Supporting Information

Theoretical insights into p-block functionalized carbon edges for efficient electrochemical CO_2 reduction

Computational details

In this work, vibrational frequencies were calculated using the finite-difference method implemented in VASP. The frequencies were obtained by displacing atoms from their optimized equilibrium positions and evaluating the corresponding forces. The vibrational calculations were performed using IBRION = 5, which activates the frozen phonon method in VASP to calculate the zone-center vibrational frequencies. The parameter NFREE was set to 0, which corresponds to the default displacement scheme used by VASP for frozen phonon calculations; under this setting, VASP automatically determines the required ionic displacements to construct the Hessian matrix. The displacement magnitude was controlled by the parameter POTIM, which defines the step width of atomic displacements in the finite-difference calculation. In this work, the displacement amplitude was 0.015 Å, a value widely used in phonon calculations to ensure the validity of the harmonic approximation while maintaining numerical stability. Regarding the displacement scheme, each atom in the system was displaced along the three Cartesian directions, and the corresponding forces were calculated. The Hessian matrix was then constructed from the resulting force constants, from which the vibrational modes and vibrational frequencies of the system were obtained. During structural optimization, the electronic self-consistent loop was converged to 10^{-7} eV, and the atomic structures were relaxed until the residual forces on each atom were smaller than 0.01 eV $Å^{-1}$.

In the vibrational frequency calculations, only the adsorbed species were considered, and the remaining atoms of the graphene nanoribbon were kept fixed.

To avoid artificial entropy divergence caused by very low-frequency modes of adsorbates, vibrational frequencies lower than 50 cm^{-1} were replaced by 50 cm^{-1} when calculating vibrational entropy contributions.

For gas-phase molecules (CO_2, CO, and H_2), thermodynamic corrections were evaluated under the ideal-gas approximation at 298.15 K and 1 atm. The entropy contributions include translational,

rotational, and vibrational terms. For adsorbed species, only vibrational entropy contributions were considered because translational and rotational motions are restricted upon adsorption. Within the computational hydrogen electrode (CHE) framework, the chemical potential of the proton–electron pair ($H^+ + e^-$) was referenced to $1/2H_2$ under standard conditions (U = 0 V vs. RHE and pH = 0).

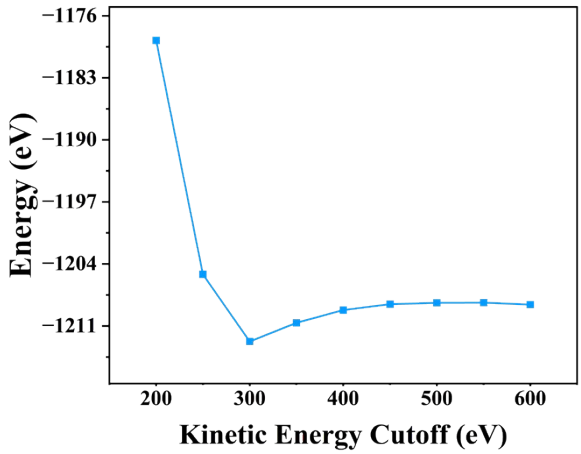

Fig. S1. Planewave energy cut off (using 1×1×1 k-points) convergence plots for CO chemisorption on Edge-AsH_2/C.

Supporting data for vibrational calculations

Representative VASP input and output files used for the vibrational frequency calculations are provided as separate supporting data files. These files correspond to the frequency calculation of the CO intermediate adsorbed on the Edge-AsH_2/C system and include the INCAR, KPOINTS, and POSCAR input files as well as an example OUTCAR file. These files illustrate the workflow used to obtain the vibrational frequencies and compute the zero-point energy (ZPE) and entropy corrections. The same computational settings were applied to all intermediates studied in this work.

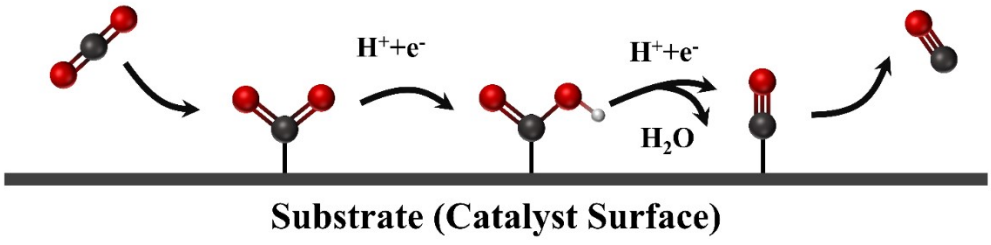

Fig. S2. Reaction Pathways and Energy Evolution Mechanisms of CO_2-to-CO Reduction

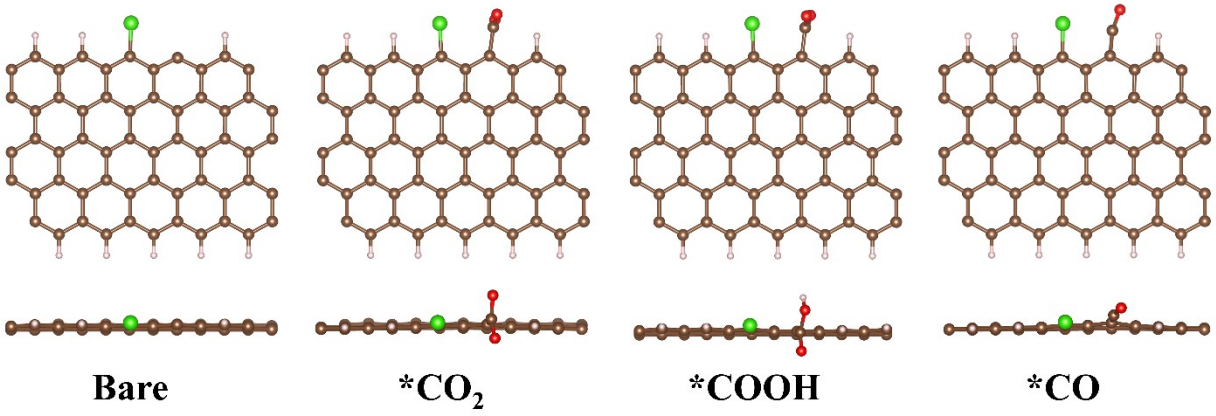

Fig. S3. Optimized geometric structures of intermediates over Edge-Cl/C.

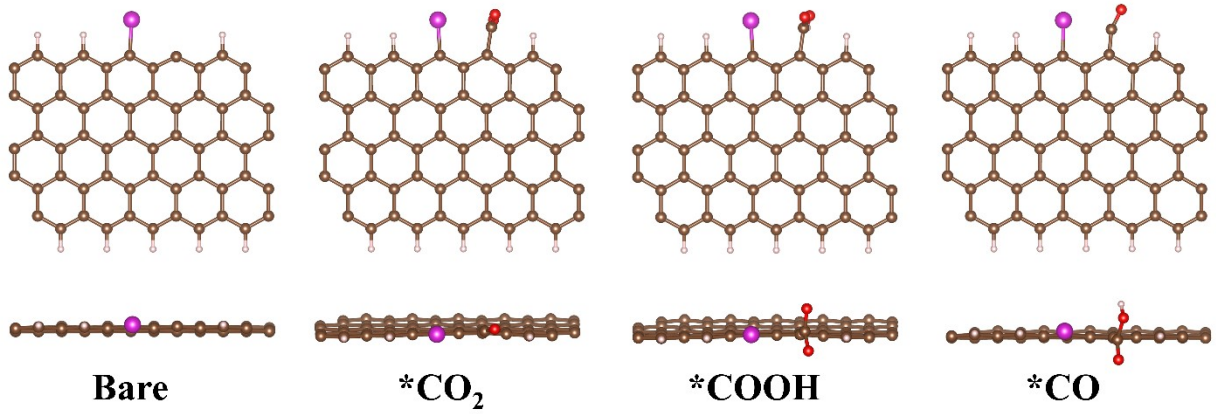

Fig. S4. Optimized geometric structures of intermediates over Edge-Br/C.

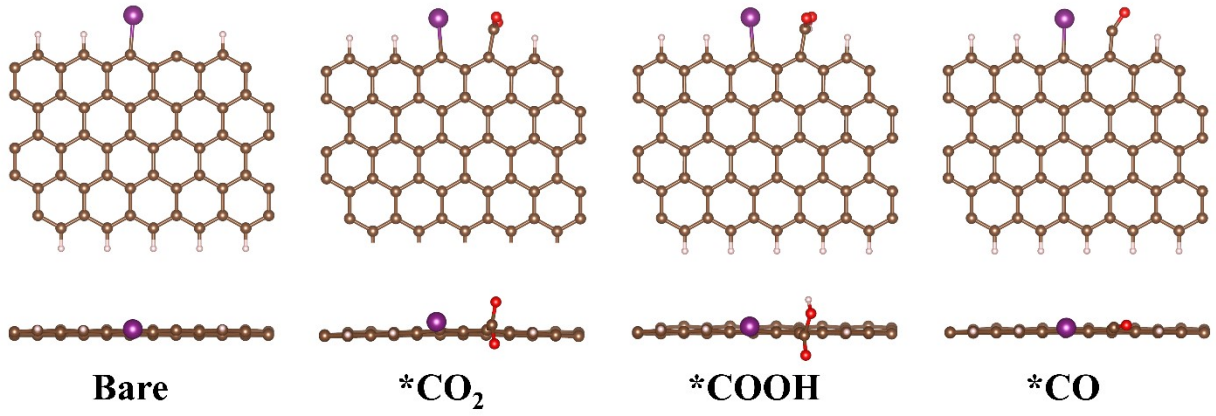

Fig. S5. Optimized geometric structures of intermediates over Edge-I/C.

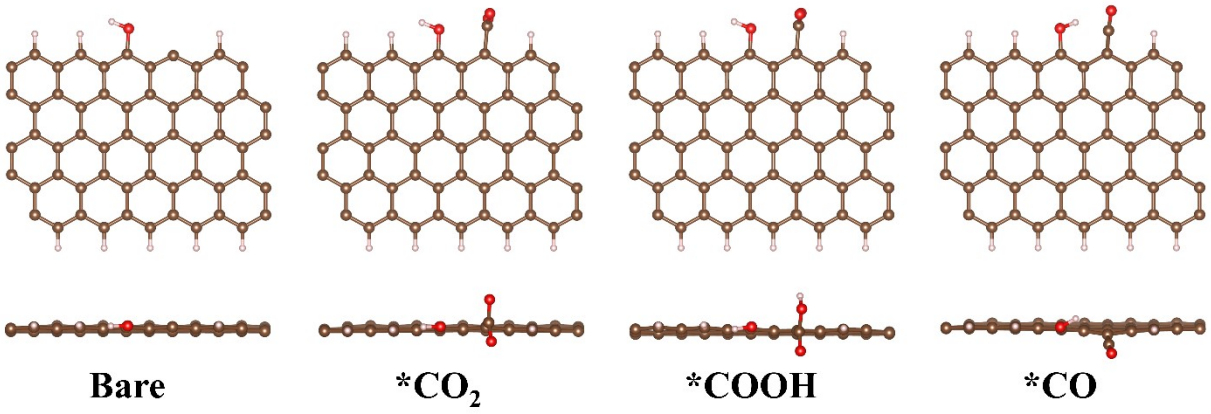

Fig. S6. Optimized geometric structures of intermediates over Edge-OH/C.

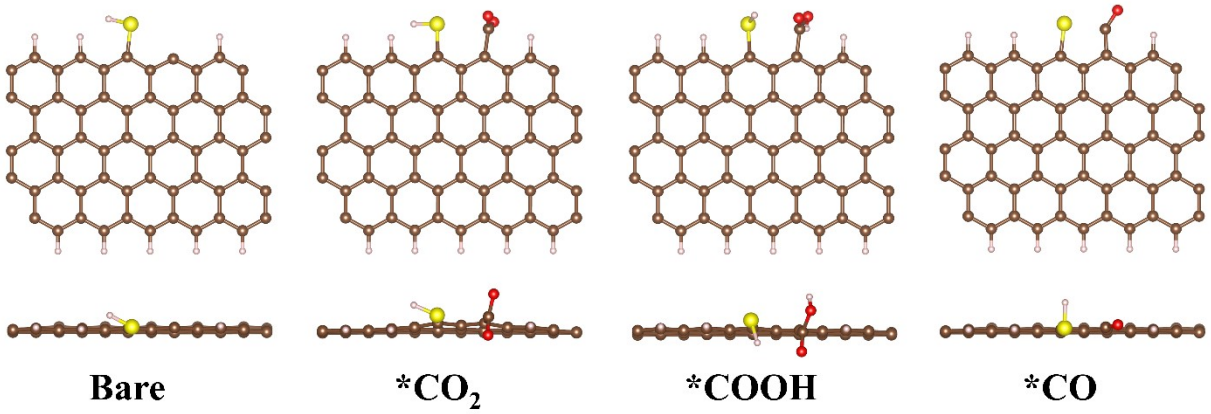

Fig. S7. Optimized geometric structures of intermediates over Edge-SH/C.

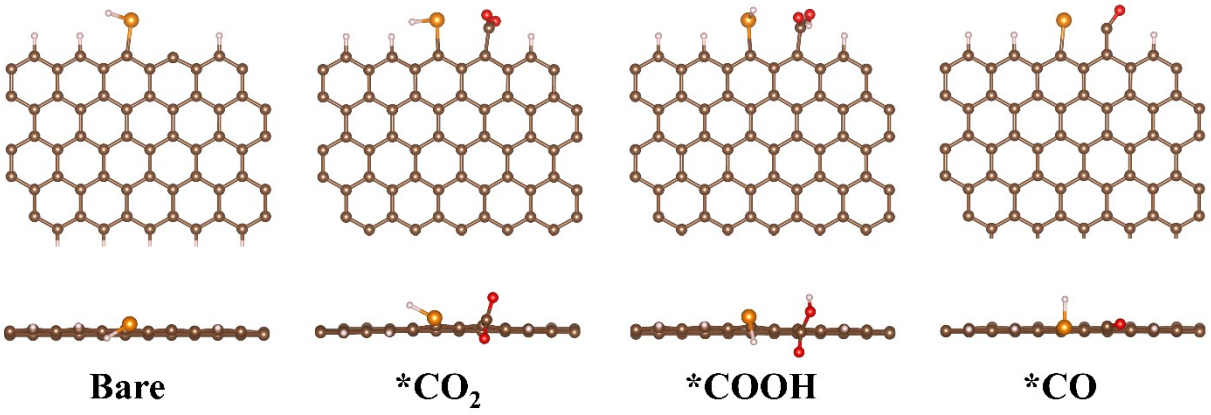

Fig. S8. Optimized geometric structures of intermediates over Edge-SeH/C.

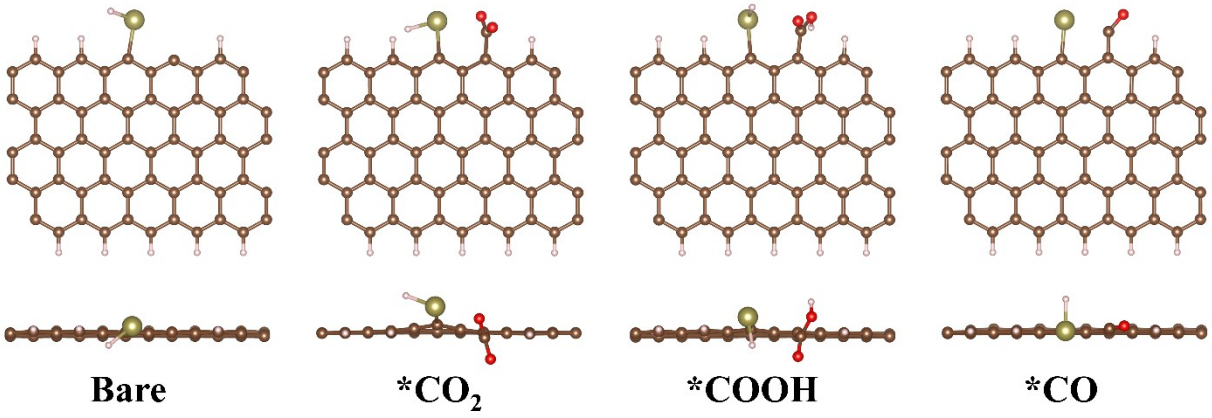

Fig. S9. Optimized geometric structures of intermediates over Edge-TeH/C.

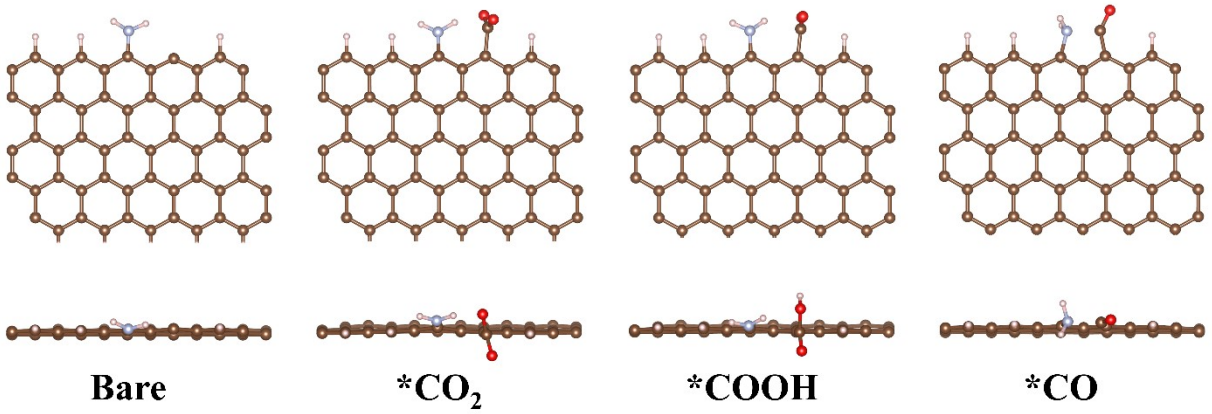

Fig. S10. Optimized geometric structures of intermediates over Edge-NH_2/C.

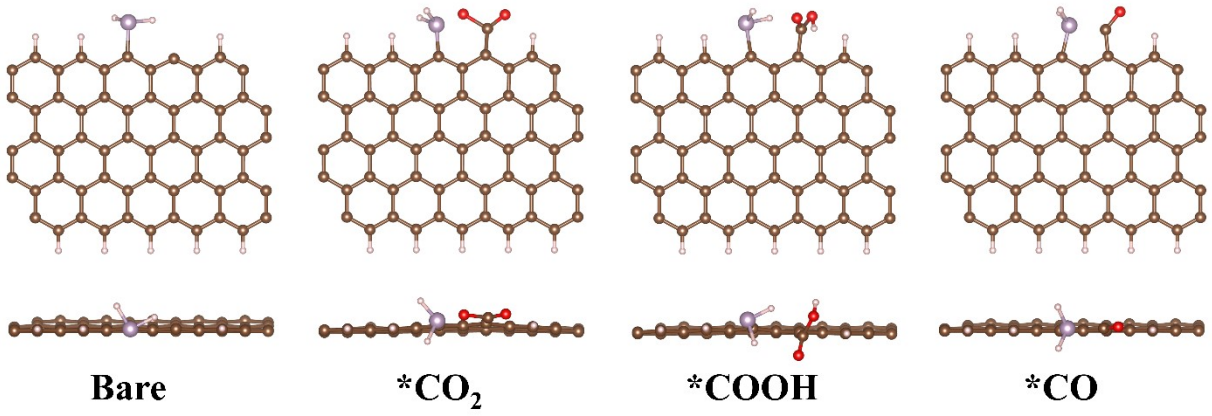

Fig. S11. Optimized geometric structures of intermediates over Edge-PH_2/C.

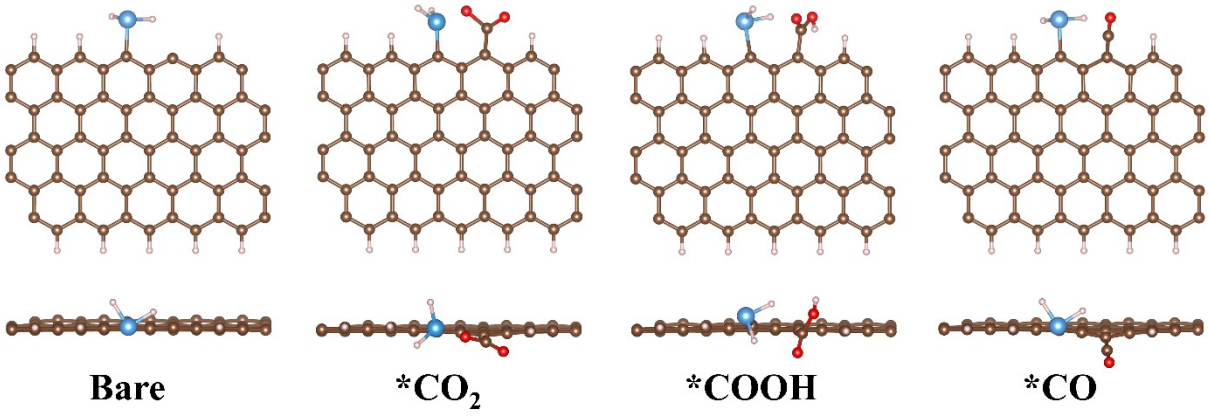

Fig. S12. Optimized geometric structures of intermediates over Edge-AsH_2/C.

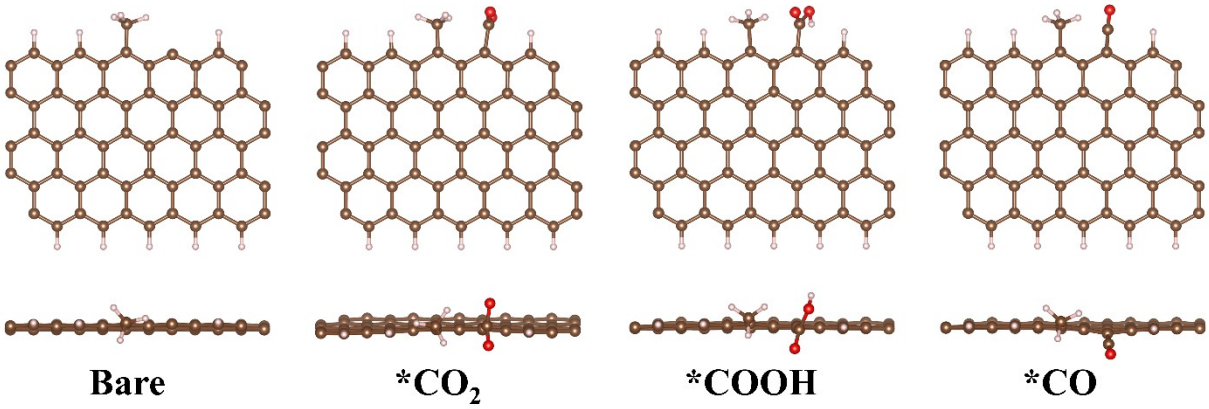

Fig. S13. Optimized geometric structures of intermediates over Edge-CH_3/C.

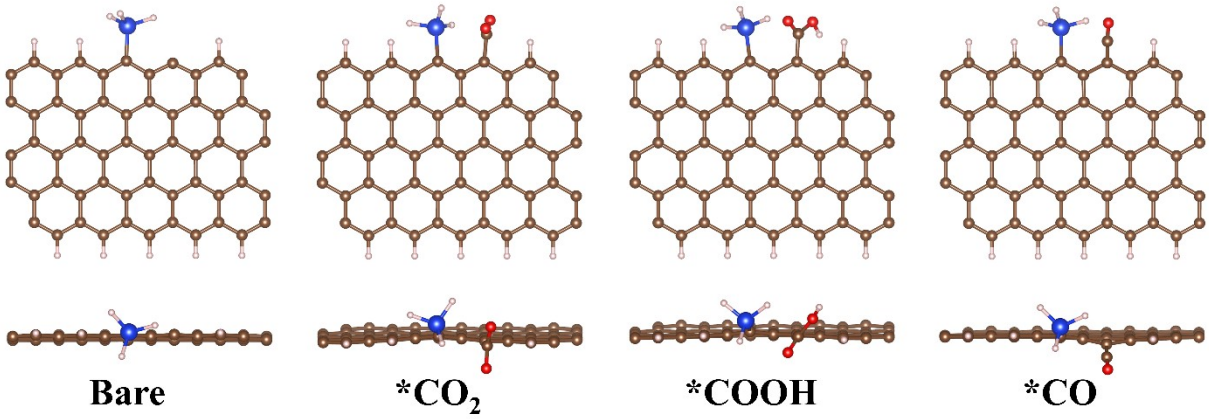

Fig. S14. Optimized geometric structures of intermediates over Edge-SiH_3/C.

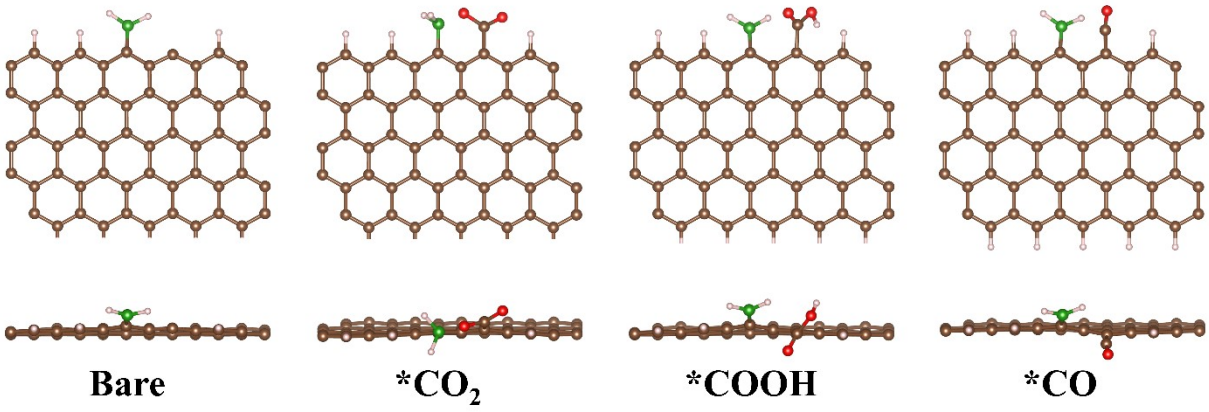

Fig. S15. Optimized geometric structures of intermediates over Edge-BH_2/C.

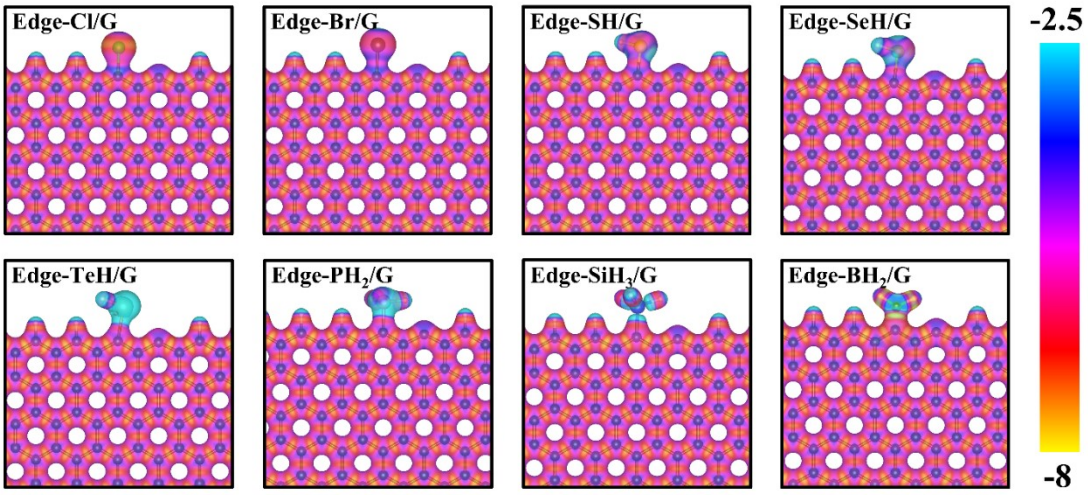

Fig. S16. Electrostatic potential distribution of Edge-Cl/C,Edge-Br/C,Edge-SH/C,Edge-SeH/C Edge-TeH/C,Edge-PH_2/C,Edge-SiH_3/C and Edge-BH_2/C.

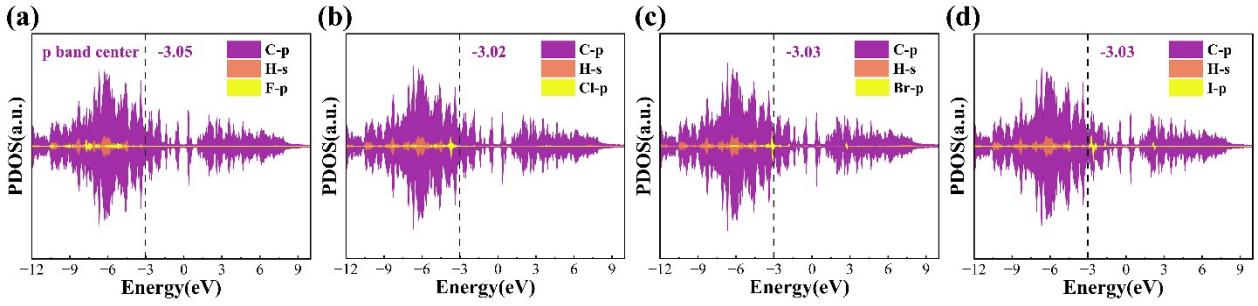

Fig. S17. Projected density of states of (a) Edge-F/C; (b) Edge-Cl/C; (c) Edge-Br/C; (d) Edge-Br/C.

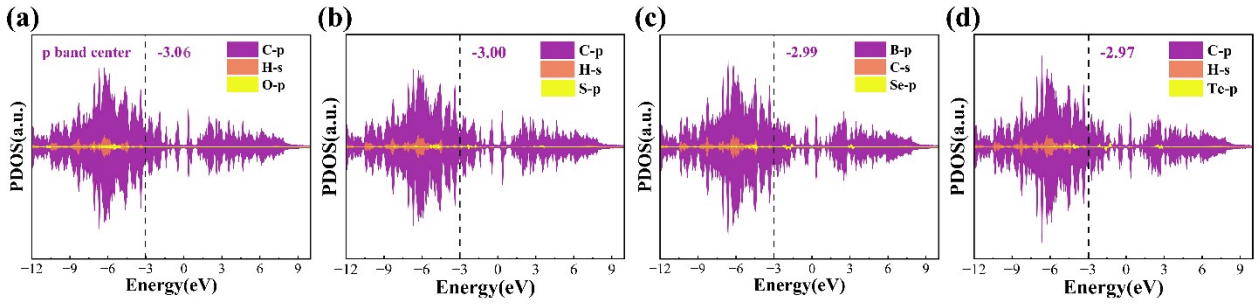

Fig. S18. Projected density of states of (a) Edge-OH/C; (b) Edge-SH/C; (c) Edge-SeH/C; (d) Edge-TeH/C.

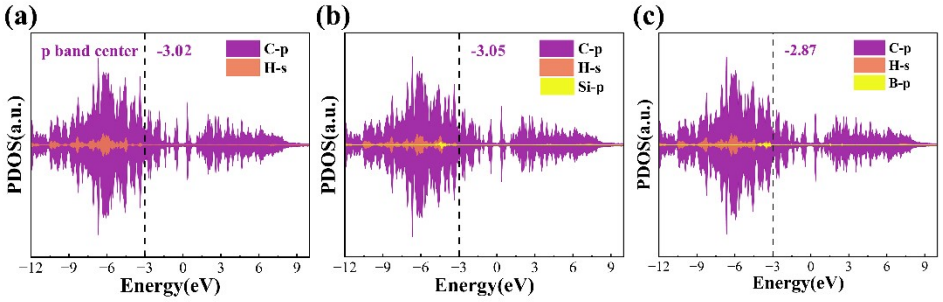

Fig. S19. Projected density of states of (a) Edge-CH_3/C; (b) Edge-SiH_3/C; (c) Edge-BH_2/C.

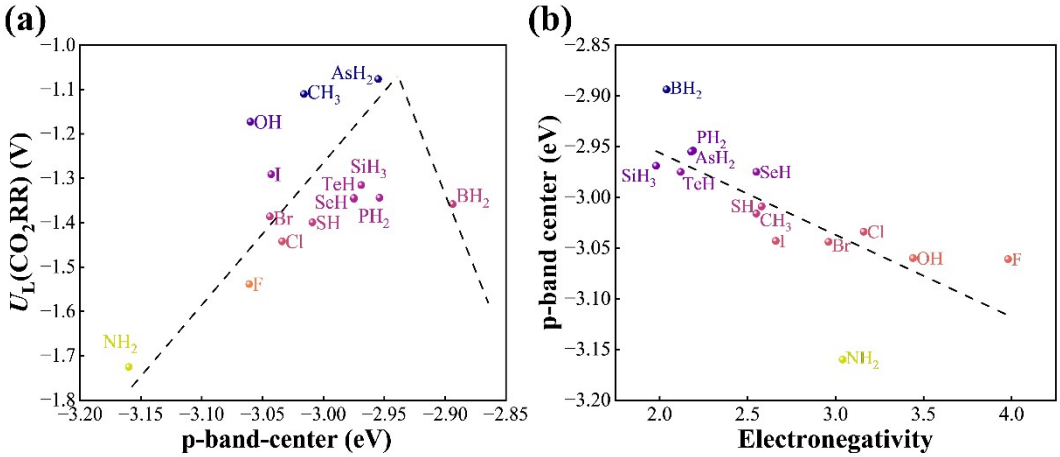

Fig. S20. Validation of the structure-activity relationships using the RPBE functional. (a) Relationship between the U_L and the p-band center of the carbon active sites. (b) Relationship between the p-band center of the carbon active sites and the electronegativity of the functional groups.

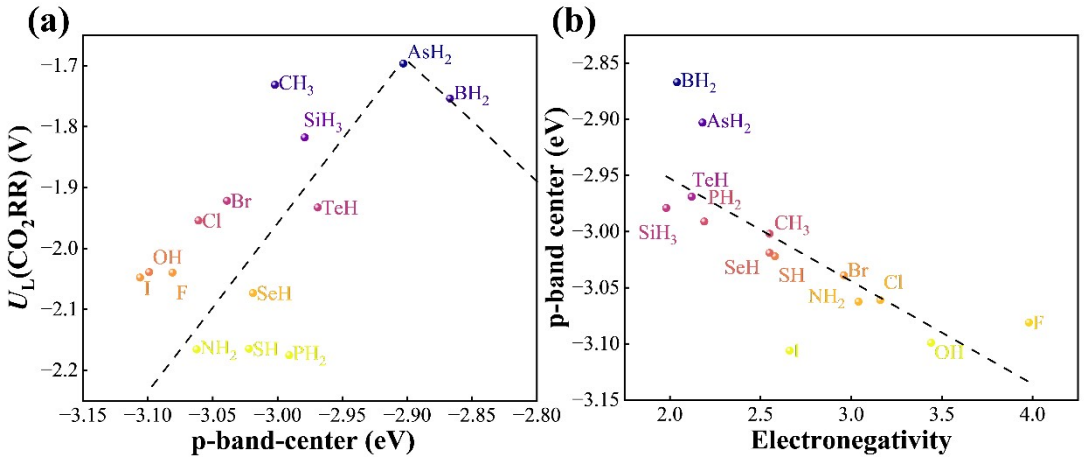

Fig. S21. Validation of structure-activity relationships incorporating the VASPsol implicit solvation model (EB_K = 78.4). (a) Relationship between the U_L and the p-band center of carbon active sites. (b) Correlation between the p-band center of carbon active sites and the electronegativity of the introduced functional groups. The results demonstrate that the trends remain robust in an aqueous environment.

Representative computational files

To illustrate the computational workflow, representative VASP input and output files (including INCAR, KPOINTS, POSCAR, and an example OUTCAR) are provided for the vibrational frequency calculation of the CO intermediate adsorbed on the Edge-AsH2/C system.

INCAR

NCORE = 1

ISTART = 1

ICHARG = 1

LWAVE = .FALSE.

LCHARG = .FALSE.

