.20212277E-01 0.20142961E-01 0.20074596E-01 0.20007145E-01 0.19940570E-01
0.19874829E-01 0.19809879E-01 0.19745671E-01 0.19682157E-01 0.19619288E-01
0.19557010E-01 0.19495272E-01 0.19434019E-01 0.19373197E-01 0.19312752E-01
0.19252631E-01 0.19192779E-01 0.19133145E-01 0.19073678E-01 0.19014330E-01
0.18955052E-01 0.18895801E-01 0.18836535E-01 0.18777215E-01 0.18717807E-01
0.18658276E-01 0.18598597E-01 0.18538743E-01 0.18478695E-01 0.18418436E-01
0.18357952E-01 0.18297236E-01 0.18236282E-01 0.18175090E-01 0.18113662E-01
0.18052006E-01 0.17990131E-01 0.17928052E-01 0.17865786E-01 0.17803353E-01
0.17740776E-01 0.17678083E-01 0.17615302E-01 0.17552465E-01 0.17489605E-01
0.17426758E-01 0.17363961E-01 0.17301252E-01 0.17238671E-01 0.17176257E-01
0.17114051E-01 0.17052093E-01 0.16990421E-01 0.16929075E-01 0.16868092E-01
0.16807509E-01 0.16747361E-01 0.16687679E-01 0.16628495E-01 0.16569837E-01
0.16511731E-01 0.16454200E-01 0.16397265E-01 0.16340944E-01 0.16285251E-01
0.16230198E-01 0.16175795E-01 0.16122045E-01 0.16068953E-01 0.16016516E-01
0.15964731E-01 0.15913591E-01 0.15863086E-01 0.15813203E-01 0.15763925E-01
0.15715233E-01 0.15667108E-01 0.15619524E-01 0.15572456E-01 0.15525877E-01
0.15479757E-01 0.15434066E-01 0.15388772E-01 0.15343843E-01 0.15299247E-01
0.15254950E-01 0.15210918E-01 0.15167120E-01 0.15123523E-01 0.15080096E-01
0.15036808E-01 0.14993629E-01 0.14950531E-01 0.14907489E-01 0.14864477E-01
0.14821471E-01 0.14778452E-01 0.14735401E-01 0.14692301E-01 0.14649137E-01
0.14605900E-01 0.14562579E-01 0.14519170E-01 0.14475668E-01 0.14432074E-01
0.14388389E-01 0.14344618E-01 0.14300768E-01 0.14256849E-01 0.14212873E-01

0.14168854E-01 0.14124809E-01 0.14080754E-01 0.14036711E-01 0.13992698E-01
0.13948738E-01 0.13904855E-01 0.13861071E-01 0.13817411E-01 0.13773899E-01
0.13730559E-01 0.13687417E-01 0.13644497E-01 0.13601821E-01 0.13559414E-01
0.13517297E-01 0.13475492E-01 0.13434017E-01 0.13392892E-01 0.13352133E-01
0.13311754E-01 0.13271768E-01 0.13232186E-01 0.13193015E-01 0.13154262E-01
0.13115931E-01 0.13078021E-01 0.13040533E-01 0.13003461E-01 0.12966801E-01
0.12930543E-01 0.12894678E-01 0.12859191E-01 0.12824070E-01 0.12789297E-01
0.12754855E-01 0.12720724E-01 0.12686882E-01 0.12653308E-01 0.12619978E-01
0.12586868E-01 0.12553954E-01 0.12521209E-01 0.12488609E-01 0.12456127E-01
0.12423738E-01 0.12391416E-01 0.12359137E-01 0.12326878E-01 0.12294614E-01
0.12262325E-01 0.12229990E-01 0.12197591E-01 0.12165110E-01 0.12132533E-01
0.12099848E-01 0.12067043E-01 0.12034110E-01 0.12001043E-01 0.11967838E-01
0.11934493E-01 0.11901011E-01 0.11867393E-01 0.11833645E-01 0.11799774E-01
0.11765791E-01 0.11731706E-01 0.11697535E-01 0.11663292E-01 0.11628994E-01
0.11594661E-01 0.11560313E-01 0.11525972E-01 0.11491660E-01 0.11457402E-01
0.11423222E-01 0.11389145E-01 0.11355197E-01 0.11321403E-01 0.11287788E-01
0.11254378E-01 0.11221197E-01 0.11188268E-01 0.11155613E-01 0.11123255E-01
0.11091211E-01 0.11059502E-01 0.11028142E-01 0.10997147E-01 0.10966530E-01
0.10936299E-01 0.10906465E-01 0.10877032E-01 0.10848006E-01 0.10819387E-01
0.10791175E-01 0.10763367E-01 0.10735959E-01 0.10708941E-01 0.10682306E-01
0.10656041E-01 0.10630132E-01 0.10604563E-01 0.10579317E-01 0.10554374E-01
0.10529714E-01 0.10505313E-01 0.10481148E-01 0.10457195E-01 0.10433428E-01
0.10409822E-01 0.10386350E-01 0.10362985E-01 0.10339702E-01 0.10316474E-01
0.10293277E-01 0.10270085E-01 0.10246875E-01 0.10223624E-01 0.10200311E-01
0.10176916E-01 0.10153420E-01 0.10129806E-01 0.10106059E-01 0.10082167E-01
0.10058116E-01 0.10033900E-01 0.10009509E-01 0.99849389E-02 0.99601874E-02
0.99352536E-02 0.99101391E-02 0.98848478E-02 0.98593856E-02 0.98337608E-02
0.98079834E-02 0.97820656E-02 0.97560211E-02 0.97298656E-02 0.97036159E-02
0.96772903E-02 0.96509083E-02 0.96244901E-02 0.95980569E-02 0.95716303E-02
0.95452325E-02 0.95188855E-02 0.94926116E-02 0.94664330E-02 0.94403714E-02
0.94144481E-02 0.93886836E-02 0.93630977E-02 0.93377094E-02 0.93125363E-02
0.92875950E-02 0.92629004E-02 0.92384663E-02 0.92143045E-02 0.91904252E-02
0.91668370E-02 0.91435462E-02 0.91205575E-02 0.90978735E-02 0.90754949E-02
0.90534203E-02 0.90316465E-02 0.90101684E-02 0.89889792E-02 0.89680703E-02
0.89474315E-02 0.89270514E-02 0.89069168E-02 0.88870137E-02 0.88673270E-02
0.88478404E-02 0.88285371E-02 0.88093996E-02 0.87904098E-02 0.87715495E-02
0.87528000E-02 0.87341429E-02 0.87155597E-02 0.86970321E-02 0.86785424E-02
0.86600734E-02 0.86416084E-02 0.86231320E-02 0.86046294E-02 0.85860872E-02
0.85674930E-02 0.85488358E-02 0.85301063E-02 0.85112964E-02 0.84923997E-02
0.84734114E-02 0.84543282E-02 0.84351485E-02 0.84158722E-02 0.83965008E-02
0.83770372E-02 0.83574859E-02 0.83378525E-02 0.83181439E-02 0.82983685E-02
0.82785352E-02 0.82586544E-02 0.82387371E-02 0.82187952E-02 0.81988412E-02
0.81788880E-02 0.81589493E-02 0.81390387E-02 0.81191702E-02 0.80993578E-02
0.80796153E-02 0.80599563E-02 0.80403940E-02 0.80209411E-02 0.80016097E-02
0.79824109E-02 0.79633552E-02 0.79444518E-02 0.79257089E-02 0.79071337E-02
0.78887320E-02 0.78705084E-02 0.78524662E-02 0.78346073E-02 0.78169327E-02
0.77994416E-02 0.77821323E-02 0.77650018E-02 0.77480461E-02 0.77312597E-02
0.77146366E-02 0.76981692E-02 0.76818496E-02 0.76656686E-02 0.76496164E-02
0.76336827E-02 0.76178563E-02 0.76021257E-02 0.75864791E-02 0.75709043E-02
0.75553893E-02 0.75399216E-02 0.75244892E-02 0.75090803E-02 0.74936835E-02
0.74782877E-02 0.74628829E-02 0.74474592E-02 0.74320081E-02 0.74165217E-02
0.74009930E-02 0.73854163E-02 0.73697867E-02 0.73541005E-02 0.73383551E-02

0.73225489E-02 0.73066816E-02 0.72907538E-02 0.72747672E-02 0.72587245E-02
0.72426295E-02 0.72264869E-02 0.72103023E-02 0.71940821E-02 0.71778338E-02
0.71615653E-02 0.71452853E-02 0.71290031E-02 0.71127286E-02 0.70964719E-02
0.70802435E-02 0.70640541E-02 0.70479144E-02 0.70318352E-02 0.70158268E-02
0.69998996E-02 0.69840634E-02 0.69683274E-02 0.69527005E-02 0.69371907E-02
0.69218054E-02 0.69065510E-02 0.68914332E-02 0.68764567E-02 0.68616255E-02
0.68469424E-02 0.68324093E-02 0.68180272E-02 0.68037962E-02 0.67897153E-02
0.67757826E-02 0.67619954E-02 0.67483499E-02 0.67348415E-02 0.67214650E-02
0.67082139E-02 0.66950815E-02 0.66820600E-02 0.66691414E-02 0.66563167E-02
0.66435770E-02 0.66309126E-02 0.66183138E-02 0.66057709E-02 0.65932738E-02
0.65808130E-02 0.65683787E-02 0.65559616E-02 0.65435530E-02 0.65311442E-02
0.65187274E-02 0.65062953E-02 0.64938412E-02 0.64813592E-02 0.64688439E-02
0.64562910E-02 0.64436966E-02 0.64310580E-02 0.64183730E-02 0.64056404E-02
0.63928596E-02 0.63800311E-02 0.63671561E-02 0.63542365E-02 0.63412751E-02
0.63282753E-02 0.63152413E-02 0.63021781E-02 0.62890910E-02 0.62759860E-02

gradient corrections used for XC

5

atomic pseudo charge-density

0.10000000E+01 0.99507271E+00 0.98052707E+00 0.95704568E+00 0.92568373E+00
0.88776197E+00 0.84474519E+00 0.79812454E+00 0.74931839E+00 0.69959966E+00
0.65005177E+00 0.60155049E+00 0.55476631E+00 0.51018082E+00 0.46811135E+00
0.42873902E+00 0.39213662E+00 0.35829427E+00 0.32714173E+00 0.29856681E+00
0.27243019E+00 0.24857680E+00 0.22684441E+00 0.20706984E+00 0.18909339E+00
0.17276170E+00 0.15792970E+00 0.14446162E+00 0.13223147E+00 0.12112317E+00
0.11103030E+00 0.10185573E+00 0.93511122E-01 0.85916370E-01 0.78998981E-01
0.72693483E-01 0.66940835E-01 0.61687850E-01 0.56886663E-01 0.52494223E-01
0.48471824E-01 0.44784673E-01 0.41401501E-01 0.38294197E-01 0.35437485E-01
0.32808629E-01 0.30387170E-01 0.28154684E-01 0.26094570E-01 0.24191860E-01
0.22433043E-01 0.20805918E-01 0.19299454E-01 0.17903669E-01 0.16609522E-01
0.15408814E-01 0.14294104E-01 0.13258632E-01 0.12296247E-01 0.11401351E-01
0.10568838E-01 0.97940489E-02 0.90727275E-02 0.84009799E-02 0.77752401E-02
0.71922383E-02 0.66489732E-02 0.61426860E-02 0.56708380E-02 0.52310902E-02
0.48212851E-02 0.44394298E-02 0.40836812E-02 0.37523329E-02 0.34438028E-02
0.31566226E-02 0.28894274E-02 0.26409474E-02 0.24099994E-02 0.21954799E-02
0.19963586E-02 0.18116719E-02 0.16405184E-02 0.14820533E-02 0.13354843E-02
0.12000676E-02 0.10751045E-02 0.95993760E-03 0.85394820E-03 0.75655353E-03
0.66720422E-03 0.58538210E-03 0.51059815E-03 0.44239061E-03 0.38032331E-03
0.32398414E-03 0.27298355E-03 0.22695333E-03 0.18554536E-03 0.14843054E-03
0.11529778E-03 0.85853022E-04 0.59818447E-04 0.36931616E-04 0.16944752E-04
-0.37596258E-06 -0.15251030E-04 -0.27888246E-04 -0.38483271E-04 -0.47220171E-04
-0.54271921E-04 -0.59800894E-04 -0.63959316E-04 -0.66889705E-04 -0.68725292E-04
-0.69590421E-04 -0.69600935E-04 -0.68864550E-04 -0.67481212E-04 -0.65543450E-04
-0.63136706E-04 -0.60339669E-04 -0.57224588E-04 -0.53857585E-04 -0.50298952E-04
-0.46603449E-04 -0.42820588E-04 -0.38994910E-04 -0.35166258E-04 -0.31370042E-04
-0.27637496E-04 -0.23995929E-04 -0.20468969E-04 -0.17076800E-04 -0.13836396E-04
-0.10761738E-04 -0.78640368E-05 -0.51519400E-05 -0.26317346E-05 -0.30754321E-06
0.18184879E-05 0.37460076E-05 0.54762863E-05 0.70120494E-05 0.83573183E-05
0.95172586E-05 0.10498036E-04 0.11306680E-04 0.11950953E-04 0.12439230E-04
0.12780382E-04 0.12983670E-04 0.13058643E-04 0.13015047E-04 0.12862735E-04
0.12611591E-04 0.12271451E-04 0.11852046E-04 0.11362931E-04 0.10813439E-04
0.10212627E-04 0.95692387E-05 0.88916613E-05 0.81878987E-05 0.74655424E-05
0.67317501E-05 0.59932278E-05 0.52562170E-05 0.45264854E-05 0.38093217E-05

0.31095337E-05 0.24314501E-05 0.17789246E-05 0.11553436E-05 0.56363617E-06
0.62857840E-08 -0.51465502E-06 -0.99754876E-06 -0.14411553E-05 -0.18446129E-05
-0.22074179E-05 -0.25294036E-05 -0.28107184E-05 -0.30518031E-05 -0.32533685E-05
-0.34163715E-05 -0.35419928E-05 -0.36316130E-05 -0.36867901E-05 -0.37092371E-05
-0.37007994E-05 -0.36634337E-05 -0.35991871E-05 -0.35101767E-05 -0.33985706E-05
-0.32665695E-05 -0.31163891E-05 -0.29502438E-05 -0.27703314E-05 -0.25788184E-05
-0.23778274E-05 -0.21694244E-05 -0.19556080E-05 -0.17382998E-05 -0.15193351E-05
-0.13004558E-05 -0.10833033E-05 -0.86941326E-06 -0.66021104E-06 -0.45700811E-06
-0.26099955E-06 -0.73262361E-07 0.10524527E-06 0.27368393E-06 0.43133217E-06
0.57758491E-06 0.71195121E-06 0.83405141E-06 0.94361370E-06 0.10404702E-05
0.11245524E-05 0.11958865E-05 0.12545883E-05 0.13008573E-05 0.13349715E-05
0.13572809E-05 0.13682019E-05 0.13682106E-05 0.13578370E-05 0.13376583E-05
0.13082928E-05 0.12703935E-05 0.12246421E-05 0.11717430E-05 0.11124172E-05
0.10473968E-05 0.97741954E-06 0.90322336E-06 0.82554157E-06 0.74509805E-06
0.66260285E-06 0.57874797E-06 0.49420362E-06 0.40961464E-06 0.32559736E-06
0.24273670E-06 0.16158369E-06 0.82653234E-07 0.64222964E-08 -0.66671676E-07
-0.13623195E-06 -0.20190340E-06 -0.26337311E-06 -0.32037069E-06 -0.37266826E-06
-0.42008018E-06 -0.46246260E-06 -0.49971262E-06 -0.53176732E-06 -0.55860258E-06
-0.58023163E-06 -0.59670348E-06 -0.60810117E-06 -0.61453985E-06 -0.61616476E-06
-0.61314909E-06 -0.60569171E-06 -0.59401487E-06 -0.57836181E-06 -0.55899437E-06
-0.53619045E-06 -0.51024163E-06 -0.48145066E-06 -0.45012905E-06 -0.41659460E-06
-0.38116908E-06 -0.34417591E-06 -0.30593794E-06 -0.26677524E-06 -0.22700311E-06
-0.18693007E-06 -0.14685601E-06 -0.10707051E-06 -0.67851159E-07 -0.29462157E-07
0.78470792E-08 0.43843091E-07 0.78309435E-07 0.11104760E-06 0.14187775E-06
0.17063939E-06 0.19719177E-06 0.22141426E-06 0.24320654E-06 0.26248861E-06
0.27920072E-06 0.29330316E-06 0.30477589E-06 0.31361809E-06 0.31984759E-06
0.32350017E-06 0.32462878E-06 0.32330264E-06 0.31960635E-06 0.31363875E-06
0.30551194E-06 0.29535001E-06 0.28328790E-06 0.26947017E-06 0.25404964E-06
0.23718618E-06 0.21904536E-06 0.19979715E-06 0.17961459E-06 0.15867254E-06
0.13714637E-06 0.11521074E-06 0.93038375E-07 0.70798934E-07 0.48657882E-07
0.26775443E-07 0.53056120E-08 -0.15604769E-07 -0.35816858E-07 -0.55200584E-07
-0.73635344E-07 -0.91010610E-07 -0.10722645E-06 -0.12219399E-06 -0.13583572E-06
-0.14808582E-06 -0.15889027E-06 -0.16820699E-06 -0.17600582E-06 -0.18226846E-06
-0.18698826E-06 -0.19017006E-06 -0.19182979E-06 -0.19199416E-06 -0.19070014E-06
-0.18799451E-06 -0.18393323E-06 -0.17858085E-06 -0.17200983E-06 -0.16429983E-06
-0.15553695E-06 -0.14581297E-06 -0.13522454E-06 -0.12387237E-06 -0.11186039E-06
-0.99294934E-07 -0.86283897E-07 -0.72935913E-07 -0.59359547E-07 -0.45662502E-07
-0.31950844E-07 -0.18328268E-07 -0.48953878E-08 0.82509363E-08 0.21018222E-07
0.33318948E-07 0.45071091E-07 0.56198605E-07 0.66631854E-07 0.76307979E-07
0.85171220E-07 0.93173168E-07 0.10027296E-06 0.10643744E-06 0.11164119E-06
0.11586660E-06 0.11910380E-06 0.12135058E-06 0.12261224E-06 0.12290138E-06
0.12223765E-06 0.12064748E-06 0.11816369E-06 0.11482516E-06 0.11067637E-06
0.10576697E-06 0.10015128E-06 0.93887835E-07 0.87038777E-07 0.79669378E-07
0.71847455E-07 0.63642813E-07 0.55126678E-07 0.46371129E-07 0.37448538E-07
0.28431017E-07 0.19389877E-07 0.10395110E-07 0.15148814E-08 -0.71849464E-08
-0.15641266E-07 -0.23794146E-07 -0.31587224E-07 -0.38968060E-07 -0.45888456E-07
-0.52304733E-07 -0.58177979E-07 -0.63474241E-07 -0.68164690E-07 -0.72225732E-07
-0.75639090E-07 -0.78391829E-07 -0.80476351E-07 -0.81890351E-07 -0.82636719E-07
-0.82723424E-07 -0.82163347E-07 -0.80974088E-07 -0.79177732E-07 -0.76800598E-07
-0.73872950E-07 -0.70428689E-07 -0.66505018E-07 -0.62142096E-07 -0.57382670E-07
-0.52271694E-07 -0.46855946E-07 -0.41183626E-07 -0.35303965E-07 -0.29266821E-07
-0.23122287E-07 -0.16920298E-07 -0.10710252E-07 -0.45406409E-08 0.15413071E-08