LORBIT = 11

ENCUT = 400

ISMEAR = 0

SIGMA = 0.05

EDIFF = 1E-7

NELMIN = 5

NELM = 200

GGA = PE

LREAL = Auto

ALGO = Fast

ISPIN = 2

EDIFFG = -0.01

IBRION = 5

NSW = 3000

ISIF = 2

IVDW = 11

KPOINTS

K

Gamma

1 1 1

0.0 0.0 0.0

POSCAR

14.7805999999999997 0.0000000000000000 0.0000000000000000

0.0000000000000000 21.3338999999999999 0.0000000000000000

0.0000000000000000 0.0000000000000000 18.4256999999999991

H C As O

24 121 1 1

Selective Dynamics

Direct

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0.0818803154246983 0.1910486376296957 0.4579073784134210 F F F H002

0.2509113506189883 0.1888495025507219 0.2952206162936981 F F F H003

0.2489737289082186 0.1911198846268702 0.4578876144763527 F F F H004

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0.5820728436739949	0.1915880137649009	0.4575615531931824	F	F	F	H008
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0.7482922101179702	0.1915351155090610	0.4575667773295219	F	F	F	H010
0.9176294706953719	0.1888106576394027	0.2952246513867149	F	F	F	H011
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0.9985355489683677	0.2737370569394882	0.4680603585328877	F	F	F	C027
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0.2509635562931184	0.3722909194187376	0.2797404144651786	F	F	F	C044
0.2486971242465456	0.4415368992105962	0.4805490419699406	F	F	F	C045
0.3316938477312448	0.5420976784918367	0.4825249550688998	F	F	F	C046

0.3342790803368405	0.3392862601658221	0.2814289084801485	F	F	F	C047
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0.4153171641060418	0.3745420881125773	0.4774024042484859	F	F	F	C049
0.4984779607753970	0.4751875434801400	0.4827351016208030	F	F	F	C050
0.3343544776161380	0.4728069700178834	0.2782525485006686	F	F	F	C051
0.4176309262158837	0.3722706878977521	0.2799164253947181	F	F	F	C052
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0.6651070052304692	0.4754340107095823	0.4845632470536068	F	F	F	C058
0.5010305699395168	0.4727812902735594	0.2789928389603737	F	F	F	C059
0.5843044865863175	0.3722554119640999	0.2803447706195842	F	F	F	C060
0.5818960423987584	0.4421387781564420	0.4822244703754562	F	F	F	C061
0.6650115255329112	0.5429123475129605	0.4885002900130555	F	F	F	C062
0.6676355825409546	0.3392663391746272	0.2819372349795559	F	F	F	C063
0.7510564252584299	0.4396661147953611	0.2795854841679201	F	F	F	C064
0.7485019132708155	0.3747138412995796	0.4780380030634245	F	F	F	C065
0.8320466549820991	0.4748044637235345	0.4832055790041310	F	F	F	C066
0.6677200287018262	0.4727655559097856	0.2798433247671959	F	F	F	C067
0.7509985003104263	0.3722595741176703	0.2805113457155740	F	F	F	C068

0.7484173210833667	0.4420487150532820	0.4823909968547150	F	F	F	C069
0.8323442745838756	0.5421215533234636	0.4855684901576776	F	F	F	C070
0.8343161946307757	0.3392719973822945	0.2819143393262035	F	F	F	C071
0.9177142131142438	0.4396855957677991	0.2791941258854080	F	F	F	C072
0.9152224682187599	0.3743125385744329	0.4776866471177007	F	F	F	C073
0.9987637083020692	0.4745121839579621	0.4820904337443102	F	F	F	C074
0.8343752338398105	0.4727858347939105	0.2797783658481017	F	F	F	C075
0.9176557484917762	0.3722780318220071	0.2803069253055866	F	F	F	C076
0.9152069631099504	0.4415697402200363	0.4813520209748164	F	F	F	C077
0.9988974230458147	0.5417326303004982	0.4833717622278816	F	F	F	C078
0.0010896780846690	0.5402276665027511	0.2803806383541929	F	F	F	C079
0.0844147168852616	0.6410149111951463	0.2834132444208290	F	F	F	C080
0.0820106104157512	0.5748294800260626	0.4827003746536826	F	F	F	C081
0.1650800245777449	0.6743856811896054	0.4812563292692176	F	F	F	C082
0.0011494012863688	0.6728296037949901	0.2861737160777795	F	F	F	C083
0.0844307225588043	0.5732487457008156	0.2807354436850225	F	F	F	C084
0.0821580148593087	0.6425536721413083	0.4823542477369118	F	F	F	C085
0.1677592695793439	0.5402575854331063	0.2792549674160965	F	F	F	C086
0.2511522226894682	0.6410621507413529	0.2819623339502237	F	F	F	C087
0.2482524468811301	0.5747886199692562	0.4820355518945587	F	F	F	C088
0.3310894556168500	0.6743206642344781	0.4808907867040684	F	F	F	C089
0.1677878060508511	0.6729179153511682	0.2839232726264277	F	F	F	C090

0.2511060033166664	0.5732762179091631	0.2798277671851040	F	F	F	C091
0.2477654464606527	0.6423421525785887	0.4814565102811118	F	F	F	C092
0.3344178943117345	0.5402397009034856	0.2791485183732506	F	F	F	C093
0.4178635621144234	0.6410009842767775	0.2822321098769078	F	F	F	C094
0.4148312621881781	0.5755679370607518	0.4833416827996023	F	F	F	C095
0.4983657027601222	0.6763728314508386	0.4820456198405735	F	F	F	C096
0.3344566898103963	0.6729322336450400	0.2829606707649748	F	F	F	C097
0.4177728326796091	0.5732272168778322	0.2803815870930451	F	F	F	C098
0.4139741384250105	0.6432655878378722	0.4818082207565502	F	F	F	C099
0.5010793168915446	0.5401792369072015	0.2802431741513018	F	F	F	C100
0.5844660091159987	0.6409158459353231	0.2845898335966948	F	F	F	C101
0.5811262452300987	0.5761097509266384	0.4885608240760924	F	F	F	C102
0.6656396947682662	0.6745356900818470	0.5048953595958274	F	F	F	C103
0.5011108073220597	0.6728193717325276	0.2841301664540008	F	F	F	C104
0.5844282219860871	0.5731619353484558	0.2821061671165912	F	F	F	C105
0.5788470526464320	0.6438561446626188	0.4909435083319301	F	F	F	C106
0.6677568875063171	0.5401441420250156	0.2816134613100255	F	F	F	C107
0.7510514107661362	0.6409290916309890	0.2863765329253803	F	F	F	C108
0.7492107067537678	0.5752971665939300	0.4889315600807242	F	F	F	C109
0.8326413334360783	0.6744647722074566	0.4886288399503115	F	F	F	C110
0.6677222754227965	0.6727789703487070	0.2874048586811460	F	F	F	C111
0.7510930446089144	0.5731739521599354	0.2831097843424180	F	F	F	C112

0.7519749777972990 0.6424683607715013 0.4927229580240037 F F F C113

0.8344220003513751 0.5401781120239486 0.2815713586922216 F F F C114

0.9177095991819042 0.6409514564631540 0.2854679817641615 F F F C115

0.9158125874241838 0.5749538427496481 0.4849675997714241 F F F C116

0.9987865695199720 0.6744691937682290 0.4832521880393058 F F F C117

0.8344702960803131 0.6727731682349518 0.2880270509960479 F F F C118

0.9177605701781296 0.5732049976545137 0.2822715888391425 F F F C119

0.9166888736983309 0.6424936828583906 0.4854086109118846 F F F C120

0.6705584984527109 0.7280360755646152 0.5424337562991518 T T T C121

0.4931222923355237 0.7691437895169553 0.4720648768797336 F F F As001

0.6782713065519286 0.7735881776657597 0.5777243945157891 T T T O001

OUTCAR

INCAR:

POTCAR: PAW_PBE H 15Jun2001

POTCAR: PAW_PBE C 08Apr2002

POTCAR: PAW_PBE As 22Sep2009

POTCAR: PAW_PBE O 08Apr2002

| |

| W W AA RRRRR N N II N N GGGG !!! |

| W W A A R R NN N II NN N G G !!! |

| W W A A R R N N N II N N N G !!! |

```
|               W WW W    AAAAAA    RRRRR     N   N N   II   N   N N   G   GGG    !
|
|               WW   WW   A      A   R    R    N    NN   II   N    NN   G     G
|
|               W     W   A      A   R     R   N     N   II   N     N   GGGG    !!!              |
|                                                                                                 |
|          For optimal performance we recommend to set                                            |
|            NCORE= 4 - approx SQRT( number of cores)                                             |
|          NCORE specifies how many cores store one orbital (NPAR=cpu/NCORE).          |
|          This setting can    greatly improve the performance of VASP for DFT.          |
|          The default,      NCORE=1                    might be grossly inefficient              |
|          on modern multi-core architectures or massively parallel machines.          |
|          Do your own testing !!!!                                                               |
|          Unfortunately you need to use the default for GW and RPA calculations. |
|          (for HF NCORE is supported but not extensively tested yet)                  |
|                                                                                                 |
 ----------------------------------------------------------------------------


 POTCAR:       PAW_PBE H 15Jun2001

    SHA256 =    030f79b5d3ab3cf0e668861823c8fb652ff669f3e15e46930bd03bfd63a607b6 H/

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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

l	E	TYP	RCUT	TYP	RCUT
0	-6.4927494	23	1.100		
0	6.8029130	23	1.100		
1	-4.0817478	23	1.100		

local pseudopotential read in

atomic valenz-charges read in

non local Contribution for L= 0 read in

real space projection operators read in

non local Contribution for L= 0 read in

real space projection operators read in

non local Contribution for L= 1 read in

real space projection operators read in

PAW grid and wavefunctions read in

number of l-projection operators is LMAX = 3

number of lm-projection operators is LMMAX = 5

POTCAR: PAW_PBE C 08Apr2002

SHA256 = 253f7b50bb8d59471dbedb8285d89021f4a42ed1a2c5d38a03a736e69125dd95 C/

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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		

local pseudopotential read in

partial core-charges read in

partial kinetic energy density read in

atomic valenz-charges read in

non local Contribution for L= 0 read in

real space projection operators read in

non local Contribution for L= 0 read in

real space projection operators read in

non local Contribution for L= 1 read in

real space projection operators read in

non local Contribution for L= 1 read in

real space projection operators read in

PAW grid and wavefunctions read in

number of l-projection operators is LMAX = 4

number of lm-projection operators is LMMAX = 8

POTCAR: PAW_PBE As 22Sep2009

SHA256 = bc8fb55b00baa90d383a523722e1771deb40ea3f17a5ce25913641995975acad As

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VRHFIN =As: s2p3

LEXCH = PE

EATOM = 170.1867 eV, 12.5084 Ry

TITEL = PAW_PBE As 22Sep2009

LULTRA = F use ultrasoft PP ?

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

RPACOR = 1.900 partial core radius

POMASS = 74.922; ZVAL = 5.000 mass and valenz

RCORE = 2.100 outmost cutoff radius

RWIGS = 2.300; RWIGS = 1.217 wigner-seitz radius (au A)

ENMAX = 208.702; ENMIN = 156.526 eV

ICORE = 3 local potential

LCOR = T correct aug charges

LPAW = T paw PP

EAUG = 462.758

DEXC = 0.000

RMAX = 2.144 core radius for proj-oper

RAUG = 1.300 factor for augmentation sphere

RDEP = 2.140 radius for radial grids

RDEPT = 1.956 core radius for aug-charge

Atomic configuration

10 entries

n	l	j	E	occ.
1	0	0.50	-11718.0418	2.0000
2	0	0.50	-1486.5454	2.0000
2	1	1.50	-1303.3889	6.0000
3	0	0.50	-190.2849	2.0000
3	1	1.50	-133.6555	6.0000
3	2	2.50	-40.6443	10.0000
4	0	0.50	-14.4936	2.0000
4	1	0.50	-5.1947	3.0000
4	2	1.50	-5.4423	0.0000
4	3	2.50	-5.4423	0.0000

Description

l	E	TYP	RCUT	TYP	RCUT
0	-14.4935570	23	2.100		
0	-11.9212055	23	2.100		
1	-5.1947127	23	2.100		
1	27.2116520	23	2.100		
2	-5.4423304	23	2.100		
3	-1.3605826	7	2.100		

local pseudopotential read in

partial core-charges read in

partial kinetic energy density read in

atomic valenz-charges read in

non local Contribution for L= 0 read in

real space projection operators read in

non local Contribution for L= 0 read in

real space projection operators read in

non local Contribution for L= 1 read in

real space projection operators read in

non local Contribution for L= 1 read in

real space projection operators read in

non local Contribution for L= 2 read in

real space projection operators read in

PAW grid and wavefunctions read in

number of l-projection operators is LMAX = 5

number of lm-projection operators is LMMAX = 13

POTCAR: PAW_PBE O 08Apr2002

SHA256 = 818f92134a0a090dccd8ba1447fa70422a3b330e708bb4f08108d8ae51209ddf O/

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VRHFIN =O: s2p4

LEXCH = PE

EATOM = 432.3788 eV, 31.7789 Ry

TITEL = PAW_PBE O 08Apr2002

LULTRA = F use ultrasoft PP ?

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

RPACOR = 1.200 partial core radius

POMASS = 16.000; ZVAL = 6.000 mass and valenz

RCORE = 1.520 outmost cutoff radius

RWIGS = 1.550; RWIGS = 0.820 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 = 605.392

DEXC = 0.000

RMAX = 1.553 core radius for proj-oper

RAUG = 1.300 factor for augmentation sphere

RDEP = 1.550 radius for radial grids

RDEPT = 1.329 core radius for aug-charge

Atomic configuration

4 entries

n	l	j	E	occ.
1	0	0.50	-514.6923	2.0000
2	0	0.50	-23.9615	2.0000
2	1	0.50	-9.0305	4.0000
3	2	1.50	-9.5241	0.0000

Description

l	E	TYP	RCUT	TYP	RCUT
0	-23.9615318	23	1.200		
0	-9.5240782	23	1.200		
1	-9.0304911	23	1.520		
1	8.1634956	23	1.520		
2	-9.5240782	7	1.500		

local pseudopotential read in

partial core-charges read in

partial kinetic energy density read in

kinetic energy density of atom read in

atomic valenz-charges read in

non local Contribution for L= 0 read in

real space projection operators read in

non local Contribution for L= 0 read in

real space projection operators read in

non local Contribution for L= 1 read in

real space projection operators read in

non local Contribution for L= 1 read in

real space projection operators read in

PAW grid and wavefunctions read in

number of l-projection operators is LMAX = 4

number of lm-projection operators is LMMAX = 8

Optimization of the real space projectors (new method)

maximal supplied QI-value = 34.20

optimisation between [QCUT,QGAM] = [9.92, 20.18] = [27.55,114.04] Ry

Optimized for a Real-space Cutoff 1.26 Angstroem

l	n(q)	QCUT	max X(q)	W(low)/X(q)	W(high)/X(q)	e(spline)
0	8	9.919	19.460	0.50E-03	0.23E-03	0.29E-06
0	8	9.919	12.209	0.48E-03	0.23E-03	0.28E-06
1	7	9.919	4.655	0.17E-03	0.75E-03	0.30E-06

Optimization of the real space projectors (new method)

maximal supplied QI-value = 25.13

optimisation between [QCUT,QGAM] = [10.05, 20.36] = [28.30,116.06] Ry

Optimized for a Real-space Cutoff 1.30 Angstroem

l	n(q)	QCUT	max X(q)	W(low)/X(q)	W(high)/X(q)	e(spline)
0	8	10.053	115.676	0.49E-03	0.72E-03	0.18E-06
0	8	10.053	87.132	0.49E-03	0.71E-03	0.18E-06
1	7	10.053	4.429	0.32E-03	0.31E-03	0.18E-06
1	7	10.053	2.733	0.23E-03	0.19E-03	0.20E-06

Optimization of the real space projectors (new method)

maximal supplied QI-value = 17.95

optimisation between [QCUT,QGAM] = [10.23, 20.47] = [29.32,117.29] Ry

Optimized for a Real-space Cutoff 1.30 Angstroem

l	n(q)	QCUT	max X(q)	W(low)/X(q)	W(high)/X(q)	e(spline)
0	8	10.233	117.213	0.22E-03	0.22E-03	0.48E-07
0	8	10.233	98.411	0.22E-03	0.22E-03	0.48E-07
1	7	10.233	10.093	0.11E-03	0.37E-03	0.86E-07
1	7	10.233	5.228	0.12E-03	0.33E-03	0.71E-07
2	7	10.233	4.067	0.22E-03	0.22E-03	0.50E-07

Optimization of the real space projectors (new method)

maximal supplied QI-value = 24.76

optimisation between [QCUT,QGAM] = [10.15, 20.30] = [28.85,115.39] Ry

Optimized for a Real-space Cutoff 1.38 Angstroem

l	n(q)	QCUT	max X(q)	W(low)/X(q)	W(high)/X(q)	e(spline)
0	8	10.150	20.381	0.22E-03	0.32E-03	0.29E-06
0	8	10.150	15.268	0.23E-03	0.35E-03	0.30E-06
1	8	10.150	5.964	0.46E-03	0.53E-03	0.21E-06
1	8	10.150	5.382	0.38E-03	0.45E-03	0.19E-06

PAW_PBE H 15Jun2001 :

energy of atom 1 EATOM= -12.4884

kinetic energy error for atom= 0.0098 (will be added to EATOM!!)

PAW_PBE C 08Apr2002 :

energy of atom 2 EATOM= -147.1560

kinetic energy error for atom= 0.0288 (will be added to EATOM!!)

PAW_PBE As 22Sep2009 :

energy of atom 3 EATOM= -170.1867

kinetic energy error for atom= 0.0013 (will be added to EATOM!!)

PAW_PBE O 08Apr2002 :

energy of atom 4 EATOM= -432.3788

kinetic energy error for atom= 0.1156 (will be added to EATOM!!)

POSCAR: Generated by VASPKIT code

positions in direct lattice

No initial velocities read in

exchange correlation table for LEXCH = 8

RHO(1)= 0.500 N(1) = 2000

RHO(2)= 100.500 N(2) = 4000

VTST: version 3.2, (02/03/18)

CHAIN: initializing optimizer

OPT: Using VASP Dynamics algorithm

CHAIN: Read ICHAIN 0

POSCAR: Generated by VASPKIT code

positions in direct lattice

No initial velocities read in

---

ion	position			nearest neighbor table	
1	0.084	0.189	0.295-	25	1.09
2	0.082	0.191	0.458-	28	1.09
3	0.251	0.189	0.295-	30	1.09
4	0.249	0.191	0.458-	33	1.09
5	0.418	0.189	0.295-	35	1.09
6	0.416	0.191	0.458-	38	1.09
7	0.584	0.189	0.295-	40	1.09
8	0.582	0.192	0.458-	43	1.09
9	0.751	0.189	0.295-	45	1.09
10	0.748	0.192	0.458-	48	1.09
11	0.918	0.189	0.295-	50	1.09
12	0.915	0.191	0.458-	53	1.09
13	0.165	0.726	0.480-	106	1.09
14	0.001	0.724	0.289-	107	1.09
15	0.329	0.725	0.481-	113	1.09
16	0.168	0.724	0.286-	114	1.09
17	0.334	0.724	0.285-	121	1.09
18	0.833	0.726	0.489-	134	1.09
19	0.668	0.724	0.290-	135	1.09

20	0.999	0.726	0.483-	141	1.09			
21	0.834	0.724	0.291-	142	1.09			
22	0.501	0.724	0.286-	128	1.09			
23	0.436	0.766	0.402-	146	1.54			
24	0.582	0.772	0.428-	146	1.54			
25	0.084	0.240	0.291-	1	1.09	27 1.41	32	1.41
26	0.165	0.274	0.468-	33	1.41	28 1.41	29	1.45
27	0.001	0.272	0.287-	25	1.41	50 1.41	55	1.45
28	0.082	0.242	0.464-	2	1.09	26 1.41	51	1.41
29	0.165	0.341	0.475-	57	1.42	65 1.42	26	1.45
30	0.251	0.240	0.291-	3	1.09	37 1.41	32	1.41
31	0.332	0.274	0.468-	38	1.41	33 1.41	34	1.45
32	0.168	0.272	0.287-	30	1.41	25 1.41	63	1.45
33	0.249	0.242	0.463-	4	1.09	26 1.41	31	1.41
34	0.332	0.341	0.475-	65	1.42	73 1.42	31	1.45
35	0.418	0.240	0.291-	5	1.09	42 1.41	37	1.41
36	0.499	0.274	0.468-	43	1.41	38 1.41	39	1.45
37	0.334	0.272	0.287-	30	1.41	35 1.41	71	1.45
38	0.415	0.242	0.463-	6	1.09	31 1.41	36	1.41
39	0.499	0.342	0.475-	73	1.42	81 1.42	36	1.45
40	0.584	0.240	0.291-	7	1.09	42 1.41	47	1.41
41	0.665	0.274	0.468-	43	1.41	48 1.41	44	1.45

42	0.501	0.272	0.287-	35	1.41	40	1.41	79	1.45
43	0.582	0.243	0.463-	8	1.09	36	1.41	41	1.41
44	0.665	0.342	0.475-	89	1.42	81	1.42	41	1.45
45	0.751	0.240	0.291-	9	1.09	47	1.41	52	1.41
46	0.832	0.274	0.468-	48	1.41	53	1.41	49	1.45
47	0.668	0.272	0.287-	45	1.41	40	1.41	87	1.45
48	0.748	0.243	0.463-	10	1.09	46	1.41	41	1.41
49	0.832	0.342	0.475-	97	1.42	89	1.42	46	1.45
50	0.918	0.240	0.291-	11	1.09	52	1.41	27	1.41
51	0.999	0.274	0.468-	53	1.41	28	1.41	54	1.45
52	0.834	0.272	0.287-	50	1.41	45	1.41	95	1.45
53	0.915	0.242	0.463-	12	1.09	51	1.41	46	1.41
54	0.999	0.341	0.475-	57	1.42	97	1.42	51	1.45
55	0.001	0.339	0.282-	100	1.42	60	1.42	27	1.45
56	0.084	0.440	0.279-	59	1.42	67	1.42	60	1.44
57	0.082	0.374	0.477-	54	1.42	29	1.42	61	1.44
58	0.165	0.474	0.481-	61	1.42	69	1.42	62	1.43
59	0.001	0.473	0.279-	56	1.42	96	1.42	103	1.44
60	0.084	0.372	0.280-	63	1.42	55	1.42	56	1.44
61	0.082	0.441	0.481-	98	1.42	58	1.42	57	1.44
62	0.165	0.542	0.482-	112	1.42	105	1.42	58	1.43
63	0.168	0.339	0.281-	60	1.42	68	1.42	32	1.45

64 0.251 0.440 0.278- 67 1.42 75 1.42 68 1.44

65 0.249 0.374 0.477- 34 1.42 29 1.42 69 1.44

66 0.332 0.475 0.482- 69 1.42 77 1.42 70 1.44

67 0.168 0.473 0.278- 64 1.42 56 1.42 110 1.44

68 0.251 0.372 0.280- 71 1.42 63 1.42 64 1.44

69 0.249 0.442 0.481- 66 1.42 58 1.42 65 1.44

70 0.332 0.542 0.483- 112 1.42 119 1.42 66 1.44

71 0.334 0.339 0.281- 68 1.42 76 1.42 37 1.45

72 0.418 0.440 0.279- 75 1.42 83 1.42 76 1.44

73 0.415 0.375 0.477- 39 1.42 34 1.42 77 1.44

74 0.498 0.475 0.483- 77 1.42 85 1.42 78 1.44

75 0.334 0.473 0.278- 72 1.42 64 1.42 117 1.44

76 0.418 0.372 0.280- 79 1.42 71 1.42 72 1.44

77 0.415 0.442 0.481- 74 1.42 66 1.42 73 1.44

78 0.498 0.543 0.485- 119 1.42 126 1.42 74 1.44

79 0.501 0.339 0.282- 76 1.42 84 1.42 42 1.45

80 0.584 0.440 0.279- 83 1.42 91 1.42 84 1.44

81 0.582 0.375 0.478- 39 1.42 44 1.42 85 1.44

82 0.665 0.475 0.485- 85 1.42 93 1.42 86 1.44

83 0.501 0.473 0.279- 80 1.42 72 1.42 124 1.44

84 0.584 0.372 0.280- 87 1.42 79 1.42 80 1.44

85 0.582 0.442 0.482- 74 1.42 82 1.42 81 1.44

86	0.665	0.543	0.489-	133	1.42	126	1.43	82 1.44
87	0.668	0.339	0.282-	84	1.42	92	1.42	47 1.45
88	0.751	0.440	0.280-	99	1.42	91	1.42	92 1.44
89	0.749	0.375	0.478-	44	1.42	49	1.42	93 1.44
90	0.832	0.475	0.483-	101	1.42	93	1.42	94 1.44
91	0.668	0.473	0.280-	88	1.42	80	1.42	131 1.44
92	0.751	0.372	0.281-	95	1.42	87	1.42	88 1.44
93	0.748	0.442	0.482-	90	1.42	82	1.42	89 1.44
94	0.832	0.542	0.486-	140	1.42	133	1.42	90 1.44
95	0.834	0.339	0.282-	92	1.42	100	1.42	52 1.45
96	0.918	0.440	0.279-	59	1.42	99	1.42	100 1.44
97	0.915	0.374	0.478-	49	1.42	54	1.42	101 1.44
98	0.999	0.475	0.482-	61	1.42	101	1.42	102 1.43
99	0.834	0.473	0.280-	88	1.42	96	1.42	138 1.44
100	0.918	0.372	0.280-	55	1.42	95	1.42	96 1.44
101	0.915	0.442	0.481-	90	1.42	98	1.42	97 1.44
102	0.999	0.542	0.483-	105	1.42	140	1.42	98 1.43
103	0.001	0.540	0.280-	143	1.42	108	1.42	59 1.44
104	0.084	0.641	0.283-	107	1.41	114	1.41	108 1.45
105	0.082	0.575	0.483-	102	1.42	62	1.42	109 1.44
106	0.165	0.674	0.481-	13	1.09	116	1.40	109 1.40
107	0.001	0.673	0.286-	14	1.09	104	1.41	139 1.41

108 0.084 0.573 0.281- 110 1.42 103 1.42 104 1.45

109 0.082 0.643 0.482- 106 1.40 141 1.41 105 1.44

110 0.168 0.540 0.279- 108 1.42 115 1.42 67 1.44

111 0.251 0.641 0.282- 121 1.41 114 1.41 115 1.45

112 0.248 0.575 0.482- 70 1.42 62 1.42 116 1.44

113 0.331 0.674 0.481- 15 1.09 123 1.39 116 1.41

114 0.168 0.673 0.284- 16 1.09 111 1.41 104 1.41

115 0.251 0.573 0.280- 117 1.42 110 1.42 111 1.45

116 0.248 0.642 0.481- 106 1.40 113 1.41 112 1.44

117 0.334 0.540 0.279- 115 1.42 122 1.42 75 1.44

118 0.418 0.641 0.282- 128 1.41 121 1.41 122 1.45

119 0.415 0.576 0.483- 78 1.42 70 1.42 123 1.44

120 0.498 0.676 0.482- 130 1.39 123 1.43 146 1.99

121 0.334 0.673 0.283- 17 1.09 111 1.41 118 1.41

122 0.418 0.573 0.280- 124 1.42 117 1.42 118 1.45

123 0.414 0.643 0.482- 113 1.39 120 1.43 119 1.44

124 0.501 0.540 0.280- 122 1.42 129 1.42 83 1.44

125 0.584 0.641 0.285- 135 1.41 128 1.41 129 1.45

126 0.581 0.576 0.489- 78 1.42 86 1.43 130 1.45

127 0.666 0.675 0.505- 145 1.34 130 1.46 137 1.47

128 0.501 0.673 0.284- 22 1.09 118 1.41 125 1.41

129 0.584 0.573 0.282- 131 1.42 124 1.42 125 1.45

130 0.579 0.644 0.491- 120 1.39 126 1.45 127 1.46

131 0.668 0.540 0.282- 129 1.42 136 1.42 91 1.44

132 0.751 0.641 0.286- 135 1.41 142 1.41 136 1.45

133 0.749 0.575 0.489- 94 1.42 86 1.42 137 1.44

134 0.833 0.674 0.489- 18 1.09 137 1.38 144 1.42

135 0.668 0.673 0.287- 19 1.09 132 1.41 125 1.41

136 0.751 0.573 0.283- 138 1.42 131 1.42 132 1.45

137 0.752 0.642 0.493- 134 1.38 133 1.44 127 1.47

138 0.834 0.540 0.282- 136 1.42 143 1.42 99 1.44

139 0.918 0.641 0.285- 142 1.41 107 1.41 143 1.45

140 0.916 0.575 0.485- 102 1.42 94 1.42 144 1.44

141 0.999 0.674 0.483- 20 1.09 144 1.39 109 1.41

142 0.834 0.673 0.288- 21 1.09 139 1.41 132 1.41

143 0.918 0.573 0.282- 103 1.42 138 1.42 139 1.45

144 0.917 0.642 0.485- 141 1.39 134 1.42 140 1.44

145 0.671 0.728 0.542- 147 1.17 127 1.34

146 0.493 0.769 0.472- 24 1.54 23 1.54 120 1.99

147 0.678 0.774 0.578- 145 1.17

LATTYP: Found a simple orthorhombic cell.

ALAT = 14.7806000000

B/A-ratio = 1.2466138046

C/A-ratio = 1.4433717170

Lattice vectors:

A1 = (-14.7806000000, 0.0000000000, 0.0000000000)

A2 = (0.0000000000, 0.0000000000, -18.4257000000)

A3 = (0.0000000000, -21.3339000000, 0.0000000000)

Analysis of symmetry for initial positions (statically):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The static configuration has the point symmetry C_1 .

Analysis of symmetry for dynamics (positions and initial velocities):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The dynamic configuration has the point symmetry C_1 .

Analysis of constrained symmetry for selective dynamics:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The constrained configuration has the point symmetry C_1 .

Analysis of structural, dynamic, and magnetic symmetry:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The magnetic configuration has the point symmetry C_1 .

Subroutine INISYM returns: Found 1 space group operations

(whereof 1 operations are pure point group operations),

and found 1 'primitive' translations

KPOINTS: KPT-Resolved Value to Generate K-Mesh: 0

Automatic generation of k-mesh.

Space group operators:

irot	det(A)	alpha	n_x	n_y	n_z	tau_x	tau_y	tau_z
1	1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Subroutine IBZKPT returns following result:

==========

Found 1 irreducible k-points:

Following reciprocal coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

Following cartesian coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

Subroutine IBZKPT_HF returns following result:

==========

Found 1 k-points in 1st BZ

the following 1 k-points will be used (e.g. in the exchange kernel)

Following reciprocal coordinates: # in IRBZ

0.000000 0.000000 0.000000 1.00000000 1 t-inv F

Dimension of arrays:

k-points NKPTS = 1 k-points in BZ NKDIM = 1 number of bands NBANDS= 480

number of dos NEDOS = 301 number of ions NIONS = 147

non local maximal LDIM = 5 non local SUM 2l+1 LMDIM = 13

total plane-waves NPLWV = 699840

max r-space proj IRMAX = 1377 max aug-charges IRDMAX= 5183

dimension x,y,z NGX = 72 NGY = 108 NGZ = 90

dimension x,y,z NGXF= 144 NGYF= 216 NGZF= 180

support grid NGXF= 144 NGYF= 216 NGZF= 180

ions per type = 24 121 1 1

NGX,Y,Z is equivalent to a cutoff of 8.10, 8.42, 8.12 a.u.

NGXF,Y,Z is equivalent to a cutoff of 16.20, 16.83, 16.24 a.u.

SYSTEM = Al2O3 Cell opt

POSCAR = Generated by VASPKIT code

Startparameter for this run:

NWRITE = 2 write-flag & timer

PREC = normal normal or accurate (medium, high low for compatibility)

ISTART = 0 job : 0-new 1-cont 2-samecut

ICHARG = 1 charge: 1-file 2-atom 10-const

ISPIN = 2 spin polarized calculation?

LNONCOLLINEAR = F non collinear calculations

LSORBIT = F spin-orbit coupling

INIWAV = 1 electr: 0-lowe 1-rand 2-diag

LASPH = F aspherical Exc in radial PAW

METAGGA= F non-selfconsistent MetaGGA calc.

Electronic Relaxation 1

ENCUT = 400.0 eV 29.40 Ry 5.42 a.u. 24.10 34.79 30.05*2*pi/ulx,y,z

ENINI = 400.0 initial cutoff

ENAUG = 644.9 eV augmentation charge cutoff

NELM = 200; NELMIN= 5; NELMDL= 0 # of ELM steps

EDIFF = 0.1E-06 stopping-criterion for ELM

LREAL = T real-space projection

NLSPLINE = F spline interpolate recip. space projectors

LCOMPAT= F compatible to vasp.4.4

GGA_COMPAT = T GGA compatible to vasp.4.4-vasp.4.6

LMAXPAW = -100 max onsite density

LMAXMIX = 2 max onsite mixed and CHGCAR

VOSKOWN= 0 Vosko Wilk Nusair interpolation

ROPT = -0.00050 -0.00050 -0.00050 -0.00050

Ionic relaxation

EDIFFG = -.1E-01 stopping-criterion for IOM

NSW = 1801 number of steps for IOM

NBLOCK = 1; KBLOCK = 1801 inner block; outer block

IBRION = 5 ionic relax: 0-MD 1-quasi-New 2-CG

NFREE = 2 steps in history (QN), initial steepest desc. (CG)

ISIF = 2 stress and relaxation

IWAVPR = 11 prediction: 0-non 1-charg 2-wave 3-comb

ISYM = 2 0-nonsym 1-usesym 2-fastsym

LCORR = T Harris-Foulkes like correction to forces

POTIM = 0.5000 time-step for ionic-motion

TEIN = 0.0 initial temperature

TEBEG = 0.0; TEEND = 0.0 temperature during run

SMASS = -3.00 Nose mass-parameter (am)

estimated Nose-frequenzy (Omega) = 0.10E-29 period in steps =****** mass= -0.499E-26a.u.

SCALEE = 1.0000 scale energy and forces

NPACO = 256; APACO = 16.0 distance and # of slots for P.C.

PSTRESS= 0.0 pullay stress

Mass of Ions in am

POMASS = 1.00 12.01 74.92 16.00

Ionic Valenz

ZVAL = 1.00 4.00 5.00 6.00

Atomic Wigner-Seitz radii

RWIGS = -1.00 -1.00 -1.00 -1.00

virtual crystal weights

VCA = 1.00 1.00 1.00 1.00

NELECT = 519.0000 total number of electrons

NUPDOWN= -1.0000 fix difference up-down

DOS related values:

EMIN = 10.00; EMAX =-10.00 energy-range for DOS

EFERMI = 0.00

ISMEAR = 0; SIGMA = 0.05 broadening in eV -4-tet -1-fermi 0-gaus

Electronic relaxation 2 (details)

IALGO = 48 algorithm

LDIAG = T sub-space diagonalisation (order eigenvalues)

LSUBROT= F optimize rotation matrix (better conditioning)

TURBO = 0 0=normal 1=particle mesh

IRESTART = 0 0=no restart 2=restart with 2 vectors

NREBOOT = 0 no. of reboots

NMIN = 0 reboot dimension

EREF = 0.00 reference energy to select bands

IMIX = 4 mixing-type and parameters

AMIX = 0.40; BMIX = 1.00

AMIX_MAG = 1.60; BMIX_MAG = 1.00

AMIN = 0.10

WC = 100.; INIMIX= 1; MIXPRE= 1; MAXMIX= -45

Intra band minimization:

WEIMIN = 0.0010 energy-eigenvalue tresh-hold

EBREAK = 0.52E-10 absolut break condition

DEPER = 0.30 relativ break condition

TIME = 0.40 timestep for ELM

volume/ion in A,a.u. = 39.52 266.73

Fermi-wavevector in a.u.,A,eV,Ry = 0.731816 1.382932 7.286662 0.535555

Thomas-Fermi vector in A = 1.824126

Write flags

LWAVE = F write WAVECAR

LDOWNSAMPLE = F k-point downsampling of WAVECAR

LCHARG = F write CHGCAR

LVTOT = F write LOCPOT, total local potential

LVHAR = F write LOCPOT, Hartree potential only

LELF = F write electronic localiz. function (ELF)

LORBIT = 11 0 simple, 1 ext, 2 COOP (PROOUT), +10 PAW based schemes

Dipole corrections

LMONO = F monopole corrections only (constant potential shift)

LDIPOL = F correct potential (dipole corrections)

IDIPOL = 0 1-x, 2-y, 3-z, 4-all directions

EPSILON= 1.0000000 bulk dielectric constant

Exchange correlation treatment:

GGA = PE GGA type

LEXCH = 8 internal setting for exchange type

VOSKOWN= 0 Vosko Wilk Nusair interpolation

LHFCALC = F Hartree Fock is set to

LHFONE = F Hartree Fock one center treatment

AEXX = 0.0000 exact exchange contribution

Linear response parameters

LEPSILON= F determine dielectric tensor

LRPA = F only Hartree local field effects (RPA)

LNABLA = F use nabla operator in PAW spheres

LVEL = F velocity operator in full k-point grid

LINTERFAST= F fast interpolation

KINTER = 0 interpolate to denser k-point grid

CSHIFT =0.1000 complex shift for real part using Kramers Kronig

OMEGAMAX= -1.0 maximum frequency

DEG_THRESHOLD= 0.2000000E-02 threshold for treating states as degnerate

RTIME = -0.100 relaxation time in fs

(WPLASMAI= 0.000 imaginary part of plasma frequency in eV, 0.658/RTIME)

DFIELD = 0.0000000 0.0000000 0.0000000 field for delta impulse in time

Orbital magnetization related:

ORBITALMAG= F switch on orbital magnetization

LCHIMAG = F perturbation theory with respect to B field

DQ = 0.001000 dq finite difference perturbation B field

LLRAUG = F two centre corrections for induced B field

---

finite differences

using selective dynamics as specified on POSCAR

charge density and potential will be updated during run

spin polarized calculation

RMM-DIIS sequential band-by-band

perform sub-space diagonalisation

before iterative eigenvector-optimisation

modified Broyden-mixing scheme, WC = 100.0

initial mixing is a Kerker type mixing with AMIX = 0.4000 and BMIX = 1.0000

Hartree-type preconditioning will be used

using additional bands 220

real space projection scheme for non local part

use partial core corrections

calculate Harris-corrections to forces

(improved forces if not selfconsistent)

use gradient corrections

use of overlap-Matrix (Vanderbilt PP)

Gauss-broadening in eV SIGMA = 0.05

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energy-cutoff : 400.00

volume of cell : 5810.14

direct lattice vectors			reciprocal lattice vectors		
14.780600000	0.000000000	0.000000000	0.067656252	0.000000000	0.000000000
0.000000000	21.333900000	0.000000000	0.000000000	0.046873755	0.000000000
0.000000000	0.000000000	18.425700000	0.000000000	0.000000000	0.054272022

length of vectors

14.780600000 21.333900000 18.425700000 0.067656252 0.046873755 0.054272022

k-points in units of 2pi/SCALE and weight: KPT-Resolved Value to Generate K-Mesh: 0

0.00000000 0.00000000 0.00000000 1.000

k-points in reciprocal lattice and weights: KPT-Resolved Value to Generate K-Mesh: 0

0.00000000 0.00000000 0.00000000 1.000

position of ions in fractional coordinates (direct lattice)

0.08428274 0.18884013 0.29522843

0.08188032 0.19104864 0.45790738

0.25091135 0.18884950 0.29522062

0.24897373 0.19111988 0.45788761

0.41754554 0.18883267 0.29520849

0.41573565 0.19138191 0.45767334

0.58422044 0.18880781 0.29516844

0.58207284 0.19158801 0.45756155

0.75093544 0.18879988 0.29517734

0.74829221 0.19153512 0.45756678

0.91762947 0.18881066 0.29522465

0.91480770 0.19126690 0.45770229

0.16524434 0.72564005 0.48042912

0.00115985 0.72402336 0.28898145

0.32883678 0.72547845 0.48118836

0.16779839 0.72413128 0.28631851

0.33448032 0.72416441 0.28485699

0.83320760 0.72571907 0.48856265

0.66761267 0.72399155 0.28990787

0.99879534 0.72572069 0.48299467

0.83446171 0.72396973 0.29096773

0.50115880 0.72401958 0.28572238

0.43627872 0.76611746 0.40196470

0.58188711 0.77231281 0.42834152

0.08426191 0.23993778 0.29062693

0.16531700 0.27369050 0.46798354

0.00093332 0.27164729 0.28686726

0.08190675 0.24206562 0.46356484

0.16531844 0.34120845 0.47478893

0.25091382 0.23994502 0.29056680

0.33205673 0.27389030 0.46789157

0.16758530 0.27166182 0.28677155

0.24875792 0.24213689 0.46348332

0.33203235 0.34142732 0.47475906

0.41756385 0.23992798 0.29059031

0.49869141 0.27417823 0.46787590

0.33424150 0.27165580 0.28674090

0.41546358 0.24238815 0.46332848

0.49867462 0.34170159 0.47495178

0.58424078 0.23990915 0.29063785

0.66521877 0.27428917 0.46800783

0.50090929 0.27163239 0.28683393

0.58197526 0.24258483 0.46335207

0.66519898 0.34176133 0.47527063

0.75093708 0.23990639 0.29066891

0.83179889 0.27405837 0.46803355

0.66759814 0.27161833 0.28692444

0.74845506 0.24252901 0.46342529

0.83178460 0.34158282 0.47516930

0.91760701 0.23991335 0.29068386

0.99853555 0.27373706 0.46806036

0.83428146 0.27162422 0.28693203

0.91507465 0.24226414 0.46349477

0.99854996 0.34124651 0.47497731

0.00096995 0.33928635 0.28168088

0.08435990 0.43970463 0.27850255

0.08192173 0.37408030 0.47737038

0.16522605 0.47447649 0.48146927

0.00103628 0.47280922 0.27898454

0.08430353 0.37229212 0.27992142

0.08191983 0.44135945 0.48073163

0.16513023 0.54163217 0.48216009

0.16761635 0.33929188 0.28144661

0.25100251 0.43970172 0.27817991

0.24865985 0.37422137 0.47724064

0.33184537 0.47479610 0.48167398

0.16769756 0.47282154 0.27825006

0.25096356 0.37229092 0.27974041

0.24869712 0.44153690 0.48054904

0.33169385 0.54209768 0.48252496

0.33427908 0.33928626 0.28142891

0.41765439 0.43967687 0.27850948

0.41531716 0.37454209 0.47740240

0.49847796 0.47518754 0.48273510

0.33435448 0.47280697 0.27825255

0.41763093 0.37227069 0.27991643

0.41536786 0.44186011 0.48093900

0.49822737 0.54266748 0.48461371

0.50094456 0.33926955 0.28167805

0.58434713 0.43966180 0.27925273

0.58190163 0.37478741 0.47792841

0.66510701 0.47543401 0.48456325

0.50103057 0.47278129 0.27899284

0.58430449 0.37225541 0.28034477

0.58189604 0.44213878 0.48222447

0.66501153 0.54291235 0.48850029

0.66763558 0.33926634 0.28193723

0.75105643 0.43966611 0.27958548

0.74850191 0.37471384 0.47803800

0.83204665 0.47480446 0.48320558

0.66772003 0.47276556 0.27984332

0.75099850 0.37225957 0.28051135

0.74841732 0.44204872 0.48239100

0.83234427 0.54212155 0.48556849

0.83431619 0.33927200 0.28191434

0.91771421 0.43968560 0.27919413

0.91522247 0.37431254 0.47768665

0.99876371 0.47451218 0.48209043

0.83437523 0.47278583 0.27977837

0.91765575 0.37227803 0.28030693

0.91520696 0.44156974 0.48135202

0.99889742 0.54173263 0.48337176

0.00108968 0.54022767 0.28038064

0.08441472 0.64101491 0.28341324

0.08201061 0.57482948 0.48270037

0.16508002 0.67438568 0.48125633

0.00114940 0.67282960 0.28617372

0.08443072 0.57324875 0.28073544

0.08215801 0.64255367 0.48235425

0.16775927 0.54025759 0.27925497

0.25115222 0.64106215 0.28196233

0.24825245 0.57478862 0.48203555

0.33108946 0.67432066 0.48089079

0.16778781 0.67291792 0.28392327

0.25110600 0.57327622 0.27982777

0.24776545 0.64234215 0.48145651

0.33441789 0.54023970 0.27914852

0.41786356 0.64100098 0.28223211

0.41483126 0.57556794 0.48334168

0.49836570 0.67637283 0.48204562

0.33445669 0.67293223 0.28296067

0.41777283 0.57322722 0.28038159

0.41397414 0.64326559 0.48180822

0.50107932 0.54017924 0.28024317

0.58446601 0.64091585 0.28458983

0.58112625 0.57610975 0.48856082

0.66563969 0.67453569 0.50489536

0.50111081 0.67281937 0.28413017

0.58442822 0.57316194 0.28210617

0.57884705 0.64385614 0.49094351

0.66775689 0.54014414 0.28161346

0.75105141 0.64092909 0.28637653

0.74921071 0.57529717 0.48893156

0.83264133 0.67446477 0.48862884

0.66772228 0.67277897 0.28740486

0.75109304 0.57317395 0.28310978

0.75197498 0.64246836 0.49272296

0.83442200 0.54017811 0.28157136

0.91770960 0.64095146 0.28546798

0.91581259 0.57495384 0.48496760

0.99878657 0.67446919 0.48325219

0.83447030 0.67277317 0.28802705

0.91776057 0.57320500 0.28227159

0.91668887 0.64249368 0.48540861

0.67055850 0.72803608 0.54243376

0.49312229 0.76914379 0.47206488

0.67827131 0.77358818 0.57772439

position of ions in cartesian coordinates (Angst):

1.24574954 4.02869645 5.43979041

1.21024019 4.07581253 8.43726398

3.70862031 4.02889640 5.43964651

3.67998110 4.07733251 8.43689982

6.17157362 4.02853730 5.43942303

6.14482229 4.08292244 8.43295171

8.63512858 4.02800700 5.43868514

8.60338587 4.08731953 8.43089191

11.09927640 4.02783767 5.43884914

11.06020784 4.08619100 8.43098817

13.56311415 4.02806769 5.43972086

13.52140675 4.08046891 8.43348514

2.44241045 15.48073228 8.85224276

0.01714329 15.44624202 5.32468554

4.86040485 15.47728475 8.86623232

2.48016083	15.44854438	5.27561892
4.94381979	15.44925102	5.24868943
12.31530821	15.48241801	9.00210881
9.86771590	15.44556328	5.34175539
14.76279437	15.48245265	8.89951487
12.33384480	15.44509788	5.36128403
7.40742774	15.44616132	5.26463480
6.44846123	16.34427327	7.40648105
8.60064057	16.47644434	7.89249226
1.24544159	5.11880857	5.35500457
2.44348447	5.83888568	8.62292425
0.01379510	5.79529612	5.28573012
1.21063093	5.16420382	8.54150671
2.44350576	7.27930703	8.74831846
3.70865680	5.11896317	5.35389675
4.90799772	5.84314818	8.62122979
2.47701125	5.79560619	5.28396654
3.67679133	5.16572412	8.54000455
4.90763733	7.28397624	8.74776806
6.17184431	5.11859945	5.35432996
7.37095832	5.84929098	8.62094089
4.94028986	5.79547769	5.28340186

6.14080105	5.17108459	8.53715151
7.37071008	7.28982754	8.75131899
8.63542933	5.11819790	5.35520577
9.83233251	5.85165762	8.62337183
7.40373985	5.79497816	5.28511603
8.60194351	5.17528049	8.53758614
9.83203999	7.29110207	8.75719411
11.09930058	5.11813883	5.35577819
12.29448669	5.84673391	8.62384580
9.86750113	5.79467828	5.28678371
11.06261487	5.17408955	8.53893540
12.29427543	7.28729373	8.75532706
13.56278217	5.11828732	5.35605354
14.75895454	5.83987900	8.62433975
12.33118059	5.79480405	5.28692356
13.52535236	5.16843899	8.54021560
14.75916747	7.28011901	8.75178945
0.01433640	7.23830099	5.19016741
1.24688988	9.38061471	5.13160436
1.21085233	7.98059169	8.79588339
2.44214010	10.12243403	8.87140832
0.01531688	10.08686464	5.14048537

1.24605669 7.94244291 5.15774803

1.21082417 9.41591828 8.85781675

2.44072381 11.55512646 8.88413716

2.47747021 7.23841895 5.18585079

3.70996763 9.38055261 5.12565949

3.67534182 7.98360125 8.79349277

4.90487369 10.12925257 8.87518021

2.47867062 10.08712741 5.12695206

3.70939194 7.94241725 5.15441295

3.67589271 9.41970405 8.85445248

4.90263409 11.56505766 8.89086006

4.94084537 7.23829915 5.18552464

6.17318240 9.38002243 5.13173213

6.13863688 7.99044345 8.79647348

7.36780335 10.13760353 8.89473216

4.94195979 10.08681662 5.12699798

6.17283567 7.94198563 5.15765608

6.13938618 9.42659932 8.86163771

7.36409940 11.57721374 8.92934676

7.40426122 7.23794266 5.19011520

8.63700113 9.37970096 5.14542709

8.60085530 7.99567721 8.80616549

 9.83068060 10.14286164 8.92841702

 7.40553244 10.08626877 5.14063835

 8.63637089 7.94165973 5.16554864

 8.60077264 9.43254448 8.88532342

 9.82926935 11.58243773 9.00095979

 9.86805449 7.23787415 5.19489091

11.10106460 9.37979293 5.15155826

11.06330738 7.99410762 8.80818483

12.29814879 10.12943095 8.90340104

 9.86930266 10.08593309 5.15630915

11.10020843 7.94174853 5.16861790

11.06205706 9.43062308 8.88839179

12.30254778 11.56556701 8.94693933

12.33169395 7.23799486 5.19446904

13.56436670 9.38020853 5.14434721

13.52753721 7.98554627 8.80171085

14.76232687 10.12319548 8.88285371

12.33256658 10.08636572 5.15511224

13.56350256 7.94214230 5.16485131

13.52730804 9.42040468 8.86924793

14.76430325 11.55726976 8.90646308

 0.01610610 11.52516301 5.16620953

1.24770016 13.67534801 5.22208742

1.21216603 12.26335464 8.89409229

2.43998181 14.38727668 8.86748475

0.01698884 14.35407948 5.27295104

1.24793674 12.22963142 5.17274706

1.21434475 13.70817579 8.88771466

2.47958266 11.52580130 5.14546825

3.71218054 13.67635582 5.19535338

3.66932012 12.26248294 8.88184247

4.89370081 14.38588962 8.86074937

2.48000445 14.35596351 5.23148504

3.71149739 12.23021751 5.15602249

3.66212196 13.70366325 8.87117322

4.94289713 11.52541976 5.14350685

6.17627417 13.67505090 5.20032419

6.13145495 12.27910881 8.90590884

7.36614411 14.42967035 8.88202798

4.94347055 14.35626898 5.21374843

6.17493313 12.22917212 5.16622701

6.11878615 13.72336372 8.87765373

7.40625295 11.52412982 5.16367665

8.63875829 13.67323457 5.24376690

8.58939458 12.29066782 9.00207518

9.83855407 14.39047696 9.30305043

7.40671840 14.35386119 5.23529721

8.63819978 12.22777941 5.19800360

8.55570675 13.73596260 9.04597780

9.86984745 11.52338111 5.18892515

11.10099048 13.67351715 5.27668808

11.07378377 12.27333222 9.00890625

12.30693849 14.38896400 9.00332842

9.86933586 14.35299928 5.29563570

11.10160586 12.22803578 5.21649595

11.11464136 13.70635576 9.07876541

12.33325782 11.52410582 5.18814938

13.56429850 13.67399428 5.25994739

13.53625953 12.26600779 8.93586750

14.76266477 14.38905833 8.90425984

12.33397166 14.35287549 5.30710003

13.56505188 12.22869810 5.20105161

13.54921157 13.70689598 8.94399344

9.91125694 15.53184883 9.99472166

7.28864335 16.40883669 8.69812580

10.02525687 16.50365282 10.64497638

---

k-point 1 : 0.0000 0.0000 0.0000 plane waves: 105525

maximum and minimum number of plane-waves per node : 105525 105525

maximum number of plane-waves: 105525

maximum index in each direction:

IXMAX= 24 IYMAX= 34 IZMAX= 30

IXMIN= -24 IYMIN= -34 IZMIN= -30

serial 3D FFT for wavefunctions

parallel 3D FFT for charge:

minimum data exchange during FFTs selected (reduces bandwidth)

total amount of memory used by VASP MPI-rank0 132380. kBytes

==========

base : 30000. kBytes

nonlr-proj: 13792. kBytes

fftplans : 5354. kBytes

grid : 63770. kBytes

one-center: 2384. kBytes

wavefun : 17080. kBytes

INWAV: cpu time 0.0000: real time 0.0000

Broyden mixing: mesh for mixing (old mesh)

NGX = 49 NGY = 69 NGZ = 61

(NGX =144 NGY =216 NGZ =180)

gives a total of 206241 points

initial charge density was supplied:

charge density of overlapping atoms calculated

number of electron 519.0000000 magnetization 147.0000000

keeping initial charge density in first step

Maximum index for non-local projection operator 1292

Maximum index for augmentation-charges 154 (set IRDMAX)

First call to EWALD: gamma= 0.099

Maximum number of real-space cells 3x 2x 3

Maximum number of reciprocal cells 2x 3x 3

FEWALD: cpu time 0.0064: real time 0.0070

---------- Iteration 1(1) ----------

POTLOK: cpu time 0.2319: real time 0.2569

SETDIJ: cpu time 0.0110: real time 0.0112

EDDIAG: cpu time 1.9671: real time 1.9786

RMM-DIIS: cpu time 3.8414: real time 3.8654

ORTHCH: cpu time 0.3618: real time 0.3630

DOS: cpu time 0.0019: real time 0.0025

LOOP: cpu time 6.4153: real time 6.4775

eigenvalue-minimisations : 960

total energy-change (2. order) : 0.6253145E+04 (-0.1156169E+05)

number of electron 519.0000000 magnetization 147.0000000

augmentation part 519.0000000 magnetization 147.0000000

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -105102.20925185

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1690.14211936

PAW double counting = 13652.10586829 -13700.47723969

entropy T*S EENTRO = -0.05422273

eigenvalues EBANDS = -553.42276431

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = 6253.14540493 eV

energy without entropy = 6253.19962766 energy(sigma->0) = 6253.17251630

---------- Iteration 1(2) ----------

EDDIAG: cpu time 1.9617: real time 1.9683

RMM-DIIS: cpu time 3.8223: real time 3.8364

ORTHCH: cpu time 0.3571: real time 0.3584

DOS: cpu time 0.0004: real time 0.0004

LOOP: cpu time 6.1415: real time 6.1635

eigenvalue-minimisations : 960

total energy-change (2. order) :-0.3969773E+04 (-0.4892682E+04)

number of electron 519.0000000 magnetization 147.0000000

augmentation part 519.0000000 magnetization 147.0000000

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -105102.20925185

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1690.14211936

PAW double counting = 13652.10586829 -13700.47723969

entropy T*S EENTRO = -0.01417874

eigenvalues EBANDS = -4523.23543262

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = 2283.37278062 eV

energy without entropy = 2283.38695936 energy(sigma->0) = 2283.37986999

---------- Iteration 1(3) ----------

EDDIAG: cpu time 1.9257: real time 1.9378

RMM-DIIS: cpu time 3.8092: real time 3.8321

ORTHCH: cpu time 0.3619: real time 0.3631

DOS: cpu time 0.0004: real time 0.0004

LOOP: cpu time 6.0972: real time 6.1334

eigenvalue-minimisations : 960

total energy-change (2. order) :-0.1553959E+04 (-0.2326767E+04)

number of electron 519.0000000 magnetization 147.0000000

augmentation part 519.0000000 magnetization 147.0000000

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -105102.20925185

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1690.14211936

PAW double counting = 13652.10586829 -13700.47723969

entropy T*S EENTRO = -0.01300233

eigenvalues EBANDS = -6077.19580200

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = 729.41358765 eV

energy without entropy = 729.42658998 energy(sigma->0) = 729.42008881

---------- Iteration 1(4) ----------

EDDIAG: cpu time 1.9457: real time 1.9529

RMM-DIIS: cpu time 3.8199: real time 3.8331

ORTHCH: cpu time 0.3577: real time 0.3591

DOS: cpu time 0.0004: real time 0.0004

LOOP: cpu time 6.1238: real time 6.1456

eigenvalue-minimisations : 960

total energy-change (2. order) :-0.1425630E+04 (-0.1105763E+04)

number of electron 519.0000000 magnetization 147.0000000

augmentation part 519.0000000 magnetization 147.0000000

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -105102.20925185

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1690.14211936

PAW double counting = 13652.10586829 -13700.47723969

entropy T*S EENTRO = -0.01007327

eigenvalues EBANDS = -7502.82879182

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -696.21647311 eV

energy without entropy = -696.20639984 energy(sigma->0) = -696.21143648

---------- Iteration 1(5) ----------

EDDIAG: cpu time 1.9308: real time 1.9374

RMM-DIIS: cpu time 3.8115: real time 3.8324

ORTHCH: cpu time 0.3575: real time 0.3587

DOS: cpu time 0.0004: real time 0.0004

LOOP: cpu time 6.1002: real time 6.1290

eigenvalue-minimisations : 960

total energy-change (2. order) :-0.3740123E+03 (-0.3261586E+03)

number of electron 519.0000000 magnetization 147.0000000

augmentation part 519.0000000 magnetization 147.0000000

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -105102.20925185

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1690.14211936

PAW double counting = 13652.10586829 -13700.47723969

entropy T*S EENTRO = -0.02800851

eigenvalues EBANDS = -7876.82311217

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1070.22872870 eV

energy without entropy = -1070.20072019 energy(sigma->0) = -1070.21472445

---------- Iteration 1(6) ----------

EDDIAG: cpu time 1.9279: real time 1.9591

RMM-DIIS: cpu time 3.8199: real time 3.8325

ORTHCH: cpu time 0.3587: real time 0.3600

DOS: cpu time 0.0004: real time 0.0004

LOOP: cpu time 6.1070: real time 6.1520

eigenvalue-minimisations : 960

total energy-change (2. order) :-0.9724909E+02 (-0.8301419E+02)

number of electron 519.0000000 magnetization 147.0000000

augmentation part 519.0000000 magnetization 147.0000000

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -105102.20925185

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1690.14211936

PAW double counting = 13652.10586829 -13700.47723969

entropy T*S EENTRO = -0.03209245

eigenvalues EBANDS = -7974.06811402

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1167.47781449 eV

energy without entropy = -1167.44572204 energy(sigma->0) = -1167.46176826

---------- Iteration 1(7) ----------

EDDIAG: cpu time 1.9395: real time 1.9458

RMM-DIIS: cpu time 3.8170: real time 3.8308

ORTHCH: cpu time 0.3577: real time 0.3588

DOS: cpu time 0.0004: real time 0.0004

LOOP: cpu time 6.1146: real time 6.1359

eigenvalue-minimisations : 960

total energy-change (2. order) :-0.2480899E+02 (-0.2290662E+02)

number of electron 519.0000000 magnetization 147.0000000

augmentation part 519.0000000 magnetization 147.0000000

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -105102.20925185

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1690.14211936

PAW double counting = 13652.10586829 -13700.47723969

entropy T*S EENTRO = -0.04483185

eigenvalues EBANDS = -7998.86436560

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1192.28680547 eV

energy without entropy = -1192.24197362 energy(sigma->0) = -1192.26438955

---------- Iteration 1(8) ----------

```
      EDDIAG:  cpu time        1.9278: real time        1.9343
  RMM-DIIS:  cpu time        3.8175: real time        3.8316
     ORTHCH:  cpu time        0.3585: real time        0.3597
        DOS:  cpu time        0.0004: real time        0.0004
     ------------------------------------------
       LOOP:  cpu time        6.1042: real time        6.1260


eigenvalue-minimisations  :      960
total energy-change (2. order) :-0.7651671E+01  (-0.6908152E+01)
number of electron          519.0000000 magnetization          147.0000000
augmentation part           519.0000000 magnetization          147.0000000


Free energy of the ion-electron system (eV)
  ---------------------------------------------------
  alpha Z              PSCENC =            233.50077011
  Ewald energy         TEWEN  =          91329.23020906
  -Hartree energ DENC  =      -105102.20925185
  -exchange            EXHF   =                0.00000000
  -V(xc)+E(xc)         XCENC  =           1690.14211936
  PAW double counting  =          13652.10586829      -13700.47723969
  entropy T*S          EENTRO =              -0.04322998
```

eigenvalues EBANDS = -8006.51763842

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1199.93847642 eV

energy without entropy = -1199.89524644 energy(sigma->0) = -1199.91686143

---------- Iteration 1(9) ----------

EDDIAG: cpu time 1.9238: real time 1.9299

RMM-DIIS: cpu time 7.9039: real time 7.9377

ORTHCH: cpu time 0.3583: real time 0.3593

DOS: cpu time 0.0004: real time 0.0004

LOOP: cpu time 10.1865: real time 10.2273

eigenvalue-minimisations : 2041

total energy-change (2. order) :-0.3417799E+01 (-0.3288551E+01)

number of electron 519.0000000 magnetization 147.0000000

augmentation part 519.0000000 magnetization 147.0000000

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -105102.20925185

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1690.14211936

PAW double counting = 13652.10586829 -13700.47723969

entropy T*S EENTRO = -0.03758039

eigenvalues EBANDS = -8009.94108680

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1203.35627522 eV

energy without entropy = -1203.31869483 energy(sigma->0) = -1203.33748502

---------- Iteration 1(10) ----------

EDDIAG: cpu time 1.9260: real time 1.9328

RMM-DIIS: cpu time 7.9130: real time 7.9522

ORTHCH: cpu time 0.3591: real time 0.3604

DOS: cpu time 0.0004: real time 0.0004

LOOP: cpu time 10.1986: real time 10.2458

eigenvalue-minimisations : 2165

total energy-change (2. order) :-0.4509083E+00 (-0.4119970E+00)

number of electron 519.0000000 magnetization 147.0000000

augmentation part 519.0000000 magnetization 147.0000000

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -105102.20925185

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1690.14211936

PAW double counting = 13652.10586829 -13700.47723969

entropy T*S EENTRO = -0.03704897

eigenvalues EBANDS = -8010.39252652

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1203.80718351 eV

energy without entropy = -1203.77013454 energy(sigma->0) = -1203.78865903

---------- Iteration 1(11) ----------

EDDIAG: cpu time 1.9293: real time 1.9502

RMM-DIIS: cpu time 7.3453: real time 7.3948

ORTHCH: cpu time 0.3568: real time 0.3580

DOS: cpu time 0.0004: real time 0.0004

LOOP: cpu time 9.6319: real time 9.7034

eigenvalue-minimisations : 2045

total energy-change (2. order) :-0.2265513E-01 (-0.1945174E-01)

number of electron 519.0000000 magnetization 147.0000000

augmentation part 519.0000000 magnetization 147.0000000

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -105102.20925185

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1690.14211936

PAW double counting = 13652.10586829 -13700.47723969

entropy T*S EENTRO = -0.03702975

eigenvalues EBANDS = -8010.41520087

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1203.82983864 eV

energy without entropy = -1203.79280890 energy(sigma->0) = -1203.81132377

---------- Iteration 1(12) ----------

EDDIAG: cpu time 1.9226: real time 1.9288

RMM-DIIS: cpu time 7.8274: real time 7.8657

ORTHCH: cpu time 0.3577: real time 0.3586

DOS: cpu time 0.0005: real time 0.0005

CHARGE: cpu time 0.5302: real time 0.5324

MIXING: cpu time 0.0067: real time 0.0075

LOOP: cpu time 10.6450: real time 10.6935

eigenvalue-minimisations : 2073

total energy-change (2. order) :-0.4065193E-02 (-0.3871173E-02)

number of electron 518.9999725 magnetization 129.4925519

augmentation part 13.3485603 magnetization 120.1905281

Broyden mixing:

rms(total) = 0.76030E+01 rms(broyden)= 0.76014E+01

rms(prec) = 0.78880E+01

weight for this iteration 100.00

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -105102.20925185

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1690.14211936

PAW double counting = 13652.10586829 -13700.47723969

entropy T*S EENTRO = -0.03702917

eigenvalues EBANDS = -8010.41926665

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1203.83390384 eV

energy without entropy = -1203.79687467 energy(sigma->0) = -1203.81538925

---------- Iteration 1(13) ----------

POTLOK: cpu time 0.1799: real time 0.1847

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9260: real time 1.9327

RMM-DIIS: cpu time 7.1897: real time 7.2188

ORTHCH: cpu time 0.3574: real time 0.3584

DOS: cpu time 0.0005: real time 0.0005

CHARGE: cpu time 0.5246: real time 0.5263

MIXING: cpu time 0.0053: real time 0.0058

LOOP: cpu time 10.1935: real time 10.2372

eigenvalue-minimisations : 1920

total energy-change (2. order) : 0.4159608E+03 (-0.6208793E+02)

number of electron 518.9999729 magnetization 110.9003208

augmentation part 12.9165444 magnetization 99.8831001

Broyden mixing:

rms(total) = 0.43964E+01 rms(broyden)= 0.43959E+01

rms(prec) = 0.45875E+01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 0.9878

0.9878

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -105996.24158199

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1997.14669930

PAW double counting = 25040.66430253 -25099.41948414

entropy T*S EENTRO = -0.00001326

eigenvalues EBANDS = -6997.08394179

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -787.87312349 eV

energy without entropy = -787.87311023 energy(sigma->0) = -787.87311686

---------- Iteration 1(14) ----------

POTLOK: cpu time 0.1779: real time 0.2063

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9259: real time 1.9326

RMM-DIIS: cpu time 7.1390: real time 7.1728

ORTHCH: cpu time 0.3551: real time 0.3563

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5233: real time 0.5249

MIXING: cpu time 0.0049: real time 0.0050

LOOP: cpu time 10.1365: real time 10.2083

eigenvalue-minimisations : 1920

total energy-change (2. order) :-0.8155024E+02 (-0.9086178E+01)

number of electron 518.9999735 magnetization 87.6529986

augmentation part 12.5034714 magnetization 76.5462227

Broyden mixing:

rms(total) = 0.28857E+01 rms(broyden)= 0.28854E+01

rms(prec) = 0.29462E+01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.2636

0.8149 1.7123

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -106759.76097741

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1942.34566782

PAW double counting = 36802.90568802 -36867.59288628

entropy T*S EENTRO = -0.00713977

eigenvalues EBANDS = -6254.37460702

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -869.42335878 eV

energy without entropy = -869.41621901 energy(sigma->0) = -869.41978889

---------- Iteration 1(15) ----------

POTLOK: cpu time 0.1732: real time 0.1890

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9259: real time 1.9324

RMM-DIIS: cpu time 7.1674: real time 7.1933

ORTHCH: cpu time 0.3566: real time 0.3579

DOS: cpu time 0.0005: real time 0.0005

CHARGE: cpu time 0.5244: real time 0.5261

MIXING: cpu time 0.0051: real time 0.0051

LOOP: cpu time 10.1631: real time 10.2143

eigenvalue-minimisations : 1922

total energy-change (2. order) :-0.6584722E+02 (-0.5512357E+01)

number of electron 518.9999735 magnetization 71.4685680

augmentation part 12.1425180 magnetization 62.3404050

Broyden mixing:

rms(total) = 0.18281E+01 rms(broyden)= 0.18278E+01

rms(prec) = 0.18431E+01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3535

2.3106 1.0266 0.7233

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107375.79845493

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1918.66466433

PAW double counting = 49747.95946590 -49815.27733295

entropy T*S EENTRO = -0.01841236

eigenvalues EBANDS = -5677.86140301

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -935.27057716 eV

energy without entropy = -935.25216480 energy(sigma->0) = -935.26137098

---------- Iteration 1(16) ----------

POTLOK: cpu time 0.1729: real time 0.1927

```
      SETDIJ:    cpu time       0.0101: real time       0.0101
      EDDIAG:    cpu time       1.9261: real time       1.9319
    RMM-DIIS:    cpu time       7.1714: real time       7.2039
      ORTHCH:    cpu time       0.3562: real time       0.3571
         DOS:    cpu time       0.0005: real time       0.0005
      CHARGE:    cpu time       0.5248: real time       0.5264
      MIXING:    cpu time       0.0053: real time       0.0053
      ----------------------------------------
        LOOP:    cpu time      10.1673: real time      10.2280

eigenvalue-minimisations    :    1923
total energy-change (2. order) :-0.6752407E+02    (-0.2639404E+01)
number of electron          518.9999734 magnetization           51.8208336
augmentation part            11.9931659 magnetization           44.5183975

Broyden mixing:
  rms(total) = 0.13854E+01        rms(broyden)= 0.13853E+01
  rms(prec ) = 0.14006E+01
  weight for this iteration          100.00

eigenvalues of (default mixing * dielectric matrix)
  average eigenvalue GAMMA=       1.4439
```

2.6103 1.6367 0.8599 0.6689

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107519.78222990

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1880.60304409

PAW double counting = 54098.40596706 -54164.54467756

entropy T*S EENTRO = -0.01740013

eigenvalues EBANDS = -5564.52024710

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1002.79464769 eV

energy without entropy = -1002.77724756 energy(sigma->0) = -1002.78594763

---------- Iteration 1(17) ----------

POTLOK: cpu time 0.1737: real time 0.1948

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9252: real time 1.9314

RMM-DIIS: cpu time 7.1286: real time 7.1811

ORTHCH: cpu time 0.3566: real time 0.3575

DOS: cpu time 0.0005: real time 0.0004

CHARGE: cpu time 0.5250: real time 0.5266

MIXING: cpu time 0.0058: real time 0.0058

LOOP: cpu time 10.1255: real time 10.2078

eigenvalue-minimisations : 1920

total energy-change (2. order) :-0.7927338E+02 (-0.4749844E+01)

number of electron 518.9999732 magnetization 33.6768259

augmentation part 11.9369816 magnetization 30.2790873

Broyden mixing:

rms(total) = 0.99265E+00 rms(broyden)= 0.99242E+00

rms(prec) = 0.10004E+01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5377

3.1359 2.1034 1.0021 0.8184 0.6289

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107538.74966943

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1831.77837520

PAW double counting = 55680.40329255 -55744.06650899

entropy T*S EENTRO = -0.00353678

eigenvalues EBANDS = -5578.49087816

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1082.06802976 eV

energy without entropy = -1082.06449297 energy(sigma->0) = -1082.06626137

---------- Iteration 1(18) ----------

POTLOK: cpu time 0.1747: real time 0.1822

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9247: real time 1.9309

RMM-DIIS: cpu time 7.1674: real time 7.1945

ORTHCH: cpu time 0.3562: real time 0.3571

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5249: real time 0.5263

MIXING: cpu time 0.0058: real time 0.0059

LOOP: cpu time 10.1641: real time 10.2074

eigenvalue-minimisations : 1920

total energy-change (2. order) :-0.5386056E+02 (-0.3727611E+01)

number of electron 518.9999729 magnetization 24.2607392

augmentation part 11.8634838 magnetization 22.9160359

Broyden mixing:

rms(total) = 0.72623E+00 rms(broyden)= 0.72582E+00

rms(prec) = 0.73345E+00

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4669

3.4038 2.2348 0.9543 0.9543 0.6271 0.6271

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107544.34898339

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1797.98122008

PAW double counting = 55525.04609610 -55587.60449989

entropy T*S EENTRO = -0.00455933

eigenvalues EBANDS = -5594.05876335

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1135.92859392 eV

energy without entropy = -1135.92403459 energy(sigma->0) = -1135.92631425

---------- Iteration 1(19) ----------

POTLOK: cpu time 0.1729: real time 0.1845

SETDIJ: cpu time 0.0100: real time 0.0100

```
      EDDIAG:    cpu time        1.9273: real time        1.9339
    RMM-DIIS:    cpu time        7.1723: real time        7.2035
      ORTHCH:    cpu time        0.3560: real time        0.3571
         DOS:    cpu time        0.0004: real time        0.0004
      CHARGE:    cpu time        0.5253: real time        0.5269
      MIXING:    cpu time        0.0061: real time        0.0062
      -----------------------------------------
        LOOP:    cpu time       10.1703: real time       10.2225

 eigenvalue-minimisations  :    1922
 total energy-change (2. order) :-0.2906592E+02  (-0.2047657E+01)
 number of electron       518.9999725 magnetization            11.8752298
 augmentation part         11.8049912 magnetization            10.7127338

 Broyden mixing:
  rms(total) = 0.48193E+00        rms(broyden)= 0.48170E+00
  rms(prec ) = 0.49062E+00
  weight for this iteration          100.00

 eigenvalues of (default mixing * dielectric matrix)
  average eigenvalue GAMMA=       1.7204
  4.7702    2.5061    1.5519    1.1382    0.7227    0.7227    0.6311
```

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107528.38618568

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1778.38824580

PAW double counting = 54392.98229790 -54455.52857482

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5619.51119457

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1164.99451552 eV

energy without entropy = -1164.99451552 energy(sigma->0) = -1164.99451552

---------- Iteration 1(20) ----------

POTLOK: cpu time 0.1717: real time 0.1924

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9241: real time 1.9304

RMM-DIIS: cpu time 7.1662: real time 7.2026

ORTHCH: cpu time 0.3540: real time 0.3550

DOS: cpu time 0.0003: real time 0.0003

CHARGE: cpu time 0.5243: real time 0.5260

MIXING: cpu time 0.0065: real time 0.0064

LOOP: cpu time 10.1571: real time 10.2232

eigenvalue-minimisations : 1920

total energy-change (2. order) :-0.2247908E+02 (-0.2441003E+01)

number of electron 518.9999724 magnetization 7.3620543

augmentation part 11.7617118 magnetization 6.3297128

Broyden mixing:

rms(total) = 0.24810E+00 rms(broyden)= 0.24782E+00

rms(prec) = 0.25716E+00

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7966

5.8972 2.2502 2.1394 0.9155 0.9155 0.8831 0.7487 0.6235

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107480.16632979

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1761.34690267

PAW double counting = 52534.71371033 -52597.36891073

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5673.05986003

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1187.47359170 eV

energy without entropy = -1187.47359170 energy(sigma->0) = -1187.47359170

---------- Iteration 1(21) ----------

POTLOK: cpu time 0.1683: real time 0.1688

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9287: real time 1.9349

RMM-DIIS: cpu time 7.1825: real time 7.2175

ORTHCH: cpu time 0.3539: real time 0.3548

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5246: real time 0.5264

MIXING: cpu time 0.0068: real time 0.0069

LOOP: cpu time 10.1752: real time 10.2197

eigenvalue-minimisations : 1921

total energy-change (2. order) :-0.6015771E+01 (-0.2269652E+00)

number of electron 518.9999723 magnetization 4.8820893

augmentation part 11.7372508 magnetization 3.8981551

Broyden mixing:

rms(total) = 0.14986E+00 rms(broyden)= 0.14979E+00

rms(prec) = 0.15937E+00

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8615

6.7881 2.3938 2.3938 1.1785 0.9699 0.9699 0.7376 0.6938 0.6286

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107460.83206167

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1755.16201679

PAW double counting = 52318.82739995 -52381.67065872

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5692.03695447

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1193.48936226 eV

energy without entropy = -1193.48936226 energy(sigma->0) = -1193.48936226

---------- Iteration 1(22) ----------

POTLOK: cpu time 0.1701: real time 0.1859

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9344: real time 1.9414

RMM-DIIS: cpu time 7.1579: real time 7.1975

ORTHCH: cpu time 0.3539: real time 0.3550

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5250: real time 0.5270

MIXING: cpu time 0.0071: real time 0.0071

LOOP: cpu time 10.1588: real time 10.2242

eigenvalue-minimisations : 1920

total energy-change (2. order) :-0.3846462E+01 (-0.6217377E-01)

number of electron 518.9999724 magnetization 3.4287927

augmentation part 11.7352339 magnetization 2.4703433

Broyden mixing:

rms(total) = 0.86655E-01 rms(broyden)= 0.86615E-01

rms(prec) = 0.93667E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8605

7.1890 2.5393 2.5393 1.3960 1.0398 1.0398 0.7860 0.7860 0.6611 0.6285

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107425.07434742

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1750.26433371

PAW double counting = 52050.88156602 -52113.79980481

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5726.66846737

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1197.33582402 eV

energy without entropy = -1197.33582402 energy(sigma->0) = -1197.33582402

---------- Iteration 1(23) ----------

POTLOK: cpu time 0.1706: real time 0.1926

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9141: real time 1.9364

RMM-DIIS: cpu time 7.1750: real time 7.2033

ORTHCH: cpu time 0.3556: real time 0.3566

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5233: real time 0.5249

MIXING: cpu time 0.0073: real time 0.0074

LOOP: cpu time 10.1564: real time 10.2317

eigenvalue-minimisations : 1921

total energy-change (2. order) :-0.2277417E+01 (-0.1649966E-01)

number of electron 518.9999724 magnetization 2.4821834

augmentation part 11.7363931 magnetization 1.5330397

Broyden mixing:

rms(total) = 0.55902E-01 rms(broyden)= 0.55891E-01

rms(prec) = 0.60789E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8666

7.3180 2.7694 2.7694 1.6976 1.2155 0.9865 0.9865 0.7529 0.7529 0.6269

0.6565

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107396.52545828

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1747.40461145

PAW double counting = 52022.76870542 -52085.69999667

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5754.62199861

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1199.61324084 eV

energy without entropy = -1199.61324084 energy(sigma->0) = -1199.61324084

---------- Iteration 1(24) ----------

POTLOK: cpu time 0.1680: real time 0.1690

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9282: real time 1.9342

RMM-DIIS: cpu time 7.1698: real time 7.1897

ORTHCH: cpu time 0.3548: real time 0.3558

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5230: real time 0.5246

MIXING: cpu time 0.0078: real time 0.0078

LOOP: cpu time 10.1619: real time 10.1916

eigenvalue-minimisations : 1920

total energy-change (2. order) :-0.1390432E+01 (-0.5353285E-02)

number of electron 518.9999724 magnetization 1.8161170

augmentation part 11.7363030 magnetization 0.8692455

Broyden mixing:

rms(total) = 0.34897E-01 rms(broyden)= 0.34892E-01

rms(prec) = 0.37950E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8827

7.4267 3.5450 2.6389 2.0268 1.2480 1.0550 1.0550 0.8399 0.7469 0.7469

0.6215 0.6422

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107375.59696301

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1745.79516896

PAW double counting = 52128.74863518 -52191.68100635

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5775.33040336

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1201.00367271 eV

energy without entropy = -1201.00367271 energy(sigma->0) = -1201.00367271

---------- Iteration 1(25) ----------

POTLOK: cpu time 0.1679: real time 0.1689

SETDIJ: cpu time 0.0100: real time 0.0100

```
      EDDIAG:    cpu time        1.9250: real time        1.9312
    RMM-DIIS:    cpu time        7.1800: real time        7.2036
      ORTHCH:    cpu time        0.3545: real time        0.3554
         DOS:    cpu time        0.0004: real time        0.0004
      CHARGE:    cpu time        0.5222: real time        0.5241
      MIXING:    cpu time        0.0079: real time        0.0079
      ------------------------------------------
        LOOP:    cpu time       10.1679: real time       10.2015


 eigenvalue-minimisations    :    1920
 total energy-change (2. order) :-0.9019985E+00    (-0.2798415E-02)
 number of electron          518.9999724 magnetization             1.3869764
 augmentation part            11.7364323 magnetization             0.4407608


 Broyden mixing:
   rms(total) = 0.21413E-01        rms(broyden)= 0.21407E-01
   rms(prec ) = 0.23398E-01
   weight for this iteration          100.00