0.74899664E-08 0.13261634E-07 0.18814831E-07 0.24110576E-07 0.29112642E-07
0.33787780E-07 0.38105922E-07 0.42040347E-07 0.45567830E-07 0.48668748E-07
0.51327172E-07 0.53530909E-07 0.55271536E-07 0.56544387E-07 0.57348522E-07
0.57686661E-07 0.57565098E-07 0.56993581E-07 0.55985174E-07 0.54556096E-07
0.52725530E-07 0.50515426E-07 0.47950275E-07 0.45056873E-07 0.41864071E-07
0.38402512E-07 0.34704359E-07 0.30803023E-07 0.26732870E-07 0.22528949E-07
0.18226695E-07 0.13861657E-07 0.94692132E-08 0.50843006E-08 0.74115276E-09
-0.35269544E-08 -0.76879439E-08 -0.11711165E-07 -0.15567606E-07 -0.19230089E-07
-0.22673450E-07 -0.25874695E-07 -0.28813144E-07 -0.31470546E-07 -0.33831177E-07
-0.35881921E-07 -0.37612319E-07 -0.39014609E-07 -0.40083731E-07 -0.40817324E-07
-0.41215691E-07 -0.41281750E-07 -0.41020969E-07 -0.40441269E-07 -0.39552927E-07
-0.38368449E-07 -0.36902433E-07 -0.35171421E-07 -0.33193733E-07 -0.30989292E-07
-0.28579446E-07 -0.25986767E-07 -0.23234864E-07 -0.20348174E-07 -0.17351757E-07
-0.14271095E-07 -0.11131882E-07 -0.79598190E-08 -0.47804186E-08 -0.16188047E-08
0.15004740E-08 0.45536262E-08 0.75177900E-08 0.10371195E-07 0.13093314E-07
0.15664999E-07 0.18068612E-07 0.20288130E-07 0.22309248E-07 0.24119459E-07
0.25708119E-07 0.27066503E-07 0.28187838E-07 0.29067320E-07 0.29702123E-07
0.30091388E-07 0.30236191E-07 0.30139509E-07 0.29806159E-07 0.29242734E-07
0.28457522E-07 0.27460408E-07 0.26262778E-07 0.24877398E-07 0.23318296E-07
0.21600630E-07 0.19740552E-07 0.17755064E-07 0.15661872E-07 0.13479236E-07
0.11225820E-07 0.89205354E-08 0.65823942E-08 0.42303553E-08 0.18831785E-08
-0.44071890E-09 -0.27234006E-08 -0.49475436E-08 -0.70965637E-08 -0.91547332E-08
-0.11107290E-07 -0.12940538E-07 -0.14641935E-07 -0.16200176E-07 -0.17605258E-07
-0.18848540E-07 -0.19922787E-07 -0.20822206E-07 -0.21542467E-07 -0.22080716E-07
-0.22435570E-07 -0.22607110E-07 -0.22596853E-07 -0.22407720E-07 -0.22043990E-07
-0.21511249E-07 -0.20816321E-07 -0.19967200E-07 -0.18972964E-07 -0.17843696E-07
-0.16590383E-07 -0.15224817E-07 -0.13759494E-07 -0.12207503E-07 -0.10582416E-07
-0.88981730E-08 -0.71689707E-08 -0.54091445E-08 -0.36330558E-08 -0.18549793E-08
-0.88992486E-10 0.16511315E-08 0.33520271E-08 0.50008349E-08 0.65852952E-08
0.80938344E-08 0.95156468E-08 0.10840767E-07 0.12060136E-07 0.13165660E-07
0.14150260E-07 0.15007909E-07 0.15733671E-07 0.16323719E-07 0.16775349E-07
0.17086989E-07 0.17258193E-07 0.17289629E-07 0.17183056E-07 0.16941299E-07
0.16568210E-07 0.16068621E-07 0.15448296E-07 0.14713870E-07 0.13872788E-07
0.12933230E-07 0.11904041E-07 0.10794653E-07 0.96149962E-08 0.83754217E-08
0.70866094E-08 0.57594812E-08 0.44051112E-08 0.30346366E-08 0.16591692E-08
0.28970778E-09 -0.10629465E-08 -0.23882728E-08 -0.36761101E-08 -0.49167316E-08
-0.61009164E-08 -0.72200151E-08 -0.82660105E-08 -0.92315723E-08 -0.10110106E-07
-0.10895795E-07 -0.11583636E-07 -0.12169469E-07 -0.12649998E-07 -0.13022805E-07
-0.13286361E-07 -0.13440023E-07 -0.13484027E-07 -0.13419480E-07 -0.13248335E-07
-0.12973367E-07 -0.12598141E-07 -0.12126971E-07 -0.11564879E-07 -0.10917548E-07
-0.10191262E-07 -0.93928581E-08 -0.85296562E-08 -0.76094011E-08 -0.66401938E-08
-0.56304228E-08 -0.45886939E-08 -0.35237599E-08 -0.24444483E-08 -0.13595910E-08
-0.27795382E-09 0.79183266E-09 0.18413399E-08 0.28624062E-08 0.38471985E-08
0.47882708E-08 0.56786190E-08 0.65117314E-08 0.72816349E-08 0.79829364E-08
0.86108588E-08 0.91612717E-08 0.96307175E-08 0.10016430E-07 0.10316351E-07
0.10529133E-07 0.10654147E-07 0.10691479E-07 0.10641916E-07 0.10506937E-07
0.10288688E-07 0.99899618E-08 0.96141644E-08 0.91652824E-08 0.86478432E-08
0.80668725E-08 0.74278480E-08 0.67366506E-08 0.59995114E-08 0.52229582E-08
0.44137592E-08 0.35788654E-08 0.27253528E-08 0.18603638E-08 0.99104892E-09
0.12450863E-09 -0.73226315E-09 -0.15724343E-08 -0.23893876E-08 -0.31767721E-08
-0.39285512E-08 -0.46390481E-08 -0.53029871E-08 -0.59155323E-08 -0.64723211E-08
-0.69694946E-08 -0.74037231E-08 -0.77722272E-08 -0.80727937E-08 -0.83037873E-08

-0.84641576E-08 -0.85534411E-08 -0.85717582E-08 -0.85198059E-08 -0.83988454E-08
-0.82106857E-08 -0.79576630E-08 -0.76426161E-08 -0.72688572E-08 -0.68401395E-08
-0.63606227E-08 -0.58348336E-08 -0.52676259E-08 -0.46641369E-08 -0.40297417E-08
-0.33700074E-08 -0.26906450E-08 -0.19974615E-08 -0.12963111E-08 -0.59304673E-09
0.10652838E-09 0.79670732E-09 0.14719253E-08 0.21268039E-08 0.27561933E-08
0.33552124E-08 0.39192858E-08 0.44441784E-08 0.49260262E-08 0.53613640E-08
0.57471505E-08 0.60807880E-08 0.63601395E-08 0.65835407E-08 0.67498089E-08
0.68582472E-08 0.69086456E-08 0.69012769E-08 0.68368888E-08 0.67166930E-08
0.65423493E-08 0.63159472E-08 0.60399845E-08 0.57173408E-08 0.53512500E-08
0.49452691E-08 0.45032452E-08 0.40292801E-08 0.35276940E-08 0.30029865E-08
0.24597968E-08 0.19028641E-08 0.13369865E-08 0.76698121E-09 0.19764363E-09
-0.36629233E-09 -0.92019325E-09 -0.14595636E-08 -0.19800814E-08 -0.24776323E-08
-0.29483418E-08 -0.33886048E-08 -0.37951131E-08 -0.41648793E-08 -0.44952582E-08
-0.47839647E-08 -0.50290893E-08 -0.52291097E-08 -0.53828999E-08 -0.54897341E-08
-0.55492887E-08 -0.55616404E-08 -0.55272608E-08 -0.54470088E-08 -0.53221186E-08
-0.51541850E-08 -0.49451457E-08 -0.46972614E-08 -0.44130926E-08 -0.40954758E-08
-0.37474957E-08 -0.33724564E-08 -0.29738508E-08 -0.25553288E-08 -0.21206652E-08
-0.16737262E-08 -0.12184358E-08 -0.75874167E-09 -0.29858078E-09 0.15815345E-09
0.60764355E-09 0.10461794E-08 0.14701884E-08 0.18762650E-08 0.22611975E-08
0.26219934E-08 0.29559019E-08 0.32604343E-08 0.35333822E-08 0.37728334E-08
0.39771851E-08 0.41451534E-08 0.42757806E-08 0.43684391E-08 0.44228326E-08
0.44389952E-08 0.44172871E-08 0.43583880E-08 0.42632864E-08 0.41332674E-08
0.39698979E-08 0.37750103E-08 0.35506830E-08 0.32992204E-08 0.30231294E-08
0.27250951E-08 0.24079556E-08 0.20746757E-08 0.17283203E-08 0.13720269E-08
0.10089773E-08 0.64236926E-09 0.27538869E-09 -0.88817403E-10 -0.44716714E-09
-0.79666932E-09 -0.11344482E-08 -0.14577675E-08 -0.17640519E-08 -0.20509075E-08
-0.23161397E-08 -0.25577690E-08 -0.27740457E-08 -0.29634625E-08 -0.31247643E-08
-0.32569564E-08 -0.33593088E-08 -0.34313590E-08 -0.34729125E-08 -0.34840409E-08
-0.34650790E-08 -0.34166180E-08 -0.33394968E-08 -0.32347912E-08 -0.31038009E-08
-0.29480357E-08 -0.27692003E-08 -0.25691764E-08 -0.23500045E-08 -0.21138630E-08
-0.18630473E-08 -0.15999480E-08 -0.13270290E-08 -0.10468057E-08 -0.76182199E-09
-0.47462716E-09 -0.18775306E-09 0.96308187E-10 0.37512531E-09 0.64634793E-09
0.90772590E-09 0.11571279E-08 0.13925594E-08 0.16121782E-08 0.18143092E-08
0.19974559E-08 0.21603108E-08 0.23017642E-08 0.24209115E-08 0.25170591E-08
0.25897272E-08 0.26386511E-08 0.26637797E-08 0.26652723E-08 0.26434944E-08
0.25990115E-08 0.25325821E-08 0.24451476E-08 0.23378207E-08 0.22118726E-08
0.20687187E-08 0.19099044E-08 0.17370893E-08 0.15520315E-08 0.13565700E-08
0.11526064E-08 0.94208642E-09 0.72698183E-09 0.50927260E-09 0.29092981E-09
0.73898319E-10 -0.13992052E-09 -0.34868586E-09 -0.55063331E-09 -0.74408955E-09
-0.92748528E-09 -0.10993671E-08 -0.12584086E-08 -0.14034205E-08 -0.15333600E-08
-0.16473378E-08 -0.17446241E-08 -0.18246510E-08 -0.18870155E-08 -0.19314795E-08
-0.19579702E-08 -0.19665787E-08 -0.19575564E-08 -0.19313105E-08 -0.18883962E-08
-0.18295095E-08 -0.17554778E-08 -0.16672513E-08 -0.15658926E-08 -0.14525654E-08
-0.13285220E-08 -0.11950894E-08 -0.10536555E-08 -0.90565537E-09 -0.75255756E-09
-0.59585094E-09 -0.43703077E-09 -0.27758435E-09 -0.11897671E-09 0.37363169E-10
0.19005491E-09 0.33777816E-09 0.47928315E-09 0.61340079E-09 0.73905256E-09
0.85525968E-09 0.96115109E-09 0.10559696E-08 0.11390764E-08 0.12099541E-08
0.12682090E-08 0.13135729E-08 0.13459040E-08 0.13651864E-08 0.13715280E-08
0.13651565E-08 0.13464140E-08 0.13157514E-08 0.12737218E-08 0.12209744E-08
0.11582468E-08 0.10863562E-08 0.10061901E-08 0.91869452E-09 0.82486429E-09
0.72573186E-09 0.62235757E-09 0.51581957E-09 0.40720333E-09 0.29759065E-09
0.18804839E-09 0.79617864E-10 -0.26694861E-10 -0.12992735E-09 -0.22916843E-09

-0.32356550E-09 -0.41233183E-09 -0.49475360E-09 -0.57019611E-09 -0.63810863E-09
-0.69802753E-09 -0.74957813E-09 -0.79247588E-09 -0.82652720E-09 -0.85163006E-09
-0.86777396E-09 -0.87503857E-09 -0.87359079E-09 -0.86368046E-09 -0.84563529E-09
-0.81985561E-09 -0.78680923E-09 -0.74702617E-09 -0.70109273E-09 -0.64964445E-09
-0.59335802E-09 -0.53294258E-09 -0.46913126E-09 -0.40267319E-09 -0.33432629E-09
-0.26485010E-09 -0.19499832E-09 -0.12551082E-09 -0.57105287E-10 0.95305931E-11
0.73746064E-10 0.13493289E-09 0.19253002E-09 0.24602779E-09 0.29497228E-09
0.33896962E-09 0.37768995E-09 0.41087033E-09 0.43831615E-09 0.45990107E-09
0.47556609E-09 0.48531828E-09 0.48922963E-09 0.48743576E-09 0.48013408E-09
0.46758068E-09 0.45008598E-09 0.42800915E-09 0.40175226E-09 0.37175461E-09
34.2040403932785 T

Non local Part

0 2 0.594199078900351
-1.78821932145992 -2.97948220375297 -2.97948220375297
-4.86951231451956