 eigenvalues of (default mixing * dielectric matrix)
   average eigenvalue GAMMA=       1.9142
   7.5661    4.2054    2.5435    2.3925    1.5228    1.1787    1.0030    1.0030    0.7640    0.7640
```

0.6941 0.6341 0.6135

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107359.65007262

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1744.73232841

PAW double counting = 52170.11401385 -52233.03392242

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5791.12891424

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1201.90567116 eV

energy without entropy = -1201.90567116 energy(sigma->0) = -1201.90567116

---------- Iteration 1(26) ----------

POTLOK: cpu time 0.1692: real time 0.1968

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9249: real time 1.9313

RMM-DIIS: cpu time 7.2046: real time 7.2307

ORTHCH: cpu time 0.3540: real time 0.3553

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5225: real time 0.5242

MIXING: cpu time 0.0084: real time 0.0084

LOOP: cpu time 10.1940: real time 10.2572

eigenvalue-minimisations : 1923

total energy-change (2. order) :-0.5321665E+00 (-0.9657343E-03)

number of electron 518.9999723 magnetization 1.1620054

augmentation part 11.7367917 magnetization 0.2160075

Broyden mixing:

rms(total) = 0.11666E-01 rms(broyden)= 0.11660E-01

rms(prec) = 0.13045E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9608

7.7154 4.9104 2.6645 2.6645 1.8366 1.1393 1.1393 0.9758 0.9758 0.7580

0.7580 0.6747 0.6293 0.6101

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107349.79634083

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1744.13353760

PAW double counting = 52180.32743183 -52243.23662334

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5800.92673876

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.43783764 eV

energy without entropy = -1202.43783764 energy(sigma->0) = -1202.43783764

---------- Iteration 1(27) ----------

POTLOK: cpu time 0.1688: real time 0.1723

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9256: real time 1.9326

RMM-DIIS: cpu time 7.1935: real time 7.2203

ORTHCH: cpu time 0.3539: real time 0.3551

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5244: real time 0.5262

MIXING: cpu time 0.0090: real time 0.0090

LOOP: cpu time 10.1858: real time 10.2261

eigenvalue-minimisations : 1921

total energy-change (2. order) :-0.2161649E+00 (-0.4016869E-03)

number of electron 518.9999723 magnetization 1.0647759

augmentation part 11.7367477 magnetization 0.1188298

Broyden mixing:

rms(total) = 0.61180E-02 rms(broyden)= 0.61135E-02

rms(prec) = 0.70995E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9711

7.8207 5.4101 2.7776 2.7776 1.9908 1.3769 1.1214 1.0118 1.0118 0.8593

0.7485 0.7485 0.6753 0.6260 0.6100

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107344.69589719

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.93646677

PAW double counting = 52187.79399261 -52250.70504239

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5806.04441824

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.65400258 eV

energy without entropy = -1202.65400258 energy(sigma->0) = -1202.65400258

---------- Iteration 1(28) ----------

POTLOK: cpu time 0.1775: real time 0.1830

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9276: real time 1.9336

RMM-DIIS: cpu time 7.1730: real time 7.2115

ORTHCH: cpu time 0.3560: real time 0.3572

DOS: cpu time 0.0003: real time 0.0003

CHARGE: cpu time 0.5219: real time 0.5234

MIXING: cpu time 0.0096: real time 0.0097

LOOP: cpu time 10.1759: real time 10.2287

eigenvalue-minimisations : 1923

total energy-change (2. order) :-0.7630373E-01 (-0.1212697E-03)

number of electron 518.9999723 magnetization 1.0187580

augmentation part 11.7367652 magnetization 0.0729141

Broyden mixing:

rms(total) = 0.32173E-02 rms(broyden)= 0.32153E-02

rms(prec) = 0.40464E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9912

7.9282 5.8052 3.0557 2.7471 2.2371 1.6836 1.1838 1.1027 0.9836 0.9836

0.7689 0.7689 0.6973 0.6796 0.6228 0.6111

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107341.79559049

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.86152718

PAW double counting = 52181.15784311 -52244.07419286

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5808.94078911

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.73030631 eV

energy without entropy = -1202.73030631 energy(sigma->0) = -1202.73030631

---------- Iteration 1(29) ----------

POTLOK: cpu time 0.1733: real time 0.1964

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9250: real time 1.9341

RMM-DIIS: cpu time 7.2538: real time 7.2856

ORTHCH: cpu time 0.3545: real time 0.3557

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5229: real time 0.5247

MIXING: cpu time 0.0104: real time 0.0104

LOOP: cpu time 10.2504: real time 10.3175

eigenvalue-minimisations : 1931

total energy-change (2. order) :-0.3135074E-01 (-0.4043497E-04)

number of electron 518.9999723 magnetization 1.0074543

augmentation part 11.7368788 magnetization 0.0616848

Broyden mixing:

rms(total) = 0.15439E-02 rms(broyden)= 0.15429E-02

rms(prec) = 0.22919E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9913

7.9769 6.0692 3.3946 2.5652 2.5652 1.7938 1.3458 1.0473 1.0473 0.9776

0.9776 0.7592 0.7592 0.6693 0.6693 0.6229 0.6114

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107339.91903463

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.82392225

PAW double counting = 52176.27049065 -52239.18831157

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5810.80961959

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76165705 eV

energy without entropy = -1202.76165705 energy(sigma->0) = -1202.76165705

---------- Iteration 1(30) ----------

POTLOK: cpu time 0.1682: real time 0.1711

SETDIJ: cpu time 0.0129: real time 0.0129

EDDIAG: cpu time 1.9273: real time 1.9340

RMM-DIIS: cpu time 7.2982: real time 7.3234

ORTHCH: cpu time 0.3547: real time 0.3560

DOS: cpu time 0.0003: real time 0.0003

CHARGE: cpu time 0.5226: real time 0.5242

MIXING: cpu time 0.0104: real time 0.0104

LOOP: cpu time 10.2946: real time 10.3322

eigenvalue-minimisations : 1938

total energy-change (2. order) :-0.7418754E-02 (-0.1043906E-04)

number of electron 518.9999723 magnetization 1.0040893

augmentation part 11.7369592 magnetization 0.0583134

Broyden mixing:

rms(total) = 0.90440E-03 rms(broyden)= 0.90392E-03

rms(prec) = 0.15000E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9781

7.9866 6.2192 3.5364 2.6619 2.6619 1.8908 1.4758 1.2631 0.9992 0.9992

1.0021 0.8553 0.7512 0.7512 0.6562 0.6562 0.6125 0.6259

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107338.79532071

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81379259

PAW double counting = 52176.75708908 -52239.67510362

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5811.93042899

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76907580 eV

energy without entropy = -1202.76907580 energy(sigma->0) = -1202.76907580

---------- Iteration 1(31) ----------

POTLOK: cpu time 0.1658: real time 0.1668

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9251: real time 1.9320

RMM-DIIS: cpu time 7.1953: real time 7.2300

ORTHCH: cpu time 0.3541: real time 0.3554

DOS: cpu time 0.0003: real time 0.0003

CHARGE: cpu time 0.5213: real time 0.5231

MIXING: cpu time 0.0107: real time 0.0108

LOOP: cpu time 10.1827: real time 10.2284

eigenvalue-minimisations : 1926

total energy-change (2. order) :-0.9633148E-03 (-0.2475593E-05)

number of electron 518.9999723 magnetization 0.9996549

augmentation part 11.7370307 magnetization 0.0538903

Broyden mixing:

rms(total) = 0.60538E-03 rms(broyden)= 0.60505E-03

rms(prec) = 0.10420E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9635

7.9958 6.2692 3.6840 2.7397 2.7397 1.9735 1.7519 1.1702 1.1702 1.0406

0.9755 0.9755 0.7614 0.7614 0.7518 0.6697 0.6139 0.6313 0.6313

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107337.98021789

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80645195

PAW double counting = 52176.21282522 -52239.13122311

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5812.73877114

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77003911 eV

energy without entropy = -1202.77003911 energy(sigma->0) = -1202.77003911

---------- Iteration 1(32) ----------

POTLOK: cpu time 0.1695: real time 0.1977

SETDIJ: cpu time 0.0099: real time 0.0099

EDDIAG: cpu time 1.9291: real time 1.9354

RMM-DIIS: cpu time 7.1756: real time 7.1986

ORTHCH: cpu time 0.3561: real time 0.3572

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5215: real time 0.5231

MIXING: cpu time 0.0115: real time 0.0115

LOOP: cpu time 10.1738: real time 10.2338

eigenvalue-minimisations : 1920

total energy-change (2. order) :-0.3996028E-03 (-0.1591722E-05)

number of electron 518.9999723 magnetization 0.9989696

augmentation part 11.7370934 magnetization 0.0532232

Broyden mixing:

rms(total) = 0.41892E-03 rms(broyden)= 0.41858E-03

rms(prec) = 0.66842E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9756

7.9990 6.3261 4.0079 2.8835 2.8835 2.1514 1.9534 1.3239 1.3239 1.0293

1.0293 0.9220 0.9220 0.7562 0.7562 0.7065 0.6651 0.6145 0.6296 0.6296

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107337.20981452

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80042579

PAW double counting = 52176.03241224 -52238.95094585

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.50341224

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77043872 eV

energy without entropy = -1202.77043872 energy(sigma->0) = -1202.77043872

---------- Iteration 1(33) ----------

POTLOK: cpu time 0.1702: real time 0.1850

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9262: real time 1.9328

RMM-DIIS: cpu time 7.0565: real time 7.0910

ORTHCH: cpu time 0.3560: real time 0.3569

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5239: real time 0.5255

MIXING: cpu time 0.0114: real time 0.0114

LOOP: cpu time 10.0547: real time 10.1131

eigenvalue-minimisations : 1905

total energy-change (2. order) :-0.2601544E-03 (-0.8083856E-06)

number of electron 518.9999723 magnetization 0.9996984

augmentation part 11.7371163 magnetization 0.0539585

Broyden mixing:

rms(total) = 0.26943E-03 rms(broyden)= 0.26923E-03

rms(prec) = 0.41380E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9835

7.9946 6.3932 4.4348 3.0115 3.0115 2.3369 1.9837 1.5677 1.2099 1.2099

1.0037 1.0037 0.8799 0.8799 0.7528 0.7528 0.6956 0.6146 0.6549 0.6288

0.6329

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107336.70114258

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79887902

PAW double counting = 52176.74389101 -52239.66244722

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.01077496

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77069887 eV

energy without entropy = -1202.77069887 energy(sigma->0) = -1202.77069887

---------- Iteration 1(34) ----------

POTLOK: cpu time 0.1688: real time 0.1708

SETDIJ: cpu time 0.0099: real time 0.0099

EDDIAG: cpu time 1.9256: real time 1.9325

RMM-DIIS: cpu time 6.4971: real time 6.5284

ORTHCH: cpu time 0.3530: real time 0.3542

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.4805: real time 0.5304

MIXING: cpu time 0.0111: real time 0.0112

LOOP: cpu time 9.4464: real time 9.5378

eigenvalue-minimisations : 1793

total energy-change (2. order) :-0.4183618E-03 (-0.4915493E-06)

number of electron 518.9999723 magnetization 0.9993478

augmentation part 11.7371271 magnetization 0.0536153

Broyden mixing:

rms(total) = 0.16952E-03 rms(broyden)= 0.16939E-03

rms(prec) = 0.24860E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0128

7.9986 6.4847 5.2064 3.3284 2.8447 2.5972 1.9942 1.8150 1.2970 1.2970

1.0356 1.0356 0.9261 0.9261 0.7586 0.7586 0.7573 0.7016 0.6153 0.6228

0.6406 0.6406

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107336.33783538

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79747825

PAW double counting = 52176.76241682 -52239.68108251

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.37299027

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77111723 eV

energy without entropy = -1202.77111723 energy(sigma->0) = -1202.77111723

---------- Iteration 1(35) ----------

POTLOK: cpu time 0.1695: real time 0.1724

SETDIJ: cpu time 0.0099: real time 0.0099

EDDIAG: cpu time 1.9257: real time 1.9326

RMM-DIIS: cpu time 6.3972: real time 6.4315

ORTHCH: cpu time 0.3547: real time 0.3559

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5244: real time 0.5261

MIXING: cpu time 0.0116: real time 0.0117

LOOP: cpu time 9.3934: real time 9.4405

eigenvalue-minimisations : 1756

total energy-change (2. order) :-0.2705514E-03 (-0.3666622E-06)

number of electron 518.9999723 magnetization 0.9994705

augmentation part 11.7371366 magnetization 0.0537458

Broyden mixing:

rms(total) = 0.90969E-04 rms(broyden)= 0.90868E-04

rms(prec) = 0.13439E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0571

8.0056 6.9275 5.9855 3.5859 2.8690 2.7255 2.2461 1.8675 1.4614 1.1987

1.1987 1.0144 1.0144 0.8870 0.8870 0.7559 0.7559 0.7347 0.6805 0.6162

0.6226 0.6397 0.6333

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107336.10106619

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79667318

PAW double counting = 52176.69265360 -52239.61139613

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.60914809

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77138778 eV

energy without entropy = -1202.77138778 energy(sigma->0) = -1202.77138778

---------- Iteration 1(36) ----------

POTLOK: cpu time 0.1697: real time 0.1872

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9271: real time 1.9332

RMM-DIIS: cpu time 6.0623: real time 6.0913

ORTHCH: cpu time 0.3540: real time 0.3551

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5236: real time 0.5252

MIXING: cpu time 0.0125: real time 0.0125

LOOP: cpu time 9.0595: real time 9.1150

eigenvalue-minimisations : 1673

total energy-change (2. order) :-0.6923552E-04 (-0.8366979E-07)

number of electron 518.9999723 magnetization 0.9997405

augmentation part 11.7371376 magnetization 0.0540153

Broyden mixing:

rms(total) = 0.50469E-04 rms(broyden)= 0.50424E-04

rms(prec) = 0.77252E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0667

7.9959 7.5413 6.1436 3.7490 2.9506 2.7200 2.3906 1.8042 1.6345 1.2397

1.2397 1.0287 1.0287 0.9243 0.9243 0.8744 0.7543 0.7543 0.7272 0.6614

0.6543 0.6167 0.6213 0.6213

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107335.99953872

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79676887

PAW double counting = 52176.81208529 -52239.73088500

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.71078331

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77145702 eV

energy without entropy = -1202.77145702 energy(sigma->0) = -1202.77145702

---------- Iteration 1(37) ----------

POTLOK: cpu time 0.1742: real time 0.1810

SETDIJ: cpu time 0.0099: real time 0.0099

EDDIAG: cpu time 1.9262: real time 1.9325

RMM-DIIS: cpu time 5.4986: real time 5.5204

ORTHCH: cpu time 0.3530: real time 0.3539

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5235: real time 0.5254

MIXING: cpu time 0.0124: real time 0.0125

LOOP: cpu time 8.4982: real time 8.5360

eigenvalue-minimisations : 1518

total energy-change (2. order) :-0.8873205E-05 (-0.2240760E-07)

number of electron 518.9999723 magnetization 0.9998117

augmentation part 11.7371385 magnetization 0.0540852

Broyden mixing:

rms(total) = 0.31392E-04 rms(broyden)= 0.31372E-04

rms(prec) = 0.48504E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0706

7.9829 7.9829 6.2014 3.8578 3.0420 2.7016 2.4969 1.8805 1.8805 1.2451

1.2451 1.2391 1.0212 1.0212 0.8968 0.8968 0.7611 0.7611 0.7714 0.7176

0.6523 0.6523 0.6182 0.6182 0.6204

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107335.95155523

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79664123

PAW double counting = 52176.81515383 -52239.73397247

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.75862911

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77146589 eV

energy without entropy = -1202.77146589 energy(sigma->0) = -1202.77146589

---------- Iteration 1(38) ----------

POTLOK: cpu time 0.1706: real time 0.1774

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9274: real time 1.9344

RMM-DIIS: cpu time 5.2430: real time 5.2701

ORTHCH: cpu time 0.3543: real time 0.3554

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5238: real time 0.5256

MIXING: cpu time 0.0131: real time 0.0132

LOOP: cpu time 8.2425: real time 8.2865

eigenvalue-minimisations : 1437

total energy-change (2. order) :-0.4445072E-05 (-0.9338061E-08)

number of electron 518.9999723 magnetization 0.9999245

augmentation part 11.7371406 magnetization 0.0541983

Broyden mixing:

rms(total) = 0.20919E-04 rms(broyden)= 0.20905E-04

rms(prec) = 0.31789E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0666

8.1027 8.1027 6.2181 3.9574 3.1961 2.6452 2.6452 1.9964 1.9964 1.3329

1.3329 1.1482 1.1482 1.0112 1.0112 0.8794 0.8794 0.7577 0.7577 0.7612

0.6990 0.6497 0.6497 0.6145 0.6198 0.6198

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107335.92503541

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79641312

PAW double counting = 52176.80420244 -52239.72300777

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.78493857

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77147034 eV

energy without entropy = -1202.77147034 energy(sigma->0) = -1202.77147034

---------- Iteration 1(39) ----------

POTLOK: cpu time 0.1701: real time 0.1821

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9317: real time 1.9383

RMM-DIIS: cpu time 5.1461: real time 5.1646

ORTHCH: cpu time 0.3541: real time 0.3550

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5244: real time 0.5263

MIXING: cpu time 0.0134: real time 0.0134

LOOP: cpu time 8.1503: real time 8.1900

eigenvalue-minimisations : 1402

total energy-change (2. order) :-0.4926915E-05 (-0.5438121E-08)

number of electron 518.9999723 magnetization 0.9999848

augmentation part 11.7371417 magnetization 0.0542584

Broyden mixing:

rms(total) = 0.13508E-04 rms(broyden)= 0.13498E-04

rms(prec) = 0.19766E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0709

8.3031 8.0755 6.2268 4.1292 3.3724 2.7669 2.7669 2.1025 2.1025 1.5574

1.4047 1.1788 1.1788 1.0154 1.0154 0.9016 0.9016 0.8305 0.7586 0.7586

0.7391 0.6832 0.6463 0.6463 0.6229 0.6135 0.6167

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107335.91017291

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79630335

PAW double counting = 52176.82772319 -52239.74652447

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.79970027

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77147527 eV

energy without entropy = -1202.77147527 energy(sigma->0) = -1202.77147527

---------- Iteration 1(40) ----------

POTLOK: cpu time 0.1697: real time 0.1874

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9276: real time 1.9341

RMM-DIIS: cpu time 5.0390: real time 5.0634

ORTHCH: cpu time 0.3567: real time 0.3578

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5248: real time 0.5265

MIXING: cpu time 0.0145: real time 0.0145

LOOP: cpu time 8.0427: real time 8.0942

eigenvalue-minimisations : 1379

total energy-change (2. order) :-0.3339424E-05 (-0.3272575E-08)

number of electron 518.9999723 magnetization 0.9999873

augmentation part 11.7371423 magnetization 0.0542609

Broyden mixing:

rms(total) = 0.87280E-05 rms(broyden)= 0.87220E-05

rms(prec) = 0.12429E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0776

8.4403 8.0564 6.2379 4.4684 3.6043 2.8651 2.8651 2.2538 2.1186 1.6922

1.4394 1.2102 1.2102 1.0868 1.0160 1.0160 0.8817 0.8817 0.7597 0.7597

0.7835 0.7160 0.6731 0.6459 0.6348 0.6287 0.6130 0.6130

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107335.90344927

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79624664

PAW double counting = 52176.83057773 -52239.74938493

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.80636463

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77147860 eV

energy without entropy = -1202.77147860 energy(sigma->0) = -1202.77147860

---------- Iteration 1(41) ----------

POTLOK: cpu time 0.1699: real time 0.1823

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9285: real time 1.9349

RMM-DIIS: cpu time 4.9472: real time 4.9642

ORTHCH: cpu time 0.3539: real time 0.3549

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5237: real time 0.5256

MIXING: cpu time 0.0143: real time 0.0143

LOOP: cpu time 7.9480: real time 7.9867

eigenvalue-minimisations : 1349

total energy-change (2. order) :-0.2025554E-05 (-0.1765465E-08)

number of electron 518.9999723 magnetization 0.9999944

augmentation part 11.7371428 magnetization 0.0542681

Broyden mixing:

rms(total) = 0.54637E-05 rms(broyden)= 0.54601E-05

rms(prec) = 0.78213E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0999

8.5633 8.0497 6.2631 5.2176 3.8124 2.9325 2.9325 2.3727 2.2016 1.8256

1.5699 1.2330 1.2330 1.2032 1.0215 1.0215 0.9128 0.9128 0.8578 0.7601

0.7601 0.7475 0.7119 0.6573 0.6499 0.6249 0.6249 0.6169 0.6083

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107335.90146402

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79622908

PAW double counting = 52176.82928856 -52239.74810012

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.80832999

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77148063 eV

energy without entropy = -1202.77148063 energy(sigma->0) = -1202.77148063

---------- Iteration 1(42) ----------

POTLOK: cpu time 0.1664: real time 0.1672

SETDIJ: cpu time 0.0086: real time 0.0133

EDDIAG: cpu time 1.9333: real time 1.9469

RMM-DIIS: cpu time 4.8015: real time 4.8328

ORTHCH: cpu time 0.3586: real time 0.3598

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5264: real time 0.5280

MIXING: cpu time 0.0151: real time 0.0152

LOOP: cpu time 7.8102: real time 7.8637

eigenvalue-minimisations : 1314

total energy-change (2. order) :-0.1568340E-05 (-0.9289280E-09)

number of electron 518.9999723 magnetization 1.0000019

augmentation part 11.7371431 magnetization 0.0542757

Broyden mixing:

rms(total) = 0.33577E-05 rms(broyden)= 0.33552E-05

rms(prec) = 0.48066E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.1044

8.6735 8.0455 6.3433 5.8185 3.9011 2.9660 2.9660 2.5001 2.2229 1.9580

1.5833 1.3741 1.2090 1.2090 1.0228 1.0228 1.0042 0.8872 0.8872 0.8100

0.7626 0.7626 0.7475 0.6913 0.6532 0.6454 0.6296 0.6156 0.6156 0.6043

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107335.90163131

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79623707

PAW double counting = 52176.83166797 -52239.75048227

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.80816951

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77148220 eV

energy without entropy = -1202.77148220 energy(sigma->0) = -1202.77148220

---------- Iteration 1(43) ----------

POTLOK: cpu time 0.1679: real time 0.1691

SETDIJ: cpu time 0.0099: real time 0.0100

```
      EDDIAG:  cpu time        1.9252: real time        1.9311
 RMM-DIIS:  cpu time        4.5777: real time        4.5952
      ORTHCH:  cpu time        0.3533: real time        0.3543
         DOS:  cpu time        0.0004: real time        0.0004
      CHARGE:  cpu time        0.5243: real time        0.5259
      MIXING:  cpu time        0.0155: real time        0.0156
      ----------------------------------------------
        LOOP:  cpu time        7.5743: real time        7.6014

eigenvalue-minimisations  :  1175
total energy-change (2. order) :-0.3885943E-06  (-0.3893952E-09)
number of electron       518.9999723 magnetization             1.0000012
augmentation part         11.7371432 magnetization             0.0542750

Broyden mixing:
 rms(total) = 0.22296E-05        rms(broyden)= 0.22286E-05
 rms(prec ) = 0.31539E-05
 weight for this iteration         100.00

eigenvalues of (default mixing * dielectric matrix)
 average eigenvalue GAMMA=      2.1127
 8.7637   8.0390   6.5749   6.0687   3.9787   2.9883   2.9883   2.6615   2.2201   2.1514
```

1.5973 1.5973 1.2493 1.2493 1.1328 1.0218 1.0218 0.9574 0.8884 0.8884

0.7604 0.7604 0.7791 0.7291 0.6761 0.6518 0.6383 0.6304 0.6150 0.6150

0.6007

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107335.90235380

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79624880

PAW double counting = 52176.83226743 -52239.75108293

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.80745794

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77148259 eV

energy without entropy = -1202.77148259 energy(sigma->0) = -1202.77148259

---------- Iteration 1(44) ----------

POTLOK: cpu time 0.1681: real time 0.1863

SETDIJ: cpu time 0.0099: real time 0.0100

EDDIAG: cpu time 1.9231: real time 1.9298

RMM-DIIS: cpu time 4.4219: real time 4.4458

ORTHCH: cpu time 0.3568: real time 0.3578

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5239: real time 0.5256

MIXING: cpu time 0.0165: real time 0.0166

LOOP: cpu time 7.4207: real time 7.4723

eigenvalue-minimisations : 1076

total energy-change (2. order) :-0.1673689E-06 (-0.1918137E-09)

number of electron 518.9999723 magnetization 0.9999988

augmentation part 11.7371432 magnetization 0.0542726

Broyden mixing:

rms(total) = 0.11806E-05 rms(broyden)= 0.11795E-05

rms(prec) = 0.15864E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.1332

8.8850 8.0266 7.0198 6.1536 4.1491 3.4345 2.8760 2.8760 2.3982 2.2007

1.8256 1.5923 1.3052 1.2078 1.2078 1.0222 1.0222 1.0212 0.9140 0.8645

0.8645 0.7617 0.7617 0.7583 0.7109 0.6574 0.6574 0.6279 0.6279 0.6211

0.6110 0.5989

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107335.90344119

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79626514

PAW double counting = 52176.83292890 -52239.75174485

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.80638662

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77148275 eV

energy without entropy = -1202.77148275 energy(sigma->0) = -1202.77148275

---------- Iteration 1(45) ----------

POTLOK: cpu time 0.1697: real time 0.1839

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9274: real time 1.9328

RMM-DIIS: cpu time 4.1690: real time 4.1951

ORTHCH: cpu time 0.3547: real time 0.3555

DOS: cpu time 0.0003: real time 0.0003

LOOP: cpu time 6.6312: real time 6.6777

eigenvalue-minimisations : 964

total energy-change (2. order) :-0.2403976E-07 (-0.1167271E-09)

number of electron 518.9999723 magnetization 0.9999988

augmentation part 11.7371432 magnetization 0.0542726

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23020906

-Hartree energ DENC = -107335.90390815

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79627221

PAW double counting = 52176.83304683 -52239.75186274

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.80592679

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77148278 eV

energy without entropy = -1202.77148278 energy(sigma->0) = -1202.77148278

---

average (electrostatic) potential at core

the test charge radii are 0.5201 0.6991 1.0621 0.7215

(the norm of the test charge is 1.0000)

1 -40.7528	2 -40.7507	3 -40.7521	4 -40.7508	5 -40.7528
6 -40.7550	7 -40.7525	8 -40.7603	9 -40.7521	10 -40.7597
11 -40.7535	12 -40.7555	13 -40.6502	14 -40.6961	15 -40.7700
16 -40.6982	17 -40.6921	18 -40.8606	19 -40.6792	20 -40.6671
21 -40.6886	22 -40.6616	23 -40.0851	24 -40.1279	25 -57.4589
26 -57.6700	27 -57.6569	28 -57.4688	29 -57.6636	30 -57.4589
31 -57.6698	32 -57.6565	33 -57.4667	34 -57.6684	35 -57.4597
36 -57.6717	37 -57.6565	38 -57.4690	39 -57.6743	40 -57.4587

41 -57.6757	42 -57.6567	43 -57.4739	44 -57.6889	45 -57.4587
46 -57.6746	47 -57.6575	48 -57.4741	49 -57.6800	50 -57.4599
51 -57.6713	52 -57.6572	53 -57.4717	54 -57.6663	55 -57.6367
56 -57.6628	57 -57.6871	58 -57.6834	59 -57.6665	60 -57.6693
61 -57.6902	62 -57.6749	63 -57.6370	64 -57.6622	65 -57.6892
66 -57.6949	67 -57.6647	68 -57.6691	69 -57.6939	70 -57.7012
71 -57.6365	72 -57.6636	73 -57.6968	74 -57.7219	75 -57.6656
76 -57.6697	77 -57.7062	78 -57.7515	79 -57.6367	80 -57.6662
81 -57.7106	82 -57.7523	83 -57.6689	84 -57.6712	85 -57.7376
86 -57.8417	87 -57.6391	88 -57.6669	89 -57.7125	90 -57.7172
91 -57.6736	92 -57.6714	93 -57.7423	94 -57.7598	95 -57.6374
96 -57.6651	97 -57.6962	98 -57.6908	99 -57.6709	100 -57.6702
101 -57.7080	102 -57.6860	103 -57.6603	104 -57.6309	105 -57.6457
106 -57.2901	107 -57.3881	108 -57.6312	109 -57.5976	110 -57.6592
111 -57.6309	112 -57.6423	113 -57.3091	114 -57.3938	115 -57.6305
116 -57.5995	117 -57.6585	118 -57.6226	119 -57.6982	120 -57.6833
121 -57.3874	122 -57.6293	123 -57.7095	124 -57.6594	125 -57.6254
126 -57.8335	127 -58.3289	128 -57.3607	129 -57.6346	130 -58.1438
131 -57.6674	132 -57.6346	133 -57.8009	134 -57.4165	135 -57.3720
136 -57.6385	137 -58.0783	138 -57.6638	139 -57.6304	140 -57.6714
141 -57.2993	142 -57.3782	143 -57.6338	144 -57.6478	145 -60.8466
146 -57.3145	147 -81.2713			

E-fermi : -2.3578 XC(G=0): -2.7341 alpha+bet : -2.2521

spin component 1

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-26.9864	1.00000
2	-21.5687	1.00000
3	-21.4717	1.00000
4	-21.0998	1.00000
5	-21.0688	1.00000
6	-21.0149	1.00000
7	-20.9789	1.00000
8	-20.9769	1.00000
9	-20.8913	1.00000
10	-20.5579	1.00000
11	-20.5035	1.00000
12	-20.4118	1.00000

13	-20.3982	1.00000
14	-20.1266	1.00000
15	-19.9760	1.00000
16	-19.7035	1.00000
17	-19.6277	1.00000
18	-19.5998	1.00000
19	-19.5841	1.00000
20	-19.5288	1.00000
21	-19.5271	1.00000
22	-19.4988	1.00000
23	-19.4813	1.00000
24	-19.1121	1.00000
25	-19.0755	1.00000
26	-18.9787	1.00000
27	-18.9650	1.00000
28	-18.9008	1.00000
29	-18.7337	1.00000
30	-18.5049	1.00000
31	-18.3593	1.00000
32	-18.2755	1.00000
33	-18.2523	1.00000
34	-18.1838	1.00000

35	-18.1817	1.00000
36	-18.0800	1.00000
37	-18.0762	1.00000
38	-17.5619	1.00000
39	-17.3135	1.00000
40	-17.2878	1.00000
41	-17.2829	1.00000
42	-17.2102	1.00000
43	-17.2037	1.00000
44	-17.1770	1.00000
45	-17.0230	1.00000
46	-16.9505	1.00000
47	-16.9328	1.00000
48	-16.8934	1.00000
49	-16.8915	1.00000
50	-16.8503	1.00000
51	-16.8419	1.00000
52	-16.8213	1.00000
53	-16.8191	1.00000
54	-16.7296	1.00000
55	-16.7264	1.00000
56	-16.1777	1.00000

57	-15.7298	1.00000
58	-15.6923	1.00000
59	-15.6606	1.00000
60	-15.6373	1.00000
61	-15.6164	1.00000
62	-15.5539	1.00000
63	-15.5500	1.00000
64	-15.1754	1.00000
65	-14.8101	1.00000
66	-14.6086	1.00000
67	-14.5783	1.00000
68	-14.5351	1.00000
69	-14.4985	1.00000
70	-14.4688	1.00000
71	-14.4426	1.00000
72	-14.3341	1.00000
73	-14.3058	1.00000
74	-14.2799	1.00000
75	-14.2723	1.00000
76	-14.1827	1.00000
77	-14.1788	1.00000
78	-13.8905	1.00000

79	-13.7601	1.00000
80	-13.5938	1.00000
81	-13.5486	1.00000
82	-13.5296	1.00000
83	-13.4980	1.00000
84	-13.4461	1.00000
85	-13.3643	1.00000
86	-13.3457	1.00000
87	-13.1891	1.00000
88	-12.7866	1.00000
89	-12.7597	1.00000
90	-12.7275	1.00000
91	-12.6963	1.00000
92	-12.6865	1.00000
93	-12.6242	1.00000
94	-12.4613	1.00000
95	-12.4465	1.00000
96	-12.3821	1.00000
97	-12.3242	1.00000
98	-12.2132	1.00000
99	-12.2036	1.00000
100	-12.1653	1.00000

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spin component 2

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260	-2.0606	0.00000
261	-1.9145	0.00000
262	-1.7226	0.00000
263	-1.6789	0.00000
264	-1.2917	0.00000
265	-1.2791	0.00000
266	-1.1571	0.00000
267	-0.7232	0.00000
268	-0.5839	0.00000
269	-0.5094	0.00000
270	-0.2807	0.00000
271	-0.2777	0.00000
272	-0.2599	0.00000
273	-0.1564	0.00000
274	-0.0577	0.00000
275	-0.0482	0.00000

276	0.0134	0.00000
277	0.0401	0.00000
278	0.0793	0.00000
279	0.2082	0.00000
280	0.2556	0.00000
281	0.2797	0.00000
282	0.4341	0.00000
283	0.4520	0.00000
284	0.4830	0.00000
285	0.6024	0.00000
286	0.6951	0.00000
287	0.8215	0.00000
288	0.8799	0.00000
289	1.0559	0.00000
290	1.1054	0.00000
291	1.1422	0.00000
292	1.1770	0.00000
293	1.2319	0.00000
294	1.2503	0.00000
295	1.3088	0.00000
296	1.3197	0.00000
297	1.3601	0.00000

298	1.4307	0.00000
299	1.4785	0.00000
300	1.5006	0.00000
301	1.5775	0.00000
302	1.6029	0.00000
303	1.6530	0.00000
304	1.6864	0.00000
305	1.7582	0.00000
306	1.7733	0.00000
307	1.8776	0.00000
308	1.8999	0.00000
309	1.9080	0.00000
310	1.9214	0.00000
311	2.1394	0.00000
312	2.1980	0.00000
313	2.2200	0.00000
314	2.2536	0.00000
315	2.2895	0.00000
316	2.2964	0.00000
317	2.3369	0.00000
318	2.3612	0.00000
319	2.3828	0.00000

320	2.4080	0.00000
321	2.4285	0.00000
322	2.4353	0.00000
323	2.4508	0.00000
324	2.4582	0.00000
325	2.4670	0.00000
326	2.5263	0.00000
327	2.5441	0.00000
328	2.7062	0.00000
329	2.7346	0.00000
330	2.7532	0.00000
331	2.7592	0.00000
332	2.7735	0.00000
333	2.8290	0.00000
334	2.8470	0.00000
335	2.8719	0.00000
336	2.9023	0.00000
337	2.9325	0.00000
338	2.9558	0.00000
339	2.9837	0.00000
340	3.0070	0.00000
341	3.0382	0.00000

342	3.0509	0.00000
343	3.0719	0.00000
344	3.0924	0.00000
345	3.1526	0.00000
346	3.1710	0.00000
347	3.1883	0.00000
348	3.1998	0.00000
349	3.3069	0.00000
350	3.3273	0.00000
351	3.3607	0.00000
352	3.3708	0.00000
353	3.3927	0.00000
354	3.4381	0.00000
355	3.4816	0.00000
356	3.4916	0.00000
357	3.4941	0.00000
358	3.5048	0.00000
359	3.6392	0.00000
360	3.6768	0.00000
361	3.6994	0.00000
362	3.7381	0.00000
363	3.7550	0.00000

364	3.7605	0.00000
365	3.7773	0.00000
366	3.7985	0.00000
367	3.8147	0.00000
368	3.8410	0.00000
369	3.8473	0.00000
370	3.8660	0.00000
371	3.8803	0.00000
372	3.8931	0.00000
373	3.9209	0.00000
374	3.9357	0.00000
375	3.9485	0.00000
376	3.9593	0.00000
377	3.9827	0.00000
378	3.9863	0.00000
379	4.0219	0.00000
380	4.0782	0.00000
381	4.1708	0.00000
382	4.2591	0.00000
383	4.2621	0.00000
384	4.2692	0.00000
385	4.2929	0.00000

386	4.3213	0.00000
387	4.3343	0.00000
388	4.3505	0.00000
389	4.3810	0.00000
390	4.3858	0.00000
391	4.4232	0.00000
392	4.4487	0.00000
393	4.4740	0.00000
394	4.4831	0.00000
395	4.4927	0.00000
396	4.4993	0.00000
397	4.5207	0.00000
398	4.5552	0.00000
399	4.5936	0.00000
400	4.6107	0.00000
401	4.6290	0.00000
402	4.6462	0.00000
403	4.6598	0.00000
404	4.6854	0.00000
405	4.7087	0.00000
406	4.7373	0.00000
407	4.7514	0.00000

408	4.7704	0.00000
409	4.7867	0.00000
410	4.7892	0.00000
411	4.8029	0.00000
412	4.8331	0.00000
413	4.8682	0.00000
414	4.8849	0.00000
415	4.9030	0.00000
416	4.9420	0.00000
417	4.9934	0.00000
418	5.0099	0.00000
419	5.0135	0.00000
420	5.0388	0.00000
421	5.0445	0.00000
422	5.0690	0.00000
423	5.0860	0.00000
424	5.1177	0.00000
425	5.1217	0.00000
426	5.1411	0.00000
427	5.1441	0.00000
428	5.1703	0.00000
429	5.1799	0.00000

430	5.1889	0.00000
431	5.1930	0.00000
432	5.2207	0.00000
433	5.2380	0.00000
434	5.2444	0.00000
435	5.2617	0.00000
436	5.3004	0.00000
437	5.3034	0.00000
438	5.3124	0.00000
439	5.3369	0.00000
440	5.3536	0.00000
441	5.3713	0.00000
442	5.3817	0.00000
443	5.3962	0.00000
444	5.4302	0.00000
445	5.4614	0.00000
446	5.4722	0.00000
447	5.4890	0.00000
448	5.5006	0.00000
449	5.5274	0.00000
450	5.5708	0.00000
451	5.5771	0.00000

452	5.5987	0.00000
453	5.6098	0.00000
454	5.6273	0.00000
455	5.6747	0.00000
456	5.6984	0.00000
457	5.7285	0.00000
458	5.7393	0.00000
459	5.7573	0.00000
460	5.7771	0.00000
461	5.7988	0.00000
462	5.8024	0.00000
463	5.8133	0.00000
464	5.8283	0.00000
465	5.8353	0.00000
466	5.8528	0.00000
467	5.8814	0.00000
468	5.8880	0.00000
469	5.9013	0.00000
470	5.9084	0.00000
471	5.9176	0.00000
472	5.9384	0.00000
473	5.9598	0.00000

474	5.9662	0.00000
475	5.9969	0.00000
476	6.0289	0.00000
477	6.0602	0.00000
478	6.1350	0.00000
479	6.1710	0.00000
480	6.2339	0.00000

---

soft charge-density along one line, spin component 1

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

soft charge-density along one line, spin component 2

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

pseudopotential strength for first ion, spin component: 1

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

pseudopotential strength for first ion, spin component: 2

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

total augmentation occupancy for first ion, spin component: 1

3.579 -0.646 0.444 -0.034 -0.000

-0.646 0.130 -0.082 0.006 0.000

0.444 -0.082 0.056 -0.003 -0.000

-0.034 0.006 -0.003 0.011 0.000

-0.000 0.000 -0.000 0.000 0.007

total augmentation occupancy for first ion, spin component: 2

-0.000 0.000 -0.000 0.000 0.000

0.000 -0.000 0.000 -0.000 -0.000

-0.000 0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

---------- aborting loop because EDIFF is reached ----------

total charge

# of ion	s	p	d	tot
1	0.646	0.043	0.000	0.690
2	0.646	0.043	0.000	0.690
3	0.646	0.043	0.000	0.690
4	0.646	0.043	0.000	0.690
5	0.646	0.043	0.000	0.690
6	0.646	0.043	0.000	0.690
7	0.646	0.043	0.000	0.690
8	0.646	0.043	0.000	0.690

9	0.646	0.043	0.000	0.690
10	0.646	0.043	0.000	0.690
11	0.646	0.043	0.000	0.690
12	0.646	0.043	0.000	0.690
13	0.646	0.043	0.000	0.689
14	0.646	0.043	0.000	0.689
15	0.648	0.045	0.000	0.693
16	0.646	0.043	0.000	0.689
17	0.646	0.043	0.000	0.689
18	0.646	0.043	0.000	0.689
19	0.646	0.043	0.000	0.689
20	0.646	0.043	0.000	0.689
21	0.646	0.043	0.000	0.689
22	0.646	0.044	0.000	0.690
23	0.541	0.015	0.000	0.557
24	0.541	0.015	0.000	0.556
25	0.870	1.763	0.000	2.633
26	0.867	1.785	0.000	2.653
27	0.867	1.786	0.000	2.653
28	0.870	1.762	0.000	2.632
29	0.865	1.783	0.000	2.648
30	0.870	1.763	0.000	2.633

31	0.867	1.786	0.000	2.653
32	0.867	1.786	0.000	2.653
33	0.870	1.762	0.000	2.632
34	0.865	1.783	0.000	2.648
35	0.870	1.763	0.000	2.633
36	0.868	1.787	0.000	2.654
37	0.867	1.786	0.000	2.653
38	0.870	1.763	0.000	2.633
39	0.865	1.784	0.000	2.649
40	0.870	1.763	0.000	2.633
41	0.868	1.787	0.000	2.655
42	0.867	1.786	0.000	2.653
43	0.871	1.764	0.000	2.634
44	0.865	1.783	0.000	2.648
45	0.870	1.763	0.000	2.633
46	0.867	1.786	0.000	2.653
47	0.867	1.786	0.000	2.653
48	0.871	1.763	0.000	2.634
49	0.865	1.783	0.000	2.648
50	0.870	1.763	0.000	2.633
51	0.867	1.786	0.000	2.653
52	0.867	1.786	0.000	2.653

53	0.870	1.762	0.000	2.632
54	0.865	1.784	0.000	2.648
55	0.865	1.784	0.000	2.649
56	0.865	1.786	0.000	2.651
57	0.866	1.787	0.000	2.653
58	0.866	1.790	0.000	2.656
59	0.865	1.786	0.000	2.651
60	0.866	1.786	0.000	2.651
61	0.866	1.788	0.000	2.654
62	0.867	1.791	0.000	2.658
63	0.865	1.784	0.000	2.649
64	0.865	1.786	0.000	2.651
65	0.866	1.787	0.000	2.652
66	0.865	1.788	0.000	2.653
67	0.865	1.786	0.000	2.651
68	0.866	1.785	0.000	2.651
69	0.865	1.787	0.000	2.652
70	0.866	1.787	0.000	2.653
71	0.865	1.784	0.000	2.649
72	0.865	1.786	0.000	2.651
73	0.866	1.786	0.000	2.652
74	0.864	1.785	0.000	2.649

75	0.865	1.786	0.000	2.651
76	0.866	1.786	0.000	2.651
77	0.865	1.786	0.000	2.651
78	0.865	1.784	0.000	2.649
79	0.865	1.784	0.000	2.649
80	0.865	1.786	0.000	2.651
81	0.865	1.785	0.000	2.650
82	0.863	1.782	0.000	2.645
83	0.865	1.786	0.000	2.651
84	0.866	1.786	0.000	2.651
85	0.865	1.784	0.000	2.648
86	0.862	1.774	0.000	2.636
87	0.865	1.784	0.000	2.649
88	0.865	1.787	0.000	2.652
89	0.865	1.785	0.000	2.650
90	0.865	1.788	0.000	2.653
91	0.865	1.786	0.000	2.651
92	0.866	1.786	0.000	2.651
93	0.864	1.783	0.000	2.647
94	0.866	1.785	0.000	2.651
95	0.865	1.784	0.000	2.649
96	0.865	1.786	0.000	2.651

97	0.866	1.787	0.000	2.653
98	0.866	1.789	0.000	2.655
99	0.865	1.786	0.000	2.651
100	0.866	1.786	0.000	2.651
101	0.865	1.787	0.000	2.652
102	0.867	1.790	0.000	2.657
103	0.865	1.786	0.000	2.651
104	0.867	1.785	0.000	2.653
105	0.866	1.786	0.000	2.652
106	0.870	1.778	0.000	2.648
107	0.869	1.765	0.000	2.635
108	0.865	1.783	0.000	2.648
109	0.869	1.789	0.000	2.658
110	0.865	1.786	0.000	2.651
111	0.867	1.785	0.000	2.653
112	0.867	1.789	0.000	2.655
113	0.871	1.782	0.000	2.653
114	0.869	1.765	0.000	2.634
115	0.865	1.783	0.000	2.648
116	0.870	1.791	0.000	2.661
117	0.865	1.786	0.000	2.651
118	0.867	1.786	0.000	2.653

119	0.865	1.782	0.000	2.647
120	0.857	1.707	0.000	2.564
121	0.869	1.765	0.000	2.634
122	0.865	1.783	0.000	2.648
123	0.866	1.778	0.000	2.644
124	0.866	1.786	0.000	2.652
125	0.867	1.785	0.000	2.653
126	0.862	1.776	0.000	2.638
127	0.849	1.831	0.000	2.679
128	0.870	1.767	0.000	2.637
129	0.865	1.783	0.000	2.648
130	0.860	1.757	0.000	2.617
131	0.866	1.786	0.000	2.652
132	0.867	1.784	0.000	2.652
133	0.864	1.787	0.000	2.651
134	0.869	1.789	0.000	2.659
135	0.869	1.767	0.000	2.636
136	0.865	1.783	0.000	2.648
137	0.866	1.772	0.000	2.638
138	0.866	1.786	0.000	2.652
139	0.867	1.785	0.000	2.652
140	0.866	1.788	0.000	2.654

141	0.870	1.779	0.000	2.649
142	0.869	1.766	0.000	2.635
143	0.865	1.783	0.000	2.648
144	0.869	1.790	0.000	2.659
145	0.942	1.718	0.000	2.660
146	1.240	1.546	0.074	2.860
147	1.633	3.526	0.000	5.160
tot	123.062	221.548	0.074	344.685

magnetization (x)

# of ion	s	p	d	tot
1	0.000	-0.000	0.000	0.000
2	-0.000	0.000	0.000	-0.000
3	0.000	-0.000	0.000	0.000
4	-0.000	0.000	0.000	-0.000
5	0.000	-0.000	0.000	0.000
6	-0.000	0.000	0.000	-0.000

7	0.000	-0.000	0.000	0.000
8	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	0.000
10	-0.000	0.000	0.000	-0.000
11	0.000	-0.000	0.000	0.000
12	-0.000	0.000	0.000	-0.000
13	0.000	-0.000	0.000	0.000
14	-0.004	0.002	0.000	-0.002
15	0.000	-0.000	0.000	0.000
16	-0.004	0.002	0.000	-0.002
17	-0.004	0.002	0.000	-0.002
18	0.000	-0.000	0.000	0.000
19	-0.003	0.001	0.000	-0.002
20	0.000	-0.000	0.000	0.000
21	-0.003	0.002	0.000	-0.002
22	-0.003	0.002	0.000	-0.002
23	-0.000	0.000	0.000	-0.000
24	-0.000	0.000	0.000	-0.000
25	-0.000	-0.007	0.000	-0.008
26	-0.000	-0.002	0.000	-0.002
27	0.000	0.003	0.000	0.003
28	0.000	0.005	0.000	0.005

29	0.000	0.003	0.000	0.003
30	-0.000	-0.007	0.000	-0.008
31	-0.000	-0.002	0.000	-0.002
32	0.000	0.003	0.000	0.003
33	0.000	0.005	0.000	0.005
34	0.000	0.002	0.000	0.002
35	-0.000	-0.007	0.000	-0.008
36	-0.000	-0.002	0.000	-0.002
37	0.000	0.003	0.000	0.003
38	0.000	0.006	0.000	0.007
39	0.000	0.002	0.000	0.002
40	-0.000	-0.007	0.000	-0.008
41	-0.000	-0.002	0.000	-0.002
42	0.000	0.002	0.000	0.003
43	0.000	0.005	0.000	0.006
44	0.000	0.004	0.000	0.004
45	-0.000	-0.007	0.000	-0.008
46	-0.000	-0.002	0.000	-0.002
47	0.000	0.003	0.000	0.003
48	0.000	0.005	0.000	0.006
49	0.000	0.001	0.000	0.002
50	-0.000	-0.007	0.000	-0.008

51	-0.000	-0.002	0.000	-0.002
52	0.000	0.002	0.000	0.003
53	0.000	0.006	0.000	0.007
54	0.000	0.002	0.000	0.002
55	-0.000	-0.005	0.000	-0.006
56	-0.000	-0.007	0.000	-0.007
57	-0.000	-0.001	0.000	-0.001
58	-0.000	-0.001	0.000	-0.001
59	0.000	0.006	0.000	0.007
60	0.000	0.003	0.000	0.003
61	0.000	0.001	0.000	0.001
62	0.000	0.003	0.000	0.003
63	-0.000	-0.005	0.000	-0.006
64	-0.000	-0.007	0.000	-0.007
65	-0.000	-0.001	0.000	-0.001
66	-0.000	-0.001	0.000	-0.001
67	0.000	0.006	0.000	0.006
68	0.000	0.003	0.000	0.003
69	0.000	0.001	0.000	0.001
70	0.000	0.002	0.000	0.002
71	-0.000	-0.005	0.000	-0.006
72	-0.000	-0.007	0.000	-0.007

73	-0.000	-0.001	0.000	-0.001
74	-0.000	-0.002	0.000	-0.002
75	0.000	0.006	0.000	0.007
76	0.000	0.003	0.000	0.004
77	0.000	0.003	0.000	0.003
78	0.000	0.001	0.000	0.001
79	-0.000	-0.005	0.000	-0.006
80	-0.000	-0.007	0.000	-0.007
81	-0.000	-0.001	0.000	-0.002
82	-0.000	-0.002	0.000	-0.002
83	0.001	0.007	0.000	0.008
84	0.000	0.003	0.000	0.003
85	0.000	0.002	0.000	0.002
86	0.000	0.005	0.000	0.006
87	-0.000	-0.005	0.000	-0.005
88	-0.000	-0.007	0.000	-0.007
89	-0.000	-0.001	0.000	-0.002
90	-0.000	-0.002	0.000	-0.002
91	0.001	0.008	0.000	0.008
92	0.000	0.003	0.000	0.003
93	0.000	0.002	0.000	0.003
94	0.000	0.001	0.000	0.001

95	-0.000	-0.005	0.000	-0.006
96	-0.000	-0.007	0.000	-0.007
97	-0.000	-0.001	0.000	-0.001
98	-0.000	-0.001	0.000	-0.001
99	0.001	0.007	0.000	0.007
100	0.000	0.003	0.000	0.004
101	0.000	0.003	0.000	0.003
102	0.000	0.002	0.000	0.002
103	-0.001	-0.010	0.000	-0.011
104	-0.003	-0.028	0.000	-0.031
105	-0.000	-0.001	0.000	-0.002
106	-0.000	-0.004	0.000	-0.005
107	0.007	0.116	0.000	0.122
108	0.001	0.010	0.000	0.011
109	0.000	0.001	0.000	0.001
110	-0.001	-0.010	0.000	-0.011
111	-0.003	-0.028	0.000	-0.031
112	-0.000	-0.001	0.000	-0.002
113	-0.000	-0.003	0.000	-0.004
114	0.007	0.120	0.000	0.127
115	0.001	0.010	0.000	0.011
116	0.000	0.001	0.000	0.002

117	-0.001	-0.010	0.000	-0.011
118	-0.003	-0.026	0.000	-0.029
119	-0.000	-0.002	0.000	-0.002
120	-0.000	-0.002	0.000	-0.002
121	0.007	0.115	0.000	0.122
122	0.001	0.010	0.000	0.010
123	0.000	0.003	0.000	0.003
124	-0.001	-0.010	0.000	-0.011
125	-0.003	-0.024	0.000	-0.027
126	-0.000	-0.002	0.000	-0.002
127	-0.000	0.001	0.000	0.001
128	0.006	0.105	0.000	0.111
129	0.001	0.009	0.000	0.010
130	0.000	0.004	0.000	0.004
131	-0.001	-0.009	0.000	-0.010
132	-0.003	-0.024	0.000	-0.027
133	-0.000	-0.002	0.000	-0.002
134	-0.000	-0.002	0.000	-0.002
135	0.006	0.097	0.000	0.102
136	0.001	0.009	0.000	0.010
137	0.000	0.004	0.000	0.005
138	-0.001	-0.010	0.000	-0.011

139	-0.003	-0.026	0.000	-0.029
140	-0.000	-0.002	0.000	-0.002
141	-0.000	-0.003	0.000	-0.004
142	0.006	0.105	0.000	0.111
143	0.001	0.010	0.000	0.010
144	0.000	0.002	0.000	0.003
145	0.000	0.005	0.000	0.006
146	-0.000	0.000	-0.000	0.000
147	0.000	0.004	0.000	0.004

---

tot	0.001	0.513	-0.000	0.514

CHARGE: cpu time 0.5204: real time 0.5220

FORLOC: cpu time 0.0200: real time 0.0200

FORNL : cpu time 2.0683: real time 2.0775

STRESS: cpu time 6.2217: real time 6.2496

FORCOR: cpu time 0.1434: real time 0.1450

FORHAR: cpu time 0.0336: real time 0.0339

MIXING: cpu time 0.0168: real time 0.0168

OFIELD: cpu time 0.0002: real time 0.0003

DFTD3 V3.0 Rev 1

IVDW = 11

DF pbe

parameters

VDW_S6 = 1.0000

VDW_S8 = 0.7220

VDW_SR = 1.2170

rs18 = 1.0000

alpha6 = 14.0000

alpha8 = 16.0000

k1-k3 = 16.0000 1.3333 -4.0000

VDW_RADIUS = 50.2022 A

VDW_CNRADIUS = 21.1671 A

Edisp (eV) -6.61779

E6 (eV) : -3.9313

E8 (eV) : -2.6865

% E8 : 40.60

FORVDW: cpu time 1.8720: real time 1.8918

FORCE on cell =-STRESS in cart. coord. units (eV):

Direction	XX	YY	ZZ	XY	YZ	ZX
Alpha Z	233.50077	233.50077	233.50077			
Ewald	107579.64891	23477.03964	-39727.58845	9.73164	3454.91959	128.50515
Hartree	106097.76185	25032.59879	-23794.45641	-6.72712	2947.16346	93.19169
E(xc)	-1914.23720	-1916.58834	-1979.89772	0.13187	1.82225	0.13010
Local	**********	-53958.07596	57015.85839	0.37222	-6360.09120	-218.27525
n-local	-472.65371	-482.46815	-439.54636	-0.68033	-0.70340	-0.31833
augment	-38.28645	-38.59098	-34.30755	0.00971	-0.98085	0.00029
Kinetic	7635.15424	7638.79437	8713.97763	-3.08733	-41.59850	-3.19058
Fock	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
vdW	-2.64198	-1.49213	-6.59312	0.00139	-0.07446	0.01168
Total	-17.74331	-15.28199	-19.05281	-0.24794	0.45689	0.05475
in kB	-4.89282	-4.21409	-5.25392	-0.06837	0.12599	0.01510

external pressure = -4.79 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

energy-cutoff : 400.00

volume of cell : 5810.14

direct lattice vectors reciprocal lattice vectors

14.780600000 0.000000000 0.000000000 0.067656252 0.000000000 0.000000000

0.000000000 21.333900000 0.000000000 0.000000000 0.046873755 0.000000000

0.000000000 0.000000000 18.425700000 0.000000000 0.000000000 0.054272022

length of vectors

14.780600000 21.333900000 18.425700000 0.067656252 0.046873755 0.054272022

FORCES acting on ions

electron-ion (+dipol) ewald-force non-local-force convergence-correction

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0.460E-02 0.154E+03 0.361E+02 -.310E-02 -.160E+03 -.357E+02 -.180E-02 0.566E+01 -.438E+00 -.551E-07 -.125E-05 0.762E-06

-.185E-01 0.155E+03 -.340E+02 0.161E-01 -.160E+03 0.335E+02 0.115E-02 0.565E+01 0.541E+00 -.873E-08 -.122E-05 -.242E-06

0.184E+00 0.154E+03 0.360E+02 -.184E+00 -.160E+03 -.356E+02 0.832E-05 0.565E+01 -.443E+00 -.246E-06 -.116E-05 0.849E-06

0.112E+00 0.155E+03 -.341E+02 -.988E-01 -.160E+03 0.336E+02 -.175E-01 0.565E+01 0.535E+00 -.141E-06 -.130E-05 -.250E-06

0.171E+00 0.154E+03 0.362E+02 -.173E+00 -.160E+03 -.357E+02 0.116E-02 0.566E+01 -

.440E+00 -.215E-06 -.103E-05 0.882E-06

0.126E+00 0.154E+03 -.340E+02 -.108E+00 -.160E+03 0.334E+02 -.211E-01 0.565E+01 0.541E+00 -.116E-06 -.145E-05 -.121E-06

-.193E-01 0.154E+03 0.363E+02 0.181E-01 -.160E+03 -.359E+02 0.159E-02 0.566E+01 -.431E+00 -.299E-07 -.966E-06 0.876E-06

-.129E-01 0.154E+03 -.338E+02 0.197E-01 -.160E+03 0.332E+02 -.720E-02 0.565E+01 0.555E+00 0.984E-08 -.127E-05 -.560E-08

-.182E+00 0.154E+03 0.363E+02 0.182E+00 -.160E+03 -.359E+02 0.255E-03 0.566E+01 -.429E+00 0.248E-06 -.101E-05 0.794E-06

-.128E+00 0.155E+03 -.337E+02 0.115E+00 -.160E+03 0.331E+02 0.109E-01 0.565E+01 0.561E+00 0.113E-06 -.123E-05 -.515E-08

-.174E+00 0.154E+03 0.362E+02 0.176E+00 -.160E+03 -.358E+02 -.177E-02 0.566E+01 -.432E+00 0.296E-06 -.114E-05 0.704E-06

-.115E+00 0.155E+03 -.338E+02 0.958E-01 -.160E+03 0.332E+02 0.192E-01 0.565E+01 0.555E+00 0.151E-06 -.133E-05 -.125E-06

0.228E+01 -.150E+03 -.386E+02 -.227E+01 0.156E+03 0.386E+02 -.103E-01 -.566E+01 0.767E-01 -.148E-06 0.129E-05 0.217E-07

-.416E+00 -.151E+03 0.388E+02 0.417E+00 0.157E+03 -.386E+02 -.129E-02 -.567E+01 -.269E+00 -.719E-07 0.878E-06 0.952E-07

0.136E+02 -.146E+03 -.413E+02 -.138E+02 0.151E+03 0.413E+02 0.257E+00 -.567E+01 -.348E-01 -.418E-06 0.965E-06 0.569E-07

0.162E+01 -.151E+03 0.402E+02 -.162E+01 0.156E+03 -.400E+02 -.100E-02 -.567E+01 -

.229E+00 -.185E-07 0.874E-06 0.870E-07

0.352E+01 -.149E+03 0.443E+02 -.352E+01 0.155E+03 -.441E+02 -.199E-02 -.567E+01 -.180E+00 -.254E-07 0.837E-06 -.180E-06

-.148E+02 -.146E+03 -.330E+02 0.149E+02 0.151E+03 0.329E+02 -.958E-01 -.566E+01 0.487E-01 0.479E-06 0.118E-05 -.204E-06

-.297E+01 -.149E+03 0.432E+02 0.296E+01 0.155E+03 -.430E+02 0.115E-01 -.567E+01 -.241E+00 0.846E-07 0.964E-06 -.502E-06

-.379E+01 -.150E+03 -.385E+02 0.379E+01 0.156E+03 0.385E+02 -.620E-02 -.566E+01 0.240E-01 0.128E-06 0.129E-05 -.479E-07

-.207E+01 -.151E+03 0.395E+02 0.207E+01 0.156E+03 -.392E+02 0.151E-02 -.566E+01 -.282E+00 -.733E-07 0.986E-06 -.224E-06

0.162E-02 -.148E+03 0.486E+02 0.601E-02 0.154E+03 -.484E+02 -.554E-02 -.569E+01 -.158E+00 0.122E-06 0.850E-06 -.476E-06

0.196E+02 -.103E+03 0.222E+02 -.212E+02 0.103E+03 -.246E+02 0.153E+01 0.138E+00 0.238E+01 -.285E-06 0.477E-06 -.470E-06

-.192E+02 -.103E+03 0.153E+02 0.216E+02 0.103E+03 -.168E+02 -.241E+01 -.119E+00 0.152E+01 0.650E-07 0.459E-06 -.714E-06

0.713E-01 0.461E+03 0.202E+03 -.745E-01 -.462E+03 -.201E+03 0.383E-02 0.102E+01 -.219E+00 -.250E-06 -.231E-05 0.328E-05

0.212E+00 0.353E+03 -.234E+03 -.212E+00 -.353E+03 0.234E+03 0.260E-02 0.443E+00 -.370E-01 -.322E-06 -.230E-05 -.237E-05

-.249E-01 0.351E+03 0.240E+03 0.235E-01 -.351E+03 -.241E+03 0.315E-02 0.408E+00

0.564E-01 0.173E-06 -.765E-06 0.347E-05

-.173E+00 0.462E+03 -.195E+03 0.180E+00 -.463E+03 0.195E+03 -.664E-02 0.105E+01 0.233E+00 -.245E-06 -.317E-05 -.166E-05

-.622E-01 0.210E+03 -.272E+03 0.663E-01 -.210E+03 0.272E+03 -.448E-02 0.936E-01 0.560E-01 -.196E-06 -.185E-06 -.316E-05

0.562E+00 0.461E+03 0.202E+03 -.565E+00 -.462E+03 -.201E+03 0.202E-02 0.102E+01 -.214E+00 -.687E-06 -.168E-05 0.358E-05

0.106E+01 0.352E+03 -.234E+03 -.107E+01 -.353E+03 0.234E+03 0.160E-01 0.448E+00 -.425E-01 -.341E-06 -.109E-05 -.212E-05

0.413E+00 0.351E+03 0.240E+03 -.415E+00 -.351E+03 -.240E+03 0.302E-02 0.408E+00 0.491E-01 -.179E-06 -.571E-06 0.372E-05

0.578E+00 0.462E+03 -.195E+03 -.583E+00 -.463E+03 0.195E+03 0.479E-02 0.105E+01 0.235E+00 -.166E-06 -.283E-05 -.175E-05

0.689E+00 0.210E+03 -.272E+03 -.695E+00 -.210E+03 0.272E+03 0.603E-02 0.912E-01 0.616E-01 0.102E-06 -.155E-05 -.321E-05

0.426E+00 0.461E+03 0.202E+03 -.428E+00 -.462E+03 -.202E+03 0.385E-02 0.102E+01 -.214E+00 -.560E-06 -.106E-05 0.368E-05

0.939E+00 0.352E+03 -.233E+03 -.955E+00 -.352E+03 0.233E+03 0.151E-01 0.441E+00 -.377E-01 -.391E-07 -.756E-06 -.175E-05

0.478E+00 0.351E+03 0.241E+03 -.480E+00 -.351E+03 -.241E+03 0.250E-02 0.406E+00 0.512E-01 -.553E-06 -.210E-06 0.394E-05

0.705E+00 0.462E+03 -.194E+03 -.715E+00 -.463E+03 0.194E+03 0.786E-02 0.106E+01

0.242E+00 -.431E-06 -.178E-05 -.122E-05

0.725E+00 0.210E+03 -.271E+03 -.734E+00 -.210E+03 0.271E+03 0.654E-02 0.911E-01 0.592E-01 -.168E-06 -.128E-05 -.300E-05

-.181E+00 0.461E+03 0.202E+03 0.178E+00 -.462E+03 -.202E+03 0.449E-02 0.102E+01 -.218E+00 0.891E-08 -.507E-06 0.369E-05

-.294E+00 0.352E+03 -.233E+03 0.298E+00 -.352E+03 0.233E+03 -.207E-02 0.440E+00 -.299E-01 0.974E-07 -.176E-05 -.173E-05

0.404E-01 0.351E+03 0.241E+03 -.394E-01 -.351E+03 -.241E+03 0.223E-02 0.409E+00 0.557E-01 -.293E-06 0.329E-06 0.401E-05

0.502E-01 0.462E+03 -.194E+03 -.564E-01 -.463E+03 0.194E+03 0.397E-02 0.106E+01 0.232E+00 -.865E-07 -.231E-05 -.102E-05

-.478E-01 0.210E+03 -.271E+03 0.458E-01 -.210E+03 0.271E+03 -.245E-03 0.933E-01 0.324E-01 0.327E-07 0.113E-06 -.283E-05

-.552E+00 0.461E+03 0.202E+03 0.550E+00 -.462E+03 -.202E+03 0.767E-03 0.102E+01 -.220E+00 0.594E-06 -.831E-06 0.346E-05

-.119E+01 0.352E+03 -.233E+03 0.120E+01 -.353E+03 0.233E+03 -.162E-01 0.447E+00 -.330E-01 0.297E-06 -.106E-05 -.175E-05

-.352E+00 0.351E+03 0.241E+03 0.349E+00 -.351E+03 -.241E+03 0.206E-02 0.413E+00 0.624E-01 0.241E-06 0.665E-06 0.389E-05

-.412E+00 0.462E+03 -.194E+03 0.425E+00 -.463E+03 0.194E+03 -.115E-01 0.106E+01 0.230E+00 0.709E-06 -.243E-05 -.988E-06

-.561E+00 0.210E+03 -.271E+03 0.565E+00 -.210E+03 0.271E+03 -.942E-02 0.915E-01

0.525E-01 0.292E-06 -.174E-05 -.297E-05

-.475E+00 0.461E+03 0.202E+03 0.474E+00 -.462E+03 -.202E+03 0.306E-02 0.102E+01 -.220E+00 0.925E-06 -.194E-05 0.310E-05

-.805E+00 0.353E+03 -.234E+03 0.820E+00 -.353E+03 0.234E+03 -.149E-01 0.447E+00 -.393E-01 0.273E-06 -.165E-05 -.211E-05

-.374E+00 0.351E+03 0.241E+03 0.368E+00 -.351E+03 -.241E+03 0.960E-03 0.411E+00 0.626E-01 0.572E-06 -.891E-07 0.359E-05

-.594E+00 0.462E+03 -.194E+03 0.607E+00 -.463E+03 0.194E+03 -.170E-01 0.105E+01 0.234E+00 0.276E-06 -.225E-05 -.117E-05

-.588E+00 0.210E+03 -.272E+03 0.599E+00 -.210E+03 0.272E+03 -.102E-01 0.992E-01 0.566E-01 -.366E-07 -.154E-05 -.316E-05

-.881E-02 0.206E+03 0.279E+03 0.122E-01 -.206E+03 -.279E+03 -.361E-02 0.687E-01 -.412E-01 0.931E-07 -.758E-06 0.403E-05

0.668E+00 0.303E+02 0.296E+03 -.663E+00 -.302E+02 -.296E+03 -.468E-02 -.410E-01 0.752E-02 -.149E-06 0.604E-06 0.403E-05

-.846E+00 0.144E+03 -.282E+03 0.848E+00 -.144E+03 0.282E+03 -.318E-02 0.137E+00 0.286E-01 0.410E-06 0.493E-06 -.336E-05

0.534E+00 -.215E+02 -.285E+03 -.534E+00 0.214E+02 0.285E+03 -.786E-03 0.387E-01 0.186E-01 -.584E-07 0.795E-06 -.325E-05

0.499E+00 -.294E+02 0.293E+03 -.496E+00 0.294E+02 -.293E+03 -.553E-02 0.254E-01 -.303E-01 -.177E-07 0.498E-06 0.373E-05

0.524E+00 0.139E+03 0.289E+03 -.524E+00 -.139E+03 -.289E+03 0.178E-02 0.104E+00 -

.248E-01 -.118E-06 -.335E-06 0.419E-05

-.127E+01 0.364E+02 -.287E+03 0.126E+01 -.364E+02 0.287E+03 -.473E-04 -.755E-02 0.138E-01 0.481E-06 0.791E-06 -.339E-05

0.167E+01 -.130E+03 -.271E+03 -.169E+01 0.130E+03 0.271E+03 0.106E-01 -.879E-01 0.372E-01 -.823E-07 0.230E-05 -.248E-05

0.397E+00 0.207E+03 0.280E+03 -.395E+00 -.207E+03 -.280E+03 0.708E-03 0.695E-01 -.370E-01 -.206E-06 -.858E-06 0.415E-05

0.919E+00 0.312E+02 0.296E+03 -.923E+00 -.311E+02 -.296E+03 0.225E-02 -.410E-01 0.122E-01 0.155E-07 0.611E-06 0.425E-05

0.133E+01 0.144E+03 -.282E+03 -.133E+01 -.144E+03 0.282E+03 0.500E-02 0.126E+00 0.279E-01 -.553E-06 0.508E-06 -.340E-05

0.342E+01 -.199E+02 -.285E+03 -.343E+01 0.199E+02 0.285E+03 0.135E-01 0.414E-01 0.136E-01 -.212E-06 0.171E-05 -.333E-05

0.139E+01 -.287E+02 0.294E+03 -.139E+01 0.287E+02 -.294E+03 -.348E-02 0.253E-01 -.307E-01 -.274E-06 0.661E-06 0.401E-05

0.678E+00 0.139E+03 0.290E+03 -.678E+00 -.139E+03 -.290E+03 0.617E-03 0.103E+00 -.295E-01 -.525E-07 -.376E-06 0.439E-05

0.160E+01 0.367E+02 -.287E+03 -.159E+01 -.367E+02 0.287E+03 -.128E-01 -.205E-01 0.128E-01 -.501E-06 0.989E-06 -.341E-05

0.611E+01 -.125E+03 -.271E+03 -.613E+01 0.125E+03 0.271E+03 0.219E-01 -.894E-01 0.147E-01 0.196E-06 0.781E-06 -.276E-05

0.367E+00 0.207E+03 0.280E+03 -.372E+00 -.207E+03 -.280E+03 0.106E-03 0.684E-01 -

.365E-01 -.290E-06 -.304E-06 0.441E-05

-.379E-01 0.319E+02 0.296E+03 0.293E-01 -.318E+02 -.296E+03 0.106E-01 -.362E-01 0.139E-01 -.853E-07 0.512E-06 0.427E-05

0.210E+01 0.144E+03 -.281E+03 -.211E+01 -.144E+03 0.281E+03 0.121E-01 0.120E+00 0.240E-01 0.457E-07 -.744E-06 -.336E-05

0.303E+01 -.172E+02 -.283E+03 -.306E+01 0.171E+02 0.283E+03 0.244E-01 0.871E-01 0.608E-01 -.101E-05 0.125E-05 -.361E-05

0.106E+01 -.272E+02 0.294E+03 -.105E+01 0.272E+02 -.294E+03 0.288E-02 0.243E-01 -.376E-01 0.432E-07 0.426E-06 0.407E-05

0.963E-01 0.140E+03 0.290E+03 -.979E-01 -.140E+03 -.290E+03 0.130E-02 0.107E+00 -.232E-01 -.169E-06 0.187E-06 0.454E-05

0.277E+01 0.387E+02 -.286E+03 -.277E+01 -.387E+02 0.286E+03 0.117E-02 -.108E-01 0.292E-01 0.589E-07 0.185E-05 -.347E-05

0.595E+01 -.115E+03 -.267E+03 -.611E+01 0.115E+03 0.267E+03 0.154E+00 0.150E-02 0.130E+00 -.105E-05 0.338E-06 -.310E-05

-.242E+00 0.207E+03 0.280E+03 0.240E+00 -.207E+03 -.280E+03 0.438E-02 0.717E-01 -.387E-01 0.465E-07 -.835E-07 0.449E-05

-.115E+01 0.314E+02 0.294E+03 0.114E+01 -.314E+02 -.294E+03 0.918E-02 -.311E-01 0.544E-02 0.241E-06 0.935E-06 0.413E-05

0.594E+00 0.144E+03 -.281E+03 -.612E+00 -.144E+03 0.281E+03 0.178E-01 0.126E+00 0.437E-01 0.409E-06 0.335E-06 -.330E-05

-.940E+00 -.159E+02 -.286E+03 0.931E+00 0.158E+02 0.285E+03 0.600E-02 0.908E-01

0.802E-01 0.508E-07 -.589E-06 -.379E-05

-.644E+00 -.265E+02 0.293E+03 0.640E+00 0.265E+02 -.293E+03 0.491E-02 0.234E-01 -.270E-01 0.193E-06 0.679E-06 0.393E-05

-.534E+00 0.139E+03 0.289E+03 0.530E+00 -.139E+03 -.289E+03 0.655E-02 0.114E+00 -.213E-01 0.116E-06 0.243E-07 0.450E-05

0.778E+00 0.408E+02 -.287E+03 -.790E+00 -.408E+02 0.287E+03 0.515E-02 0.211E-02 -.191E-01 0.552E-06 -.117E-06 -.381E-05

-.459E+00 -.113E+03 -.276E+03 0.425E+00 0.113E+03 0.276E+03 0.348E-01 0.602E-01 -.268E+00 -.224E-08 0.568E-06 -.317E-05

-.572E+00 0.206E+03 0.279E+03 0.570E+00 -.206E+03 -.279E+03 0.115E-02 0.721E-01 -.455E-01 0.986E-07 -.209E-06 0.434E-05

-.783E+00 0.304E+02 0.294E+03 0.787E+00 -.304E+02 -.294E+03 -.755E-02 -.308E-01 -.138E-02 0.133E-06 0.911E-06 0.387E-05

-.123E+01 0.144E+03 -.281E+03 0.125E+01 -.145E+03 0.281E+03 -.158E-01 0.122E+00 0.504E-01 -.329E-06 0.379E-07 -.323E-05

-.366E+01 -.174E+02 -.283E+03 0.369E+01 0.173E+02 0.283E+03 -.308E-01 0.116E+00 0.587E-01 0.130E-05 0.142E-05 -.335E-05

-.130E+01 -.277E+02 0.291E+03 0.129E+01 0.277E+02 -.291E+03 -.132E-02 0.341E-01 -.219E-01 0.650E-07 0.820E-06 0.369E-05

-.347E+00 0.139E+03 0.289E+03 0.347E+00 -.139E+03 -.289E+03 0.164E-04 0.112E+00 -.146E-01 0.239E-06 0.270E-07 0.426E-05

-.829E+00 0.400E+02 -.287E+03 0.821E+00 -.400E+02 0.287E+03 0.126E-01 -.748E-02 -

.182E-01 -.574E-06 0.106E-06 -.365E-05

-.786E+01 -.119E+03 -.267E+03 0.805E+01 0.119E+03 0.267E+03 -.190E+00 0.324E-02 0.345E-01 0.122E-05 0.194E-06 -.276E-05

-.409E+00 0.206E+03 0.279E+03 0.410E+00 -.206E+03 -.279E+03 -.280E-02 0.716E-01 -.464E-01 0.196E-06 -.163E-06 0.407E-05

-.631E-01 0.300E+02 0.294E+03 0.728E-01 -.299E+02 -.294E+03 -.948E-02 -.347E-01 0.122E-02 -.107E-06 0.508E-06 0.384E-05

-.206E+01 0.145E+03 -.282E+03 0.208E+01 -.145E+03 0.282E+03 -.189E-01 0.132E+00 0.256E-01 -.281E-07 -.762E-06 -.325E-05

-.257E+01 -.208E+02 -.285E+03 0.259E+01 0.208E+02 0.285E+03 -.291E-01 0.409E-01 0.318E-01 -.105E-07 0.186E-05 -.316E-05

-.552E+00 -.290E+02 0.291E+03 0.557E+00 0.290E+02 -.291E+03 -.285E-02 0.292E-01 -.251E-01 -.306E-07 0.562E-06 0.359E-05

0.590E-01 0.139E+03 0.289E+03 -.592E-01 -.139E+03 -.289E+03 -.341E-03 0.109E+00 -.208E-01 0.511E-07 0.137E-07 0.406E-05

-.290E+01 0.378E+02 -.286E+03 0.291E+01 -.378E+02 0.286E+03 -.147E-01 -.368E-02 0.209E-01 -.612E-07 0.193E-05 -.328E-05

-.514E+01 -.128E+03 -.271E+03 0.518E+01 0.128E+03 0.271E+03 -.464E-01 -.862E-01 0.378E-01 -.223E-06 0.110E-05 -.242E-05

0.400E+00 -.137E+03 0.280E+03 -.392E+00 0.137E+03 -.280E+03 -.969E-02 -.127E+00 -.156E-01 -.631E-07 0.958E-06 0.306E-05

0.194E+01 -.343E+03 0.233E+03 -.194E+01 0.344E+03 -.233E+03 0.911E-02 -.461E+00 -

.546E-01 -.338E-06 0.283E-05 0.115E-05

-.253E+01 -.197E+03 -.259E+03 0.254E+01 0.197E+03 0.259E+03 -.947E-02 -.198E+00 0.369E-01 0.735E-06 0.277E-05 -.187E-05

0.691E+01 -.447E+03 -.198E+03 -.693E+01 0.448E+03 0.198E+03 0.966E-02 -.112E+01 0.881E-01 -.404E-06 0.263E-06 -.145E-06

-.464E+00 -.451E+03 0.204E+03 0.465E+00 0.452E+03 -.204E+03 -.207E-02 -.108E+01 -.112E+00 -.174E-06 0.308E-05 0.499E-06

0.171E+01 -.203E+03 0.269E+03 -.171E+01 0.203E+03 -.269E+03 -.481E-02 -.926E-01 -.320E-01 -.400E-06 0.758E-06 0.261E-05

-.211E+01 -.338E+03 -.222E+03 0.215E+01 0.338E+03 0.222E+03 -.442E-01 -.604E+00 0.538E-01 0.764E-06 -.351E-06 -.591E-06

0.218E+01 -.136E+03 0.282E+03 -.218E+01 0.136E+03 -.282E+03 -.636E-02 -.126E+00 -.941E-02 -.106E-06 0.611E-06 0.331E-05

0.672E+01 -.339E+03 0.238E+03 -.670E+01 0.340E+03 -.238E+03 -.127E-01 -.461E+00 -.459E-01 0.353E-06 0.280E-05 0.117E-05

0.678E+01 -.193E+03 -.258E+03 -.680E+01 0.193E+03 0.258E+03 0.111E-01 -.145E+00 0.633E-01 -.119E-05 0.257E-05 -.198E-05

0.313E+02 -.427E+03 -.198E+03 -.313E+02 0.428E+03 0.197E+03 0.726E-01 -.970E+00 0.135E+00 -.913E-06 0.658E-06 -.373E-06

0.544E+01 -.449E+03 0.209E+03 -.544E+01 0.450E+03 -.209E+03 0.602E-03 -.108E+01 -.798E-01 -.197E-06 0.334E-05 0.512E-06

0.368E+01 -.201E+03 0.272E+03 -.368E+01 0.201E+03 -.272E+03 -.735E-03 -.976E-01 -

.306E-01 0.225E-06 0.850E-06 0.274E-05

0.124E+02 -.332E+03 -.223E+03 -.125E+02 0.332E+03 0.223E+03 0.121E+00 -.535E+00 0.314E-01 -.124E-05 -.606E-06 -.656E-06

0.219E+01 -.133E+03 0.283E+03 -.219E+01 0.133E+03 -.283E+03 0.542E-03 -.128E+00 -.442E-02 0.321E-07 0.116E-05 0.328E-05

0.492E+01 -.332E+03 0.245E+03 -.489E+01 0.332E+03 -.245E+03 -.319E-01 -.476E+00 -.375E-01 0.363E-06 0.243E-05 0.817E-06

0.112E+02 -.182E+03 -.258E+03 -.113E+02 0.182E+03 0.258E+03 0.472E-01 -.989E-01 -.104E+00 -.100E-05 -.127E-06 -.261E-05

0.318E+02 -.399E+03 -.175E+03 -.321E+02 0.401E+03 0.174E+03 0.296E+00 -.142E+01 0.132E+01 -.126E-06 0.976E-06 -.207E-05

0.930E+01 -.443E+03 0.219E+03 -.930E+01 0.444E+03 -.219E+03 -.562E-02 -.109E+01 -.483E-01 -.722E-08 0.313E-05 0.186E-06

0.169E+01 -.196E+03 0.273E+03 -.170E+01 0.197E+03 -.273E+03 0.550E-02 -.109E+00 -.511E-01 0.389E-06 0.125E-05 0.254E-05

0.172E+02 -.310E+03 -.216E+03 -.175E+02 0.310E+03 0.216E+03 0.325E+00 -.219E+00 0.123E+00 -.213E-05 0.292E-06 -.173E-05

-.104E+01 -.132E+03 0.281E+03 0.103E+01 0.132E+03 -.281E+03 0.103E-01 -.127E+00 0.152E-03 0.215E-06 0.145E-05 0.296E-05

-.512E+01 -.332E+03 0.239E+03 0.512E+01 0.332E+03 -.239E+03 0.883E-02 -.494E+00 -.419E-01 0.231E-06 0.239E-05 0.329E-06

0.158E+01 -.170E+03 -.261E+03 -.170E+01 0.169E+03 0.261E+03 0.118E+00 0.372E+00 -

.934E-01 -.846E-06 0.469E-06 -.263E-05

-.654E+01 -.301E+03 -.189E+03 0.606E+01 0.296E+03 0.185E+03 0.473E+00 0.504E+01

0.404E+01 0.210E-06 0.343E-06 -.238E-06

-.623E+00 -.436E+03 0.227E+03 0.621E+00 0.437E+03 -.227E+03 0.164E-02 -.120E+01 -

.481E-01 0.311E-06 0.285E-05 -.330E-06

-.302E+01 -.197E+03 0.268E+03 0.301E+01 0.197E+03 -.268E+03 0.146E-01 -.112E+00 -

.428E-01 0.115E-06 0.137E-05 0.214E-05

0.333E+01 -.280E+03 -.215E+03 -.525E+01 0.280E+03 0.214E+03 0.191E+01 0.643E+00

0.821E+00 -.152E-05 -.130E-06 -.156E-05

-.274E+01 -.134E+03 0.277E+03 0.274E+01 0.134E+03 -.277E+03 0.247E-02 -.123E+00 -

.185E-01 0.580E-07 0.117E-05 0.269E-05

-.601E+01 -.338E+03 0.230E+03 0.600E+01 0.339E+03 -.230E+03 0.113E-01 -.494E+00 -

.460E-01 -.157E-06 0.258E-05 0.517E-07

-.650E+01 -.171E+03 -.257E+03 0.658E+01 0.170E+03 0.257E+03 -.775E-01 0.485E+00

0.181E-01 0.101E-05 0.306E-06 -.230E-05

-.442E+02 -.422E+03 -.184E+03 0.448E+02 0.423E+03 0.183E+03 -.563E+00 -.110E+01

0.627E+00 0.935E-06 0.202E-05 -.783E-06

-.867E+01 -.441E+03 0.211E+03 0.866E+01 0.442E+03 -.211E+03 0.144E-01 -.111E+01 -

.752E-01 0.136E-06 0.319E-05 -.816E-06

-.293E+01 -.201E+03 0.265E+03 0.294E+01 0.201E+03 -.265E+03 -.917E-02 -.110E+00 -

.204E-01 -.647E-07 0.125E-05 0.193E-05

-.145E+02 -.290E+03 -.209E+03 0.165E+02 0.289E+03 0.208E+03 -.198E+01 0.605E+00

0.784E+00 0.225E-05 0.481E-06 -.908E-06

-.139E+01 -.136E+03 0.277E+03 0.140E+01 0.136E+03 -.277E+03 -.102E-01 -.125E+00 -.239E-01 -.821E-07 0.117E-05 0.275E-05

-.279E+01 -.343E+03 0.230E+03 0.277E+01 0.343E+03 -.230E+03 0.235E-01 -.473E+00 -.592E-01 -.410E-06 0.256E-05 0.706E-06

-.104E+02 -.189E+03 -.258E+03 0.105E+02 0.189E+03 0.258E+03 -.771E-01 -.139E+00 -.526E-01 0.126E-05 0.623E-06 -.204E-05

-.149E+02 -.446E+03 -.196E+03 0.150E+02 0.447E+03 0.196E+03 -.693E-01 -.113E+01 0.998E-01 0.590E-06 0.157E-05 -.343E-06

-.549E+01 -.448E+03 0.204E+03 0.550E+01 0.449E+03 -.203E+03 -.485E-02 -.109E+01 -.125E+00 -.823E-07 0.318E-05 -.444E-06

-.912E+00 -.203E+03 0.267E+03 0.920E+00 0.203E+03 -.267E+03 -.911E-02 -.102E+00 -.317E-01 -.303E-06 0.114E-05 0.235E-05

-.163E+02 -.329E+03 -.218E+03 0.166E+02 0.329E+03 0.218E+03 -.360E+00 -.480E+00 0.429E-01 0.175E-05 0.670E-06 -.997E-06

-.335E+01 -.256E+03 -.194E+03 0.236E+01 0.248E+03 0.189E+03 0.979E+00 0.780E+01 0.489E+01 0.103E-05 0.278E-05 0.200E-05

0.531E+02 -.518E+03 -.137E+03 -.541E+02 0.522E+03 0.141E+03 0.105E+01 -.396E+01 -.382E+01 -.143E-05 0.220E-05 -.108E-05

-.466E+02 -.585E+03 -.446E+03 0.524E+02 0.636E+03 0.481E+03 -.586E+01 -.510E+02 -.343E+02 0.259E-05 0.484E-05 0.473E-05

0.436E+01 0.278E+02 0.224E+02 -.327E-12 -.216E-11 0.165E-11 -.441E+01 -.278E+02 -.224E+02 0.231E-05 0.503E-04 0.458E-04

POSITION			TOTAL-FORCE (eV/Angst)		
1.24575	4.02870	5.43979	0.000041	0.001024	-0.000410
1.21024	4.07581	8.43726	-0.000985	0.002614	-0.001142
3.70862	4.02890	5.43965	0.000308	0.001895	-0.001095
3.67998	4.07733	8.43690	-0.004035	-0.000418	-0.002900
6.17157	4.02854	5.43942	-0.000007	-0.000134	-0.001753
6.14482	4.08292	8.43295	-0.002834	-0.003301	-0.003191
8.63513	4.02801	5.43869	0.000777	-0.000438	-0.002003
8.60339	4.08732	8.43089	-0.000134	-0.001175	-0.002212
11.09928	4.02784	5.43885	0.000873	0.001976	-0.002713
11.06021	4.08619	8.43099	-0.001746	0.000706	-0.000644
13.56311	4.02807	5.43972	0.000332	0.001626	-0.001620
13.52141	4.08047	8.43349	0.000402	-0.002253	0.000295
2.44241	15.48073	8.85224	-0.000622	-0.005273	0.002324
0.01714	15.44624	5.32469	0.000346	0.001533	-0.001196
4.86040	15.47728	8.86623	0.001094	0.000213	-0.000356
2.48016	15.44854	5.27562	0.000363	-0.001207	-0.000510

4.94382	15.44925	5.24869	0.001780	-0.003002	0.000307
12.31531	15.48242	9.00211	-0.004285	0.001585	0.004161
9.86772	15.44556	5.34176	0.000427	-0.001112	0.000908
14.76279	15.48245	8.89951	-0.006129	-0.000475	0.005517
12.33384	15.44510	5.36128	0.001361	-0.003219	-0.001281
7.40743	15.44616	5.26463	0.002371	0.001542	0.001391
6.44846	16.34427	7.40648	-0.002676	-0.001174	0.002046
8.60064	16.47644	7.89249	0.005088	0.002096	0.005110
1.24544	5.11881	5.35500	0.000946	0.000163	-0.002454
2.44348	5.83889	8.62292	0.002420	-0.004431	0.001216
0.01380	5.79530	5.28573	0.002076	-0.002457	0.000473
1.21063	5.16420	8.54151	0.000256	-0.000513	-0.001897
2.44351	7.27931	8.74832	-0.000079	-0.001258	-0.000127
3.70866	5.11896	5.35390	-0.000425	-0.001626	0.000336
4.90800	5.84315	8.62123	-0.001081	0.003830	-0.000759
2.47701	5.79561	5.28397	0.001449	-0.000600	-0.002606
3.67679	5.16572	8.54000	-0.000123	0.001641	-0.000045
4.90764	7.28398	8.74777	0.000698	-0.000612	0.001031
6.17184	5.11860	5.35433	0.001477	0.000392	0.000897
7.37096	5.84929	8.62094	-0.000622	0.007087	-0.002456
4.94029	5.79548	5.28340	0.000602	-0.002691	-0.001173
6.14080	5.17108	8.53715	-0.002519	0.002538	0.002460

7.37071	7.28983	8.75132	-0.001989	0.001604	0.000134
8.63543	5.11820	5.35521	0.001240	0.001352	-0.001068
9.83233	5.85166	8.62337	0.002789	0.000655	-0.001100
7.40374	5.79498	5.28512	0.003456	-0.002691	-0.001337
8.60194	5.17528	8.53759	-0.001891	-0.000423	-0.000216
9.83204	7.29110	8.75719	-0.001834	-0.002606	-0.002436
11.09930	5.11814	5.35578	-0.000869	-0.003344	-0.001362
12.29449	5.84673	8.62385	0.000027	0.005747	-0.002203
9.86750	5.79468	5.28678	-0.000748	-0.000719	0.001552
11.06261	5.17409	8.53894	0.002659	0.002689	-0.000399
12.29428	7.28729	8.75533	-0.004530	0.001185	-0.001521
13.56278	5.11829	5.35605	0.002656	0.000536	-0.001982
14.75895	5.83988	8.62434	-0.000230	-0.002660	-0.002199
12.33118	5.79480	5.28692	-0.004505	-0.001471	0.002595
13.52535	5.16844	8.54022	-0.003506	0.003798	-0.001432
14.75917	7.28012	8.75179	0.000944	0.002537	-0.000701
0.01434	7.23830	5.19017	0.000085	-0.000210	0.000078
1.24689	9.38061	5.13160	0.000543	-0.001861	-0.000002
1.21085	7.98059	8.79588	-0.000934	-0.000483	0.001543
2.44214	10.12243	8.87141	-0.000902	0.003289	-0.005011
0.01532	10.08686	5.14049	-0.002041	-0.000138	-0.002399
1.24606	7.94244	5.15775	0.002008	-0.002604	0.000830

1.21082	9.41592	8.85782	-0.000764	0.004388	0.000185
2.44072	11.55513	8.88414	-0.006138	-0.002810	0.001634
2.47747	7.23842	5.18585	0.002795	0.002875	0.001312
3.70997	9.38055	5.12566	-0.001084	-0.003011	0.000044
3.67534	7.98360	8.79349	-0.000564	0.001046	0.000949
4.90487	10.12925	8.87518	0.000247	-0.000261	0.000031
2.47867	10.08713	5.12695	-0.002269	0.001499	0.000764
3.70939	7.94242	5.15441	0.000820	-0.004013	-0.001698
3.67589	9.41970	8.85445	-0.001460	0.001932	-0.000146
4.90263	11.56506	8.89086	-0.000411	0.001441	0.000910
4.94085	7.23830	5.18552	-0.004705	0.002249	0.000831
6.17318	9.38002	5.13173	0.002026	0.002091	0.001832
6.13864	7.99044	8.79647	0.002460	-0.000316	-0.001670
7.36780	10.13760	8.89473	-0.000643	0.003165	0.000572
4.94196	10.08682	5.12700	0.004134	0.001476	-0.001156
6.17284	7.94199	5.15766	-0.000053	0.000553	0.003032
6.13939	9.42660	8.86164	0.000767	-0.000413	-0.002183
7.36410	11.57721	8.92935	-0.000673	-0.002169	0.003500
7.40426	7.23794	5.19012	0.002142	0.001761	0.001073
8.63700	9.37970	5.14543	-0.000542	0.002943	0.000950
8.60086	7.99568	8.80617	0.001101	-0.000541	-0.001069
9.83068	10.14286	8.92842	-0.002252	0.002516	-0.000708

7.40553	10.08627	5.14064	0.001204	-0.003579	0.003145
8.63637	7.94166	5.16555	0.002611	0.001782	-0.001408
8.60077	9.43254	8.88532	-0.006062	0.002372	-0.001266
9.82927	11.58244	9.00096	0.001096	0.003285	0.001010
9.86805	7.23787	5.19489	-0.000369	0.000097	-0.000214
11.10106	9.37979	5.15156	-0.003832	-0.001035	0.000660
11.06331	7.99411	8.80818	-0.000268	-0.001629	0.000118
12.29815	10.12943	8.90340	-0.000825	-0.001085	0.001373
9.86930	10.08593	5.15631	-0.005452	-0.001463	0.001408
11.10021	7.94175	5.16862	-0.000603	-0.003080	0.001390
11.06206	9.43062	8.88839	0.004615	0.001819	0.002064
12.30255	11.56557	8.94694	0.003320	-0.000837	-0.000806
12.33169	7.23799	5.19447	-0.001031	0.000240	-0.001753
13.56437	9.38021	5.14435	0.000726	0.001642	-0.000577
13.52754	7.98555	8.80171	-0.000765	-0.002567	-0.003115
14.76233	10.12320	8.88285	-0.005205	0.000905	-0.001614
12.33257	10.08637	5.15511	0.002640	0.000532	-0.001540
13.56350	7.94214	5.16485	-0.000086	-0.000895	-0.000372
13.52731	9.42040	8.86925	-0.000161	0.003138	-0.000535
14.76430	11.55727	8.90646	-0.002221	-0.000725	0.001756
0.01611	11.52516	5.16621	-0.001078	-0.002566	0.000391
1.24770	13.67535	5.22209	0.001836	-0.002327	-0.002482

1.21217	12.26335	8.89409	0.000611	-0.000318	0.001179
2.43998	14.38728	8.86748	-0.002686	0.000864	0.000809
0.01699	14.35408	5.27295	-0.000441	-0.000665	-0.001972
1.24794	12.22963	5.17275	0.001053	0.000849	-0.001363
1.21434	13.70818	8.88771	0.002067	0.002348	0.003768
2.47958	11.52580	5.14547	-0.001616	-0.000201	-0.001483
3.71218	13.67636	5.19535	0.004633	0.000579	0.001067
3.66932	12.26248	8.88184	-0.002107	0.000018	-0.000624
4.89370	14.38589	8.86075	0.004012	-0.001493	-0.002451
2.48000	14.35596	5.23149	0.001282	-0.001176	0.001686
3.71150	12.23022	5.15602	0.000901	-0.004535	0.001008
3.66212	13.70366	8.87117	-0.005216	0.004170	-0.000652
4.94290	11.52542	5.14351	-0.000071	-0.001779	-0.001602
6.17627	13.67505	5.20032	0.000855	0.000596	0.000063
6.13145	12.27911	8.90591	0.005248	0.006535	0.004619
7.36614	14.42967	8.88203	-0.000135	-0.000458	0.000254
4.94347	14.35627	5.21375	0.000104	-0.001898	0.001066
6.17493	12.22917	5.16623	-0.001422	-0.001049	0.001554
6.11879	13.72336	8.87765	0.005259	0.001201	0.000124
7.40625	11.52413	5.16368	0.000910	-0.003354	0.000353
8.63876	13.67323	5.24377	0.001853	0.002098	-0.001322
8.58939	12.29067	9.00208	-0.000498	0.000682	-0.000838

9.83855	14.39048	9.30305	0.004608	-0.001779	0.002149
7.40672	14.35386	5.23530	-0.001144	-0.000359	-0.000752
8.63820	12.22778	5.19800	0.000308	-0.001243	0.001058
8.55571	13.73596	9.04598	0.000930	-0.004883	0.004121
9.86985	11.52338	5.18893	0.001750	-0.001978	-0.000110
11.10099	13.67352	5.27669	0.003182	-0.000864	-0.000982
11.07378	12.27333	9.00891	-0.003484	0.003910	-0.002746
12.30694	14.38896	9.00333	-0.001226	-0.001113	0.001405
9.86934	14.35300	5.29564	0.002925	0.000015	-0.000039
11.10161	12.22804	5.21650	-0.001114	-0.002727	0.001058
11.11464	13.70636	9.07877	0.001887	0.000292	-0.000060
12.33326	11.52411	5.18815	-0.000926	0.000279	0.000533
13.56430	13.67399	5.25995	0.001560	-0.000022	0.000084
13.53626	12.26601	8.93587	-0.002292	0.004248	0.002106
14.76266	14.38906	8.90426	-0.003758	0.001204	0.003635
12.33397	14.35288	5.30710	0.002775	-0.001899	-0.001764
13.56505	12.22870	5.20105	0.000101	0.000092	-0.001137
13.54921	13.70690	8.94399	-0.000579	-0.003611	0.001053
9.91126	15.53185	9.99472	0.002291	0.004294	0.005909
7.28864	16.40884	8.69813	-0.000091	-0.004292	-0.002828
10.02526	16.50365	10.64498	0.003072	-0.002275	0.000150

---

total drift: -0.044294 0.025188 -0.022834

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

---

free energy TOTEN = -1209.38927529 eV

energy without entropy= -1209.38927529 energy(sigma->0) = -1209.38927529

POTLOK: cpu time 0.1777: real time 0.1783

---

stress matrix after NEB project (eV)

-17.74331 -0.24794 0.05475

-0.24794 -15.28199 0.45689

0.05475 0.45689 -19.05281

FORCES: max atom, RMS 0.007655 0.000706

FORCE total and by dimension 0.008558 0.005909

Stress total and by dimension 30.198016 19.052805

| |

| W W AA RRRRR N N II N N GGGG !!! |

| W W A A R R NN N II NN N G G !!! |

| W W A A R R N N N II N N N G !!! |

| W WW W AAAAAA RRRRR N N N II N N N G GGG ! |

| WW WW A A R R N NN II N NN G G |

| W W A A R R N N II N N GGGG !!! |

| |

| Your timestep is larger than 0.1 Angst. |

| For finite differences this really does not make sense. I will |

| reset POTIM to 0.015. I recommend to use 0.01 to 0.02 for finite |

| differences. |

| |

Finite differences:

Step POTIM = 1.500000000000000E-002

Degrees of freedom DOF = 6

LATTYP: Found a simple orthorhombic cell.

ALAT = 14.7806000000

B/A-ratio = 1.2466138046

C/A-ratio = 1.4433717170

Lattice vectors:

A1 = (-14.7806000000, 0.0000000000, 0.0000000000)

A2 = (0.0000000000, 0.0000000000, -18.4257000000)

A3 = (0.0000000000, -21.3339000000, 0.0000000000)

Analysis of symmetry for initial positions (statically):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The static configuration has the point symmetry C_1 .

Analysis of symmetry for dynamics (positions and initial velocities):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The dynamic configuration has the point symmetry C_1 .

Analysis of constrained symmetry for selective dynamics:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The constrained configuration has the point symmetry C_1 .

Analysis of structural, dynamic, and magnetic symmetry:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The magnetic configuration has the point symmetry C_1 .

Subroutine INISYM returns: Found 1 space group operations

(whereof 1 operations are pure point group operations),

and found 1 'primitive' translations

KPOINTS: KPT-Resolved Value to Generate K-Mesh: 0

Automatic generation of k-mesh.

Space group operators:

irot	det(A)	alpha	n_x	n_y	n_z	tau_x	tau_y	tau_z
1	1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Subroutine IBZKPT returns following result:

==========

Found 1 irreducible k-points:

Following reciprocal coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

Following cartesian coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

WAVPRE: cpu time 0.1227: real time 0.1357

FEWALD: cpu time 0.0028: real time 0.0028

ORTHCH: cpu time 1.0128: real time 1.0158

LOOP+: cpu time 413.9708: real time 416.2489

---------- Iteration 2(1) ----------

POTLOK: cpu time 0.1737: real time 0.1872

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9279: real time 1.9348

RMM-DIIS: cpu time 7.1336: real time 7.1565

ORTHCH: cpu time 0.3517: real time 0.3530

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5244: real time 0.5262

MIXING: cpu time 0.0044: real time 0.0043

LOOP: cpu time 10.1260: real time 10.1724

eigenvalue-minimisations : 1927

total energy-change (2. order) : 0.2034728E-02 (-0.4345576E-01)

number of electron 518.9999724 magnetization 0.9999987

augmentation part 11.7377713 magnetization 0.0542772

Broyden mixing:

rms(total) = 0.15660E-01 rms(broyden)= 0.15501E-01

rms(prec) = 0.15951E-01

weight for this iteration 100.00

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.75640856

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79841311

PAW double counting = 52176.83292844 -52239.75174389

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.89079617

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76944803 eV

energy without entropy = -1202.76944803 energy(sigma->0) = -1202.76944803

---------- Iteration 2(2) ----------

POTLOK: cpu time 0.1684: real time 0.1876

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9253: real time 1.9318

RMM-DIIS: cpu time 7.1126: real time 7.1508

ORTHCH: cpu time 0.3522: real time 0.3532

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5254: real time 0.5272

MIXING: cpu time 0.0046: real time 0.0046

LOOP: cpu time 10.0990: real time 10.1658

eigenvalue-minimisations : 1920

total energy-change (2. order) :-0.3226761E-03 (-0.4205479E-03)

number of electron 518.9999724 magnetization 0.9999989

augmentation part 11.7373389 magnetization 0.0542768

Broyden mixing:

rms(total) = 0.86718E-02 rms(broyden)= 0.86583E-02

rms(prec) = 0.89223E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6384

1.6384

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.81461299

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80027133

PAW double counting = 52177.19011832 -52240.10950715

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.83419924

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76977070 eV

energy without entropy = -1202.76977070 energy(sigma->0) = -1202.76977070

---------- Iteration 2(3) ----------

POTLOK: cpu time 0.1693: real time 0.1849

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9225: real time 1.9289

RMM-DIIS: cpu time 7.1451: real time 7.1816

ORTHCH: cpu time 0.3542: real time 0.3553

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5247: real time 0.5266

MIXING: cpu time 0.0048: real time 0.0049

LOOP: cpu time 10.1312: real time 10.1927

eigenvalue-minimisations : 1937

total energy-change (2. order) :-0.2709967E-04 (-0.1805602E-04)

number of electron 518.9999724 magnetization 0.9999991

augmentation part 11.7379081 magnetization 0.0542765

Broyden mixing:

rms(total) = 0.36107E-02 rms(broyden)= 0.36085E-02

rms(prec) = 0.37584E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4920

0.7253 2.2588

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.84836826

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79864593

PAW double counting = 52177.61014159 -52240.52928607

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.79909003

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76979780 eV

energy without entropy = -1202.76979780 energy(sigma->0) = -1202.76979780

---------- Iteration 2(4) ----------

POTLOK: cpu time 0.1686: real time 0.1845

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9190: real time 1.9259

RMM-DIIS: cpu time 7.1347: real time 7.1617

ORTHCH: cpu time 0.3538: real time 0.3551

DOS: cpu time 0.0003: real time 0.0003

CHARGE: cpu time 0.5272: real time 0.5287

MIXING: cpu time 0.0053: real time 0.0053

LOOP: cpu time 10.1191: real time 10.1714

eigenvalue-minimisations : 1912

total energy-change (2. order) :-0.4218513E-05 (-0.2809078E-05)

number of electron 518.9999724 magnetization 0.9999992

augmentation part 11.7376711 magnetization 0.0542758

Broyden mixing:

rms(total) = 0.96218E-03 rms(broyden)= 0.96115E-03

rms(prec) = 0.10451E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3919

2.3964 0.8896 0.8896

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.88236620

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80051869

PAW double counting = 52177.92060399 -52240.84040598

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.76631156

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76980202 eV

energy without entropy = -1202.76980202 energy(sigma->0) = -1202.76980202

---------- Iteration 2(5) ----------

POTLOK: cpu time 0.1693: real time 0.1869