Reciprocal Space Part

0.18925024E+02 0.18753244E+02 0.18241190E+02 0.17398641E+02 0.16241658E+02
0.14792226E+02 0.13077777E+02 0.11130586E+02 0.89870706E+01 0.66869981E+01
0.42726328E+01 0.17878314E+01 -0.72288486E+00 -0.32152612E+01 -0.56462225E+01
-0.79747469E+01 -0.10162679E+02 -0.12175468E+02 -0.13982809E+02 -0.15559178E+02
-0.16884251E+02 -0.17943198E+02 -0.18726842E+02 -0.19231691E+02 -0.19459846E+02
-0.19418769E+02 -0.19120958E+02 -0.18583499E+02 -0.17827533E+02 -0.16877652E+02
-0.15761228E+02 -0.14507703E+02 -0.13147858E+02 -0.11713076E+02 -0.10234617E+02
-0.87429281E+01 -0.72669933E+01 -0.58337520E+01 -0.44675860E+01 -0.31898917E+01
-0.20187428E+01 -0.96864912E+00 -0.50413695E-01 0.72891258E+00 0.13659809E+01
0.18610048E+01 0.22175383E+01 0.24421811E+01 0.25442210E+01 0.25352276E+01
0.24286080E+01 0.22391400E+01 0.19824943E+01 0.16747613E+01 0.13319932E+01
0.96977378E+00 0.60282627E+00 0.24466820E+00 -0.92679993E-01 -0.39892687E+00
-0.66567918E+00 -0.88654687E+00 -0.10571842E+01 -0.11752696E+01 -0.12404272E+01
-0.12540967E+01 -0.12193576E+01 -0.11407144E+01 -0.10238539E+01 -0.87537989E+00
-0.70253781E+00 -0.51293552E+00 -0.31427052E+00 -0.11407096E+00 0.80542405E-01
0.26306687E+00 0.42779621E+00 0.56996294E+00 0.68584203E+00 0.77281476E+00
0.82939296E+00 0.85520488E+00 0.85094532E+00 0.81829337E+00 0.75980224E+00
0.67876615E+00 0.57906982E+00 0.46502638E+00 0.34120952E+00 0.21228587E+00
0.82852854E-01 -0.42712696E-01 -0.16039078E+00 -0.26663557E+00 -0.35847089E+00
-0.43356164E+00 -0.49026014E+00 -0.52762691E+00 -0.54542645E+00 -0.54409949E+00

Real Space Part

-0.40771874E+03 -0.40753896E+03 -0.40699980E+03 -0.40610179E+03 -0.40484584E+03
-0.40323317E+03 -0.40126543E+03 -0.39894456E+03 -0.39627294E+03 -0.39325326E+03
-0.38988862E+03 -0.38618249E+03 -0.38213873E+03 -0.37776160E+03 -0.37305575E+03
-0.36802623E+03 -0.36267853E+03 -0.35701856E+03 -0.35105263E+03 -0.34478754E+03
-0.33823053E+03 -0.33138928E+03 -0.32427199E+03 -0.31688731E+03 -0.30924442E+03
-0.30135300E+03 -0.29322326E+03 -0.28486596E+03 -0.27629239E+03 -0.26751445E+03
-0.25854458E+03 -0.24939585E+03 -0.24008192E+03 -0.23061710E+03 -0.22101631E+03
-0.21129516E+03 -0.20146991E+03 -0.19155749E+03 -0.18157555E+03 -0.17154243E+03
-0.16147720E+03 -0.15139966E+03 -0.14133033E+03 -0.13129052E+03 -0.12130225E+03
-0.11138833E+03 -0.10157234E+03 -0.91878614E+02 -0.82332275E+02 -0.72959210E+02
-0.63786081E+02 -0.54840313E+02 -0.46150094E+02 -0.37744362E+02 -0.29652792E+02
-0.21905789E+02 -0.14534463E+02 -0.75706153E+01 -0.10467120E+01 0.50041396E+01
0.10548223E+02 0.15551203E+02 0.19976833E+02 0.23947352E+02 0.28057103E+02
0.32338822E+02 0.36756611E+02 0.41274501E+02 0.45854087E+02 0.50457194E+02
0.55044366E+02 0.59574678E+02 0.64009290E+02 0.68302968E+02 0.72418209E+02

0.76306628E+02 0.79930545E+02 0.83241124E+02 0.86197352E+02 0.88754146E+02
0.90864763E+02 0.92488430E+02 0.93575677E+02 0.94085369E+02 0.93971950E+02
0.93189061E+02 0.91697272E+02 0.89448671E+02 0.86402820E+02 0.82519024E+02
0.77752053E+02 0.72065975E+02 0.65420062E+02 0.57774350E+02 0.49096829E+02
0.39342887E+02 0.28494130E+02 0.16679271E+02 0.24365950E+01 0.00000000E+00

Reciprocal Space Part

-0.84380410E+01 -0.83422438E+01 -0.80567334E+01 -0.75871107E+01 -0.69425723E+01
-0.61357053E+01 -0.51822091E+01 -0.41005476E+01 -0.29115427E+01 -0.16379187E+01
-0.30380665E+00 0.10657764E+01 0.24454634E+01 0.38100749E+01 0.51351445E+01
0.63974224E+01 0.75753432E+01 0.86494483E+01 0.96027546E+01 0.10421059E+02
0.11093177E+02 0.11611104E+02 0.11970108E+02 0.12168737E+02 0.12208760E+02
0.12095033E+02 0.11835297E+02 0.11439917E+02 0.10921569E+02 0.10294884E+02
0.95760537E+01 0.87824183E+01 0.79320389E+01 0.70432682E+01 0.61343304E+01
0.52229190E+01 0.43258233E+01 0.34585913E+01 0.26352349E+01 0.18679857E+01
0.11671029E+01 0.54073871E+00 -0.51398183E-02 -0.46677084E+00 -0.84256280E+00
-0.11330071E+01 -0.13405429E+01 -0.14693797E+01 -0.15252839E+01 -0.15153369E+01
-0.14476719E+01 -0.13311980E+01 -0.11753186E+01 -0.98965315E+00 -0.78376785E+00
-0.56692421E+00 -0.34784975E+00 -0.13453686E+00 0.65926241E-01 0.24748936E+00
0.40523719E+00 0.53544814E+00 0.63561572E+00 0.70443365E+00 0.74174714E+00
0.74847352E+00 0.72649622E+00 0.67853658E+00 0.60800854E+00 0.51886135E+00
0.41541576E+00 0.30219888E+00 0.18378284E+00 0.64631822E-01 -0.51038094E-01
-0.15938292E+00 -0.25703544E+00 -0.34118841E+00 -0.40965496E+00 -0.46090536E+00
-0.49408034E+00 -0.50898186E+00 -0.50604272E+00 -0.48627714E+00 -0.45121495E+00
-0.40282234E+00 -0.34341239E+00 -0.27554896E+00 -0.20194725E+00 -0.12537458E+00
-0.48554605E-01 0.25922105E-01 0.95678383E-01 0.15861958E+00 0.21298966E+00
0.25741315E+00 0.29092207E+00 0.31296789E+00 0.32341870E+00 0.32254242E+00

Real Space Part

0.25837316E+03 0.25826205E+03 0.25792885E+03 0.25737389E+03 0.25659772E+03
0.25560112E+03 0.25438510E+03 0.25295089E+03 0.25129994E+03 0.24943396E+03
0.24735486E+03 0.24506480E+03 0.24256618E+03 0.23986166E+03 0.23695411E+03
0.23384669E+03 0.23054280E+03 0.22704609E+03 0.22336050E+03 0.21949022E+03
0.21543976E+03 0.21121386E+03 0.20681758E+03 0.20225630E+03 0.19753567E+03
0.19266166E+03 0.18764058E+03 0.18247905E+03 0.17718404E+03 0.17176285E+03
0.16622314E+03 0.16057294E+03 0.15482062E+03 0.14897495E+03 0.14304509E+03
0.13704057E+03 0.13097133E+03 0.12484773E+03 0.11868051E+03 0.11248087E+03
0.10626040E+03 0.10003117E+03 0.93805629E+02 0.87596714E+02 0.81417789E+02
0.75282668E+02 0.69205618E+02 0.63201357E+02 0.57285056E+02 0.51472335E+02
0.45779265E+02 0.40222362E+02 0.34818582E+02 0.29585317E+02 0.24540384E+02
0.19702020E+02 0.15088866E+02 0.10719959E+02 0.66147158E+01 0.27929175E+01
-0.72531069E+00 -0.39194941E+01 -0.67680320E+01 -0.93444442E+01 -0.12005009E+02
-0.14768401E+02 -0.17612181E+02 -0.20513962E+02 -0.23449994E+02 -0.26396758E+02
-0.29330056E+02 -0.32224898E+02 -0.35057623E+02 -0.37800836E+02 -0.40431827E+02
-0.42921481E+02 -0.45247126E+02 -0.47379523E+02 -0.49294153E+02 -0.50964143E+02
-0.52361696E+02 -0.53462620E+02 -0.54237620E+02 -0.54662401E+02 -0.54710098E+02
-0.54353424E+02 -0.53569243E+02 -0.52329443E+02 -0.50610382E+02 -0.48388306E+02
-0.45636819E+02 -0.42335059E+02 -0.38459367E+02 -0.33986566E+02 -0.28898211E+02
-0.23168446E+02 -0.16786908E+02 -0.98299898E+01 -0.14364499E+01 0.00000000E+00

Non local Part

1 1 0.594199078900351
-0.477478817810334

Reciprocal Space Part

0.00000000E+00 0.15279168E+00 0.30752124E+00 0.46604653E+00 0.63006765E+00

0.80105405E+00 0.98017828E+00 0.11682588E+01 0.13657131E+01 0.15725231E+01
0.17882131E+01 0.20118422E+01 0.22420100E+01 0.24768769E+01 0.27141978E+01
0.29513677E+01 0.31854799E+01 0.34133929E+01 0.36318064E+01 0.38373418E+01
0.40266279E+01 0.41963873E+01 0.43435215E+01 0.44651933E+01 0.45589034E+01
0.46225593E+01 0.46545348E+01 0.46537180E+01 0.46195474E+01 0.45520344E+01
0.44517717E+01 0.43199273E+01 0.41582255E+01 0.39689131E+01 0.37547138E+01
0.35187715E+01 0.32645831E+01 0.29959239E+01 0.27167668E+01 0.24311973E+01
0.21433272E+01 0.18572087E+01 0.15767505E+01 0.13056396E+01 0.10472690E+01
0.80467403E+00 0.58047788E+00 0.37684898E+00 0.19546929E+00 0.37515357E-01
-0.96348385E-01 -0.20596384E+00 -0.29166167E+00 -0.35423266E+00 -0.39488898E+00
-0.41521676E+00 -0.41712134E+00 -0.40276697E+00 -0.37451262E+00 -0.33484566E+00
-0.28631536E+00 -0.23146775E+00 -0.17278367E+00 -0.11262148E+00 -0.53165628E-01
0.36175780E-02 0.56016277E-01 0.10260074E+00 0.14224207E+00 0.17412178E+00
0.19773248E+00 0.21286995E+00 0.21961732E+00 0.21832218E+00 0.20956746E+00
0.19413743E+00 0.17297989E+00 0.14716579E+00 0.11784774E+00 0.86218533E-01
0.53470926E-01 0.20759875E-01 -0.10831888E-01 -0.40323998E-01 -0.66863680E-01
-0.89745523E-01 -0.10842549E+00 -0.12252907E+00 -0.13185353E+00 -0.13636468E+00
-0.13618832E+00 -0.13159712E+00 -0.12299346E+00 -0.11088897E+00 -0.95881731E-01
-0.78631844E-01 -0.59836272E-01 -0.40203856E-01 -0.20431252E-01 -0.11805371E-02

Real Space Part

0.00000000E+00 0.36016470E+01 0.71942522E+01 0.10768800E+02 0.14316325E+02
0.17827942E+02 0.21294866E+02 0.24708440E+02 0.28060163E+02 0.31341709E+02
0.34544954E+02 0.37662004E+02 0.40685209E+02 0.43607194E+02 0.46420881E+02
0.49119503E+02 0.51696633E+02 0.54146202E+02 0.56462517E+02 0.58640278E+02
0.60674600E+02 0.62561027E+02 0.64295548E+02 0.65874613E+02 0.67295142E+02
0.68554544E+02 0.69650724E+02 0.70582093E+02 0.71347581E+02 0.71946638E+02
0.72379246E+02 0.72645920E+02 0.72747716E+02 0.72686227E+02 0.72463589E+02
0.72082479E+02 0.71546110E+02 0.70858231E+02 0.70023121E+02 0.69045580E+02
0.67930924E+02 0.66684975E+02 0.65314048E+02 0.63824939E+02 0.62224913E+02
0.60521687E+02 0.58723413E+02 0.56838660E+02 0.54876394E+02 0.52845959E+02
0.50757054E+02 0.48619706E+02 0.46444251E+02 0.44241304E+02 0.42021734E+02
0.39796636E+02 0.37577302E+02 0.35375190E+02 0.33201894E+02 0.31069116E+02
0.28988627E+02 0.26972250E+02 0.25032102E+02 0.23146954E+02 0.21198081E+02
0.19186272E+02 0.17126556E+02 0.15033706E+02 0.12922679E+02 0.10808038E+02
0.87042218E+01 0.66255492E+01 0.45854845E+01 0.25982885E+01 0.67621131E+00
-0.11668827E+01 -0.29197381E+01 -0.45694937E+01 -0.61053510E+01 -0.75163038E+01
-0.87916195E+01 -0.99222707E+01 -0.10898201E+02 -0.11711497E+02 -0.12354019E+02
-0.12818083E+02 -0.13097844E+02 -0.13186511E+02 -0.13079209E+02 -0.12771576E+02
-0.12258995E+02 -0.11539032E+02 -0.10608916E+02 -0.94665225E+01 -0.81115752E+01
-0.65421253E+01 -0.47610403E+01 -0.27960553E+01 -0.41220264E+00 0.00000000E+00

PAW radial sets

363 0.520134355386775

(5E20.12)

augmentation charges (non spherical)

0.136235920566E-01 0.259291988841E-01 0.160051128787E-02 0.259291988841E-01
0.489927346999E-01

0.414104798650E-02 0.160051128787E-02 0.414104798650E-02 -0.308695800982E-02

occupancies in atom

0.999999998693E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00

0.000000000000E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00

grid

0.116365397438E-04	0.120001524756E-04	0.123751271949E-04	0.127618189353E-04
0.131605938244E-04			
0.135718294303E-04	0.139959151194E-04	0.144332524243E-04	0.148842554251E-04
0.153493511404E-04			
0.158289799324E-04	0.163235959232E-04	0.168336674253E-04	0.173596773848E-04
0.179021238385E-04			
0.184615203857E-04	0.190383966745E-04	0.196332989028E-04	0.202467903364E-04
0.208794518411E-04			
0.215318824339E-04	0.222046998492E-04	0.228985411241E-04	0.236140632016E-04
0.243519435526E-04			
0.251128808170E-04	0.258975954658E-04	0.267068304825E-04	0.275413520675E-04
0.284019503625E-04			
0.292894401994E-04	0.302046618718E-04	0.311484819298E-04	0.321217940016E-04
0.331255196387E-04			
0.341606091889E-04	0.352280426958E-04	0.363288308273E-04	0.374640158317E-04
0.386346725253E-04			
0.398419093096E-04	0.410868692207E-04	0.423707310119E-04	0.436947102696E-04
0.450600605642E-04			
0.464680746370E-04	0.479200856242E-04	0.494174683192E-04	0.509616404744E-04
0.525540641432E-04			
0.541962470646E-04	0.558897440906E-04	0.576361586586E-04	0.594371443092E-04
0.612944062521E-04			
0.632097029807E-04	0.651848479365E-04	0.672217112269E-04	0.693222213953E-04
0.714883672472E-04			
0.737221997335E-04	0.760258338920E-04	0.784014508502E-04	0.808512998904E-04
0.833777005792E-04			
0.859830449641E-04	0.886697998377E-04	0.914405090742E-04	0.942977960371E-04
0.972443660636E-04			
0.100283009026E-03	0.103416601973E-03	0.106648111853E-03	0.109980598327E-03
0.113417216659E-03			
0.116961220709E-03	0.120615966013E-03	0.124384912957E-03	0.128271630056E-03
0.132279797333E-03			
0.136413209802E-03	0.140675781061E-03	0.145071547000E-03	0.149604669619E-03
0.154279440969E-03			
0.159100287220E-03	0.164071772845E-03	0.169198604950E-03	0.174485637720E-03
0.179937877028E-03			
0.185560485163E-03	0.191358785724E-03	0.197338268660E-03	0.203504595467E-03
0.209863604547E-03			
0.216421316740E-03	0.223183941020E-03	0.230157880376E-03	0.237349737876E-03
0.244766322917E-03			
0.252414657670E-03	0.260301983735E-03	0.268435768991E-03	0.276823714672E-03
0.285473762654E-03			
0.294394102977E-03	0.303593181601E-03	0.313079708400E-03	0.322862665409E-03
0.332951315330E-03			
0.343355210302E-03	0.354084200943E-03	0.365148445678E-03	0.376558420359E-03
0.388324928181E-03			
0.400459109912E-03	0.412972454440E-03	0.425876809655E-03	0.439184393661E-03
0.452907806348E-03			
0.467060041321E-03	0.481654498203E-03	0.496704995321E-03	0.512225782792E-03
0.528231556011E-03			
0.544737469568E-03	0.561759151596E-03	0.579312718570E-03	0.597414790562E-03
0.616082506980E-03			

0.635333542796E-03	0.655186125282E-03	0.675659051264E-03	0.696771704924E-03
0.718544076149E-03			
0.740996779462E-03	0.764151073538E-03	0.788028881330E-03	0.812652810832E-03
0.838046176477E-03			
0.864233021221E-03	0.891238139296E-03	0.919087099697E-03	0.947806270383E-03
0.977422843248E-03			
0.100796485986E-02	0.103946123802E-02	0.107194179914E-02	0.110543729647E-02
0.113997944423E-02			
0.117560094762E-02	0.121233553381E-02	0.125021798383E-02	0.128928416557E-02
0.132957106768E-02			
0.137111683461E-02	0.141396080274E-02	0.145814353760E-02	0.150370687229E-02
0.155069394712E-02			
0.159914925040E-02	0.164911866057E-02	0.170064948971E-02	0.175379052823E-02
0.180859209116E-02			
0.186510606572E-02	0.192338596048E-02	0.198348695604E-02	0.204546595723E-02
0.210938164702E-02			
0.217529454209E-02	0.224326705010E-02	0.231336352880E-02	0.238565034695E-02
0.246019594719E-02			
0.253707091078E-02	0.261634802451E-02	0.269810234955E-02	0.278241129256E-02
0.286935467894E-02			
0.295901482847E-02	0.305147663317E-02	0.314682763778E-02	0.324515812254E-02
0.334656118875E-02			
0.345113284689E-02	0.355897210752E-02	0.367018107505E-02	0.378486504437E-02
0.390313260059E-02			
0.402509572182E-02	0.415086988523E-02	0.428057417634E-02	0.441433140179E-02
0.455226820564E-02			
0.469451518925E-02	0.484120703495E-02	0.499248263354E-02	0.514848521583E-02
0.530936248822E-02			
0.547526677257E-02	0.564635515043E-02	0.582278961173E-02	0.600473720819E-02
0.619237021149E-02			
0.638586627635E-02	0.658540860877E-02	0.679118613947E-02	0.700339370278E-02
0.72223222113E-02			
0.744790889526E-02	0.768063740041E-02	0.792063808866E-02	0.816813819750E-02
0.842337206506E-02			
0.868658135194E-02	0.895801527002E-02	0.923793081843E-02	0.952659302689E-02
0.982427520662E-02			
0.101312592091E-01	0.104478356931E-01	0.107743043996E-01	0.111109744357E-01
0.114581645676E-01			
0.118162035217E-01	0.121854302968E-01	0.125661944841E-01	0.129588565989E-01
0.133637884217E-01			
0.137813733500E-01	0.142120067619E-01	0.146560963897E-01	0.151140627064E-01
0.155863393239E-01			
0.160733734032E-01	0.165756260781E-01	0.170935728915E-01	0.176277042461E-01
0.181785258681E-01			
0.187465592867E-01	0.193323423274E-01	0.199364296215E-01	0.205593931310E-01
0.212018226904E-01			
0.218643265651E-01	0.225475320271E-01	0.232520859492E-01	0.239786554173E-01
0.247279283622E-01			
0.255006142105E-01	0.262974445570E-01	0.271191738568E-01	0.279665801397E-01
0.288404657473E-01			
0.297416580921E-01	0.306710104413E-01	0.316294027246E-01	0.326177423671E-01
0.336369651489E-01			

0.346880360907E-01	0.357719503678E-01	0.368897342522E-01	0.380424460843E-01
0.392311772750E-01			
0.404570533392E-01	0.417212349610E-01	0.430249190933E-01	0.443693400906E-01
0.457557708780E-01			
0.471855241562E-01	0.486599536446E-01	0.501804553628E-01	0.517484689527E-01
0.533654790415E-01			
0.550330166468E-01	0.567526606272E-01	0.585260391764E-01	0.603548313652E-01
0.622407687309E-01			
0.641856369174E-01	0.661912773653E-01	0.682595890554E-01	0.703925303074E-01
0.725921206330E-01			
0.748604426491E-01	0.771996440488E-01	0.796119396355E-01	0.820996134194E-01
0.846650207805E-01			
0.873105906985E-01	0.900388280525E-01	0.928523159930E-01	0.957537183872E-01
0.987457823419E-01			
0.101831340804E+00	0.105013315242E+00	0.108294718414E+00	0.111678657220E+00
0.115168335641E+00			
0.118767057775E+00	0.122478230966E+00	0.126305369027E+00	0.130252095570E+00
0.134322147435E+00			
0.138519378231E+00	0.142847761981E+00	0.147311396886E+00	0.151914509205E+00
0.156661457259E+00			
0.161556735555E+00	0.166604979041E+00	0.171810967496E+00	0.177179630055E+00
0.182716049878E+00			
0.188425468959E+00	0.194313293090E+00	0.200385096984E+00	0.206646629548E+00
0.213103819326E+00			
0.219762780118E+00	0.226629816762E+00	0.233711431108E+00	0.241014328171E+00
0.248545422483E+00			
0.256311844636E+00	0.264320948036E+00	0.272580315864E+00	0.281097768257E+00
0.289881369712E+00			
0.298939436720E+00	0.308280545644E+00	0.317913540832E+00	0.327847543002E+00
0.338091957867E+00			
0.348656485048E+00	0.359551127251E+00	0.370786199746E+00	0.382372340126E+00
0.394320518384E+00			
0.406642047297E+00	0.419348593138E+00	0.432452186723E+00	0.445965234799E+00
0.459900531793E+00			
0.474271271928E+00	0.489091061712E+00	0.504373932821E+00	0.520134355387E+00
0.536387251698E+00			
0.553148010325E+00	0.570432500694E+00	0.588257088111E+00	0.606638649257E+00
0.625594588164E+00			
0.645142852702E+00	0.665301951562E+00	0.686090971788E+00	0.707529596845E+00
0.729638125257E+00			
0.752437489828E+00	0.775949277458E+00	0.800195749583E+00	
aepotential			
0.568167509245E+05	0.550635481897E+05	0.524115275846E+05	0.499018713441E+05
0.475237204497E+05			
0.451515547378E+05	0.430200164382E+05	0.409238097938E+05	0.389890217306E+05
0.368813865094E+05			
0.350615246282E+05	0.333557092279E+05	0.316173241956E+05	0.300729091537E+05
0.286886799447E+05			
0.272489939628E+05	0.259465437732E+05	0.248400202732E+05	0.235396741163E+05
0.223170218821E+05			
0.213328748534E+05	0.203294079803E+05	0.194844222350E+05	0.185710568927E+05
0.176709429315E+05			

0.167671510199E+05	0.160243622565E+05	0.152818091117E+05	0.146690277682E+05
0.138258389832E+05			
0.134189698578E+05	0.126725443221E+05	0.123038676256E+05	0.119831142764E+05
0.113066884034E+05			
0.109542752362E+05	0.105045026707E+05	0.101224377086E+05	0.974218310199E+04
0.935878435724E+04			
0.898430881262E+04	0.863162335351E+04	0.834109909528E+04	0.802614032693E+04
0.765474863659E+04			
0.737958797444E+04	0.710461943105E+04	0.684124268882E+04	0.657256357790E+04
0.634080972021E+04			
0.611883238911E+04	0.588776114841E+04	0.567061153551E+04	0.546806596497E+04
0.527334245377E+04			
0.508202990632E+04	0.489948715094E+04	0.472473624177E+04	0.455158263083E+04
0.439380708114E+04			
0.423918224458E+04	0.409513459489E+04	0.395420396787E+04	0.381489630690E+04
0.368299767628E+04			
0.356065917645E+04	0.344808656759E+04	0.332059296355E+04	0.320340159630E+04
0.308841817339E+04			
0.298656692828E+04	0.289151173890E+04	0.278932022020E+04	0.269860643300E+04
0.260963295288E+04			
0.252369425395E+04	0.244027743974E+04	0.235675162269E+04	0.227998960265E+04
0.220500647734E+04			
0.213360027980E+04	0.206507687815E+04	0.199794153830E+04	0.193259130823E+04
0.187002537936E+04			
0.180928697676E+04	0.175002211291E+04	0.169313737953E+04	0.163803960546E+04
0.158539968194E+04			
0.153386090079E+04	0.148425513654E+04	0.143657002851E+04	0.139061558403E+04
0.134610494542E+04			
0.130289436224E+04	0.126122212897E+04	0.122102031708E+04	0.118215352244E+04
0.114447797219E+04			
0.110798464935E+04	0.107278404419E+04	0.103876475250E+04	0.100569435470E+04
0.973994994213E+03			
0.943496118508E+03	0.913601133424E+03	0.884368745084E+03	0.856377178574E+03
0.829284208704E+03			
0.803218610485E+03	0.778000642091E+03	0.753540985318E+03	0.729760315842E+03
0.706813187509E+03			
0.684588297547E+03	0.663084401005E+03	0.642266135539E+03	0.622145759815E+03
0.602604001613E+03			
0.583767205221E+03	0.565471068185E+03	0.547758863981E+03	0.530608539213E+03
0.513970586017E+03			
0.497866957727E+03	0.482290300210E+03	0.467205520126E+03	0.452603639977E+03
0.438446185809E+03			
0.424735989962E+03	0.411454977271E+03	0.398592550498E+03	0.386131640032E+03
0.374064605946E+03			
0.362373286107E+03	0.351044213533E+03	0.340068051205E+03	0.329433845745E+03
0.319134048467E+03			
0.309149644115E+03	0.299487029885E+03	0.290127192243E+03	0.281044793509E+03
0.272245103681E+03			
0.263725213549E+03	0.255462407793E+03	0.247455143583E+03	0.239704879539E+03
0.232184929110E+03			
0.224899820685E+03	0.217837606539E+03	0.210994023374E+03	0.204364206949E+03
0.197938229036E+03			

0.191708799370E+03	0.185670997314E+03	0.179820456426E+03	0.174149726407E+03
0.168652754948E+03			
0.163326590424E+03	0.158163091260E+03	0.153157588893E+03	0.148306699724E+03
0.143604779095E+03			
0.139046607489E+03	0.134629057361E+03	0.130346510366E+03	0.126195683197E+03
0.122171984941E+03			
0.118271582517E+03	0.114490256495E+03	0.110824578770E+03	0.107271016470E+03
0.103826131339E+03			
0.100486939601E+03	0.972496474930E+02	0.941112617705E+02	0.910688157695E+02
0.881183294491E+02			
0.852582835944E+02	0.824865483648E+02	0.797986769210E+02	0.771921574428E+02
0.746652114120E+02			
0.722153653278E+02	0.698406104858E+02	0.675378771122E+02	0.653049180667E+02
0.631403153303E+02			
0.610415851152E+02	0.590064415061E+02	0.570331440351E+02	0.551198864034E+02
0.532594415948E+02			
0.514567312679E+02	0.497167994242E+02	0.480262228740E+02	0.463814095189E+02
0.447917181876E+02			
0.432498169270E+02	0.417546208464E+02	0.403054640044E+02	0.388992758341E+02
0.375349740621E+02			
0.362124635070E+02	0.349306291423E+02	0.336869443383E+02	0.324814397445E+02
0.313100087425E+02			
0.301767426114E+02	0.290753781389E+02	0.280084558665E+02	0.269725471906E+02
0.259693347023E+02			
0.249948801144E+02	0.240502968713E+02	0.231336866599E+02	0.222438647082E+02
0.213822880378E+02			
0.205459542447E+02	0.197336290054E+02	0.189463412224E+02	0.181816945021E+02
0.174408862092E+02			
0.167210511930E+02	0.160240511476E+02	0.153460686204E+02	0.146892408360E+02
0.140510311724E+02			
0.134327459069E+02	0.128311284555E+02	0.122486578950E+02	0.116821075902E+02
0.111327310512E+02			
0.105997234406E+02	0.100818813024E+02	0.957910573785E+01	0.909110837013E+01
0.861710351187E+01			
0.815666139425E+01	0.770969115698E+01	0.727563373976E+01	0.685365938987E+01
0.644399715789E+01			
0.604555582198E+01	0.565869169298E+01	0.528250018497E+01	0.491691343928E+01
0.456181226095E+01			
0.421605205641E+01	0.388029822947E+01	0.355353593873E+01	0.323577162745E+01
0.292654903710E+01			
0.262607615453E+01	0.233295412816E+01	0.204845397889E+01	0.177062722040E+01
0.150114356179E+01			
0.123765152926E+01	0.981878863997E+00	0.731952146227E+00	0.488975790051E+00
0.251903371338E+00			
0.209078273758E-01	-0.204480442105E+00	-0.424462383510E+00	-0.638633203133E+00 -
0.848176627864E+00			
-0.105234460716E+01	-0.125184141922E+01	-0.144656118854E+01	-0.163708683529E+01 -
0.182289825149E+01			
-0.200469780342E+01	-0.218254162819E+01	-0.235628649195E+01	-0.252640591990E+01 -
0.269290796311E+01			
-0.285574659210E+01	-0.301535768816E+01	-0.317162135008E+01	-0.332467859460E+01 -
0.347473929943E+01			

-0.362179442613E+01	-0.376601399967E+01	-0.390740306908E+01	-0.404617161618E+01	-
0.418226540348E+01				
-0.431585470976E+01	-0.444698240445E+01	-0.457569584972E+01	-0.470208217807E+01	-
0.482620917633E+01				
-0.494808565161E+01	-0.506779772342E+01	-0.518537029025E+01	-0.530086011134E+01	-
0.541426215957E+01				
-0.552565816017E+01	-0.563501364100E+01	-0.574239753105E+01	-0.584777592621E+01	-
0.595122575761E+01				
-0.605264787394E+01	-0.615217618516E+01	-0.624969186829E+01	-0.634522873672E+01	-
0.643879964711E+01				
-0.653029619518E+01	-0.661979302919E+01	-0.670720794367E+01	-0.679254061638E+01	-
0.687569280278E+01				
-0.695670920370E+01	-0.703546681630E+01	-0.711195648576E+01	-0.718611572365E+01	-
0.725789767596E+01				
-0.732722792337E+01	-0.739404316527E+01	-0.745830295716E+01	-0.751990886320E+01	-
0.757879898400E+01				
-0.763492317934E+01	-0.768818647270E+01	-0.773852374220E+01	-0.778586547210E+01	-
0.783014132776E+01				
-0.787126564785E+01	-0.790918193518E+01	-0.794381778947E+01	-0.797511601153E+01	-
0.800299906906E+01				
-0.802741824207E+01	-0.804832384000E+01	-0.806566339383E+01	-0.807939749303E+01	-
0.808949045218E+01				
-0.809591723488E+01	-0.809865883865E+01	-0.809770895816E+01	-0.809306453381E+01	-
0.808473836730E+01				
-0.807275471800E+01	-0.805714718044E+01	-0.803796037344E+01	-0.801525501883E+01	-
0.798910219636E+01				
-0.795958822936E+01	-0.792680814028E+01	-0.789087460601E+01	-0.785191062927E+01	-
0.781004819483E+01				
-0.776543219354E+01	-0.771821750745E+01	-0.766856247326E+01	-0.761663264758E+01	-
0.756259230646E+01				
-0.750660579095E+01	-0.744883026007E+01	-0.738941079276E+01		
core charge-density				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				

-0.623208146421E+02 -0.623208668963E+02 -0.623209174513E+02 -0.623209663512E+02 -
0.623210136383E+02
-0.623210593532E+02 -0.623211035347E+02 -0.623211462198E+02 -0.623211874439E+02 -
0.623212272406E+02
-0.623212656418E+02 -0.623213026778E+02 -0.623213383772E+02 -0.623213727668E+02 -
0.623214058719E+02
-0.623214377159E+02 -0.623214683208E+02 -0.623214977066E+02 -0.623215258918E+02 -
0.623215528932E+02
-0.623215787254E+02 -0.623216034020E+02 -0.623216269340E+02 -0.623216493309E+02 -
0.623216706006E+02
-0.623216907485E+02 -0.623217097784E+02 -0.623217276919E+02 -0.623217444888E+02 -
0.623217601662E+02
-0.623217747195E+02 -0.623217881414E+02 -0.623218004223E+02 -0.623218115505E+02 -
0.623218215112E+02
-0.623218302870E+02 -0.623218378578E+02 -0.623218442005E+02 -0.623218492889E+02 -
0.623218530937E+02
-0.623218555821E+02 -0.623218567176E+02 -0.623218564603E+02 -0.623218547661E+02 -
0.623218515868E+02
-0.623218468700E+02 -0.623218405584E+02 -0.623218325903E+02 -0.623218228984E+02 -
0.623218114102E+02
-0.623217980476E+02 -0.623217827264E+02 -0.623217653557E+02 -0.623217458382E+02 -
0.623217240694E+02
-0.623216999368E+02 -0.623216733204E+02 -0.623216440913E+02 -0.623216121118E+02 -
0.623215772343E+02
-0.623215393012E+02 -0.623214981442E+02 -0.623214535833E+02 -0.623214054267E+02 -
0.623213534692E+02
-0.623212974922E+02 -0.623212372626E+02 -0.623211725317E+02 -0.623211030343E+02 -
0.623210284880E+02
-0.623209485917E+02 -0.623208630245E+02 -0.623207714450E+02 -0.623206734891E+02 -
0.623205687693E+02
-0.623204568730E+02 -0.623203373610E+02 -0.623202097655E+02 -0.623200735888E+02 -
0.623199283011E+02
-0.623197733384E+02 -0.623196081008E+02 -0.623194319497E+02 -0.623192442055E+02 -
0.623190441455E+02
-0.623188310005E+02 -0.623186039521E+02 -0.623183621298E+02 -0.623181046078E+02 -
0.623178304006E+02
-0.623175384605E+02 -0.623172276729E+02 -0.623168968522E+02 -0.623165447374E+02 -
0.623161699874E+02
-0.623157711755E+02 -0.623153467847E+02 -0.623148952016E+02 -0.623144147101E+02 -
0.623139034855E+02
-0.623133595870E+02 -0.623127809510E+02 -0.623121653828E+02 -0.623115105487E+02 -
0.623108139671E+02
-0.623100729990E+02 -0.623092848385E+02 -0.623084465020E+02 -0.623075548169E+02 -
0.623066064102E+02
-0.623055976952E+02 -0.623045248586E+02 -0.623033838462E+02 -0.623021703472E+02 -
0.623008797791E+02
-0.622995072699E+02 -0.622980476399E+02 -0.622964953831E+02 -0.622948446459E+02 -
0.622930892063E+02
-0.622912224500E+02 -0.622892373465E+02 -0.622871264231E+02 -0.622848817368E+02 -
0.622824948461E+02
-0.622799567789E+02 -0.622772580001E+02 -0.622743883771E+02 -0.622713371422E+02 -
0.622680928535E+02