```
      SETDIJ:    cpu time       0.0101: real time       0.0101
      EDDIAG:    cpu time       1.9233: real time       1.9298
    RMM-DIIS:    cpu time       6.8986: real time       6.9251
      ORTHCH:    cpu time       0.3550: real time       0.3561
         DOS:    cpu time       0.0003: real time       0.0003
      CHARGE:    cpu time       0.5267: real time       0.5284
      MIXING:    cpu time       0.0055: real time       0.0055
      ----------------------------------------
        LOOP:    cpu time       9.8888: real time       9.9421

eigenvalue-minimisations    :    1834
total energy-change (2. order) : 0.9294272E-06    (-0.3759198E-06)
number of electron          518.9999724 magnetization             0.9999993
augmentation part            11.7376290 magnetization             0.0542760

Broyden mixing:
  rms(total) = 0.38644E-03        rms(broyden)= 0.38595E-03
  rms(prec ) = 0.42825E-03
  weight for this iteration          100.00

eigenvalues of (default mixing * dielectric matrix)
  average eigenvalue GAMMA=      1.4407
```

2.5248 1.5808 0.8286 0.8286

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.89409020

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80059952

PAW double counting = 52177.99190555 -52240.91173807

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.75463692

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76980109 eV

energy without entropy = -1202.76980109 energy(sigma->0) = -1202.76980109

---------- Iteration 2(6) ----------

POTLOK: cpu time 0.1698: real time 0.1724

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9250: real time 1.9316

RMM-DIIS: cpu time 6.1534: real time 6.1870

ORTHCH: cpu time 0.3530: real time 0.3539

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5247: real time 0.5267

MIXING: cpu time 0.0057: real time 0.0057

LOOP: cpu time 9.1421: real time 9.1878

eigenvalue-minimisations : 1669

total energy-change (2. order) :-0.1401640E-06 (-0.9823190E-07)

number of electron 518.9999724 magnetization 0.9999994

augmentation part 11.7376232 magnetization 0.0542761

Broyden mixing:

rms(total) = 0.14241E-03 rms(broyden)= 0.14219E-03

rms(prec) = 0.17035E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4054

2.6001 1.8029 0.7808 0.9216 0.9216

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.90292855

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80059148

PAW double counting = 52178.01482352 -52240.93464714

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.74579958

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76980123 eV

energy without entropy = -1202.76980123 energy(sigma->0) = -1202.76980123

---------- Iteration 2(7) ----------

POTLOK: cpu time 0.1678: real time 0.1821

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9246: real time 1.9311

RMM-DIIS: cpu time 5.2369: real time 5.2618

ORTHCH: cpu time 0.3511: real time 0.3523

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5236: real time 0.5252

MIXING: cpu time 0.0059: real time 0.0059

LOOP: cpu time 8.2203: real time 8.2688

eigenvalue-minimisations : 1431

total energy-change (2. order) :-0.5946604E-06 (-0.1179023E-07)

number of electron 518.9999724 magnetization 0.9999995

augmentation part 11.7376277 magnetization 0.0542761

Broyden mixing:

rms(total) = 0.67703E-04 rms(broyden)= 0.67665E-04

rms(prec) = 0.91649E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3648

2.6525 1.9604 1.1376 0.9464 0.8452 0.6469

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.90839516

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80062546

PAW double counting = 52178.00997774 -52240.92979539

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.74037352

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76980183 eV

energy without entropy = -1202.76980183 energy(sigma->0) = -1202.76980183

---------- Iteration 2(8) ----------

POTLOK: cpu time 0.1698: real time 0.1782

SETDIJ: cpu time 0.0100: real time 0.0101

```
      EDDIAG:  cpu time        1.9274: real time        1.9340
 RMM-DIIS:  cpu time        5.0093: real time        5.0402
      ORTHCH:  cpu time        0.3514: real time        0.3525
         DOS:  cpu time        0.0004: real time        0.0004
      CHARGE:  cpu time        0.5243: real time        0.5258
      MIXING:  cpu time        0.0064: real time        0.0065
      ------------------------------------------
        LOOP:  cpu time        7.9990: real time        8.0476

eigenvalue-minimisations  :  1364
total energy-change (2. order) :-0.5621332E-06  (-0.3141435E-08)
number of electron       518.9999724 magnetization             0.9999996
augmentation part          11.7376309 magnetization             0.0542761

Broyden mixing:
  rms(total) = 0.39841E-04        rms(broyden)= 0.39819E-04
  rms(prec ) = 0.63226E-04
  weight for this iteration        100.00

eigenvalues of (default mixing * dielectric matrix)
  average eigenvalue GAMMA=      1.4149
  2.6942   2.1882   1.6357   0.9775   0.9775   0.8118   0.6192
```

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.91265226

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80065401

PAW double counting = 52178.00486372 -52240.92467918

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.73614771

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76980239 eV

energy without entropy = -1202.76980239 energy(sigma->0) = -1202.76980239

---------- Iteration 2(9) ----------

POTLOK: cpu time 0.1694: real time 0.1886

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9205: real time 1.9274

RMM-DIIS: cpu time 4.9396: real time 4.9751

ORTHCH: cpu time 0.3504: real time 0.3516

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5230: real time 0.5250

MIXING: cpu time 0.0066: real time 0.0066

LOOP: cpu time 7.9200: real time 7.9849

eigenvalue-minimisations : 1325

total energy-change (2. order) :-0.8886709E-06 (-0.2720626E-08)

number of electron 518.9999724 magnetization 0.9999997

augmentation part 11.7376323 magnetization 0.0542762

Broyden mixing:

rms(total) = 0.22297E-04 rms(broyden)= 0.22286E-04

rms(prec) = 0.39994E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4647

2.9513 2.5559 1.8787 1.1176 0.9431 0.8275 0.8275 0.6164

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.91972256

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80070755

PAW double counting = 52177.99823772 -52240.91805542

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.72912960

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76980328 eV

energy without entropy = -1202.76980328 energy(sigma->0) = -1202.76980328

---------- Iteration 2(10) ----------

POTLOK: cpu time 0.1661: real time 0.1666

SETDIJ: cpu time 0.0099: real time 0.0100

EDDIAG: cpu time 1.9235: real time 1.9296

RMM-DIIS: cpu time 4.7922: real time 4.8156

ORTHCH: cpu time 0.3519: real time 0.3531

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5238: real time 0.5257

MIXING: cpu time 0.0072: real time 0.0072

LOOP: cpu time 7.7749: real time 7.8081

eigenvalue-minimisations : 1269

total energy-change (2. order) :-0.7842609E-06 (-0.2213326E-08)

number of electron 518.9999724 magnetization 0.9999997

augmentation part 11.7376313 magnetization 0.0542762

Broyden mixing:

rms(total) = 0.13628E-04 rms(broyden)= 0.13618E-04

rms(prec) = 0.25121E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4639

3.2135 2.6013 1.9541 1.2963 0.9770 0.9770 0.7989 0.7392 0.6172

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.92576374

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80075501

PAW double counting = 52177.99521374 -52240.91503648

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.72313163

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76980406 eV

energy without entropy = -1202.76980406 energy(sigma->0) = -1202.76980406

---------- Iteration 2(11) ----------

POTLOK: cpu time 0.1689: real time 0.1758

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9232: real time 1.9288

RMM-DIIS: cpu time 4.6007: real time 4.6243

ORTHCH: cpu time 0.3520: real time 0.3529

DOS: cpu time 0.0005: real time 0.0005

CHARGE: cpu time 0.5279: real time 0.5292

MIXING: cpu time 0.0076: real time 0.0077

LOOP: cpu time 7.5908: real time 7.6292

eigenvalue-minimisations : 1181

total energy-change (2. order) :-0.6158807E-06 (-0.1217587E-08)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7376314 magnetization 0.0542763

Broyden mixing:

rms(total) = 0.95468E-05 rms(broyden)= 0.95418E-05

rms(prec) = 0.16991E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6262

4.3777 2.6665 2.2188 1.8145 1.1745 0.9207 0.9207 0.8699 0.6798 0.6192

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.92948116

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80077316

PAW double counting = 52177.99493738 -52240.91476137

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.71943173

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76980468 eV

energy without entropy = -1202.76980468 energy(sigma->0) = -1202.76980468

---------- Iteration 2(12) ----------

POTLOK: cpu time 0.1685: real time 0.1871

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9230: real time 1.9293

RMM-DIIS: cpu time 4.5978: real time 4.6228

ORTHCH: cpu time 0.3517: real time 0.3527

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5237: real time 0.5252

MIXING: cpu time 0.0079: real time 0.0080

LOOP: cpu time 7.5831: real time 7.6357

eigenvalue-minimisations : 1195

total energy-change (2. order) :-0.6314949E-06 (-0.1359869E-08)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7376324 magnetization 0.0542763

Broyden mixing:

rms(total) = 0.54234E-05 rms(broyden)= 0.54136E-05

rms(prec) = 0.89231E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6816

5.2514 2.7091 2.3542 1.8953 1.2622 1.0255 1.0255 0.8419 0.8419 0.6199

0.6701

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.93357540

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80078645

PAW double counting = 52177.99503682 -52240.91486068

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.71535153

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76980531 eV

energy without entropy = -1202.76980531 energy(sigma->0) = -1202.76980531

---------- Iteration 2(13) ----------

POTLOK: cpu time 0.1678: real time 0.1932

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9196: real time 1.9262

RMM-DIIS: cpu time 4.2400: real time 4.2578

ORTHCH: cpu time 0.3531: real time 0.3542

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5231: real time 0.5248

MIXING: cpu time 0.0080: real time 0.0080

LOOP: cpu time 7.2221: real time 7.2748

eigenvalue-minimisations : 1002

total energy-change (2. order) :-0.2837805E-06 (-0.3662040E-09)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7376323 magnetization 0.0542762

Broyden mixing:

rms(total) = 0.30415E-05 rms(broyden)= 0.30394E-05

rms(prec) = 0.53779E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7360

6.0236 2.7920 2.5284 1.9857 1.5709 1.0683 1.0683 0.8703 0.8703 0.7748

0.6207 0.6586

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.93498881

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80079288

PAW double counting = 52177.99511446 -52240.91493910

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.71394407

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76980559 eV

energy without entropy = -1202.76980559 energy(sigma->0) = -1202.76980559

---------- Iteration 2(14) ----------

POTLOK: cpu time 0.1664: real time 0.1777

SETDIJ: cpu time 0.0101: real time 0.0102

```
      EDDIAG:  cpu time        1.9267: real time        1.9332
 RMM-DIIS:  cpu time        4.2924: real time        4.3065
     ORTHCH:  cpu time        0.3516: real time        0.3527
        DOS:  cpu time        0.0004: real time        0.0004
     CHARGE:  cpu time        0.5234: real time        0.5253
     MIXING:  cpu time        0.0085: real time        0.0085
     ------------------------------------------
       LOOP:  cpu time        7.2795: real time        7.3144

eigenvalue-minimisations  :  1017
total energy-change (2. order) :-0.1640437E-06  (-0.3044374E-09)
number of electron       518.9999724 magnetization             0.9999998
augmentation part         11.7376321 magnetization             0.0542763

Broyden mixing:
 rms(total) = 0.22556E-05        rms(broyden)= 0.22544E-05
 rms(prec ) = 0.35974E-05
 weight for this iteration         100.00