-0.622646433538E+02 -0.622609757258E+02 -0.622570762463E+02 -0.622529303363E+02 -
0.622485225086E+02
-0.622438363127E+02 -0.622388542762E+02 -0.622335578424E+02 -0.622279273050E+02 -
0.622219417391E+02
-0.622155789273E+02 -0.622088152826E+02 -0.622016257668E+02 -0.621939838041E+02 -
0.621858611900E+02
-0.621772279957E+02 -0.621680524669E+02 -0.621583009169E+02 -0.621479376157E+02 -
0.621369246707E+02
-0.621252219041E+02 -0.621127867224E+02 -0.620995739802E+02 -0.620855358368E+02 -
0.620706216070E+02
-0.620547776042E+02 -0.620379469768E+02 -0.620200695374E+02 -0.620010815845E+02 -
0.619809157178E+02
-0.619595006448E+02 -0.619367609812E+02 -0.619126170442E+02 -0.618869846376E+02 -
0.618597748315E+02
-0.618308937345E+02 -0.618002422600E+02 -0.617677158863E+02 -0.617332044128E+02 -
0.616965917096E+02
-0.616577554648E+02 -0.616165669285E+02 -0.615728906540E+02 -0.615265842395E+02 -
0.614774980684E+02
-0.614254750528E+02 -0.613703503796E+02 -0.613119512613E+02 -0.612500966930E+02 -
0.611845972187E+02
-0.611152547069E+02 -0.610418621387E+02 -0.609642034098E+02 -0.608820531485E+02 -
0.607951765519E+02
-0.607033292405E+02 -0.606062571352E+02 -0.605036963548E+02 -0.603953731371E+02 -
0.602810037826E+02
-0.601602946211E+02 -0.600329419990E+02 -0.598986322862E+02 -0.597570418987E+02 -
0.596078373338E+02
-0.594506752098E+02 -0.592852023064E+02 -0.591110555939E+02 -0.589278622427E+02 -
0.587352396007E+02
-0.585327951230E+02 -0.583201262402E+02 -0.580968201448E+02 -0.578624534779E+02 -
0.576165918931E+02
-0.573587894748E+02 -0.570885879856E+02 -0.568055159149E+02 -0.565090873026E+02 -
0.561988003053E+02
-0.558741354762E+02 -0.555345537248E+02 -0.551794939215E+02 -0.548083701134E+02 -
0.544205683110E+02
-0.540154428098E+02 -0.535923120034E+02 -0.531504536506E+02 -0.526890995562E+02 -
0.522074296313E+02
-0.517045653109E+02 -0.511795623204E+02 -0.506314028138E+02 -0.500589869481E+02 -
0.494611240177E+02
-0.488365233585E+02 -0.481837853353E+02 -0.475013928548E+02 -0.467877039944E+02 -
0.460409464789E+02
-0.452592148634E+02 -0.444404713407E+02 -0.435825510393E+02 -0.426831724667E+02 -
0.417399533181E+02
-0.407504312143E+02 -0.397120881008E+02 -0.386223762173E+02 -0.375238282596E+02 -
0.364583488277E+02
-0.354223615172E+02 -0.344120532299E+02 -0.334233282092E+02 -0.324518753275E+02 -
0.314932332910E+02
-0.305430031328E+02 -0.295972189875E+02 -0.286529121405E+02 -0.277138961731E+02 -
0.268807027160E+02
-0.260664130351E+02 -0.252730858705E+02 -0.245093210951E+02 -0.237369804927E+02 -
0.230177326346E+02
-0.223202792622E+02 -0.216439601545E+02 -0.209881352061E+02 -0.203521808893E+02 -
0.197354951450E+02

-0.191374976575E+02 -0.185576198385E+02 -0.179953113192E+02
pspotential valence only
-0.835364443183E+01 -0.835480471514E+01 -0.835592983867E+01 -0.835702087007E+01 -
0.835807884224E+01
-0.835910475745E+01 -0.836009958644E+01 -0.836106427094E+01 -0.836199972487E+01 -
0.836290683408E+01
-0.836378645693E+01 -0.836463942654E+01 -0.836546655033E+01 -0.836626861160E+01 -
0.836704636979E+01
-0.836780056104E+01 -0.836853189944E+01 -0.836924107781E+01 -0.836992876738E+01 -
0.837059561908E+01
-0.837124226465E+01 -0.837186931595E+01 -0.837247736699E+01 -0.837306699323E+01 -
0.837363875307E+01
-0.837419318797E+01 -0.837473082266E+01 -0.837525216614E+01 -0.837575771220E+01 -
0.837624793930E+01
-0.837672331183E+01 -0.837718427960E+01 -0.837763127942E+01 -0.837806473403E+01 -
0.837848505413E+01
-0.837889263748E+01 -0.837928787009E+01 -0.837967112602E+01 -0.838004276847E+01 -
0.838040314880E+01
-0.838075260865E+01 -0.838109147855E+01 -0.838142007940E+01 -0.838173872233E+01 -
0.838204770903E+01
-0.838234733196E+01 -0.838263787479E+01 -0.838291961258E+01 -0.838319281205E+01 -
0.838345773176E+01
-0.838371462259E+01 -0.838396372759E+01 -0.838420528259E+01 -0.838443951627E+01 -
0.838466665035E+01
-0.838488689980E+01 -0.838510047314E+01 -0.838530757244E+01 -0.838550839365E+01 -
0.838570312694E+01
-0.838589195655E+01 -0.838607506113E+01 -0.838625261389E+01 -0.838642478299E+01 -
0.838659173124E+01
-0.838675361656E+01 -0.838691059214E+01 -0.838706280638E+01 -0.838721040324E+01 -
0.838735352234E+01
-0.838749229913E+01 -0.838762686466E+01 -0.838775734613E+01 -0.838788386698E+01 -
0.838800654673E+01
-0.838812550132E+01 -0.838824084303E+01 -0.838835268091E+01 -0.838846112051E+01 -
0.838856626418E+01
-0.838866821125E+01 -0.838876705775E+01 -0.838886289691E+01 -0.838895581929E+01 -
0.838904591216E+01
-0.838913326065E+01 -0.838921794676E+01 -0.838930005033E+01 -0.838937964851E+01 -
0.838945681606E+01
-0.838953162551E+01 -0.838960414700E+01 -0.838967444854E+01 -0.838974259597E+01 -
0.838980865298E+01
-0.838987268138E+01 -0.838993474093E+01 -0.838999488940E+01 -0.839005318268E+01 -
0.839010967509E+01
-0.839016441888E+01 -0.839021746471E+01 -0.839026886165E+01 -0.839031865690E+01 -
0.839036689617E+01
-0.839041362371E+01 -0.839045888209E+01 -0.839050271250E+01 -0.839054515454E+01 -
0.839058624645E+01
-0.839062602512E+01 -0.839066452601E+01 -0.839070178326E+01 -0.839073782960E+01 -
0.839077269660E+01
-0.839080641434E+01 -0.839083901186E+01 -0.839087051687E+01 -0.839090095570E+01 -
0.839093035370E+01
-0.839095873478E+01 -0.839098612190E+01 -0.839101253651E+01 -0.839103799908E+01 -
0.839106252886E+01

-0.839108614388E+01 -0.839110886091E+01 -0.839113069563E+01 -0.839115166254E+01 -
0.839117177470E+01
-0.839119104418E+01 -0.839120948165E+01 -0.839122709654E+01 -0.839124389719E+01 -
0.839125989033E+01
-0.839127508150E+01 -0.839128947488E+01 -0.839130307320E+01 -0.839131587777E+01 -
0.839132788850E+01
-0.839133910356E+01 -0.839134951977E+01 -0.839135913215E+01 -0.839136793406E+01 -
0.839137591712E+01
-0.839138307106E+01 -0.839138938381E+01 -0.839139484120E+01 -0.839139942698E+01 -
0.839140312271E+01
-0.839140590779E+01 -0.839140775907E+01 -0.839140865094E+01 -0.839140855513E+01 -
0.839140744065E+01
-0.839140527342E+01 -0.839140201653E+01 -0.839139762959E+01 -0.839139206899E+01 -
0.839138528722E+01
-0.839137723318E+01 -0.839136785168E+01 -0.839135708308E+01 -0.839134486358E+01 -
0.839133112416E+01
-0.839131579102E+01 -0.839129878494E+01 -0.839128002095E+01 -0.839125940810E+01 -
0.839123684905E+01
-0.839121223965E+01 -0.839118546856E+01 -0.839115641684E+01 -0.839112495749E+01 -
0.839109095480E+01
-0.839105426415E+01 -0.839101473099E+01 -0.839097219072E+01 -0.839092646773E+01 -
0.839087737479E+01
-0.839082471244E+01 -0.839076826815E+01 -0.839070781547E+01 -0.839064311316E+01 -
0.839057390440E+01
-0.839049991574E+01 -0.839042085596E+01 -0.839033641510E+01 -0.839024626330E+01 -
0.839015004933E+01
-0.839004739951E+01 -0.838993791623E+01 -0.838982117647E+01 -0.838969673001E+01 -
0.838956409812E+01
-0.838942277124E+01 -0.838927220763E+01 -0.838911183092E+01 -0.838894102811E+01 -
0.838875914737E+01
-0.838856549542E+01 -0.838835933502E+01 -0.838813988229E+01 -0.838790630374E+01 -
0.838765771312E+01
-0.838739316829E+01 -0.838711166753E+01 -0.838681214591E+01 -0.838649347164E+01 -
0.838615444150E+01
-0.838579377646E+01 -0.838541011741E+01 -0.838500201972E+01 -0.838456794809E+01 -
0.838410627128E+01
-0.838361525580E+01 -0.838309305977E+01 -0.838253772635E+01 -0.838194717663E+01 -
0.838131920226E+01
-0.838065145751E+01 -0.837994145100E+01 -0.837918653680E+01 -0.837838390521E+01 -
0.837753057294E+01
-0.837662337253E+01 -0.837565894157E+01 -0.837463371106E+01 -0.837354389330E+01 -
0.837238546864E+01
-0.837115417245E+01 -0.836984548046E+01 -0.836845459399E+01 -0.836697642402E+01 -
0.836540557461E+01
-0.836373632572E+01 -0.836196261482E+01 -0.836007801782E+01 -0.835807572911E+01 -
0.835594854109E+01
-0.835368882185E+01 -0.835128849308E+01 -0.834873900633E+01 -0.834603131868E+01 -
0.834315586743E+01
-0.834010254432E+01 -0.833686066826E+01 -0.833341895804E+01 -0.832976550409E+01 -
0.832588773939E+01
-0.832177241045E+01 -0.831740554780E+01 -0.831277243594E+01 -0.830785758371E+01 -
0.830264469495E+01

-0.829711663949E+01	-0.829125542484E+01	-0.828504216962E+01	-0.827845707784E+01	-
0.827147941596E+01				
-0.826408749197E+01	-0.825625863814E+01	-0.824796919746E+01	-0.823919451474E+01	-
0.822990893335E+01				
-0.822008579863E+01	-0.820969746880E+01	-0.819871533457E+01	-0.818710984941E+01	-
0.817485057107E+01				
-0.816190621669E+01	-0.814824473295E+01	-0.813383338323E+01	-0.811863885406E+01	-
0.810262738249E+01				
-0.808576490830E+01	-0.806801725156E+01	-0.804935032004E+01	-0.802973034831E+01	-
0.800912417210E+01				
-0.798749954069E+01	-0.796482547035E+01	-0.794107264255E+01	-0.791621384903E+01	-
0.789022448811E+01				
-0.786308311389E+01	-0.783477204132E+01	-0.780527800950E+01	-0.777459290460E+01	-
0.774271454385E+01				
-0.770964752036E+01	-0.767540410909E+01	-0.764000523083E+01	-0.760348147294E+01	-
0.756587416102E+01				
-0.752723647588E+01	-0.748763460806E+01	-0.744714893951E+01	-0.740587524014E+01	-
0.736392586472E+01				
-0.732143093256E+01	-0.727853946978E+01	-0.723542049159E+01	-0.719226399780E+01	-
0.714928185317E+01				
-0.710670851951E+01	-0.706480160447E+01	-0.702384218697E+01	-0.698413487725E+01	-
0.694600756435E+01				
-0.690981080034E+01	-0.687591676636E+01	-0.684471775960E+01	-0.681662413693E+01	-
0.679206164257E+01				
-0.677146804349E+01	-0.675528898808E+01	-0.674397299915E+01	-0.673796550700E+01	-
0.673770182678E+01				
-0.674359898675E+01	-0.675604632403E+01	-0.677539478319E+01	-0.680194488747E+01	-
0.683593340293E+01				
-0.687751878849E+01	-0.692676562062E+01	-0.698362829905E+01	-0.704793447378E+01	-
0.711936876866E+01				
-0.719745748841E+01	-0.728155504693E+01	-0.737083279537E+01	-0.746427070562E+01	-
0.756065192903E+01				
-0.765855958948E+01	-0.775637434022E+01	-0.785227039992E+01	-0.794420735060E+01	-
0.802991551862E+01				
-0.810687506150E+01	-0.817229377835E+01	-0.822309665426E+01	-0.825595081217E+01	-
0.826736090807E+01				
-0.825387848207E+01	-0.821247059100E+01	-0.814108762803E+01	-0.804444361476E+01	-
0.802396209553E+01				
-0.799360565649E+01	-0.795629702880E+01	-0.792149596577E+01	-0.785191062927E+01	-
0.781004819483E+01				
-0.776543219354E+01	-0.771821750745E+01	-0.766856247326E+01	-0.761663264758E+01	-
0.756259230646E+01				
-0.750660579095E+01	-0.744883026007E+01	-0.738941079276E+01		
core charge-density (pseudized)				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
0.000000000000E+00				

0.165635813850E-03	0.170811518247E-03	0.176148950441E-03	0.181653164020E-03
0.187329370483E-03			
0.193182944178E-03	0.199219427384E-03	0.205444535565E-03	0.211864162779E-03
0.218484387257E-03			
0.225311477159E-03	0.232351896512E-03	0.239612311324E-03	0.247099595901E-03
0.254820839354E-03			
0.262783352309E-03	0.270994673833E-03	0.279462578567E-03	0.288195084092E-03
0.297200458517E-03			
0.306487228309E-03	0.316064186364E-03	0.325940400336E-03	0.336125221219E-03
0.346628292200E-03			
0.357459557795E-03	0.368629273256E-03	0.380148014289E-03	0.392026687062E-03
0.404276538534E-03			
0.416909167100E-03	0.429936533579E-03	0.443370972532E-03	0.457225203944E-03
0.471512345266E-03			
0.486245923835E-03	0.501439889685E-03	0.517108628749E-03	0.533266976484E-03
0.549930231917E-03			
0.567114172129E-03	0.584835067193E-03	0.603109695579E-03	0.621955360039E-03
0.641389903992E-03			
0.661431728415E-03	0.682099809267E-03	0.703413715453E-03	0.725393627355E-03
0.748060355938E-03			
0.771435362451E-03	0.795540778750E-03	0.820399428249E-03	0.846034847532E-03
0.872471308636E-03			
0.899733842030E-03	0.927848260314E-03	0.956841182660E-03	0.986740060012E-03
0.101757320108E-02			
0.104936979913E-02	0.108215995964E-02	0.111597472880E-02	0.115084612288E-02
0.118680715859E-02			
0.122389188428E-02	0.126213541224E-02	0.130157395188E-02	0.134224484406E-02
0.138418659640E-02			
0.142743891978E-02	0.147204276590E-02	0.151804036608E-02	0.156547527119E-02
0.161439239296E-02			
0.166483804643E-02	0.171685999380E-02	0.177050748970E-02	0.182583132776E-02
0.188288388872E-02			
0.194171919003E-02	0.200239293696E-02	0.206496257533E-02	0.212948734592E-02
0.219602834053E-02			
0.226464855980E-02	0.233541297287E-02	0.240838857884E-02	0.248364447025E-02
0.256125189841E-02			
0.264128434088E-02	0.272381757101E-02	0.280892972967E-02	0.289670139919E-02
0.298721567961E-02			
0.308055826737E-02	0.317681753640E-02	0.327608462172E-02	0.337845350573E-02
0.348402110710E-02			
0.359288737254E-02	0.370515537131E-02	0.382093139279E-02	0.394032504703E-02
0.406344936843E-02			
0.419042092274E-02	0.432135991728E-02	0.445639031465E-02	0.459563995005E-02
0.473924065212E-02			
0.488732836767E-02	0.504004329024E-02	0.519752999266E-02	0.535993756379E-02
0.552741974947E-02			
0.570013509785E-02	0.587824710933E-02	0.606192439106E-02	0.625134081632E-02
0.644667568884E-02			
0.664811391223E-02	0.685584616468E-02	0.707006907908E-02	0.729098542879E-02
0.751880431907E-02			
0.775374138462E-02	0.799601899308E-02	0.824586645497E-02	0.850352024011E-02
0.876922420069E-02			