eigenvalues of (default mixing * dielectric matrix)
 average eigenvalue GAMMA=      1.7838
 6.7009   3.0268   2.6331   2.0662   1.7634   1.1894   1.0709   1.0709   0.8545   0.8545
```

0.6972 0.6220 0.6400

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.93568583

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80079534

PAW double counting = 52177.99506715 -52240.91489231

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.71324914

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76980576 eV

energy without entropy = -1202.76980576 energy(sigma->0) = -1202.76980576

---------- Iteration 2(15) ----------

POTLOK: cpu time 0.1699: real time 0.1809

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9216: real time 1.9282

RMM-DIIS: cpu time 4.0614: real time 4.0863

ORTHCH: cpu time 0.3542: real time 0.3554

DOS: cpu time 0.0003: real time 0.0003

LOOP: cpu time 6.5175: real time 6.5612

eigenvalue-minimisations : 944

total energy-change (2. order) :-0.8215648E-07 (-0.1877201E-09)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7376321 magnetization 0.0542763

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.16747224

-Hartree energ DENC = -107335.93596240

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80079460

PAW double counting = 52177.99489018 -52240.91471538

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.71297187

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76980584 eV

energy without entropy = -1202.76980584 energy(sigma->0) = -1202.76980584

---

average (electrostatic) potential at core

the test charge radii are 0.5201 0.6991 1.0621 0.7215

(the norm of the test charge is 1.0000)

1 -40.7525	2 -40.7504	3 -40.7517	4 -40.7504	5 -40.7524
6 -40.7546	7 -40.7521	8 -40.7599	9 -40.7518	10 -40.7596
11 -40.7532	12 -40.7552	13 -40.6495	14 -40.6956	15 -40.7691
16 -40.6977	17 -40.6915	18 -40.8662	19 -40.6786	20 -40.6668
21 -40.6882	22 -40.6608	23 -40.0822	24 -40.1244	25 -57.4585
26 -57.6696	27 -57.6565	28 -57.4684	29 -57.6631	30 -57.4585
31 -57.6694	32 -57.6561	33 -57.4664	34 -57.6680	35 -57.4593
36 -57.6713	37 -57.6561	38 -57.4686	39 -57.6740	40 -57.4584
41 -57.6754	42 -57.6563	43 -57.4734	44 -57.6885	45 -57.4584
46 -57.6743	47 -57.6571	48 -57.4739	49 -57.6797	50 -57.4595
51 -57.6710	52 -57.6569	53 -57.4714	54 -57.6660	55 -57.6363
56 -57.6623	57 -57.6867	58 -57.6829	59 -57.6660	60 -57.6689
61 -57.6897	62 -57.6743	63 -57.6366	64 -57.6618	65 -57.6888
66 -57.6945	67 -57.6643	68 -57.6687	69 -57.6935	70 -57.7007
71 -57.6361	72 -57.6632	73 -57.6965	74 -57.7218	75 -57.6651
76 -57.6693	77 -57.7059	78 -57.7520	79 -57.6362	80 -57.6658
81 -57.7102	82 -57.7520	83 -57.6684	84 -57.6708	85 -57.7370
86 -57.8415	87 -57.6387	88 -57.6665	89 -57.7122	90 -57.7166
91 -57.6731	92 -57.6710	93 -57.7423	94 -57.7588	95 -57.6370
96 -57.6646	97 -57.6958	98 -57.6902	99 -57.6704	100 -57.6698

101 -57.7074	102 -57.6856	103 -57.6598	104 -57.6304	105 -57.6450
106 -57.2892	107 -57.3875	108 -57.6308	109 -57.5969	110 -57.6587
111 -57.6303	112 -57.6418	113 -57.3082	114 -57.3932	115 -57.6300
116 -57.5989	117 -57.6580	118 -57.6221	119 -57.6982	120 -57.6828
121 -57.3868	122 -57.6288	123 -57.7089	124 -57.6589	125 -57.6248
126 -57.8356	127 -58.3295	128 -57.3601	129 -57.6341	130 -58.1470
131 -57.6669	132 -57.6341	133 -57.7981	134 -57.4165	135 -57.3714
136 -57.6380	137 -58.0758	138 -57.6633	139 -57.6299	140 -57.6707
141 -57.2983	142 -57.3777	143 -57.6334	144 -57.6476	145 -60.8535
146 -57.3121	147 -81.2845			

E-fermi : -2.3010 XC(G=0): -2.7344 alpha+bet : -2.2521

spin component 1

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-27.0142	1.00000
2	-21.5683	1.00000

3	-21.4713	1.00000
4	-21.0995	1.00000
5	-21.0684	1.00000
6	-21.0145	1.00000
7	-20.9784	1.00000
8	-20.9764	1.00000
9	-20.8908	1.00000
10	-20.5577	1.00000
11	-20.5030	1.00000
12	-20.4114	1.00000
13	-20.3978	1.00000
14	-20.1262	1.00000
15	-19.9756	1.00000
16	-19.7031	1.00000
17	-19.6272	1.00000
18	-19.5994	1.00000
19	-19.5837	1.00000
20	-19.5284	1.00000
21	-19.5266	1.00000
22	-19.4984	1.00000
23	-19.4808	1.00000
24	-19.1119	1.00000

25	-19.0749	1.00000
26	-18.9782	1.00000
27	-18.9646	1.00000
28	-18.9004	1.00000
29	-18.7332	1.00000
30	-18.5044	1.00000
31	-18.3589	1.00000
32	-18.2751	1.00000
33	-18.2519	1.00000
34	-18.1836	1.00000
35	-18.1809	1.00000
36	-18.0796	1.00000
37	-18.0757	1.00000
38	-17.5611	1.00000
39	-17.3131	1.00000
40	-17.2874	1.00000
41	-17.2825	1.00000
42	-17.2097	1.00000
43	-17.2033	1.00000
44	-17.1767	1.00000
45	-17.0224	1.00000
46	-16.9501	1.00000

47	-16.9324	1.00000
48	-16.8929	1.00000
49	-16.8911	1.00000
50	-16.8499	1.00000
51	-16.8415	1.00000
52	-16.8209	1.00000
53	-16.8187	1.00000
54	-16.7292	1.00000
55	-16.7259	1.00000
56	-16.1763	1.00000
57	-15.7294	1.00000
58	-15.6918	1.00000
59	-15.6597	1.00000
60	-15.6369	1.00000
61	-15.6160	1.00000
62	-15.5534	1.00000
63	-15.5496	1.00000
64	-15.1748	1.00000
65	-14.8087	1.00000
66	-14.6082	1.00000
67	-14.5778	1.00000
68	-14.5347	1.00000

69	-14.4981	1.00000
70	-14.4684	1.00000
71	-14.4421	1.00000
72	-14.3336	1.00000
73	-14.3055	1.00000
74	-14.2795	1.00000
75	-14.2720	1.00000
76	-14.1822	1.00000
77	-14.1784	1.00000
78	-13.8890	1.00000
79	-13.7599	1.00000
80	-13.5932	1.00000
81	-13.5482	1.00000
82	-13.5292	1.00000
83	-13.4975	1.00000
84	-13.4455	1.00000
85	-13.3639	1.00000
86	-13.3453	1.00000
87	-13.1889	1.00000
88	-12.7863	1.00000
89	-12.7592	1.00000
90	-12.7277	1.00000

91	-12.6959	1.00000
92	-12.6864	1.00000
93	-12.6234	1.00000
94	-12.4610	1.00000
95	-12.4460	1.00000
96	-12.3820	1.00000
97	-12.3232	1.00000
98	-12.2127	1.00000
99	-12.2031	1.00000
100	-12.1648	1.00000
101	-11.9493	1.00000
102	-11.6845	1.00000
103	-11.6282	1.00000
104	-11.6108	1.00000
105	-11.5807	1.00000
106	-11.1072	1.00000
107	-11.0765	1.00000
108	-10.8985	1.00000
109	-10.8874	1.00000
110	-10.8318	1.00000
111	-10.7107	1.00000
112	-10.6805	1.00000

113	-10.6623	1.00000
114	-10.6463	1.00000
115	-10.5892	1.00000
116	-10.5808	1.00000
117	-10.5715	1.00000
118	-10.5677	1.00000
119	-10.5260	1.00000
120	-10.5251	1.00000
121	-10.5103	1.00000
122	-10.5025	1.00000
123	-10.3783	1.00000
124	-10.2944	1.00000
125	-10.2566	1.00000
126	-10.1874	1.00000
127	-10.1863	1.00000
128	-10.0809	1.00000
129	-10.0404	1.00000
130	-9.8918	1.00000
131	-9.8656	1.00000
132	-9.7945	1.00000
133	-9.7859	1.00000
134	-9.7591	1.00000

135	-9.6910	1.00000
136	-9.4501	1.00000
137	-9.4250	1.00000
138	-9.3949	1.00000
139	-9.3878	1.00000
140	-9.3797	1.00000
141	-9.3690	1.00000
142	-9.3104	1.00000
143	-9.3040	1.00000
144	-9.3002	1.00000
145	-9.2856	1.00000
146	-9.2703	1.00000
147	-9.0927	1.00000
148	-9.0041	1.00000
149	-8.9859	1.00000
150	-8.9569	1.00000
151	-8.9558	1.00000
152	-8.7938	1.00000
153	-8.7454	1.00000
154	-8.7343	1.00000
155	-8.7178	1.00000
156	-8.7083	1.00000

157	-8.6868	1.00000
158	-8.6779	1.00000
159	-8.6681	1.00000
160	-8.6535	1.00000
161	-8.5943	1.00000
162	-8.5824	1.00000
163	-8.5758	1.00000
164	-8.5674	1.00000
165	-8.4876	1.00000
166	-8.4571	1.00000
167	-8.4356	1.00000
168	-8.3450	1.00000
169	-8.2972	1.00000
170	-8.2750	1.00000
171	-8.2631	1.00000
172	-8.2328	1.00000
173	-8.2318	1.00000
174	-8.1511	1.00000
175	-8.1447	1.00000
176	-8.0769	1.00000
177	-8.0443	1.00000
178	-8.0259	1.00000

179	-8.0212	1.00000
180	-7.9728	1.00000
181	-7.9642	1.00000
182	-7.9236	1.00000
183	-7.9003	1.00000
184	-7.8847	1.00000
185	-7.8719	1.00000
186	-7.8004	1.00000
187	-7.7969	1.00000
188	-7.7473	1.00000
189	-7.7101	1.00000
190	-7.6660	1.00000
191	-7.5993	1.00000
192	-7.5844	1.00000
193	-7.5755	1.00000
194	-7.5466	1.00000
195	-7.4801	1.00000
196	-7.4795	1.00000
197	-7.4275	1.00000
198	-7.3239	1.00000
199	-7.2489	1.00000
200	-7.1559	1.00000

201	-7.0656	1.00000
202	-7.0417	1.00000
203	-7.0277	1.00000
204	-7.0131	1.00000
205	-6.9961	1.00000
206	-6.9892	1.00000
207	-6.9749	1.00000
208	-6.8665	1.00000
209	-6.8202	1.00000
210	-6.8011	1.00000
211	-6.7926	1.00000
212	-6.7315	1.00000
213	-6.6856	1.00000
214	-6.4706	1.00000
215	-6.4244	1.00000
216	-6.3957	1.00000
217	-6.3906	1.00000
218	-6.3735	1.00000
219	-6.3721	1.00000
220	-6.3166	1.00000
221	-6.3067	1.00000
222	-6.2366	1.00000

223	-6.2292	1.00000
224	-6.2287	1.00000
225	-6.0773	1.00000
226	-6.0371	1.00000
227	-5.7920	1.00000
228	-5.7520	1.00000
229	-5.6935	1.00000
230	-5.6407	1.00000
231	-5.6366	1.00000
232	-5.5584	1.00000
233	-5.5299	1.00000
234	-5.4675	1.00000
235	-5.4386	1.00000
236	-5.1649	1.00000
237	-5.0582	1.00000
238	-5.0502	1.00000
239	-5.0177	1.00000
240	-4.9885	1.00000
241	-4.9099	1.00000
242	-4.8531	1.00000
243	-4.8217	1.00000
244	-4.7893	1.00000

245	-4.6802	1.00000
246	-4.5721	1.00000
247	-4.5708	1.00000
248	-4.5051	1.00000
249	-4.4451	1.00000
250	-4.3833	1.00000
251	-4.2924	1.00000
252	-4.2651	1.00000
253	-4.2123	1.00000
254	-3.5574	1.00000
255	-3.3541	1.00000
256	-3.1998	1.00000
257	-2.9389	1.00000
258	-2.8479	1.00000
259	-2.8231	1.00000
260	-2.6060	1.00000
261	-1.9082	0.00000
262	-1.7672	0.00000
263	-1.7183	0.00000
264	-1.3434	0.00000
265	-1.2946	0.00000
266	-1.1841	0.00000

267	-0.7445	0.00000
268	-0.5843	0.00000
269	-0.5009	0.00000
270	-0.3074	0.00000
271	-0.3054	0.00000
272	-0.2895	0.00000
273	-0.1825	0.00000
274	-0.0576	0.00000
275	-0.0485	0.00000
276	-0.0097	0.00000
277	0.0354	0.00000
278	0.0851	0.00000
279	0.1733	0.00000
280	0.2207	0.00000
281	0.2486	0.00000
282	0.4207	0.00000
283	0.4489	0.00000
284	0.4820	0.00000
285	0.5984	0.00000
286	0.6753	0.00000
287	0.8191	0.00000
288	0.8714	0.00000

289	1.0451	0.00000
290	1.0826	0.00000
291	1.1209	0.00000
292	1.1628	0.00000
293	1.2232	0.00000
294	1.2444	0.00000
295	1.2874	0.00000
296	1.3144	0.00000
297	1.3456	0.00000
298	1.4113	0.00000
299	1.4657	0.00000
300	1.4839	0.00000
301	1.5526	0.00000
302	1.5870	0.00000
303	1.6251	0.00000
304	1.6775	0.00000
305	1.7507	0.00000
306	1.7634	0.00000
307	1.8729	0.00000
308	1.8949	0.00000
309	1.9049	0.00000
310	1.9130	0.00000

311	2.1241	0.00000
312	2.1866	0.00000
313	2.2084	0.00000
314	2.2355	0.00000
315	2.2757	0.00000
316	2.2917	0.00000
317	2.3313	0.00000
318	2.3535	0.00000
319	2.3726	0.00000
320	2.3976	0.00000
321	2.4199	0.00000
322	2.4297	0.00000
323	2.4392	0.00000
324	2.4537	0.00000
325	2.4613	0.00000
326	2.5236	0.00000
327	2.5372	0.00000
328	2.7006	0.00000
329	2.7284	0.00000
330	2.7533	0.00000
331	2.7564	0.00000
332	2.7642	0.00000

333	2.8140	0.00000
334	2.8345	0.00000
335	2.8583	0.00000
336	2.8911	0.00000
337	2.9242	0.00000
338	2.9464	0.00000
339	2.9783	0.00000
340	3.0049	0.00000
341	3.0340	0.00000
342	3.0442	0.00000
343	3.0661	0.00000
344	3.0851	0.00000
345	3.1496	0.00000
346	3.1625	0.00000
347	3.1795	0.00000
348	3.1922	0.00000
349	3.3000	0.00000
350	3.3228	0.00000
351	3.3512	0.00000
352	3.3673	0.00000
353	3.3893	0.00000
354	3.4328	0.00000

355	3.4762	0.00000
356	3.4852	0.00000
357	3.4852	0.00000
358	3.4985	0.00000
359	3.6343	0.00000
360	3.6729	0.00000
361	3.6862	0.00000
362	3.7322	0.00000
363	3.7512	0.00000
364	3.7589	0.00000
365	3.7720	0.00000
366	3.7934	0.00000
367	3.8121	0.00000
368	3.8341	0.00000
369	3.8381	0.00000
370	3.8519	0.00000
371	3.8767	0.00000
372	3.8838	0.00000
373	3.9102	0.00000
374	3.9241	0.00000
375	3.9336	0.00000
376	3.9575	0.00000

377	3.9726	0.00000
378	3.9840	0.00000
379	4.0162	0.00000
380	4.0690	0.00000
381	4.1645	0.00000
382	4.2464	0.00000
383	4.2574	0.00000
384	4.2581	0.00000
385	4.2852	0.00000
386	4.3129	0.00000
387	4.3274	0.00000
388	4.3406	0.00000
389	4.3713	0.00000
390	4.3809	0.00000
391	4.4174	0.00000
392	4.4441	0.00000
393	4.4684	0.00000
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395	4.4864	0.00000
396	4.4963	0.00000
397	4.5177	0.00000
398	4.5502	0.00000

399	4.5906	0.00000
400	4.6076	0.00000
401	4.6272	0.00000
402	4.6430	0.00000
403	4.6567	0.00000
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406	4.7317	0.00000
407	4.7461	0.00000
408	4.7670	0.00000
409	4.7829	0.00000
410	4.7835	0.00000
411	4.7968	0.00000
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417	4.9835	0.00000
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420	5.0350	0.00000

421	5.0392	0.00000
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425	5.1170	0.00000
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427	5.1408	0.00000
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429	5.1751	0.00000
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431	5.1879	0.00000
432	5.2154	0.00000
433	5.2353	0.00000
434	5.2407	0.00000
435	5.2558	0.00000
436	5.2895	0.00000
437	5.2956	0.00000
438	5.3090	0.00000
439	5.3315	0.00000
440	5.3491	0.00000
441	5.3671	0.00000
442	5.3729	0.00000

443	5.3929	0.00000
444	5.4209	0.00000
445	5.4539	0.00000
446	5.4643	0.00000
447	5.4817	0.00000
448	5.4951	0.00000
449	5.5190	0.00000
450	5.5503	0.00000
451	5.5698	0.00000
452	5.5755	0.00000
453	5.5968	0.00000
454	5.6160	0.00000
455	5.6584	0.00000
456	5.6830	0.00000
457	5.7143	0.00000
458	5.7295	0.00000
459	5.7531	0.00000
460	5.7782	0.00000
461	5.7908	0.00000
462	5.7934	0.00000
463	5.8009	0.00000
464	5.8107	0.00000

465	5.8202	0.00000
466	5.8457	0.00000
467	5.8545	0.00000
468	5.8837	0.00000
469	5.8931	0.00000
470	5.9038	0.00000
471	5.9142	0.00000
472	5.9411	0.00000
473	5.9444	0.00000
474	5.9631	0.00000
475	6.0043	0.00000
476	6.0304	0.00000
477	6.0458	0.00000
478	6.0548	0.00000
479	6.1070	0.00000
480	6.2715	0.00000

spin component 2

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-27.0075	1.00000

2	-21.5671	1.00000
3	-21.4697	1.00000
4	-21.0977	1.00000
5	-21.0675	1.00000
6	-21.0118	1.00000
7	-20.9770	1.00000
8	-20.9746	1.00000
9	-20.8803	1.00000
10	-20.5547	1.00000
11	-20.4996	1.00000
12	-20.4003	1.00000
13	-20.3881	1.00000
14	-20.1221	1.00000
15	-19.9524	1.00000
16	-19.7004	1.00000
17	-19.6260	1.00000
18	-19.5973	1.00000
19	-19.5773	1.00000
20	-19.5271	1.00000
21	-19.5248	1.00000
22	-19.4758	1.00000
23	-19.4613	1.00000

24	-19.1094	1.00000
25	-19.0725	1.00000
26	-18.9683	1.00000
27	-18.9550	1.00000
28	-18.8956	1.00000
29	-18.7036	1.00000
30	-18.5014	1.00000
31	-18.3519	1.00000
32	-18.2469	1.00000
33	-18.2267	1.00000
34	-18.1783	1.00000
35	-18.1755	1.00000
36	-18.0595	1.00000
37	-18.0562	1.00000
38	-17.5578	1.00000
39	-17.2969	1.00000
40	-17.2868	1.00000
41	-17.2731	1.00000
42	-17.2074	1.00000
43	-17.2063	1.00000
44	-17.1737	1.00000
45	-17.0184	1.00000

46	-16.9412	1.00000
47	-16.9220	1.00000
48	-16.8704	1.00000
49	-16.8693	1.00000
50	-16.8291	1.00000
51	-16.8226	1.00000
52	-16.8176	1.00000
53	-16.8152	1.00000
54	-16.7308	1.00000
55	-16.7248	1.00000
56	-16.1736	1.00000
57	-15.7287	1.00000
58	-15.6569	1.00000
59	-15.6432	1.00000
60	-15.6208	1.00000
61	-15.5663	1.00000
62	-15.5275	1.00000
63	-15.5248	1.00000
64	-15.1711	1.00000
65	-14.8065	1.00000
66	-14.6060	1.00000
67	-14.5602	1.00000

68	-14.5000	1.00000
69	-14.4984	1.00000
70	-14.4644	1.00000
71	-14.4378	1.00000
72	-14.3302	1.00000
73	-14.2979	1.00000
74	-14.2678	1.00000
75	-14.2636	1.00000
76	-14.1641	1.00000
77	-14.1608	1.00000
78	-13.8882	1.00000
79	-13.7575	1.00000
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81	-13.5376	1.00000
82	-13.5181	1.00000
83	-13.4939	1.00000
84	-13.4437	1.00000
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86	-13.3407	1.00000
87	-13.1873	1.00000
88	-12.7800	1.00000
89	-12.7497	1.00000

90	-12.7190	1.00000
91	-12.6773	1.00000
92	-12.6705	1.00000
93	-12.6212	1.00000
94	-12.4484	1.00000
95	-12.4312	1.00000
96	-12.3784	1.00000
97	-12.3224	1.00000
98	-12.2081	1.00000
99	-12.1979	1.00000
100	-12.1633	1.00000
101	-11.9466	1.00000
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104	-11.5917	1.00000
105	-11.5729	1.00000
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107	-11.0740	1.00000
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110	-10.8289	1.00000
111	-10.7047	1.00000

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113	-10.6593	1.00000
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132	-9.7868	1.00000
133	-9.7768	1.00000

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171	-8.2329	1.00000
172	-8.2291	1.00000
173	-8.2270	1.00000
174	-8.1410	1.00000
175	-8.1335	1.00000
176	-8.0736	1.00000
177	-8.0422	1.00000

178	-8.0130	1.00000
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182	-7.9194	1.00000
183	-7.8907	1.00000
184	-7.8708	1.00000
185	-7.8631	1.00000
186	-7.7915	1.00000
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199	-7.2356	1.00000

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216	-6.3825	1.00000
217	-6.3779	1.00000
218	-6.3627	1.00000
219	-6.3381	1.00000
220	-6.3029	1.00000
221	-6.2752	1.00000

222	-6.2291	1.00000
223	-6.2276	1.00000
224	-6.2222	1.00000
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231	-5.6222	1.00000
232	-5.5436	1.00000
233	-5.5228	1.00000
234	-5.4410	1.00000
235	-5.4112	1.00000
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244	-4.7772	1.00000
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249	-4.4208	1.00000
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251	-4.2962	1.00000
252	-4.2262	1.00000
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258	-2.7988	1.00000
259	-2.7395	1.00000
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262	-1.7219	0.00000
263	-1.6784	0.00000
264	-1.2856	0.00000
265	-1.2714	0.00000

266	-1.1532	0.00000
267	-0.7231	0.00000
268	-0.5836	0.00000
269	-0.5084	0.00000
270	-0.2804	0.00000
271	-0.2773	0.00000
272	-0.2594	0.00000
273	-0.1558	0.00000
274	-0.0567	0.00000
275	-0.0478	0.00000
276	0.0139	0.00000
277	0.0405	0.00000
278	0.0801	0.00000
279	0.2085	0.00000
280	0.2558	0.00000
281	0.2802	0.00000
282	0.4348	0.00000
283	0.4528	0.00000
284	0.4832	0.00000
285	0.6030	0.00000
286	0.6956	0.00000
287	0.8219	0.00000

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289	1.0522	0.00000
290	1.1023	0.00000
291	1.1428	0.00000
292	1.1772	0.00000
293	1.2318	0.00000
294	1.2505	0.00000
295	1.3085	0.00000
296	1.3201	0.00000
297	1.3595	0.00000
298	1.4302	0.00000
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300	1.5014	0.00000
301	1.5770	0.00000
302	1.6033	0.00000
303	1.6535	0.00000
304	1.6863	0.00000
305	1.7581	0.00000
306	1.7736	0.00000
307	1.8769	0.00000
308	1.9004	0.00000
309	1.9082	0.00000

310	1.9206	0.00000
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312	2.1977	0.00000
313	2.2200	0.00000
314	2.2541	0.00000
315	2.2895	0.00000
316	2.2963	0.00000
317	2.3366	0.00000
318	2.3612	0.00000
319	2.3833	0.00000
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326	2.5262	0.00000
327	2.5429	0.00000
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329	2.7344	0.00000
330	2.7535	0.00000
331	2.7593	0.00000

332	2.7727	0.00000
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341	3.0379	0.00000
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343	3.0717	0.00000
344	3.0926	0.00000
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346	3.1711	0.00000
347	3.1884	0.00000
348	3.2003	0.00000
349	3.3057	0.00000
350	3.3274	0.00000
351	3.3595	0.00000
352	3.3709	0.00000
353	3.3925	0.00000

354	3.4383	0.00000
355	3.4815	0.00000
356	3.4914	0.00000
357	3.4943	0.00000
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360	3.6768	0.00000
361	3.6986	0.00000
362	3.7380	0.00000
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365	3.7769	0.00000
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370	3.8661	0.00000
371	3.8805	0.00000
372	3.8932	0.00000
373	3.9208	0.00000
374	3.9358	0.00000
375	3.9484	0.00000

376	3.9593	0.00000
377	3.9828	0.00000
378	3.9866	0.00000
379	4.0221	0.00000
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381	4.1709	0.00000
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384	4.2686	0.00000
385	4.2929	0.00000
386	4.3210	0.00000
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391	4.4233	0.00000
392	4.4481	0.00000
393	4.4735	0.00000
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399	4.5937	0.00000
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405	4.7085	0.00000
406	4.7374	0.00000
407	4.7512	0.00000
408	4.7704	0.00000
409	4.7866	0.00000
410	4.7888	0.00000
411	4.8025	0.00000
412	4.8337	0.00000
413	4.8675	0.00000
414	4.8853	0.00000
415	4.9024	0.00000
416	4.9417	0.00000
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419	5.0127	0.00000

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427	5.1441	0.00000
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429	5.1797	0.00000
430	5.1887	0.00000
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432	5.2204	0.00000
433	5.2377	0.00000
434	5.2439	0.00000
435	5.2615	0.00000
436	5.2982	0.00000
437	5.3029	0.00000
438	5.3120	0.00000
439	5.3358	0.00000
440	5.3530	0.00000
441	5.3709	0.00000

442	5.3805	0.00000
443	5.3955	0.00000
444	5.4289	0.00000
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446	5.4703	0.00000
447	5.4871	0.00000
448	5.4991	0.00000
449	5.5258	0.00000
450	5.5683	0.00000
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456	5.6934	0.00000
457	5.7204	0.00000
458	5.7295	0.00000
459	5.7514	0.00000
460	5.7686	0.00000
461	5.7926	0.00000
462	5.7963	0.00000
463	5.8022	0.00000

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467	5.8666	0.00000
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469	5.8894	0.00000
470	5.8986	0.00000
471	5.9009	0.00000
472	5.9150	0.00000
473	5.9462	0.00000
474	5.9571	0.00000
475	5.9755	0.00000
476	6.0044	0.00000
477	6.0307	0.00000
478	6.0909	0.00000
479	6.1220	0.00000
480	6.1916	0.00000

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soft charge-density along one line, spin component 1

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

soft charge-density along one line, spin component 2

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

pseudopotential strength for first ion, spin component: 1

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

pseudopotential strength for first ion, spin component: 2

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

total augmentation occupancy for first ion, spin component: 1

3.579	-0.646	0.444	-0.034	-0.000
-0.646	0.130	-0.082	0.006	0.000
0.444	-0.082	0.056	-0.003	-0.000
-0.034	0.006	-0.003	0.011	0.000
-0.000	0.000	-0.000	0.000	0.007

total augmentation occupancy for first ion, spin component: 2

-0.000	0.000	-0.000	0.000	0.000
0.000	-0.000	0.000	-0.000	-0.000
-0.000	0.000	-0.000	-0.000	-0.000
0.000	-0.000	-0.000	-0.000	-0.000
0.000	-0.000	-0.000	-0.000	-0.000

---------- aborting loop because EDIFF is reached ----------

total charge

# of ion	s	p	d	tot
1	0.646	0.043	0.000	0.690
2	0.646	0.043	0.000	0.690
3	0.646	0.043	0.000	0.690
4	0.646	0.043	0.000	0.690
5	0.646	0.043	0.000	0.690
6	0.646	0.043	0.000	0.690
7	0.646	0.043	0.000	0.690
8	0.646	0.043	0.000	0.690
9	0.646	0.043	0.000	0.690
10	0.646	0.043	0.000	0.690
11	0.646	0.043	0.000	0.690
12	0.646	0.043	0.000	0.690
13	0.646	0.043	0.000	0.689
14	0.646	0.043	0.000	0.689
15	0.648	0.045	0.000	0.693
16	0.646	0.043	0.000	0.689
17	0.646	0.043	0.000	0.689
18	0.646	0.043	0.000	0.689
19	0.646	0.043	0.000	0.689
20	0.646	0.043	0.000	0.689

21	0.646	0.043	0.000	0.689
22	0.646	0.044	0.000	0.690
23	0.541	0.015	0.000	0.557
24	0.541	0.015	0.000	0.556
25	0.870	1.763	0.000	2.633
26	0.867	1.785	0.000	2.653
27	0.867	1.786	0.000	2.653
28	0.870	1.762	0.000	2.632
29	0.865	1.783	0.000	2.648
30	0.870	1.763	0.000	2.633
31	0.867	1.786	0.000	2.653
32	0.867	1.786	0.000	2.653
33	0.870	1.762	0.000	2.632
34	0.865	1.783	0.000	2.648
35	0.870	1.763	0.000	2.633
36	0.868	1.787	0.000	2.654
37	0.867	1.786	0.000	2.653
38	0.870	1.763	0.000	2.633
39	0.865	1.784	0.000	2.649
40	0.870	1.763	0.000	2.633
41	0.868	1.787	0.000	2.655
42	0.867	1.786	0.000	2.653

43	0.871	1.764	0.000	2.634
44	0.865	1.783	0.000	2.648
45	0.870	1.763	0.000	2.633
46	0.867	1.786	0.000	2.653
47	0.867	1.786	0.000	2.653
48	0.871	1.763	0.000	2.634
49	0.865	1.783	0.000	2.648
50	0.870	1.763	0.000	2.633
51	0.867	1.786	0.000	2.653
52	0.867	1.786	0.000	2.653
53	0.870	1.762	0.000	2.632
54	0.865	1.784	0.000	2.648
55	0.865	1.784	0.000	2.649
56	0.865	1.786	0.000	2.651
57	0.866	1.787	0.000	2.653
58	0.866	1.790	0.000	2.656
59	0.865	1.786	0.000	2.651
60	0.866	1.786	0.000	2.651
61	0.866	1.788	0.000	2.654
62	0.867	1.791	0.000	2.658
63	0.865	1.784	0.000	2.649
64	0.865	1.786	0.000	2.651

65	0.866	1.787	0.000	2.652
66	0.865	1.788	0.000	2.653
67	0.865	1.786	0.000	2.651
68	0.866	1.785	0.000	2.651
69	0.865	1.787	0.000	2.652
70	0.866	1.787	0.000	2.653
71	0.865	1.784	0.000	2.649
72	0.865	1.786	0.000	2.651
73	0.866	1.786	0.000	2.652
74	0.864	1.785	0.000	2.649
75	0.865	1.786	0.000	2.651
76	0.866	1.786	0.000	2.651
77	0.865	1.786	0.000	2.651
78	0.865	1.784	0.000	2.649
79	0.865	1.784	0.000	2.649
80	0.865	1.786	0.000	2.651
81	0.865	1.785	0.000	2.650
82	0.863	1.782	0.000	2.645
83	0.865	1.786	0.000	2.651
84	0.866	1.786	0.000	2.651
85	0.865	1.784	0.000	2.648
86	0.862	1.774	0.000	2.636

87	0.865	1.784	0.000	2.649
88	0.865	1.787	0.000	2.652
89	0.865	1.785	0.000	2.650
90	0.865	1.788	0.000	2.653
91	0.865	1.786	0.000	2.651
92	0.866	1.786	0.000	2.651
93	0.864	1.783	0.000	2.647
94	0.866	1.785	0.000	2.651
95	0.865	1.784	0.000	2.649
96	0.865	1.786	0.000	2.651
97	0.866	1.787	0.000	2.653
98	0.866	1.789	0.000	2.655
99	0.865	1.786	0.000	2.651
100	0.866	1.786	0.000	2.651
101	0.865	1.787	0.000	2.652
102	0.867	1.790	0.000	2.657
103	0.865	1.786	0.000	2.651
104	0.867	1.785	0.000	2.653
105	0.866	1.786	0.000	2.652
106	0.870	1.778	0.000	2.648
107	0.869	1.765	0.000	2.635
108	0.865	1.783	0.000	2.648

109	0.869	1.789	0.000	2.658
110	0.865	1.786	0.000	2.651
111	0.867	1.785	0.000	2.653
112	0.867	1.789	0.000	2.655
113	0.871	1.782	0.000	2.653
114	0.869	1.765	0.000	2.634
115	0.865	1.783	0.000	2.648
116	0.870	1.791	0.000	2.661
117	0.865	1.786	0.000	2.651
118	0.867	1.786	0.000	2.653
119	0.865	1.782	0.000	2.647
120	0.857	1.707	0.000	2.564
121	0.869	1.765	0.000	2.634
122	0.865	1.783	0.000	2.648
123	0.866	1.778	0.000	2.644
124	0.866	1.786	0.000	2.652
125	0.867	1.785	0.000	2.653
126	0.862	1.776	0.000	2.637
127	0.849	1.830	0.000	2.678
128	0.870	1.767	0.000	2.637
129	0.865	1.783	0.000	2.648
130	0.860	1.757	0.000	2.617

131	0.866	1.786	0.000	2.652
132	0.867	1.784	0.000	2.652
133	0.864	1.787	0.000	2.651
134	0.869	1.790	0.000	2.659
135	0.869	1.767	0.000	2.636
136	0.865	1.783	0.000	2.648
137	0.866	1.772	0.000	2.638
138	0.866	1.786	0.000	2.652
139	0.867	1.785	0.000	2.652
140	0.866	1.788	0.000	2.654
141	0.870	1.779	0.000	2.649
142	0.869	1.766	0.000	2.635
143	0.865	1.783	0.000	2.648
144	0.869	1.790	0.000	2.659
145	0.942	1.719	0.000	2.662
146	1.240	1.546	0.074	2.860
147	1.634	3.528	0.000	5.162
---	---	---	---	---
tot	123.063	221.551	0.074	344.688

magnetization (x)

# of ion	s	p	d	tot
1	0.000	-0.000	0.000	0.000
2	-0.000	0.000	0.000	-0.000
3	0.000	-0.000	0.000	0.000
4	-0.000	0.000	0.000	-0.000
5	0.000	-0.000	0.000	0.000
6	-0.000	0.000	0.000	-0.000
7	0.000	-0.000	0.000	0.000
8	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	0.000
10	-0.000	0.000	0.000	-0.000
11	0.000	-0.000	0.000	0.000
12	-0.000	0.000	0.000	-0.000
13	0.000	-0.000	0.000	0.000
14	-0.004	0.002	0.000	-0.002
15	0.000	-0.000	0.000	0.000
16	-0.004	0.002	0.000	-0.002
17	-0.004	0.002	0.000	-0.002
18	0.000	-0.000	0.000	0.000

19	-0.003	0.001	0.000	-0.002
20	0.000	-0.000	0.000	0.000
21	-0.003	0.002	0.000	-0.002
22	-0.003	0.002	0.000	-0.002
23	-0.000	0.000	0.000	-0.000
24	-0.000	0.000	0.000	-0.000
25	-0.000	-0.007	0.000	-0.008
26	-0.000	-0.002	0.000	-0.002
27	0.000	0.003	0.000	0.003
28	0.000	0.005	0.000	0.005
29	0.000	0.003	0.000	0.003
30	-0.000	-0.007	0.000	-0.008
31	-0.000	-0.002	0.000	-0.002
32	0.000	0.003	0.000	0.003
33	0.000	0.005	0.000	0.005
34	0.000	0.002	0.000	0.002
35	-0.000	-0.007	0.000	-0.008
36	-0.000	-0.002	0.000	-0.002
37	0.000	0.003	0.000	0.003
38	0.000	0.006	0.000	0.007
39	0.000	0.002	0.000	0.002
40	-0.000	-0.007	0.000	-0.008

41	-0.000	-0.002	0.000	-0.002
42	0.000	0.002	0.000	0.003
43	0.000	0.005	0.000	0.006
44	0.000	0.004	0.000	0.004
45	-0.000	-0.007	0.000	-0.008
46	-0.000	-0.002	0.000	-0.002
47	0.000	0.003	0.000	0.003
48	0.000	0.005	0.000	0.006
49	0.000	0.001	0.000	0.002
50	-0.000	-0.007	0.000	-0.008
51	-0.000	-0.002	0.000	-0.002
52	0.000	0.002	0.000	0.003
53	0.000	0.006	0.000	0.007
54	0.000	0.002	0.000	0.002
55	-0.000	-0.005	0.000	-0.006
56	-0.000	-0.007	0.000	-0.007
57	-0.000	-0.001	0.000	-0.001
58	-0.000	-0.001	0.000	-0.001
59	0.000	0.006	0.000	0.007
60	0.000	0.003	0.000	0.003
61	0.000	0.001	0.000	0.001
62	0.000	0.003	0.000	0.003

63	-0.000	-0.005	0.000	-0.006
64	-0.000	-0.007	0.000	-0.007
65	-0.000	-0.001	0.000	-0.001
66	-0.000	-0.001	0.000	-0.001
67	0.000	0.006	0.000	0.006
68	0.000	0.003	0.000	0.003
69	0.000	0.001	0.000	0.001
70	0.000	0.002	0.000	0.002
71	-0.000	-0.005	0.000	-0.006
72	-0.000	-0.007	0.000	-0.007
73	-0.000	-0.001	0.000	-0.001
74	-0.000	-0.002	0.000	-0.002
75	0.000	0.006	0.000	0.007
76	0.000	0.003	0.000	0.004
77	0.000	0.003	0.000	0.003
78	0.000	0.001	0.000	0.001
79	-0.000	-0.005	0.000	-0.006
80	-0.000	-0.007	0.000	-0.007
81	-0.000	-0.001	0.000	-0.002
82	-0.000	-0.002	0.000	-0.002
83	0.001	0.007	0.000	0.008
84	0.000	0.003	0.000	0.003

85	0.000	0.002	0.000	0.002
86	0.000	0.005	0.000	0.006
87	-0.000	-0.005	0.000	-0.005
88	-0.000	-0.007	0.000	-0.007
89	-0.000	-0.001	0.000	-0.002
90	-0.000	-0.002	0.000	-0.002
91	0.001	0.008	0.000	0.008
92	0.000	0.003	0.000	0.003
93	0.000	0.002	0.000	0.003
94	0.000	0.001	0.000	0.001
95	-0.000	-0.005	0.000	-0.006
96	-0.000	-0.007	0.000	-0.007
97	-0.000	-0.001	0.000	-0.001
98	-0.000	-0.001	0.000	-0.001
99	0.001	0.007	0.000	0.007
100	0.000	0.003	0.000	0.004
101	0.000	0.003	0.000	0.003
102	0.000	0.002	0.000	0.002
103	-0.001	-0.010	0.000	-0.011
104	-0.003	-0.028	0.000	-0.031
105	-0.000	-0.001	0.000	-0.002
106	-0.000	-0.004	0.000	-0.005

107	0.007	0.116	0.000	0.122
108	0.001	0.010	0.000	0.011
109	0.000	0.001	0.000	0.001
110	-0.001	-0.010	0.000	-0.011
111	-0.003	-0.028	0.000	-0.031
112	-0.000	-0.001	0.000	-0.002
113	-0.000	-0.003	0.000	-0.004
114	0.007	0.120	0.000	0.127
115	0.001	0.010	0.000	0.011
116	0.000	0.001	0.000	0.002
117	-0.001	-0.010	0.000	-0.011
118	-0.003	-0.026	0.000	-0.029
119	-0.000	-0.002	0.000	-0.002
120	-0.000	-0.002	0.000	-0.002
121	0.007	0.115	0.000	0.122
122	0.001	0.010	0.000	0.010
123	0.000	0.003	0.000	0.003
124	-0.001	-0.010	0.000	-0.011
125	-0.003	-0.024	0.000	-0.027
126	-0.000	-0.002	0.000	-0.002
127	-0.000	0.001	0.000	0.001
128	0.006	0.105	0.000	0.111

129	0.001	0.009	0.000	0.010
130	0.000	0.004	0.000	0.004
131	-0.001	-0.009	0.000	-0.010
132	-0.003	-0.024	0.000	-0.027
133	-0.000	-0.002	0.000	-0.002
134	-0.000	-0.002	0.000	-0.002
135	0.006	0.097	0.000	0.102
136	0.001	0.009	0.000	0.010
137	0.000	0.004	0.000	0.005
138	-0.001	-0.010	0.000	-0.011
139	-0.003	-0.026	0.000	-0.029
140	-0.000	-0.002	0.000	-0.002
141	-0.000	-0.003	0.000	-0.004
142	0.006	0.105	0.000	0.111
143	0.001	0.010	0.000	0.010
144	0.000	0.002	0.000	0.003
145	0.000	0.005	0.000	0.006
146	-0.000	0.000	-0.000	0.000
147	0.000	0.004	0.000	0.004
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tot	0.001	0.513	-0.000	0.514

CHARGE: cpu time 0.5249: real time 0.5267

FORLOC: cpu time 0.0200: real time 0.0200

FORNL : cpu time 2.0735: real time 2.0804

STRESS: cpu time 6.2313: real time 6.2518

FORCOR: cpu time 0.1401: real time 0.1405

FORHAR: cpu time 0.0331: real time 0.0332

MIXING: cpu time 0.0088: real time 0.0088

OFIELD: cpu time 0.0001: real time 0.0001

DFTD3 V3.0 Rev 1

Edisp (eV) -6.61789

E6 (eV) : -3.9313

E8 (eV) : -2.6866

% E8 : 40.60

FORVDW: cpu time 1.8566: real time 1.8872

FORCE on cell =-STRESS in cart. coord. units (eV):

Direction XX YY ZZ XY YZ ZX

Alpha Z	233.50077	233.50077	233.50077			
Ewald	107579.24971	23477.46510	-39727.67744	7.74370	3455.47796	126.44025
Hartree	106097.93807	25032.61944	-23794.62156	-7.53039	2947.26437	92.23252
E(xc)	-1914.24398	-1916.59145	-1979.90240	0.12713	1.82431	0.12322
Local	**********	-53958.39074	57016.14852	2.90662	-6360.67159	-215.40322
n-local	-472.65576	-482.49050	-439.56543	-0.61282	-0.71870	-0.26624
augment	-38.27908	-38.59493	-34.30895	0.02903	-0.98329	0.00810
Kinetic	7635.26017	7638.75065	8713.99126	-3.01273	-41.61923	-3.14433
Fock	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
vdW	-2.64127	-1.49211	-6.59328	0.00094	-0.07429	0.01123
Total	-17.74472	-15.22377	-19.02851	-0.34852	0.49954	0.00153
in kB	-4.89321	-4.19804	-5.24722	-0.09611	0.13775	0.00042

external pressure = -4.78 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

energy-cutoff : 400.00

volume of cell : 5810.14

direct lattice vectors			reciprocal lattice vectors		
14.780600000	0.000000000	0.000000000	0.067656252	0.000000000	0.000000000

0.000000000 21.333900000 0.000000000 0.000000000 0.046873755 0.000000000

0.000000000 0.000000000 18.425700000 0.000000000 0.000000000 0.054272022

length of vectors

14.780600000 21.333900000 18.425700000 0.067656252 0.046873755 0.054272022

FORCES acting on ions

electron-ion (+dipol) ewald-force non-local-force convergence-correction

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0.428E-02 0.154E+03 0.361E+02 -.278E-02 -.160E+03 -.357E+02 -.180E-02 0.566E+01 -.438E+00 -.285E-06 0.232E-06 0.114E-06

-.190E-01 0.155E+03 -.340E+02 0.166E-01 -.160E+03 0.335E+02 0.115E-02 0.565E+01 0.541E+00 -.128E-05 -.152E-06 -.306E-06

0.184E+00 0.154E+03 0.360E+02 -.184E+00 -.160E+03 -.356E+02 0.758E-05 0.565E+01 -.443E+00 -.225E-06 0.908E-06 -.770E-06

0.112E+00 0.155E+03 -.341E+02 -.983E-01 -.160E+03 0.336E+02 -.175E-01 0.565E+01 0.535E+00 -.579E-06 0.151E-05 -.640E-06

0.171E+00 0.154E+03 0.362E+02 -.173E+00 -.160E+03 -.357E+02 0.116E-02 0.566E+01 -.440E+00 0.420E-07 0.105E-05 -.691E-06

0.126E+00 0.154E+03 -.340E+02 -.108E+00 -.160E+03 0.334E+02 -.211E-01 0.565E+01

0.541E+00 0.663E-06 0.143E-05 -.455E-06

-.189E-01 0.154E+03 0.363E+02 0.178E-01 -.160E+03 -.359E+02 0.159E-02 0.566E+01 -.431E+00 0.241E-06 0.533E-06 0.261E-06

-.124E-01 0.154E+03 -.338E+02 0.192E-01 -.160E+03 0.332E+02 -.719E-02 0.565E+01 0.555E+00 0.124E-05 0.369E-07 0.194E-07

-.181E+00 0.154E+03 0.363E+02 0.182E+00 -.160E+03 -.359E+02 0.256E-03 0.566E+01 -.429E+00 0.235E-06 -.108E-06 0.113E-05

-.127E+00 0.155E+03 -.337E+02 0.114E+00 -.160E+03 0.331E+02 0.109E-01 0.565E+01 0.561E+00 0.590E-06 -.144E-05 0.336E-06

-.174E+00 0.154E+03 0.362E+02 0.176E+00 -.160E+03 -.358E+02 -.177E-02 0.566E+01 -.432E+00 -.178E-07 -.260E-06 0.106E-05

-.115E+00 0.155E+03 -.338E+02 0.958E-01 -.160E+03 0.332E+02 0.192E-01 0.565E+01 0.555E+00 -.622E-06 -.163E-05 0.191E-06

0.227E+01 -.150E+03 -.386E+02 -.226E+01 0.156E+03 0.386E+02 -.103E-01 -.566E+01 0.767E-01 0.368E-06 -.254E-06 -.510E-06

-.419E+00 -.151E+03 0.388E+02 0.420E+00 0.157E+03 -.386E+02 -.129E-02 -.567E+01 -.269E+00 0.979E-06 -.380E-06 0.192E-06

0.136E+02 -.146E+03 -.413E+02 -.138E+02 0.151E+03 0.413E+02 0.257E+00 -.567E+01 -.349E-01 -.665E-07 -.585E-06 -.840E-06

0.162E+01 -.151E+03 0.402E+02 -.162E+01 0.156E+03 -.400E+02 -.101E-02 -.567E+01 -.229E+00 0.733E-06 -.330E-06 0.458E-06

0.352E+01 -.149E+03 0.443E+02 -.352E+01 0.155E+03 -.441E+02 -.200E-02 -.567E+01 -

.180E+00 0.239E-06 -.226E-06 0.291E-06

-.149E+02 -.146E+03 -.329E+02 0.150E+02 0.151E+03 0.329E+02 -.979E-01 -.566E+01 0.496E-01 -.658E-10 -.223E-05 -.164E-05

-.297E+01 -.149E+03 0.432E+02 0.296E+01 0.155E+03 -.430E+02 0.115E-01 -.567E+01 -.241E+00 -.129E-05 -.400E-06 -.151E-06

-.381E+01 -.150E+03 -.385E+02 0.381E+01 0.156E+03 0.385E+02 -.635E-02 -.566E+01 0.241E-01 0.229E-05 -.753E-06 -.623E-06

-.207E+01 -.151E+03 0.395E+02 0.207E+01 0.156E+03 -.392E+02 0.151E-02 -.566E+01 -.282E+00 -.582E-07 -.663E-06 -.312E-06

0.250E-02 -.148E+03 0.486E+02 0.515E-02 0.154E+03 -.484E+02 -.553E-02 -.570E+01 -.158E+00 -.584E-06 -.687E-07 0.164E-06

0.196E+02 -.103E+03 0.222E+02 -.212E+02 0.103E+03 -.246E+02 0.154E+01 0.138E+00 0.238E+01 -.567E-06 -.553E-06 -.113E-05

-.192E+02 -.103E+03 0.153E+02 0.216E+02 0.103E+03 -.168E+02 -.241E+01 -.119E+00 0.152E+01 -.800E-06 -.408E-06 -.126E-05

0.701E-01 0.461E+03 0.202E+03 -.733E-01 -.462E+03 -.201E+03 0.382E-02 0.102E+01 -.219E+00 -.601E-07 0.570E-06 -.268E-06

0.209E+00 0.353E+03 -.234E+03 -.210E+00 -.353E+03 0.234E+03 0.264E-02 0.443E+00 -.370E-01 -.111E-05 0.478E-06 -.200E-05

-.256E-01 0.351E+03 0.240E+03 0.243E-01 -.351E+03 -.241E+03 0.314E-02 0.408E+00 0.564E-01 0.456E-06 0.574E-06 0.606E-06

-.175E+00 0.462E+03 -.195E+03 0.181E+00 -.463E+03 0.195E+03 -.665E-02 0.105E+01

0.233E+00 -.230E-05 -.632E-06 -.180E-05

-.654E-01 0.210E+03 -.272E+03 0.696E-01 -.210E+03 0.272E+03 -.450E-02 0.935E-01 0.560E-01 -.450E-06 -.928E-07 -.174E-05

0.561E+00 0.461E+03 0.202E+03 -.563E+00 -.462E+03 -.201E+03 0.202E-02 0.102E+01 -.214E+00 -.169E-06 0.198E-05 -.267E-05

0.106E+01 0.352E+03 -.234E+03 -.107E+01 -.353E+03 0.234E+03 0.160E-01 0.448E+00 -.424E-01 0.264E-07 0.153E-05 -.180E-05

0.411E+00 0.351E+03 0.240E+03 -.413E+00 -.351E+03 -.240E+03 0.302E-02 0.408E+00 0.491E-01 0.350E-06 0.143E-05 -.177E-05

0.577E+00 0.462E+03 -.195E+03 -.582E+00 -.463E+03 0.195E+03 0.480E-02 0.105E+01 0.235E+00 -.903E-06 0.307E-05 -.225E-05

0.687E+00 0.210E+03 -.272E+03 -.693E+00 -.210E+03 0.272E+03 0.614E-02 0.913E-01 0.616E-01 0.161E-06 -.302E-06 -.171E-05

0.426E+00 0.461E+03 0.202E+03 -.428E+00 -.462E+03 -.202E+03 0.385E-02 0.102E+01 -.214E+00 -.217E-06 0.235E-05 -.244E-05

0.940E+00 0.352E+03 -.233E+03 -.956E+00 -.352E+03 0.233E+03 0.150E-01 0.441E+00 -.377E-01 0.130E-05 0.239E-06 -.123E-05

0.477E+00 0.351E+03 0.241E+03 -.479E+00 -.351E+03 -.241E+03 0.250E-02 0.406E+00 0.512E-01 -.844E-07 0.198E-05 -.275E-05

0.705E+00 0.462E+03 -.194E+03 -.715E+00 -.463E+03 0.194E+03 0.784E-02 0.106E+01 0.242E+00 0.134E-05 0.308E-05 -.156E-05

0.726E+00 0.210E+03 -.271E+03 -.735E+00 -.210E+03 0.271E+03 0.655E-02 0.910E-01

0.593E-01 0.343E-06 -.729E-06 -.148E-05

-.180E+00 0.461E+03 0.202E+03 0.177E+00 -.462E+03 -.202E+03 0.450E-02 0.102E+01 -.218E+00 -.960E-07 0.129E-05 0.221E-06

-.292E+00 0.352E+03 -.233E+03 0.296E+00 -.352E+03 0.233E+03 -.181E-02 0.440E+00 -.299E-01 0.111E-05 -.288E-05 -.111E-05

0.411E-01 0.351E+03 0.241E+03 -.401E-01 -.351E+03 -.241E+03 0.224E-02 0.409E+00 0.557E-01 -.520E-06 0.186E-05 -.146E-05

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-.443E-01 0.210E+03 -.271E+03 0.420E-01 -.210E+03 0.271E+03 -.181E-03 0.933E-01 0.324E-01 0.151E-06 -.121E-05 -.156E-05

-.550E+00 0.461E+03 0.202E+03 0.548E+00 -.462E+03 -.202E+03 0.772E-03 0.102E+01 -.220E+00 0.197E-06 -.254E-07 0.262E-05

-.119E+01 0.352E+03 -.233E+03 0.120E+01 -.353E+03 0.233E+03 -.164E-01 0.447E+00 -.330E-01 -.169E-06 -.346E-05 -.131E-05

-.351E+00 0.351E+03 0.241E+03 0.348E+00 -.351E+03 -.241E+03 0.207E-02 0.413E+00 0.624E-01 -.299E-06 0.117E-05 0.824E-06

-.410E+00 0.462E+03 -.194E+03 0.424E+00 -.463E+03 0.194E+03 -.114E-01 0.106E+01 0.230E+00 0.916E-06 -.463E-05 -.482E-06

-.559E+00 0.210E+03 -.271E+03 0.564E+00 -.210E+03 0.271E+03 -.954E-02 0.914E-01 0.525E-01 -.454E-08 -.138E-05 -.166E-05

-.475E+00 0.461E+03 0.202E+03 0.474E+00 -.462E+03 -.202E+03 0.306E-02 0.102E+01 -

.220E+00 0.292E-06 -.500E-06 0.239E-05

-.806E+00 0.353E+03 -.234E+03 0.821E+00 -.353E+03 0.234E+03 -.150E-01 0.447E+00 -.393E-01 -.120E-05 -.174E-05 -.165E-05

-.373E+00 0.351E+03 0.241E+03 0.367E+00 -.351E+03 -.241E+03 0.957E-03 0.411E+00 0.626E-01 0.140E-06 0.462E-06 0.187E-05

-.594E+00 0.462E+03 -.194E+03 0.607E+00 -.463E+03 0.194E+03 -.171E-01 0.105E+01 0.234E+00 -.137E-05 -.448E-05 -.924E-06

-.590E+00 0.210E+03 -.272E+03 0.600E+00 -.210E+03 0.272E+03 -.102E-01 0.990E-01 0.566E-01 -.153E-06 -.641E-06 -.161E-05

-.984E-02 0.206E+03 0.279E+03 0.132E-01 -.206E+03 -.279E+03 -.361E-02 0.686E-01 -.412E-01 0.780E-06 0.496E-06 -.584E-07

0.665E+00 0.303E+02 0.296E+03 -.660E+00 -.302E+02 -.296E+03 -.468E-02 -.410E-01 0.750E-02 0.974E-06 0.948E-07 -.568E-06

-.849E+00 0.144E+03 -.282E+03 0.852E+00 -.144E+03 0.282E+03 -.325E-02 0.137E+00 0.287E-01 -.866E-06 -.299E-06 -.146E-05