0.904322980136E-02	0.932579635636E-02	0.961719127403E-02	0.991769030887E-02
0.102275778214E-01			
0.105471470461E-01	0.108767003676E-01	0.112165496050E-01	0.115670163059E-01
0.119284320486E-01			
0.123011387538E-01	0.126854890063E-01	0.130818463860E-01	0.134905858093E-01
0.139120938812E-01			
0.143467692580E-01	0.147950230206E-01	0.152572790602E-01	0.157339744748E-01
0.162255599782E-01			
0.167325003215E-01	0.172552747271E-01	0.177943773362E-01	0.183503176692E-01
0.189236211007E-01			
0.195148293481E-01	0.201245009754E-01	0.207532119118E-01	0.214015559855E-01
0.220701454738E-01			
0.227596116692E-01	0.234706054626E-01	0.242037979426E-01	0.249598810139E-01
0.257395680323E-01			
0.265435944586E-01	0.273727185319E-01	0.282277219614E-01	0.291094106381E-01
0.300186153670E-01			
0.309561926200E-01	0.319230253087E-01	0.329200235802E-01	0.339481256339E-01
0.350082985601E-01			
0.361015392022E-01	0.372288750413E-01	0.383913651041E-01	0.395901008945E-01
0.408262073491E-01			
0.421008438169E-01	0.434152050633E-01	0.447705222981E-01	0.461680642294E-01
0.476091381406E-01			
0.490950909928E-01	0.506273105521E-01	0.522072265401E-01	0.538363118098E-01
0.555160835441E-01			
0.572481044777E-01	0.590339841421E-01	0.608753801312E-01	0.627739993889E-01
0.647315995152E-01			
0.667499900910E-01	0.688310340195E-01	0.709766488824E-01	0.731888083088E-01
0.754695433540E-01			
0.778209438860E-01	0.802451599766E-01	0.827444032925E-01	0.853209484837E-01
0.879771345639E-01			
0.907153662777E-01	0.935381154496E-01	0.964479223078E-01	0.994473967758E-01
0.102539219724E+00			
0.105726144173E+00	0.109010996438E+00	0.112396677203E+00	0.115886162516E+00
0.119482504687E+00			
0.123188833080E+00	0.127008354774E+00	0.130944355091E+00	0.135000197951E+00
0.139179326050E+00			
0.143485260827E+00	0.147921602201E+00	0.152492028045E+00	0.157200293368E+00
0.162050229166E+00			
0.167045740922E+00	0.172190806688E+00	0.177489474731E+00	0.182945860675E+00
0.188564144105E+00			
0.194348564557E+00	0.200303416853E+00	0.206433045696E+00	0.212741839465E+00
0.219234223136E+00			
0.225914650223E+00	0.232787593684E+00	0.239857535657E+00	0.247128955958E+00
0.254606319203E+00			
0.262294060450E+00	0.270196569233E+00	0.278318171849E+00	0.286663111765E+00
0.295235527991E+00			
0.304039431264E+00	0.313078677880E+00	0.322356941004E+00	0.331877679291E+00
0.341644102622E+00			
0.351659134795E+00	0.361925372969E+00	0.372445043698E+00	0.383219955360E+00
0.394251446830E+00			
0.405540332228E+00	0.417086841608E+00	0.428890557474E+00	0.440950347037E+00
0.453264290164E+00			

0.465829603023E+00	0.478642557491E+00	0.491698396446E+00	0.504991245181E+00
0.518514019247E+00			
0.532258329181E+00	0.546214382699E+00	0.560370885106E+00	0.574714938854E+00
0.589231943403E+00			
0.603905496772E+00	0.618717300433E+00	0.633647069500E+00	0.648672450501E+00
0.663768949338E+00			
0.678909872439E+00	0.694066284487E+00	0.709206986479E+00	0.724298518283E+00
0.739305190214E+00			
0.754189148450E+00	0.768910479380E+00	0.783427358095E+00	0.797696246219E+00
0.811672144064E+00			
0.825308901556E+00	0.838559591593E+00	0.851376948150E+00	0.863713869646E+00
0.875523985597E+00			
0.886762281306E+00	0.897385771145E+00	0.907354205780E+00	0.916630792245E+00
0.925182898117E+00			
0.932982701978E+00	0.940007741963E+00	0.946241302505E+00	0.951672566592E+00
0.956296447395E+00			
0.960112999468E+00	0.963126296910E+00	0.965342654966E+00	0.966768064320E+00
0.967404705877E+00			
0.967246420825E+00	0.966273029454E+00	0.964433274187E+00	0.961700484870E+00
0.958043687182E+00			
0.953448253882E+00	0.947902101021E+00	0.941395881254E+00	0.933923173003E+00
0.925480666844E+00			
0.916068344042E+00	0.905689647106E+00	0.894351638945E+00	
ae wavefunction			
0.581013143449E-04	0.599167371659E-04	0.617888830471E-04	0.637195242216E-04
0.657104882907E-04			
0.677636599495E-04	0.698809827764E-04	0.720644610598E-04	0.743161617065E-04
0.766382161862E-04			
0.790328225642E-04	0.815022475620E-04	0.840488287137E-04	0.866749765768E-04
0.893831770074E-04			
0.921759935143E-04	0.950560696908E-04	0.980261317024E-04	0.101088990872E-03
0.104247546347E-03			
0.107504787832E-03	0.110863798413E-03	0.114327757490E-03	0.117899943761E-03
0.121583738344E-03			
0.125382627964E-03	0.129300208258E-03	0.133340187159E-03	0.137506388430E-03
0.141802755229E-03			
0.146233353933E-03	0.150802377851E-03	0.155514151317E-03	0.160373133683E-03
0.165383923581E-03			
0.170551263291E-03	0.175880043150E-03	0.181375306262E-03	0.187042253193E-03
0.192886246927E-03			
0.198912817940E-03	0.205127669385E-03	0.211536682530E-03	0.218145922283E-03
0.224961642924E-03			
0.231990294059E-03	0.239238526646E-03	0.246713199325E-03	0.254421384879E-03
0.262370376936E-03			
0.270567696823E-03	0.279021100692E-03	0.287738586859E-03	0.296728403326E-03
0.305999055594E-03			
0.315559314673E-03	0.325418225387E-03	0.335585114891E-03	0.346069601487E-03
0.356881603708E-03			
0.368031349657E-03	0.379529386682E-03	0.391386591315E-03	0.403614179537E-03
0.416223717368E-03			
0.429227131760E-03	0.442636721876E-03	0.456465170605E-03	0.470725556669E-03
0.485431366819E-03			

0.500596508616E-03	0.516235323526E-03	0.532362600390E-03	0.548993589469E-03
0.566144016696E-03			
0.583830098569E-03	0.602068557377E-03	0.620876636957E-03	0.640272118991E-03
0.660273339634E-03			
0.680899206869E-03	0.702169218257E-03	0.724103479274E-03	0.746722722256E-03
0.770048325886E-03			
0.794102335271E-03	0.818907482703E-03	0.844487209013E-03	0.870865685584E-03
0.898067837081E-03			
0.926119364831E-03	0.955046771002E-03	0.984877383438E-03	0.101563938133E-02
0.104736182165E-02			
0.108007466639E-02	0.111380881070E-02	0.114859611181E-02	0.118446941889E-02
0.122146260383E-02			
0.125961059297E-02	0.129894939981E-02	0.133951615865E-02	0.138134915941E-02
0.142448788339E-02			
0.146897304021E-02	0.151484660577E-02	0.156215186156E-02	0.161093343507E-02
0.166123734132E-02			
0.171311102592E-02	0.176660340918E-02	0.182176493184E-02	0.187864760193E-02
0.193730504326E-02			
0.199779254529E-02	0.206016711458E-02	0.212448752770E-02	0.219081438592E-02
0.225921017140E-02			
0.232973930523E-02	0.240246820706E-02	0.247746535673E-02	0.255480135765E-02
0.263454900211E-02			
0.271678333861E-02	0.280158174119E-02	0.288902398086E-02	0.297919229917E-02
0.307217148403E-02			
0.316804894779E-02	0.326691480767E-02	0.336886196859E-02	0.347398620851E-02
0.358238626627E-02			
0.369416393215E-02	0.380942414102E-02	0.392827506835E-02	0.405082822902E-02
0.417719857913E-02			
0.430750462074E-02	0.444186850982E-02	0.458041616720E-02	0.472327739308E-02
0.487058598463E-02			
0.502247985724E-02	0.517910116915E-02	0.534059644991E-02	0.550711673245E-02
0.567881768901E-02			
0.585585977118E-02	0.603840835367E-02	0.622663388261E-02	0.642071202781E-02
0.662082383960E-02			
0.682715591007E-02	0.703990053892E-02	0.725925590407E-02	0.748542623707E-02
0.771862200347E-02			
0.795906008839E-02	0.820696398706E-02	0.846256400093E-02	0.872609743914E-02
0.899780882560E-02			
0.927795011168E-02	0.956678089500E-02	0.986456864395E-02	0.101715889285E-01
0.104881256572E-01			
0.108144713206E-01	0.111509272409E-01	0.114978038291E-01	0.118554208479E-01
0.122241076822E-01			
0.126042036164E-01	0.129960581193E-01	0.134000311356E-01	0.138164933858E-01
0.142458266728E-01			
0.146884241969E-01	0.151446908786E-01	0.156150436887E-01	0.160999119876E-01
0.165997378717E-01			
0.171149765292E-01	0.176460966034E-01	0.181935805649E-01	0.187579250929E-01
0.193396414644E-01			
0.199392559524E-01	0.205573102336E-01	0.211943618041E-01	0.218509844046E-01
0.225277684540E-01			
0.232253214936E-01	0.239442686372E-01	0.246852530338E-01	0.254489363364E-01
0.262359991824E-01			

0.270471416785E-01	0.278830838993E-01	0.287445663912E-01	0.296323506855E-01
0.305472198214E-01			
0.314899788745E-01	0.324614554933E-01	0.334625004450E-01	0.344939881698E-01
0.355568173317E-01			
0.366519113986E-01	0.377802191940E-01	0.389427154917E-01	0.401404015838E-01
0.413743058773E-01			
0.426454844691E-01	0.439550217526E-01	0.453040309991E-01	0.466936549603E-01
0.481250664644E-01			
0.495994689941E-01	0.511180972926E-01	0.526822179489E-01	0.542931299699E-01
0.559521653734E-01			
0.576606897241E-01	0.594201027368E-01	0.612318387654E-01	0.630973673905E-01
0.650181938885E-01			
0.669958597653E-01	0.690319431776E-01	0.711280594635E-01	0.732858614799E-01
0.755070400653E-01			
0.777933243748E-01	0.801464821699E-01	0.825683201490E-01	0.850606842124E-01
0.876254595424E-01			
0.902645708336E-01	0.929799823656E-01	0.957736979628E-01	0.986477609665E-01
0.101604254134E+00			
0.104645299328E+00	0.107773057354E+00	0.110989727457E+00	0.114297546877E+00
0.117698790200E+00			
0.121195768643E+00	0.124790829246E+00	0.128486353803E+00	0.132284757798E+00
0.136188489067E+00			
0.140200026383E+00	0.144321877735E+00	0.148556578675E+00	0.152906690045E+00
0.157374796055E+00			
0.161963501408E+00	0.166675429109E+00	0.171513216966E+00	0.176479514850E+00
0.181576980773E+00			
0.186808277349E+00	0.192176067521E+00	0.197683010140E+00	0.203331755211E+00
0.209124938444E+00			
0.215065176077E+00	0.221155058470E+00	0.227397144013E+00	0.233793951962E+00
0.240347955506E+00			
0.247061573443E+00	0.253937162213E+00	0.260977006986E+00	0.268183312042E+00
0.275558191029E+00			
0.283103656298E+00	0.290821607553E+00	0.298713820386E+00	0.306781933498E+00
0.315027435637E+00			
0.323451651936E+00	0.332055729185E+00	0.340840620821E+00	0.349807070743E+00
0.358955596902E+00			
0.368286473661E+00	0.377799713787E+00	0.387495049476E+00	0.397371912762E+00
0.407429415080E+00			
0.417666326327E+00	0.428081052860E+00	0.438671615195E+00	0.449435624879E+00
0.460370260569E+00			
0.471472243884E+00	0.482737814816E+00	0.494162705515E+00	0.505742115924E+00
0.517470686530E+00			
0.529342473001E+00	0.541350918903E+00	0.553488830424E+00	0.565748349051E+00
0.578120925768E+00			
0.590597296001E+00	0.603167452957E+00	0.615820624933E+00	0.628545250357E+00
0.641328956406E+00			
0.654158536652E+00	0.667019933024E+00	0.679898216491E+00	0.692777572575E+00
0.705641287323E+00			
0.718471736808E+00	0.731250379454E+00	0.743957750865E+00	0.756573463830E+00
0.769076210373E+00			
0.781443768947E+00	0.793653016795E+00	0.805679945611E+00	0.817499683877E+00
0.829086524254E+00			

0.840413957026E+00	0.851454708954E+00	0.862180790299E+00	0.872563546945E+00
0.882573721409E+00			
0.892181519094E+00	0.901356683888E+00	0.910068580871E+00	0.918286286730E+00
0.925978688500E+00			
0.933114590020E+00	0.939662826945E+00	0.945592389127E+00	0.950872551925E+00
0.955473014163E+00			
0.959364044237E+00	0.962516633930E+00	0.964902658425E+00	0.966495042899E+00
0.967267935838E+00			
0.967196886985E+00	0.966259031101E+00	0.964433274187E+00	0.961700484870E+00
0.958043687182E+00			
0.953448253882E+00	0.947902101021E+00	0.941395881254E+00	0.933923173003E+00
0.925480666844E+00			
0.916068344042E+00	0.905689647106E+00	0.894351638945E+00	
pseudo wavefunction			
0.751002279840E-04	0.774469220727E-04	0.798669444758E-04	0.823625865196E-04
0.849362111285E-04			
0.875902550623E-04	0.903272312236E-04	0.931497310368E-04	0.960604269020E-04
0.990620747247E-04			
0.102157516526E-03	0.105349683133E-03	0.108641596953E-03	0.112036374837E-03
0.115537231030E-03			
0.119147480213E-03	0.122870540642E-03	0.126709937387E-03	0.130669305667E-03
0.134752394291E-03			
0.138963069210E-03	0.143305317176E-03	0.147783249518E-03	0.152401106033E-03
0.157163258999E-03			
0.162074217320E-03	0.167138630791E-03	0.172361294501E-03	0.177747153372E-03
0.183301306845E-03			
0.189029013705E-03	0.194935697061E-03	0.201026949478E-03	0.207308538278E-03
0.213786410996E-03			
0.220466701012E-03	0.227355733361E-03	0.234460030715E-03	0.241786319568E-03
0.249341536597E-03			
0.257132835234E-03	0.265167592437E-03	0.273453415676E-03	0.281998150135E-03
0.290809886141E-03			
0.299896966822E-03	0.309267996009E-03	0.318931846380E-03	0.328897667862E-03
0.339174896296E-03			
0.349773262367E-03	0.360702800820E-03	0.371973859962E-03	0.383597111455E-03
0.395583560427E-03			
0.407944555887E-03	0.420691801471E-03	0.433837366526E-03	0.447393697535E-03
0.461373629900E-03			
0.475790400100E-03	0.490657658218E-03	0.505989480868E-03	0.521800384524E-03
0.538105339260E-03			
0.554919782928E-03	0.572259635776E-03	0.590141315516E-03	0.608581752872E-03
0.627598407611E-03			
0.647209285072E-03	0.667432953216E-03	0.688288560204E-03	0.709795852528E-03
0.731975193707E-03			
0.754847583568E-03	0.778434678127E-03	0.802758810097E-03	0.827843010027E-03
0.853711028113E-03			
0.880387356683E-03	0.907897253384E-03	0.936266765101E-03	0.965522752614E-03
0.995692916031E-03			
0.102680582102E-02	0.105889092584E-02	0.109197860925E-02	0.112610019927E-02
0.116128800282E-02			
0.119757533634E-02	0.123499655731E-02	0.127358709678E-02	0.131338349295E-02
0.135442342572E-02			

0.139674575237E-02	0.144039054439E-02	0.148539912538E-02	0.153181411017E-02
0.157967944521E-02			
0.162904045013E-02	0.167994386068E-02	0.173243787297E-02	0.178657218908E-02
0.184239806415E-02			
0.189996835488E-02	0.195933756958E-02	0.202056191980E-02	0.208369937350E-02
0.214880970997E-02			
0.221595457643E-02	0.228519754635E-02	0.235660417968E-02	0.243024208490E-02
0.250618098303E-02			
0.258449277364E-02	0.266525160291E-02	0.274853393383E-02	0.283441861857E-02
0.292298697317E-02			
0.301432285448E-02	0.310851273955E-02	0.320564580753E-02	0.330581402403E-02
0.340911222824E-02			
0.351563822268E-02	0.362549286577E-02	0.373878016732E-02	0.385560738699E-02
0.397608513580E-02			
0.410032748085E-02	0.422845205327E-02	0.436058015957E-02	0.449683689648E-02
0.463735126931E-02			
0.478225631408E-02	0.493168922342E-02	0.508579147641E-02	0.524470897250E-02
0.540859216955E-02			
0.557759622622E-02	0.575188114883E-02	0.593161194273E-02	0.611695876847E-02
0.630809710279E-02			
0.650520790464E-02	0.670847778642E-02	0.691809919048E-02	0.713427057126E-02
0.735719658295E-02			
0.758708827309E-02	0.782416328225E-02	0.806864604981E-02	0.832076802627E-02
0.858076789211E-02			
0.884889178350E-02	0.912539352502E-02	0.941053486964E-02	0.970458574621E-02
0.100078245146E-01			
0.103205382286E-01	0.106430229078E-01	0.109755838165E-01	0.113185357528E-01
0.116722033456E-01			
0.120369213616E-01	0.124130350211E-01	0.128009003242E-01	0.132008843868E-01
0.136133657874E-01			
0.140387349240E-01	0.144773943829E-01	0.149297593181E-01	0.153962578431E-01
0.158773314347E-01			
0.163734353489E-01	0.168850390499E-01	0.174126266528E-01	0.179566973792E-01
0.185177660276E-01			
0.190963634574E-01	0.196930370889E-01	0.203083514178E-01	0.209428885461E-01
0.215972487287E-01			
0.222720509377E-01	0.229679334428E-01	0.236855544106E-01	0.244255925217E-01
0.251887476061E-01			
0.259757412995E-01	0.267873177176E-01	0.276242441526E-01	0.284873117896E-01
0.293773364458E-01			
0.302951593306E-01	0.312416478303E-01	0.322176963148E-01	0.332242269695E-01
0.342621906517E-01			
0.353325677728E-01	0.364363692060E-01	0.375746372220E-01	0.387484464515E-01
0.399589048760E-01			
0.412071548482E-01	0.424943741416E-01	0.438217770308E-01	0.451906154027E-01
0.466021799005E-01			
0.480578010988E-01	0.495588507139E-01	0.511067428465E-01	0.527029352602E-01
0.543489306952E-01			
0.560462782185E-01	0.577965746098E-01	0.596014657865E-01	0.614626482651E-01
0.633818706629E-01			
0.653609352370E-01	0.674016994648E-01	0.695060776627E-01	0.716760426471E-01
0.739136274343E-01			

0.762209269825E-01	0.786000999743E-01	0.810533706401E-01	0.835830306224E-01
0.861914408808E-01			
0.888810336368E-01	0.916543143582E-01	0.945138637823E-01	0.974623399766E-01
0.100502480436E+00			
0.103637104214E+00	0.106869114090E+00	0.110201498761E+00	0.113637335069E+00
0.117179790247E+00			
0.120832124194E+00	0.124597691759E+00	0.128479945046E+00	0.132482435721E+00
0.136608817329E+00			
0.140862847598E+00	0.145248390737E+00	0.149769419713E+00	0.154430018495E+00
0.159234384268E+00			
0.164186829582E+00	0.169291784445E+00	0.174553798341E+00	0.179977542142E+00
0.185567809913E+00			
0.191329520589E+00	0.197267719491E+00	0.203387579665E+00	0.209694403017E+00
0.216193621216E+00			
0.222890796323E+00	0.229791621126E+00	0.236901919126E+00	0.244227644144E+00
0.251774879488E+00			
0.259549836648E+00	0.267558853436E+00	0.275808391535E+00	0.284305033365E+00
0.293055478216E+00			
0.302066537544E+00	0.311345129353E+00	0.320898271570E+00	0.330733074297E+00
0.340856730834E+00			
0.351276507342E+00	0.361999731024E+00	0.373033776658E+00	0.384386051345E+00
0.396063977286E+00			
0.408074972409E+00	0.420426428650E+00	0.433125687674E+00	0.446180013796E+00
0.459596563876E+00			
0.473382353906E+00	0.487544222024E+00	0.502088787645E+00	0.517022406403E+00
0.532351120562E+00			
0.548080604554E+00	0.564216105259E+00	0.580762376663E+00	0.597723608473E+00
0.615103348293E+00			
0.632904416927E+00	0.651128816381E+00	0.669777630136E+00	0.688850915254E+00
0.708347585907E+00			
0.728265287917E+00	0.748600263931E+00	0.769347208906E+00	0.790499115597E+00
0.812047109854E+00			
0.833980275581E+00	0.856285469339E+00	0.878947124699E+00	0.901947046622E+00
0.925264196314E+00			
0.948874467257E+00	0.972750453348E+00	0.996861210430E+00	0.102117201281E+01
0.104564410679E+01			
0.107023446371E+01	0.109489553541E+01	0.111957501580E+01	0.114421561257E+01
0.116875483398E+01			
0.119312479622E+01	0.121725205764E+01	0.124105748696E+01	0.126445617314E+01
0.128735738551E+01			
0.130966459320E+01	0.133127555356E+01	0.135208247936E+01	0.137197229487E+01
0.139082699014E+01			
0.140852408242E+01	0.142493719179E+01	0.143993673606E+01	0.145339074673E+01
0.146516580336E+01			
0.147512807827E+01	0.148314447612E+01	0.148908384397E+01	0.149281821698E+01
0.149422405190E+01			
0.149318338614E+01	0.148958484370E+01	0.148332439172E+01	0.147430573249E+01
0.146244019801E+01			
0.144764599698E+01	0.142984665161E+01	0.140896845461E+01	0.138493678002E+01
0.135767109845E+01			
0.132707858311E+01	0.129304625414E+01	0.125543191107E+01	0.121408357465E+01
0.116888602410E+01			

0.111973616312E+01	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00
0.000000000000E+00			
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
ae wavefunction			
0.106329947500E-03	0.109652313188E-03	0.113078486510E-03	0.116611710791E-03
0.120255330686E-03			
0.124012795332E-03	0.127887661631E-03	0.131883597587E-03	0.136004385802E-03
0.140253927030E-03			
0.144636243903E-03	0.149155484700E-03	0.153815927290E-03	0.158621983181E-03
0.163578201685E-03			
0.168689274223E-03	0.173960038778E-03	0.179395484445E-03	0.185000756165E-03
0.190781159604E-03			
0.196742166158E-03	0.202889418110E-03	0.209228734014E-03	0.215766114143E-03
0.222507746208E-03			
0.229460011185E-03	0.236629489376E-03	0.244022966583E-03	0.251647440593E-03
0.259510127694E-03			
0.267618469674E-03	0.275980140614E-03	0.284603054385E-03	0.293495371948E-03
0.302665509160E-03			
0.312122144766E-03	0.321874228460E-03	0.331930989520E-03	0.342301945386E-03
0.352996910739E-03			
0.364026006781E-03	0.375399670728E-03	0.387128665760E-03	0.399224091134E-03
0.411697392668E-03			
0.424560373645E-03	0.437825205839E-03	0.451504441095E-03	0.465611023160E-03
0.480158299943E-03			
0.495160036056E-03	0.510630425867E-03	0.526584106915E-03	0.543036173691E-03
0.560002191923E-03			
0.577498213244E-03	0.595540790388E-03	0.614146992779E-03	0.633334422655E-03
0.653121231710E-03			
0.673526138165E-03	0.694568444495E-03	0.716268055597E-03	0.738645497594E-03
0.761721937202E-03			
0.785519201673E-03	0.810059799435E-03	0.835366941162E-03	0.861464561933E-03
0.888377343555E-03			
0.916130737944E-03	0.944750991103E-03	0.974265167758E-03	0.100470117708E-02
0.103608779874E-02			
0.106845471019E-02	0.110183251453E-02	0.113625276931E-02	0.117174801640E-02
0.120835181238E-02			
0.124609876033E-02	0.128502454229E-02	0.132516595285E-02	0.136656093379E-02
0.140924860975E-02			
0.145326932500E-02	0.149866468137E-02	0.154547757740E-02	0.159375224860E-02
0.164353430903E-02			
0.169487079409E-02	0.174781020479E-02	0.180240255321E-02	0.185869940942E-02
0.191675394991E-02			
0.197662100745E-02	0.203835712251E-02	0.210202059627E-02	0.216767154524E-02
0.223537195755E-02			
0.230518575110E-02	0.237717883329E-02	0.245141916276E-02	0.252797681294E-02
0.260692403765E-02			
0.268833533852E-02	0.277228753467E-02	0.285885983447E-02	0.294813390958E-02
0.304019397094E-02			
0.313512684756E-02	0.323302206731E-02	0.333397194044E-02	0.343807164552E-02
0.354541931811E-02			
0.365611614200E-02	0.377026644333E-02	0.388797778758E-02	0.400936107948E-02
0.413453066590E-02			

0.426360444206E-02	0.439670396072E-02	0.453395454487E-02	0.467548540375E-02
0.482142975239E-02			
0.497192493481E-02	0.512711255086E-02	0.528713858700E-02	0.545215355089E-02
0.562231261015E-02			
0.579777573527E-02	0.597870784672E-02	0.616527896665E-02	0.635766437489E-02
0.655604476990E-02			
0.676060643429E-02	0.697154140542E-02	0.718904765102E-02	0.741332925006E-02
0.764459657897E-02			
0.788306650339E-02	0.812896257563E-02	0.838251523781E-02	0.864396203124E-02
0.891354781178E-02			
0.919152497151E-02	0.947815366701E-02	0.977370205421E-02	0.100784465302E-01
0.103926719819E-01			
0.107166720421E-01	0.110507493531E-01	0.113952158372E-01	0.117503929761E-01
0.121166120974E-01			
0.124942146696E-01	0.128835526058E-01	0.132849885758E-01	0.136988963267E-01
0.141256610131E-01			
0.145656795368E-01	0.150193608951E-01	0.154871265395E-01	0.159694107445E-01
0.164666609863E-01			
0.169793383318E-01	0.175079178389E-01	0.180528889670E-01	0.186147559995E-01
0.191940384769E-01			
0.197912716418E-01	0.204070068966E-01	0.210418122722E-01	0.216962729098E-01
0.223709915551E-01			
0.230665890657E-01	0.237837049314E-01	0.245229978077E-01	0.252851460634E-01
0.260708483418E-01			
0.268808241360E-01	0.277158143787E-01	0.285765820459E-01	0.294639127764E-01
0.303786155052E-01			
0.313215231129E-01	0.322934930901E-01	0.332954082164E-01	0.343281772570E-01
0.353927356733E-01			
0.364900463502E-01	0.376211003396E-01	0.387869176192E-01	0.399885478684E-01
0.412270712593E-01			
0.425035992665E-01	0.438192754875E-01	0.451752764868E-01	0.465728126490E-01
0.480131290551E-01			
0.494975063637E-01	0.510272617206E-01	0.526037496734E-01	0.542283631063E-01
0.559025341896E-01			
0.576277353405E-01	0.594054801961E-01	0.612373246050E-01	0.631248676312E-01
0.650697525521E-01			
0.670736679094E-01	0.691383485053E-01	0.712655764789E-01	0.734571823289E-01
0.757150459909E-01			
0.780410978707E-01	0.804373199360E-01	0.829057467582E-01	0.854484665921E-01
0.880676224407E-01			
0.907654130862E-01	0.935440941668E-01	0.964059792156E-01	0.993534406698E-01
0.102388910916E+00			
0.105514883229E+00	0.108733912823E+00	0.112048617698E+00	0.115461679656E+00
0.118975845096E+00			
0.122593925921E+00	0.126318800236E+00	0.130153413230E+00	0.134100777712E+00
0.138163974850E+00			
0.142346154683E+00	0.146650536527E+00	0.151080409452E+00	0.155639132627E+00
0.160330135323E+00			
0.165156917123E+00	0.170123047900E+00	0.175232167565E+00	0.180487985756E+00
0.185894281437E+00			
0.191454902021E+00	0.197173762826E+00	0.203054845825E+00	0.209102198465E+00
0.215319932166E+00			

0.221712220537E+00	0.228283297465E+00	0.235037454673E+00	0.241979039227E+00
0.249112450514E+00			
0.256442136998E+00	0.263972592385E+00	0.271708351825E+00	0.279653986935E+00
0.287814101360E+00			
0.296193324533E+00	0.304796306584E+00	0.313627710758E+00	0.322692207130E+00
0.331994464016E+00			
0.341539139991E+00	0.351330874403E+00	0.361374277475E+00	0.371673919653E+00
0.382234319480E+00			
0.393059931809E+00	0.404155133537E+00	0.415524209705E+00	0.427171337395E+00
0.439100569784E+00			
0.451315817376E+00	0.463820829574E+00	0.476619174200E+00	0.489714215357E+00
0.503109090678E+00			
0.516806686480E+00	0.530809611196E+00	0.545120168129E+00	0.559740325255E+00
0.574671683966E+00			
0.589915446086E+00	0.605472378290E+00	0.621342775296E+00	0.637526420157E+00
0.654022543319E+00			
0.670829778555E+00	0.687946117289E+00	0.705368860153E+00	0.723094566336E+00
0.741119000235E+00			
0.759437075969E+00	0.778042798638E+00	0.796929203636E+00	0.816088292970E+00
0.835510968560E+00			
0.855186963442E+00	0.875104770396E+00	0.895251565733E+00	0.915613134465E+00
0.936173788144E+00			
0.956916283932E+00	0.977821737871E+00	0.998869539391E+00	0.102003725958E+01
0.104130055961E+01			
0.106263309773E+01	0.108400643066E+01	0.110538991914E+01	0.112675062646E+01
0.114805322047E+01			
0.116925987066E+01	0.119033014998E+01	0.121122093124E+01	0.123188628907E+01
0.125227739974E+01			
0.127234244432E+01	0.129202651415E+01	0.131127151808E+01	0.133001609671E+01
0.134819553807E+01			
0.136574170088E+01	0.138258294566E+01	0.139864407108E+01	0.141384626207E+01
0.142810704760E+01			
0.144134027076E+01	0.145345607108E+01	0.146436088503E+01	0.147395746070E+01
0.148214489478E+01			
0.148881868737E+01	0.149387082350E+01	0.149718987981E+01	0.149866115989E+01
0.149816686218E+01			
0.149558628224E+01	0.149079605449E+01	0.148367043500E+01	0.147408163206E+01
0.146190018542E+01			
0.144699540142E+01	0.142923584870E+01	0.140848991784E+01	0.138462645170E+01
0.135751545337E+01			
0.132702887546E+01	0.129304149987E+01	0.125543191107E+01	0.121408357465E+01
0.116888602410E+01			
0.111973616312E+01	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00
0.000000000000E+00			
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
pseudo wavefunction			
0.118327813132E-08	0.125838244909E-08	0.133825374294E-08	0.142319457951E-08
0.151352672977E-08			
0.160959238792E-08	0.171175546774E-08	0.182040298110E-08	0.193594650407E-08
0.205882373603E-08			
0.218950015773E-08	0.232847079466E-08	0.247626209225E-08	0.263343391018E-08
0.280058164318E-08			

0.297833847653E-08	0.316737778468E-08	0.336841568206E-08	0.358221373592E-08
0.380958185123E-08			
0.405138133876E-08	0.430852817789E-08	0.458199648649E-08	0.487282221103E-08
0.518210705099E-08			
0.551102263223E-08	0.586081494534E-08	0.623280906568E-08	0.662841417300E-08
0.704912888965E-08			
0.749654695765E-08	0.797236327603E-08	0.847838032146E-08	0.901651497629E-08
0.958880579009E-08			
0.101974207020E-07	0.108446652534E-07	0.115329913214E-07	0.122650064073E-07
0.130434835141E-07			
0.138713716514E-07	0.147518070061E-07	0.156881248237E-07	0.166838720422E-07
0.177428207287E-07			
0.188689823687E-07	0.200666230623E-07	0.213402796849E-07	0.226947770737E-07
0.241352463052E-07			
0.256671441322E-07	0.272962736555E-07	0.290288063066E-07	0.308713052266E-07
0.328307501280E-07			
0.349145637357E-07	0.371306399052E-07	0.394873735258E-07	0.419936923225E-07
0.446590906752E-07			
0.474936655853E-07	0.505081549252E-07	0.537139781147E-07	0.571232793803E-07
0.607489737593E-07			
0.646047960246E-07	0.687053527141E-07	0.730661774629E-07	0.777037898478E-07
0.826357579658E-07			
0.878807649855E-07	0.934586799223E-07	0.993906329055E-07	0.105699095223E-06
0.112407964446E-06			
0.119542654959E-06	0.127130194232E-06	0.135199325205E-06	0.143780615174E-06
0.152906571581E-06			
0.162611765163E-06	0.172932960908E-06	0.183909257328E-06	0.195582234573E-06
0.207996111941E-06			
0.221197915390E-06	0.235237655681E-06	0.250168517826E-06	0.266047062561E-06
0.282933440613E-06			
0.300891620554E-06	0.319989631132E-06	0.340299818970E-06	0.361899122630E-06
0.384869364070E-06			
0.409297558598E-06	0.435276244501E-06	0.462903833597E-06	0.492284984034E-06
0.523530996752E-06			
0.556760237114E-06	0.592098583288E-06	0.629679903099E-06	0.669646561139E-06
0.712149958071E-06			
0.757351104157E-06	0.805421229191E-06	0.856542431149E-06	0.910908365999E-06
0.968724981308E-06			
0.103021129640E-05	0.109560023203E-05	0.116513949275E-05	0.123909250522E-05
0.131773941611E-05			
0.140137815338E-05	0.149032555482E-05	0.158491856832E-05	0.168551552827E-05
0.179249751297E-05			
0.190626978821E-05	0.202726334249E-05	0.215593651965E-05	0.229277675516E-05
0.243830242256E-05			
0.259306479715E-05	0.275765014428E-05	0.293268194023E-05	0.311882323394E-05
0.331677915882E-05			
0.352729960377E-05	0.375118205394E-05	0.398927461162E-05	0.424247920898E-05
0.451175502465E-05			
0.479812211718E-05	0.510266528916E-05	0.542653819646E-05	0.577096771844E-05
0.613725860540E-05			
0.652679842111E-05	0.694106279892E-05	0.738162103157E-05	0.785014201573E-05
0.834840057382E-05			

0.887828417707E-05	0.944180009531E-05	0.100410830005E-04	0.106784030528E-04
0.113561745000E-04			
0.120769648224E-04	0.128435044586E-04	0.136586971481E-04	0.145256309301E-04
0.154475898413E-04			
0.164280663552E-04	0.174707746109E-04	0.185796644821E-04	0.197589365384E-04
0.210130579560E-04			
0.223467794389E-04	0.237651532131E-04	0.252735521630E-04	0.268776901827E-04
0.285836438179E-04			
0.303978752822E-04	0.323272569329E-04	0.343790973011E-04	0.365611687725E-04
0.388817370257E-04			
0.413495923379E-04	0.439740828772E-04	0.467651501075E-04	0.497333664398E-04
0.528899752727E-04			
0.562469335732E-04	0.598169571591E-04	0.636135688548E-04	0.676511497021E-04
0.719449934200E-04			
0.765113643192E-04	0.813675588912E-04	0.865319713044E-04	0.920241630544E-04
0.978649370331E-04			
0.104076416295E-03	0.110682127823E-03	0.117707091599E-03	0.125177915334E-03
0.133122895200E-03			
0.141572122947E-03	0.150557599820E-03	0.160113357695E-03	0.170275587895E-03
0.181082778173E-03			
0.192575858386E-03	0.204798355389E-03	0.217796557764E-03	0.231619690975E-03
0.246320103636E-03			
0.261953465570E-03	0.278578978429E-03	0.296259599650E-03	0.315062280603E-03
0.335058219818E-03			
0.356323132255E-03	0.378937535623E-03	0.402987054822E-03	0.428562745666E-03
0.455761439090E-03			
0.484686107136E-03	0.515446252101E-03	0.548158320297E-03	0.582946141982E-03
0.619941399101E-03			
0.659284122599E-03	0.701123221161E-03	0.745617043359E-03	0.792933975297E-03
0.843253076002E-03			
0.896764752916E-03	0.953671480001E-03	0.101418856116E-02	0.107854494174E-02
0.114698407128E-02			
0.121976482045E-02	0.129716245587E-02	0.137946967621E-02	0.146699771341E-02
0.156007750323E-02			
0.165906092922E-02	0.176432214488E-02	0.187625897867E-02	0.199529442718E-02
0.212187824179E-02			
0.225648861458E-02	0.239963396977E-02	0.255185486695E-02	0.271372602313E-02
0.288585846082E-02			
0.306890178989E-02	0.326354663125E-02	0.347052719110E-02	0.369062399481E-02
0.392466679009E-02			
0.417353762962E-02	0.443817414395E-02	0.471957301603E-02	0.501879366933E-02
0.533696218230E-02			
0.567527544247E-02	0.603500555427E-02	0.641750451538E-02	0.682420917723E-02
0.725664650606E-02			
0.771643916171E-02	0.820531141230E-02	0.872509540374E-02	0.927773780395E-02
0.986530684262E-02			
0.104899997682E-01	0.111541507450E-01	0.118602392138E-01	0.126108987407E-01
0.134089263801E-01			
0.142572925781E-01	0.151591516438E-01	0.161178528164E-01	0.171369519591E-01
0.182202239074E-01			
0.193716755044E-01	0.205955593537E-01	0.218963883218E-01	0.232789508226E-01
0.247483269158E-01			

0.263099052532E-01	0.279694009027E-01	0.297328740839E-01	0.316067498460E-01
0.335978387164E-01			
0.357133583497E-01	0.379609562036E-01	0.403487332639E-01	0.428852688407E-01
0.455796464527E-01			
0.484414808110E-01	0.514809459116E-01	0.547088042361E-01	0.581364370557E-01
0.617758758255E-01			
0.656398346448E-01	0.697417437521E-01	0.740957840104E-01	0.787169223245E-01
0.836209479227E-01			
0.888245094151E-01	0.943451525289E-01	0.100201358401E+00	0.106412582293E+00
0.112999292571E+00			
0.119983009784E+00	0.127386345635E+00	0.135233041653E+00	0.143548007321E+00
0.152357357433E+00			
0.161688448430E+00	0.171569913443E+00	0.182031695815E+00	0.193105080837E+00
0.204822725487E+00			
0.217218685991E+00	0.230328443055E+00	0.244188924746E+00	0.258838527022E+00
0.274317132128E+00			
0.290666125161E+00	0.307928409376E+00	0.326148421018E+00	0.345372144785E+00
0.365647131381E+00			
0.387022519055E+00	0.409549061477E+00	0.433279164885E+00	0.458266938014E+00
0.484568259012E+00			
0.512240864216E+00	0.541344464400E+00	0.571940894800E+00	0.604094305836E+00
0.637871401978E+00			
0.673341736465E+00	0.710578069529E+00	0.749656797302E+00	0.790658457353E+00
0.833668314849E+00			
0.878777030158E+00	0.926081404196E+00	0.975685191588E+00	0.102769996336E+01
0.108224599010E+01			
0.113945310298E+01	0.119946147334E+01	0.126242223145E+01	0.132849782195E+01
0.139786196669E+01			
0.147069907700E+01	0.154720292676E+01	0.162757436790E+01	0.171201784271E+01
0.180073642719E+01			
0.189392513081E+01	0.199176218669E+01	0.209439843751E+01	0.220199046886E+01
0.231476530812E+01			
0.243297201266E+01	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00
0.000000000000E+00			
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
ae wavefunction			
0.156129193110E-08	0.167471969820E-08	0.179374313658E-08	0.191874928226E-08
0.205014431376E-08			
0.218835752479E-08	0.233383899029E-08	0.248706852523E-08	0.264855047021E-08
0.281882172533E-08			
0.299844420032E-08	0.318801835329E-08	0.338817819307E-08	0.359959350817E-08
0.382297633410E-08			
0.405908139977E-08	0.430870465052E-08	0.457269481425E-08	0.485195220172E-08
0.514742673695E-08			
0.546012710894E-08	0.579112972789E-08	0.614156739323E-08	0.651265230789E-08
0.690566372839E-08			
0.732196401425E-08	0.776299217947E-08	0.823028688741E-08	0.872546972858E-08
0.925028356912E-08			
0.980654150301E-08	0.103962155119E-07	0.110213600048E-07	0.116841845903E-07
0.123870319376E-07			
0.131323666810E-07	0.139228438409E-07	0.147612524651E-07	0.156505764128E-07
0.165939817838E-07			

0.175948183015E-07	0.186566669596E-07	0.197833164151E-07	0.209788007610E-07
0.222474146697E-07			
0.235936948046E-07	0.250224908914E-07	0.265389446593E-07	0.281485253022E-07
0.298570325914E-07			
0.316706501238E-07	0.335959429357E-07	0.356398799915E-07	0.378098787849E-07
0.401138174555E-07			
0.425600778971E-07	0.451575610818E-07	0.479157327820E-07	0.508446575767E-07
0.539550226940E-07			
0.572582050135E-07	0.607662866454E-07	0.644921186936E-07	0.684493597679E-07
0.726525273084E-07			
0.771170589717E-07	0.818593507297E-07	0.868968890434E-07	0.922481860298E-07
0.979329662648E-07			
0.103972192543E-06	0.110388142873E-06	0.117204541670E-06	0.124446549927E-06
0.132140968020E-06			
0.140316262851E-06	0.149002713907E-06	0.158232524253E-06	0.168039887055E-06
0.178461212952E-06			
0.189535179929E-06	0.201302922335E-06	0.213808184301E-06	0.227097465336E-06
0.241220201736E-06			
0.256228974055E-06	0.272179676165E-06	0.289131738503E-06	0.307148356643E-06
0.326296720431E-06			
0.346648285410E-06	0.368279007957E-06	0.391269666362E-06	0.415706146819E-06
0.441679779253E-06			
0.469287668582E-06	0.498633066359E-06	0.529825763445E-06	0.562982504910E-06
0.598227425721E-06			
0.635692520777E-06	0.675518141408E-06	0.717853530627E-06	0.762857388480E-06
0.810698445133E-06			
0.861556139184E-06	0.915621278975E-06	0.973096754285E-06	0.103419825977E-05
0.109915522188E-05			
0.116821154660E-05	0.124162664411E-05	0.131967631281E-05	0.140265385638E-05
0.149087112126E-05			
0.158465974213E-05	0.168437234718E-05	0.179038391549E-05	0.190309317628E-05
0.202292413440E-05			
0.215032763217E-05	0.228578311155E-05	0.242980035774E-05	0.258292147382E-05
0.274572291404E-05			
0.291881763557E-05	0.310285744938E-05	0.329853545929E-05	0.350658868643E-05
0.372780084523E-05			
0.396300530717E-05	0.421308824295E-05	0.447899197448E-05	0.476171850601E-05
0.506233334431E-05			
0.538196949575E-05	0.572183174711E-05	0.608320120898E-05	0.646744015127E-05
0.687599714616E-05			
0.731041252893E-05	0.777232420701E-05	0.826347384528E-05	0.878571343987E-05
0.934101228733E-05			
0.993146439367E-05	0.105592964272E-04	0.112268760757E-04	0.119367209440E-04
0.126915081297E-04			
0.134940842165E-04	0.143474760727E-04	0.152549022137E-04	0.162197849362E-04
0.172457632522E-04			
0.183367065298E-04	0.194967291111E-04	0.207302057797E-04	0.220417882595E-04
0.234364226952E-04			
0.249193682707E-04	0.264962170353E-04	0.281729148931E-04	0.299557839892E-04
0.318515465048E-04			
0.338673499058E-04	0.360107938188E-04	0.382899586077E-04	0.407134357207E-04
0.432903599758E-04			

0.460304438587E-04	0.489440140060E-04	0.520420499664E-04	0.553362254012E-04
0.588389518893E-04			
0.625634254771E-04	0.665236761707E-04	0.707346205138E-04	0.752121175117E-04
0.799730279837E-04			
0.850352778242E-04	0.904179249792E-04	0.961412308489E-04	0.102226736082E-03
0.108697341112E-03			
0.115577391737E-03	0.122892770144E-03	0.130670991590E-03	0.138941307051E-03
0.147734812453E-03			
0.157084564634E-03	0.167025704620E-03	0.177595588540E-03	0.188833926777E-03
0.200782931826E-03			
0.213487475331E-03	0.226995254949E-03	0.241356971616E-03	0.256626517870E-03
0.272861177927E-03			
0.290121840160E-03	0.308473222832E-03	0.327984113873E-03	0.348727625559E-03
0.370781465007E-03			
0.394228221438E-03	0.419155671211E-03	0.445657101928E-03	0.473831656458E-03
0.503784698193E-03			
0.535628199174E-03	0.569481151767E-03	0.605470006212E-03	0.643729134743E-03
0.684401324594E-03			
0.727638301181E-03	0.773601283502E-03	0.822461573726E-03	0.874401182845E-03
0.929613494760E-03			
0.988303970860E-03	0.105069089806E-02	0.111700618206E-02	0.118749618936E-02
0.126242264053E-02			
0.134206355724E-02	0.142671426831E-02	0.151668847463E-02	0.161231938096E-02
0.171396089420E-02			
0.182198889551E-02	0.193680258768E-02	0.205882592581E-02	0.218850913101E-02
0.232633029797E-02			
0.247279709658E-02	0.262844857576E-02	0.279385707599E-02	0.296963025469E-02
0.315641323123E-02			
0.335489086061E-02	0.356579014125E-02	0.378988276394E-02	0.402798781109E-02
0.428097461611E-02			
0.454976578681E-02	0.483534040945E-02	0.513873743598E-02	0.546105926992E-02
0.580347555949E-02			
0.616722720804E-02	0.655363061962E-02	0.696408218089E-02	0.740006300714E-02
0.786314395198E-02			
0.835499090638E-02	0.887737038987E-02	0.943215547103E-02	0.100213319958E-01
0.106470051965E-01			
0.113114066244E-01	0.120169015238E-01	0.127659965432E-01	0.135613479394E-01
0.144057701645E-01			
0.153022449693E-01	0.162539309664E-01	0.172641737190E-01	0.183365163721E-01
0.194747108158E-01			
0.206827294967E-01	0.219647777721E-01	0.233253069736E-01	0.247690280862E-01
0.263009261950E-01			
0.279262755752E-01	0.296506556303E-01	0.314799675852E-01	0.334204519851E-01
0.354787071067E-01			
0.376617082253E-01	0.399768277987E-01	0.424318566793E-01	0.450350262414E-01
0.477950315890E-01			
0.507210558482E-01	0.538227955120E-01	0.571104869927E-01	0.605949342810E-01
0.642875379032E-01			
0.682003250481E-01	0.723459810417E-01	0.767378821101E-01	0.813901295144E-01
0.863175850601E-01			
0.915359080696E-01	0.970615937396E-01	0.102912013062E+00	0.109105454230E+00
0.115661165538E+00			

0.122599399952E+00	0.129941461278E+00	0.137709751696E+00	0.145927821472E+00
0.154620419709E+00			
0.163813547346E+00	0.173534511342E+00	0.183811981229E+00	0.194676046741E+00
0.206158277610E+00			
0.218291785302E+00	0.231111285812E+00	0.244653165461E+00	0.258955547394E+00
0.274058360952E+00			
0.290003412020E+00	0.306834456562E+00	0.324597274865E+00	0.343339749134E+00
0.363111942441E+00			
0.383966180451E+00	0.405957135504E+00	0.429141912959E+00	0.453580141175E+00
0.479334063520E+00			
0.506468634141E+00	0.535051617718E+00	0.565153692202E+00	0.596848556805E+00
0.630213044573E+00			
0.665327240551E+00	0.702274605488E+00	0.741142107651E+00	0.782020361249E+00
0.825003775130E+00			
0.870190709861E+00	0.917683647717E+00	0.967589375296E+00	0.102001918070E+01
0.107508906802E+01			
0.113291999068E+01	0.119363810728E+01	0.125737506164E+01	0.132426829259E+01
0.139446137480E+01			
0.146810439728E+01	0.154535438475E+01	0.162637576604E+01	0.171134089743E+01
0.180043064949E+01			
0.189383506419E+01	0.199175409507E+01	0.209439843751E+01	0.220199046886E+01
0.231476530812E+01			
0.243297201266E+01	0.000000000000E+00	0.000000000000E+00	0.000000000000E+00
0.000000000000E+00			
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00	
End of Dataset			