0.524E+00 -.215E+02 -.285E+03 -.524E+00 0.214E+02 0.285E+03 -.657E-03 0.386E-01 0.186E-01 -.102E-05 0.129E-06 -.163E-05

0.496E+00 -.294E+02 0.293E+03 -.493E+00 0.294E+02 -.293E+03 -.554E-02 0.254E-01 -.304E-01 0.917E-06 -.194E-06 0.333E-07

0.522E+00 0.139E+03 0.289E+03 -.522E+00 -.139E+03 -.289E+03 0.178E-02 0.103E+00 -.248E-01 0.842E-06 0.294E-06 -.824E-06

-.127E+01 0.364E+02 -.287E+03 0.127E+01 -.364E+02 0.287E+03 -.162E-04 -.770E-02

0.140E-01 -.396E-06 0.128E-06 -.105E-05

0.165E+01 -.130E+03 -.271E+03 -.167E+01 0.130E+03 0.271E+03 0.108E-01 -.880E-01 0.372E-01 -.114E-05 0.147E-05 -.178E-05

0.395E+00 0.207E+03 0.280E+03 -.393E+00 -.207E+03 -.280E+03 0.709E-03 0.695E-01 -.371E-01 0.671E-06 0.762E-06 -.164E-05

0.916E+00 0.312E+02 0.296E+03 -.920E+00 -.311E+02 -.296E+03 0.225E-02 -.410E-01 0.122E-01 0.581E-06 0.302E-06 -.146E-05

0.132E+01 0.144E+03 -.282E+03 -.133E+01 -.144E+03 0.282E+03 0.498E-02 0.126E+00 0.279E-01 -.575E-06 -.275E-06 -.178E-05

0.341E+01 -.199E+02 -.285E+03 -.342E+01 0.199E+02 0.285E+03 0.137E-01 0.412E-01 0.136E-01 -.755E-06 0.318E-06 -.243E-05

0.139E+01 -.287E+02 0.294E+03 -.138E+01 0.287E+02 -.294E+03 -.349E-02 0.252E-01 -.307E-01 0.924E-06 0.294E-06 -.830E-06

0.676E+00 0.139E+03 0.290E+03 -.676E+00 -.139E+03 -.290E+03 0.617E-03 0.103E+00 -.295E-01 0.422E-06 0.521E-06 -.199E-05

0.159E+01 0.367E+02 -.287E+03 -.158E+01 -.366E+02 0.287E+03 -.126E-01 -.206E-01 0.128E-01 -.103E-05 -.436E-06 -.208E-05

0.609E+01 -.125E+03 -.271E+03 -.612E+01 0.125E+03 0.271E+03 0.223E-01 -.894E-01 0.150E-01 -.243E-06 0.186E-05 -.252E-05

0.366E+00 0.207E+03 0.280E+03 -.371E+00 -.207E+03 -.280E+03 0.105E-03 0.684E-01 -.365E-01 -.493E-09 0.992E-06 -.241E-05

-.384E-01 0.319E+02 0.296E+03 0.298E-01 -.318E+02 -.296E+03 0.106E-01 -.362E-01

0.139E-01 -.305E-06 0.477E-06 -.165E-05

0.210E+01 0.144E+03 -.281E+03 -.211E+01 -.144E+03 0.281E+03 0.122E-01 0.121E+00 0.241E-01 0.378E-06 -.127E-05 -.177E-05

0.304E+01 -.172E+02 -.283E+03 -.306E+01 0.171E+02 0.283E+03 0.248E-01 0.891E-01 0.606E-01 0.147E-06 -.201E-06 -.169E-05

0.105E+01 -.272E+02 0.294E+03 -.105E+01 0.272E+02 -.294E+03 0.287E-02 0.243E-01 -.376E-01 0.175E-06 0.610E-06 -.139E-05

0.962E-01 0.140E+03 0.290E+03 -.977E-01 -.140E+03 -.290E+03 0.129E-02 0.107E+00 -.232E-01 -.355E-06 0.678E-06 -.207E-05

0.276E+01 0.387E+02 -.286E+03 -.277E+01 -.387E+02 0.286E+03 0.170E-02 -.103E-01 0.295E-01 0.569E-06 -.634E-06 -.207E-05

0.595E+01 -.115E+03 -.267E+03 -.611E+01 0.115E+03 0.267E+03 0.158E+00 0.559E-02 0.129E+00 -.116E-05 0.274E-05 -.120E-05

-.241E+00 0.207E+03 0.280E+03 0.239E+00 -.207E+03 -.280E+03 0.438E-02 0.716E-01 -.387E-01 -.678E-06 0.106E-05 -.161E-05

-.114E+01 0.314E+02 0.294E+03 0.113E+01 -.314E+02 -.294E+03 0.919E-02 -.311E-01 0.542E-02 -.101E-05 0.382E-06 -.887E-06

0.599E+00 0.144E+03 -.281E+03 -.616E+00 -.144E+03 0.281E+03 0.178E-01 0.126E+00 0.437E-01 0.188E-06 -.950E-06 -.147E-05

-.923E+00 -.159E+02 -.286E+03 0.914E+00 0.158E+02 0.285E+03 0.616E-02 0.909E-01 0.802E-01 0.169E-05 -.177E-05 -.167E-05

-.642E+00 -.265E+02 0.293E+03 0.638E+00 0.265E+02 -.293E+03 0.491E-02 0.234E-01 -

.270E-01 -.732E-06 0.573E-06 -.112E-05

-.532E+00 0.139E+03 0.289E+03 0.528E+00 -.139E+03 -.289E+03 0.656E-02 0.114E+00 -.214E-01 -.776E-06 0.642E-06 -.927E-06

0.786E+00 0.408E+02 -.287E+03 -.798E+00 -.408E+02 0.287E+03 0.496E-02 0.236E-02 -.190E-01 0.198E-06 -.114E-05 -.149E-05

-.408E+00 -.113E+03 -.276E+03 0.379E+00 0.113E+03 0.276E+03 0.310E-01 0.604E-01 -.268E+00 -.545E-07 -.819E-06 -.270E-05

-.570E+00 0.206E+03 0.279E+03 0.568E+00 -.206E+03 -.279E+03 0.118E-02 0.720E-01 -.455E-01 -.693E-06 0.914E-06 -.809E-07

-.779E+00 0.304E+02 0.294E+03 0.783E+00 -.304E+02 -.294E+03 -.754E-02 -.309E-01 -.137E-02 -.689E-06 0.105E-06 0.125E-07

-.123E+01 0.144E+03 -.281E+03 0.124E+01 -.145E+03 0.281E+03 -.157E-01 0.123E+00 0.505E-01 0.666E-06 -.347E-07 -.153E-05

-.365E+01 -.174E+02 -.283E+03 0.368E+01 0.173E+02 0.283E+03 -.307E-01 0.115E+00 0.591E-01 0.137E-06 -.316E-06 -.146E-05

-.129E+01 -.277E+02 0.291E+03 0.129E+01 0.277E+02 -.291E+03 -.131E-02 0.340E-01 -.219E-01 -.961E-06 0.473E-07 -.409E-06

-.345E+00 0.139E+03 0.289E+03 0.344E+00 -.139E+03 -.289E+03 0.220E-04 0.112E+00 -.146E-01 -.521E-06 0.396E-06 0.253E-06

-.820E+00 0.400E+02 -.287E+03 0.812E+00 -.400E+02 0.287E+03 0.122E-01 -.762E-02 -.182E-01 0.450E-06 -.467E-06 -.139E-05

-.786E+01 -.119E+03 -.267E+03 0.805E+01 0.119E+03 0.267E+03 -.186E+00 -.916E-03

0.351E-01 0.271E-05 -.263E-05 -.350E-05

-.408E+00 0.206E+03 0.279E+03 0.409E+00 -.206E+03 -.279E+03 -.281E-02 0.715E-01 -.464E-01 -.568E-07 0.594E-06 0.712E-06

-.634E-01 0.300E+02 0.294E+03 0.732E-01 -.299E+02 -.294E+03 -.948E-02 -.348E-01 0.120E-02 0.393E-06 -.718E-08 0.183E-06

-.206E+01 0.145E+03 -.282E+03 0.208E+01 -.145E+03 0.282E+03 -.190E-01 0.132E+00 0.256E-01 0.178E-06 -.802E-06 -.141E-05

-.257E+01 -.208E+02 -.285E+03 0.260E+01 0.208E+02 0.285E+03 -.291E-01 0.410E-01 0.319E-01 -.113E-06 0.430E-06 -.688E-06

-.549E+00 -.290E+02 0.291E+03 0.554E+00 0.290E+02 -.291E+03 -.285E-02 0.292E-01 -.251E-01 -.235E-06 -.320E-06 0.187E-06

0.589E-01 0.139E+03 0.289E+03 -.591E-01 -.139E+03 -.289E+03 -.353E-03 0.109E+00 -.208E-01 0.367E-06 0.201E-06 0.295E-06

-.290E+01 0.378E+02 -.286E+03 0.291E+01 -.378E+02 0.286E+03 -.145E-01 -.431E-02 0.207E-01 0.228E-06 0.267E-06 -.862E-06

-.515E+01 -.128E+03 -.271E+03 0.520E+01 0.128E+03 0.271E+03 -.464E-01 -.862E-01 0.375E-01 0.141E-06 0.514E-06 -.131E-05

0.395E+00 -.137E+03 0.280E+03 -.387E+00 0.137E+03 -.280E+03 -.971E-02 -.128E+00 -.157E-01 0.134E-05 -.368E-06 0.371E-06

0.192E+01 -.343E+03 0.233E+03 -.193E+01 0.344E+03 -.233E+03 0.906E-02 -.461E+00 -.547E-01 0.264E-05 0.108E-06 0.103E-05

-.255E+01 -.197E+03 -.259E+03 0.256E+01 0.197E+03 0.259E+03 -.932E-02 -.198E+00

0.367E-01 0.948E-07 0.121E-05 -.138E-05

0.688E+01 -.447E+03 -.198E+03 -.690E+01 0.448E+03 0.198E+03 0.958E-02 -.112E+01 0.884E-01 0.159E-05 0.204E-05 -.213E-05

-.474E+00 -.451E+03 0.204E+03 0.475E+00 0.452E+03 -.204E+03 -.212E-02 -.108E+01 -.113E+00 0.303E-05 -.101E-05 0.724E-06

0.170E+01 -.203E+03 0.269E+03 -.170E+01 0.203E+03 -.269E+03 -.482E-02 -.927E-01 -.320E-01 0.176E-05 0.458E-07 0.399E-06

-.214E+01 -.338E+03 -.222E+03 0.218E+01 0.338E+03 0.222E+03 -.441E-01 -.604E+00 0.539E-01 0.161E-05 0.171E-05 -.190E-05

0.218E+01 -.136E+03 0.282E+03 -.217E+01 0.136E+03 -.282E+03 -.636E-02 -.126E+00 -.944E-02 0.125E-05 0.478E-06 -.226E-06

0.671E+01 -.339E+03 0.238E+03 -.669E+01 0.340E+03 -.238E+03 -.128E-01 -.462E+00 -.460E-01 0.135E-05 0.146E-05 0.791E-06

0.676E+01 -.193E+03 -.259E+03 -.678E+01 0.193E+03 0.258E+03 0.114E-01 -.146E+00 0.634E-01 -.711E-06 0.311E-05 -.251E-05

0.312E+02 -.427E+03 -.198E+03 -.313E+02 0.428E+03 0.197E+03 0.725E-01 -.971E+00 0.135E+00 -.103E-05 0.369E-05 -.225E-05

0.543E+01 -.449E+03 0.209E+03 -.543E+01 0.450E+03 -.209E+03 0.566E-03 -.108E+01 -.798E-01 0.266E-05 0.102E-05 0.153E-05

0.368E+01 -.201E+03 0.272E+03 -.367E+01 0.201E+03 -.272E+03 -.739E-03 -.977E-01 -.306E-01 0.107E-05 0.102E-05 -.151E-06

0.124E+02 -.332E+03 -.223E+03 -.125E+02 0.332E+03 0.223E+03 0.121E+00 -.535E+00

0.315E-01 -.381E-06 0.420E-05 -.252E-05

0.218E+01 -.133E+03 0.283E+03 -.219E+01 0.133E+03 -.283E+03 0.541E-03 -.128E+00 -.443E-02 0.297E-06 0.100E-05 -.709E-06

0.492E+01 -.332E+03 0.245E+03 -.488E+01 0.332E+03 -.245E+03 -.319E-01 -.476E+00 -.375E-01 -.733E-06 0.168E-05 0.163E-06

0.112E+02 -.182E+03 -.258E+03 -.112E+02 0.183E+03 0.258E+03 0.482E-01 -.999E-01 -.104E+00 0.118E-05 0.312E-05 -.125E-05

0.316E+02 -.399E+03 -.175E+03 -.319E+02 0.401E+03 0.174E+03 0.297E+00 -.142E+01 0.132E+01 -.285E-05 -.129E-05 -.142E-05

0.929E+01 -.443E+03 0.219E+03 -.929E+01 0.444E+03 -.219E+03 -.565E-02 -.109E+01 -.481E-01 0.538E-06 0.215E-05 0.815E-06

0.169E+01 -.196E+03 0.273E+03 -.169E+01 0.197E+03 -.273E+03 0.549E-02 -.109E+00 -.511E-01 -.420E-06 0.112E-05 -.427E-06

0.171E+02 -.310E+03 -.216E+03 -.175E+02 0.310E+03 0.216E+03 0.326E+00 -.221E+00 0.122E+00 0.176E-05 0.386E-05 -.814E-06

-.103E+01 -.132E+03 0.281E+03 0.102E+01 0.132E+03 -.281E+03 0.103E-01 -.127E+00 0.180E-03 -.112E-05 0.765E-06 -.650E-06

-.511E+01 -.332E+03 0.239E+03 0.510E+01 0.332E+03 -.239E+03 0.888E-02 -.494E+00 -.419E-01 -.276E-05 0.719E-06 -.552E-07

0.162E+01 -.170E+03 -.261E+03 -.173E+01 0.169E+03 0.261E+03 0.122E+00 0.383E+00 -.937E-01 -.273E-05 0.444E-05 -.205E-05

-.519E+01 -.301E+03 -.189E+03 0.464E+01 0.296E+03 0.185E+03 0.672E+00 0.505E+01

0.404E+01 -.554E-05 -.251E-05 -.534E-05

-.619E+00 -.436E+03 0.227E+03 0.617E+00 0.437E+03 -.227E+03 0.166E-02 -.120E+01 -.484E-01 -.204E-05 0.212E-05 0.259E-06

-.301E+01 -.197E+03 0.268E+03 0.300E+01 0.197E+03 -.268E+03 0.146E-01 -.112E+00 -.427E-01 -.190E-05 0.362E-06 -.407E-06

0.331E+01 -.281E+03 -.215E+03 -.526E+01 0.280E+03 0.214E+03 0.194E+01 0.675E+00 0.823E+00 -.371E-05 0.576E-06 -.278E-05

-.273E+01 -.134E+03 0.277E+03 0.273E+01 0.134E+03 -.277E+03 0.250E-02 -.123E+00 -.185E-01 -.141E-05 -.227E-06 -.382E-06

-.599E+01 -.338E+03 0.230E+03 0.598E+01 0.339E+03 -.230E+03 0.113E-01 -.494E+00 -.460E-01 -.191E-05 -.158E-05 -.399E-06

-.645E+01 -.171E+03 -.257E+03 0.653E+01 0.170E+03 0.257E+03 -.730E-01 0.475E+00 0.187E-01 0.212E-07 -.425E-06 -.468E-05

-.444E+02 -.422E+03 -.184E+03 0.450E+02 0.423E+03 0.183E+03 -.562E+00 -.109E+01 0.649E+00 -.362E-05 -.897E-05 -.776E-05

-.865E+01 -.441E+03 0.211E+03 0.864E+01 0.442E+03 -.211E+03 0.145E-01 -.111E+01 -.754E-01 -.389E-05 -.168E-06 -.361E-06

-.292E+01 -.201E+03 0.265E+03 0.293E+01 0.201E+03 -.265E+03 -.916E-02 -.110E+00 -.204E-01 -.131E-05 -.106E-05 -.186E-06

-.145E+02 -.289E+03 -.209E+03 0.164E+02 0.289E+03 0.208E+03 -.195E+01 0.575E+00 0.791E+00 0.128E-06 0.205E-06 -.698E-05

-.138E+01 -.136E+03 0.277E+03 0.139E+01 0.136E+03 -.277E+03 -.102E-01 -.125E+00 -

.239E-01 -.312E-06 -.911E-06 0.188E-06

-.279E+01 -.343E+03 0.230E+03 0.277E+01 0.343E+03 -.230E+03 0.235E-01 -.473E+00 -.593E-01 0.145E-05 -.163E-05 0.118E-06

-.104E+02 -.189E+03 -.258E+03 0.105E+02 0.189E+03 0.258E+03 -.768E-01 -.138E+00 -.534E-01 0.223E-05 -.203E-05 -.381E-05

-.150E+02 -.446E+03 -.196E+03 0.151E+02 0.447E+03 0.196E+03 -.703E-01 -.112E+01 0.101E+00 0.568E-05 -.369E-05 -.380E-05

-.549E+01 -.448E+03 0.204E+03 0.549E+01 0.449E+03 -.204E+03 -.484E-02 -.109E+01 -.125E+00 -.273E-06 -.253E-05 -.642E-06

-.914E+00 -.203E+03 0.267E+03 0.923E+00 0.203E+03 -.267E+03 -.912E-02 -.102E+00 -.317E-01 0.818E-06 -.102E-05 0.380E-06

-.164E+02 -.329E+03 -.218E+03 0.167E+02 0.329E+03 0.218E+03 -.360E+00 -.478E+00 0.447E-01 0.400E-05 -.370E-05 -.646E-05

-.715E+01 -.256E+03 -.193E+03 0.601E+01 0.248E+03 0.188E+03 0.922E+00 0.778E+01 0.490E+01 -.942E-05 0.318E-05 0.117E-05

0.529E+02 -.518E+03 -.137E+03 -.540E+02 0.522E+03 0.141E+03 0.106E+01 -.396E+01 -.382E+01 -.341E-05 -.370E-05 -.378E-05

-.443E+02 -.586E+03 -.447E+03 0.493E+02 0.637E+03 0.481E+03 -.497E+01 -.511E+02 -.344E+02 -.746E-05 0.113E-04 0.832E-05

0.325E+01 0.279E+02 0.224E+02 -.327E-12 0.227E-12 0.182E-11 -.329E+01 -.279E+02 -.225E+02 -.208E-04 0.193E-04 -.146E-03

POSITION			TOTAL-FORCE (eV/Angst)		
1.24575	4.02870	5.43979	0.000041	0.001020	-0.000406
1.21024	4.07581	8.43726	-0.000984	0.002610	-0.001139
3.70862	4.02890	5.43965	0.000307	0.001892	-0.001092
3.67998	4.07733	8.43690	-0.004034	-0.000421	-0.002910
6.17157	4.02854	5.43942	-0.000009	-0.000136	-0.001750
6.14482	4.08292	8.43295	-0.002835	-0.003304	-0.003193
8.63513	4.02801	5.43869	0.000775	-0.000440	-0.001998
8.60339	4.08732	8.43089	-0.000137	-0.001171	-0.002214
11.09928	4.02784	5.43885	0.000872	0.001970	-0.002714
11.06021	4.08619	8.43099	-0.001748	0.000698	-0.000655
13.56311	4.02807	5.43972	0.000332	0.001622	-0.001618
13.52141	4.08047	8.43349	0.000401	-0.002254	0.000286
2.44241	15.48073	8.85224	-0.000598	-0.005263	0.002322
0.01714	15.44624	5.32469	0.000352	0.001544	-0.001197
4.86040	15.47728	8.86623	0.001143	0.000145	-0.000606
2.48016	15.44854	5.27562	0.000368	-0.001202	-0.000502
4.94382	15.44925	5.24869	0.001792	-0.002997	0.000305
12.31531	15.48242	9.00211	-0.003355	0.004352	-0.001236

9.86772	15.44556	5.34176	0.000404	-0.001132	0.000943
14.76279	15.48245	8.89951	-0.005991	-0.000398	0.005533
12.33384	15.44510	5.36128	0.001355	-0.003205	-0.001290
7.40743	15.44616	5.26463	0.002388	0.001483	0.001465
6.44846	16.34427	7.40648	-0.001008	-0.000792	0.003208
8.60064	16.47644	7.89249	0.006080	0.001464	0.006137
1.24544	5.11881	5.35500	0.000958	0.000166	-0.002466
2.44348	5.83889	8.62292	0.002380	-0.004432	0.001216
0.01380	5.79530	5.28573	0.002067	-0.002450	0.000472
1.21063	5.16420	8.54151	0.000268	-0.000518	-0.001879
2.44351	7.27931	8.74832	-0.000034	-0.001253	-0.000121
3.70866	5.11896	5.35390	-0.000415	-0.001627	0.000332
4.90800	5.84315	8.62123	-0.001046	0.003852	-0.000745
2.47701	5.79561	5.28397	0.001435	-0.000594	-0.002608
3.67679	5.16572	8.54000	-0.000109	0.001654	-0.000039
4.90764	7.28398	8.74777	0.000691	-0.000537	0.001049
6.17184	5.11860	5.35433	0.001478	0.000385	0.000898
7.37096	5.84929	8.62094	-0.000549	0.007021	-0.002466
4.94029	5.79548	5.28340	0.000591	-0.002687	-0.001176
6.14080	5.17108	8.53715	-0.002558	0.002551	0.002468
7.37071	7.28983	8.75132	-0.001915	0.001598	0.000125
8.63543	5.11820	5.35521	0.001241	0.001357	-0.001081

9.83233	5.85166	8.62337	0.002659	0.000617	-0.001102
7.40374	5.79498	5.28512	0.003455	-0.002680	-0.001337
8.60194	5.17528	8.53759	-0.001887	-0.000467	-0.000191
9.83204	7.29110	8.75719	-0.002112	-0.002547	-0.002432
11.09930	5.11814	5.35578	-0.000867	-0.003344	-0.001365
12.29449	5.84673	8.62385	0.000108	0.005736	-0.002189
9.86750	5.79468	5.28678	-0.000754	-0.000715	0.001551
11.06261	5.17409	8.53894	0.002649	0.002824	-0.000385
12.29428	7.28729	8.75533	-0.004446	0.001264	-0.001506
13.56278	5.11829	5.35605	0.002656	0.000544	-0.001993
14.75895	5.83988	8.62434	-0.000206	-0.002713	-0.002213
12.33118	5.79480	5.28692	-0.004506	-0.001478	0.002594
13.52535	5.16844	8.54022	-0.003520	0.003811	-0.001411
14.75917	7.28012	8.75179	0.000938	0.002469	-0.000711
0.01434	7.23830	5.19017	0.000095	-0.000206	0.000078
1.24689	9.38061	5.13160	0.000551	-0.001855	-0.000003
1.21085	7.98059	8.79588	-0.000925	-0.000436	0.001578
2.44214	10.12243	8.87141	-0.000839	0.003224	-0.005016
0.01532	10.08686	5.14049	-0.002048	-0.000125	-0.002397
1.24606	7.94244	5.15775	0.002002	-0.002604	0.000832
1.21082	9.41592	8.85782	-0.000786	0.004445	0.000204
2.44072	11.55513	8.88414	-0.006571	-0.002745	0.001637

2.47747	7.23842	5.18585	0.002790	0.002881	0.001310
3.70997	9.38055	5.12566	-0.001072	-0.003009	0.000046
3.67534	7.98360	8.79349	-0.000540	0.000972	0.000927
4.90487	10.12925	8.87518	0.000267	-0.000292	0.000109
2.47867	10.08713	5.12695	-0.002287	0.001510	0.000768
3.70939	7.94242	5.15441	0.000810	-0.004003	-0.001698
3.67589	9.41970	8.85445	-0.001480	0.001957	-0.000140
4.90263	11.56506	8.89086	-0.000932	0.001278	0.001043
4.94085	7.23830	5.18552	-0.004695	0.002258	0.000827
6.17318	9.38002	5.13173	0.002042	0.002090	0.001834
6.13864	7.99044	8.79647	0.002504	-0.000392	-0.001629
7.36780	10.13760	8.89473	0.000561	0.002854	0.000286
4.94196	10.08682	5.12700	0.004115	0.001483	-0.001153
6.17284	7.94199	5.15766	-0.000063	0.000558	0.003034
6.13939	9.42660	8.86164	0.000628	-0.000046	-0.002219
7.36410	11.57721	8.92935	-0.001361	0.000040	0.003244
7.40426	7.23794	5.19012	0.002161	0.001767	0.001070
8.63700	9.37970	5.14543	-0.000523	0.002956	0.000939
8.60086	7.99568	8.80617	0.001168	-0.000698	-0.001061
9.83068	10.14286	8.92842	-0.002964	0.002355	-0.000795
7.40553	10.08627	5.14064	0.001191	-0.003591	0.003144
8.63637	7.94166	5.16555	0.002596	0.001775	-0.001406

8.60077	9.43254	8.88532	-0.006080	0.002507	-0.001209
9.82927	11.58244	9.00096	0.001741	0.003850	0.001037
9.86805	7.23787	5.19489	-0.000376	0.000098	-0.000215
11.10106	9.37979	5.15156	-0.003817	-0.001037	0.000670
11.06331	7.99411	8.80818	-0.000258	-0.001604	0.000136
12.29815	10.12943	8.90340	0.000531	-0.000879	0.001578
9.86930	10.08593	5.15631	-0.005473	-0.001467	0.001410
11.10021	7.94175	5.16862	-0.000613	-0.003071	0.001393
11.06206	9.43062	8.88839	0.004557	0.001907	0.002010
12.30255	11.56557	8.94694	0.001982	-0.003028	-0.000593
12.33169	7.23799	5.19447	-0.001013	0.000244	-0.001756
13.56437	9.38021	5.14435	0.000715	0.001652	-0.000578
13.52754	7.98555	8.80171	-0.000682	-0.002506	-0.003157
14.76233	10.12320	8.88285	-0.005213	0.000806	-0.001712
12.33257	10.08637	5.15511	0.002643	0.000523	-0.001539
13.56350	7.94214	5.16485	-0.000095	-0.000890	-0.000371
13.52731	9.42040	8.86925	-0.000247	0.002810	-0.000472
14.76430	11.55727	8.90646	-0.002561	-0.000348	0.001434
0.01611	11.52516	5.16621	-0.001074	-0.002552	0.000393
1.24770	13.67535	5.22209	0.001868	-0.002255	-0.002478
1.21217	12.26335	8.89409	0.001231	-0.000354	0.001231
2.43998	14.38728	8.86748	-0.003225	0.000705	0.000773

0.01699	14.35408	5.27295	-0.000466	-0.000739	-0.001970
1.24794	12.22963	5.17275	0.001037	0.000864	-0.001362
1.21434	13.70818	8.88771	0.002383	0.002676	0.003652
2.47958	11.52580	5.14547	-0.001624	-0.000197	-0.001487
3.71218	13.67636	5.19535	0.004603	0.000625	0.001088
3.66932	12.26248	8.88184	-0.001520	-0.000009	-0.000681
4.89370	14.38589	8.86075	0.003475	-0.002024	-0.001900
2.48000	14.35596	5.23149	0.001279	-0.001238	0.001695
3.71150	12.23022	5.15602	0.000878	-0.004495	0.001009
3.66212	13.70366	8.87117	-0.004369	0.004351	-0.000506
4.94290	11.52542	5.14351	-0.000044	-0.001784	-0.001601
6.17627	13.67505	5.20032	0.000880	0.000658	0.000051
6.13145	12.27911	8.90591	0.005097	0.007294	0.004543
7.36614	14.42967	8.88203	0.000279	0.002624	0.002095
4.94347	14.35627	5.21375	0.000140	-0.001856	0.001121
6.17493	12.22917	5.16623	-0.001437	-0.001052	0.001575
6.11879	13.72336	8.87765	0.005052	-0.000549	-0.001617
7.40625	11.52413	5.16368	0.000934	-0.003341	0.000351
8.63876	13.67323	5.24377	0.001841	0.002203	-0.001386
8.58939	12.29067	9.00208	0.007868	0.000969	0.000570
9.83855	14.39048	9.30305	0.124328	0.030014	0.019181
7.40672	14.35386	5.23530	-0.001104	-0.000374	-0.000837

8.63820	12.22778	5.19800	0.000300	-0.001261	0.001099
8.55571	13.73596	9.04598	-0.003791	0.033742	0.020132
9.86985	11.52338	5.18893	0.001757	-0.001964	-0.000106
11.10099	13.67352	5.27669	0.003165	-0.000838	-0.000926
11.07378	12.27333	9.00891	0.005784	0.002379	-0.003230
12.30694	14.38896	9.00333	0.004106	-0.005874	-0.000735
9.86934	14.35300	5.29564	0.002859	-0.000010	-0.000115
11.10161	12.22804	5.21650	-0.001121	-0.002729	0.001035
11.11464	13.70636	9.07877	-0.008515	-0.037394	-0.015751
12.33326	11.52411	5.18815	-0.000912	0.000301	0.000538
13.56430	13.67399	5.25995	0.001586	0.000062	0.000094
13.53626	12.26601	8.93587	-0.002051	0.003976	0.002018
14.76266	14.38906	8.90426	-0.003853	0.000476	0.003482
12.33397	14.35288	5.30710	0.002778	-0.001993	-0.001762
13.56505	12.22870	5.20105	0.000074	0.000096	-0.001144
13.54921	13.70690	8.94399	0.000545	-0.001114	0.005111
9.92626	15.53185	9.99472	-0.211795	-0.122620	-0.077663
7.28864	16.40884	8.69813	0.002159	-0.007091	-0.001038
10.02526	16.50365	10.64498	0.081920	0.093832	0.065033

---

total drift:	-0.044162	0.024444	-0.023016

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

---

free energy TOTEN = -1209.38769450 eV

energy without entropy= -1209.38769450 energy(sigma->0) = -1209.38769450

d Force =-0.1571278E-02[-0.318E-02, 0.344E-04] d Energy =-0.1580786E-02 0.951E-05

d Force = 0.6276743E-01[0.901E-01, 0.354E-01] d Ewald = 0.6273682E-01 0.306E-04

POTLOK: cpu time 0.1773: real time 0.1779

---

stress matrix after NEB project (eV)

-17.74472 -0.34852 0.00153

-0.34852 -15.22377 0.49954

0.00153 0.49954 -19.02851

FORCES: max atom, RMS 0.256757 0.024141

FORCE total and by dimension 0.292692 0.211795

Stress total and by dimension 30.157331 19.028513

Finite differences progress:

Degree of freedom: 1/ 6

Displacement: 1/ 2

Total: 1/ 12

LATTYP: Found a simple orthorhombic cell.

ALAT = 14.7806000000

B/A-ratio = 1.2466138046

C/A-ratio = 1.4433717170

Lattice vectors:

A1 = (-14.7806000000, 0.0000000000, 0.0000000000)

A2 = (0.0000000000, 0.0000000000, -18.4257000000)

A3 = (0.0000000000, -21.3339000000, 0.0000000000)

Analysis of symmetry for initial positions (statically):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The static configuration has the point symmetry C_1 .

Analysis of symmetry for dynamics (positions and initial velocities):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The dynamic configuration has the point symmetry C_1 .

Analysis of constrained symmetry for selective dynamics:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The constrained configuration has the point symmetry C_1 .

Analysis of structural, dynamic, and magnetic symmetry:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The magnetic configuration has the point symmetry C_1 .

Subroutine INISYM returns: Found 1 space group operations

(whereof 1 operations are pure point group operations),

and found 1 'primitive' translations

KPOINTS: KPT-Resolved Value to Generate K-Mesh: 0

Automatic generation of k-mesh.

Space group operators:

irot	det(A)	alpha	n_x	n_y	n_z	tau_x	tau_y	tau_z
1	1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Subroutine IBZKPT returns following result:

==========

Found 1 irreducible k-points:

Following reciprocal coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

Following cartesian coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

WAVPRE: cpu time 0.1261: real time 0.1524

FEWALD: cpu time 0.0027: real time 0.0027

ORTHCH: cpu time 0.9988: real time 1.0024

LOOP+: cpu time 139.8593: real time 140.6961

---------- Iteration 3(1) ----------

POTLOK: cpu time 0.1710: real time 0.1817

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9259: real time 1.9322

RMM-DIIS: cpu time 7.1062: real time 7.1411

ORTHCH: cpu time 0.3532: real time 0.3546

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5254: real time 0.5274

MIXING: cpu time 0.0041: real time 0.0042

LOOP: cpu time 10.0962: real time 10.1516

eigenvalue-minimisations : 1926

total energy-change (2. order) : 0.1071462E-02 (-0.1737306E+00)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7369393 magnetization 0.0542611

Broyden mixing:

rms(total) = 0.31450E-01 rms(broyden)= 0.31133E-01

rms(prec) = 0.32034E-01

weight for this iteration 100.00

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107336.19594189

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79571325

PAW double counting = 52177.99462844 -52240.91445342

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.51782601

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76873429 eV

energy without entropy = -1202.76873429 energy(sigma->0) = -1202.76873429

---------- Iteration 3(2) ----------

POTLOK: cpu time 0.1695: real time 0.1859

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9220: real time 1.9288

RMM-DIIS: cpu time 7.1130: real time 7.1459

ORTHCH: cpu time 0.3571: real time 0.3582

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5285: real time 0.5305

MIXING: cpu time 0.0041: real time 0.0041

LOOP: cpu time 10.1046: real time 10.1639

eigenvalue-minimisations : 1920

total energy-change (2. order) :-0.1204141E-02 (-0.1752344E-02)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7356168 magnetization 0.0542644

Broyden mixing:

rms(total) = 0.18632E-01 rms(broyden)= 0.18599E-01

rms(prec) = 0.19331E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3448

1.3448

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107336.11104457

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79504063

PAW double counting = 52176.83471691 -52239.75364393

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.60415280

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76993844 eV

energy without entropy = -1202.76993844 energy(sigma->0) = -1202.76993844

---------- Iteration 3(3) ----------

POTLOK: cpu time 0.1697: real time 0.1706

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9254: real time 1.9315

RMM-DIIS: cpu time 7.1618: real time 7.1829

ORTHCH: cpu time 0.3527: real time 0.3536

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5290: real time 0.5305

MIXING: cpu time 0.0046: real time 0.0046

LOOP: cpu time 10.1537: real time 10.1843

eigenvalue-minimisations : 1938

total energy-change (2. order) : 0.6142153E-04 (-0.9674131E-04)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7371533 magnetization 0.0542693

Broyden mixing:

rms(total) = 0.89295E-02 rms(broyden)= 0.89245E-02

rms(prec) = 0.92532E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4396

0.6837 2.1955

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.95073222

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78726345

PAW double counting = 52175.69830551 -52238.61483394

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.75902513

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76987701 eV

energy without entropy = -1202.76987701 energy(sigma->0) = -1202.76987701

---------- Iteration 3(4) ----------

POTLOK: cpu time 0.1665: real time 0.1969

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9233: real time 1.9297

RMM-DIIS: cpu time 7.1976: real time 7.2287

ORTHCH: cpu time 0.3544: real time 0.3554

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5279: real time 0.5298

MIXING: cpu time 0.0050: real time 0.0050

LOOP: cpu time 10.1852: real time 10.2560

eigenvalue-minimisations : 1931

total energy-change (2. order) :-0.5861691E-04 (-0.1259898E-04)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7368151 magnetization 0.0542705

Broyden mixing:

rms(total) = 0.30786E-02 rms(broyden)= 0.30773E-02

rms(prec) = 0.33603E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3263

2.3462 0.8163 0.8163

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.88536523

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78977604

PAW double counting = 52175.01693708 -52237.93420591

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.82622293

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76993563 eV

energy without entropy = -1202.76993563 energy(sigma->0) = -1202.76993563

---------- Iteration 3(5) ----------

POTLOK: cpu time 0.1695: real time 0.1820

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9228: real time 1.9296

RMM-DIIS: cpu time 7.2937: real time 7.3229

ORTHCH: cpu time 0.3534: real time 0.3544

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5283: real time 0.5301

MIXING: cpu time 0.0052: real time 0.0052

LOOP: cpu time 10.2833: real time 10.3347

eigenvalue-minimisations : 1946

total energy-change (2. order) : 0.1584532E-04 (-0.2433704E-05)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7366427 magnetization 0.0542711

Broyden mixing:

rms(total) = 0.12011E-02 rms(broyden)= 0.12000E-02

rms(prec) = 0.13201E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4212

2.5062 0.8362 0.8362 1.5061

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.88673614

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79023957

PAW double counting = 52175.01469511 -52237.93217141

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.82509224

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76991979 eV

energy without entropy = -1202.76991979 energy(sigma->0) = -1202.76991979

---------- Iteration 3(6) ----------

POTLOK: cpu time 0.1680: real time 0.1833

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9227: real time 1.9295

RMM-DIIS: cpu time 7.1509: real time 7.2082

ORTHCH: cpu time 0.3530: real time 0.3541

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5289: real time 0.5307

MIXING: cpu time 0.0054: real time 0.0055

LOOP: cpu time 10.1393: real time 10.2218

eigenvalue-minimisations : 1912

total energy-change (2. order) :-0.4936155E-06 (-0.1347551E-05)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7365199 magnetization 0.0542715

Broyden mixing:

rms(total) = 0.43920E-03 rms(broyden)= 0.43697E-03

rms(prec) = 0.50106E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3953

2.6039 1.7450 0.7589 0.9344 0.9344

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.87967128

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79045287

PAW double counting = 52175.08736342 -52238.00499975

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.83221087

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76992028 eV

energy without entropy = -1202.76992028 energy(sigma->0) = -1202.76992028

---------- Iteration 3(7) ----------

POTLOK: cpu time 0.1680: real time 0.1842

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9281: real time 1.9348

RMM-DIIS: cpu time 6.0661: real time 6.0854

ORTHCH: cpu time 0.3545: real time 0.3555

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5299: real time 0.5318

MIXING: cpu time 0.0054: real time 0.0054

LOOP: cpu time 9.0625: real time 9.1077

eigenvalue-minimisations : 1645

total energy-change (2. order) :-0.2457935E-05 (-0.8603353E-07)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7365382 magnetization 0.0542715

Broyden mixing:

rms(total) = 0.17744E-03 rms(broyden)= 0.17737E-03

rms(prec) = 0.22576E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3489

2.6474 1.8893 1.0314 1.0314 0.7811 0.7128

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.86469088

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79024390

PAW double counting = 52175.11532475 -52238.03292380

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.84702203

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76992274 eV

energy without entropy = -1202.76992274 energy(sigma->0) = -1202.76992274

---------- Iteration 3(8) ----------

POTLOK: cpu time 0.1691: real time 0.1726

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9207: real time 1.9275

RMM-DIIS: cpu time 5.5063: real time 5.5282

ORTHCH: cpu time 0.3525: real time 0.3537

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5287: real time 0.5305

MIXING: cpu time 0.0056: real time 0.0056

LOOP: cpu time 8.4935: real time 8.5286

eigenvalue-minimisations : 1500

total energy-change (2. order) :-0.2662993E-05 (-0.3195138E-07)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7365551 magnetization 0.0542716

Broyden mixing:

rms(total) = 0.92055E-04 rms(broyden)= 0.91961E-04

rms(prec) = 0.13709E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3620

2.6845 2.1033 1.3198 1.0061 1.0061 0.7885 0.6259

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.85396107

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79010523

PAW double counting = 52175.13541466 -52238.05298089

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.85764866

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76992540 eV

energy without entropy = -1202.76992540 energy(sigma->0) = -1202.76992540

---------- Iteration 3(9) ----------

POTLOK: cpu time 0.1676: real time 0.1797

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9225: real time 1.9290

RMM-DIIS: cpu time 5.1299: real time 5.1529

ORTHCH: cpu time 0.3551: real time 0.3563

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5301: real time 0.5321

MIXING: cpu time 0.0063: real time 0.0064

LOOP: cpu time 8.1221: real time 8.1671

eigenvalue-minimisations : 1403

total energy-change (2. order) :-0.2710083E-05 (-0.7781662E-08)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7365532 magnetization 0.0542716

Broyden mixing:

rms(total) = 0.55446E-04 rms(broyden)= 0.55433E-04

rms(prec) = 0.95243E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4259

2.7928 2.3930 1.7127 1.2509 0.9257 0.9257 0.7901 0.6166

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.84459273

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79004264

PAW double counting = 52175.15399774 -52238.07155471

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.86696638

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76992811 eV

energy without entropy = -1202.76992811 energy(sigma->0) = -1202.76992811

---------- Iteration 3(10) ----------

POTLOK: cpu time 0.1670: real time 0.1739

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9202: real time 1.9267

RMM-DIIS: cpu time 5.3305: real time 5.3505

ORTHCH: cpu time 0.3552: real time 0.3564

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5301: real time 0.5319

MIXING: cpu time 0.0063: real time 0.0064

LOOP: cpu time 8.3199: real time 8.3563

eigenvalue-minimisations : 1452

total energy-change (2. order) :-0.3777714E-05 (-0.1367793E-07)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7365464 magnetization 0.0542718

Broyden mixing:

rms(total) = 0.40167E-04 rms(broyden)= 0.40124E-04

rms(prec) = 0.63298E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4518

3.1651 2.5987 1.9214 1.1724 1.0173 1.0173 0.7795 0.7795 0.6153

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.83148901

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78997561

PAW double counting = 52175.17054541 -52238.08809802

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.88001121

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76993189 eV

energy without entropy = -1202.76993189 energy(sigma->0) = -1202.76993189

---------- Iteration 3(11) ----------

POTLOK: cpu time 0.1697: real time 0.1858

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9235: real time 1.9303

RMM-DIIS: cpu time 5.0579: real time 5.0801

ORTHCH: cpu time 0.3527: real time 0.3538

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5305: real time 0.5323

MIXING: cpu time 0.0069: real time 0.0069

LOOP: cpu time 8.0517: real time 8.0999

eigenvalue-minimisations : 1379

total energy-change (2. order) :-0.2854365E-05 (-0.9419120E-08)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7365491 magnetization 0.0542718

Broyden mixing:

rms(total) = 0.20919E-04 rms(broyden)= 0.20899E-04

rms(prec) = 0.36261E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5036

3.7613 2.6553 1.9757 1.3139 1.3139 0.9495 0.9495 0.7905 0.7081 0.6181

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.82207478

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78990411

PAW double counting = 52175.17217854 -52238.08972298

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.88936497

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76993474 eV

energy without entropy = -1202.76993474 energy(sigma->0) = -1202.76993474

---------- Iteration 3(12) ----------

POTLOK: cpu time 0.1681: real time 0.1749

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9238: real time 1.9301

RMM-DIIS: cpu time 4.9250: real time 4.9407

ORTHCH: cpu time 0.3546: real time 0.3558

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5267: real time 0.5288

MIXING: cpu time 0.0072: real time 0.0072

LOOP: cpu time 7.9158: real time 7.9479

eigenvalue-minimisations : 1334

total energy-change (2. order) :-0.1966080E-05 (-0.5816063E-08)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7365500 magnetization 0.0542718

Broyden mixing:

rms(total) = 0.18909E-04 rms(broyden)= 0.18900E-04

rms(prec) = 0.27045E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6442

4.9393 2.6954 2.3360 1.8825 1.1177 1.1177 1.0252 0.8404 0.8404 0.6203

0.6711

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.81609427

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78986839

PAW double counting = 52175.16979994 -52238.08734286

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.89531323

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76993671 eV

energy without entropy = -1202.76993671 energy(sigma->0) = -1202.76993671

---------- Iteration 3(13) ----------

POTLOK: cpu time 0.1702: real time 0.1911

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9253: real time 1.9320

RMM-DIIS: cpu time 4.7861: real time 4.8320

ORTHCH: cpu time 0.3530: real time 0.3543

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5273: real time 0.5291

MIXING: cpu time 0.0078: real time 0.0078

LOOP: cpu time 7.7802: real time 7.8568

eigenvalue-minimisations : 1298

total energy-change (2. order) :-0.1561362E-05 (-0.4296533E-08)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7365479 magnetization 0.0542718

Broyden mixing:

rms(total) = 0.79623E-05 rms(broyden)= 0.79376E-05

rms(prec) = 0.12969E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6938

5.8249 2.7357 2.5238 1.8980 1.1912 1.1912 1.0100 1.0100 0.8288 0.8288

0.6212 0.6620

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.81159034

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78985729

PAW double counting = 52175.16731007 -52238.08485638

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.89980423

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76993827 eV

energy without entropy = -1202.76993827 energy(sigma->0) = -1202.76993827

---------- Iteration 3(14) ----------

POTLOK: cpu time 0.1659: real time 0.1663

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9209: real time 1.9264

RMM-DIIS: cpu time 4.5824: real time 4.6030

ORTHCH: cpu time 0.3613: real time 0.3622

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5280: real time 0.5295

MIXING: cpu time 0.0081: real time 0.0081

LOOP: cpu time 7.5772: real time 7.6061

eigenvalue-minimisations : 1184

total energy-change (2. order) :-0.8497373E-06 (-0.1475422E-08)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7365481 magnetization 0.0542718

Broyden mixing:

rms(total) = 0.48157E-05 rms(broyden)= 0.48136E-05

rms(prec) = 0.79916E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7524

6.5696 2.8955 2.6349 1.9967 1.7573 1.0881 1.0881 1.0630 0.8377 0.8377

0.7427 0.6226 0.6475

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.80989949

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78985257

PAW double counting = 52175.16732847 -52238.08487422

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.90149178

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76993912 eV

energy without entropy = -1202.76993912 energy(sigma->0) = -1202.76993912

---------- Iteration 3(15) ----------

POTLOK: cpu time 0.1662: real time 0.1850

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9242: real time 1.9299

RMM-DIIS: cpu time 4.5528: real time 4.5665

ORTHCH: cpu time 0.3519: real time 0.3530

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5272: real time 0.5289

MIXING: cpu time 0.0082: real time 0.0082

LOOP: cpu time 7.5409: real time 7.5821

eigenvalue-minimisations : 1176

total energy-change (2. order) :-0.6345217E-06 (-0.7310934E-09)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7365483 magnetization 0.0542718

Broyden mixing:

rms(total) = 0.30820E-05 rms(broyden)= 0.30805E-05

rms(prec) = 0.51410E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7950

7.0186 3.2769 2.6575 2.2298 1.7728 1.2812 1.1003 1.1003 1.0347 0.8486

0.8486 0.6997 0.6244 0.6365

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.80917557

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78985150

PAW double counting = 52175.16782645 -52238.08537157

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.90221589

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76993975 eV

energy without entropy = -1202.76993975 energy(sigma->0) = -1202.76993975

---------- Iteration 3(16) ----------

POTLOK: cpu time 0.1645: real time 0.1657

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9226: real time 1.9289

RMM-DIIS: cpu time 4.5657: real time 4.5815

ORTHCH: cpu time 0.3561: real time 0.3573

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5279: real time 0.5299

MIXING: cpu time 0.0089: real time 0.0089

LOOP: cpu time 7.5563: real time 7.5827

eigenvalue-minimisations : 1190

total energy-change (2. order) :-0.5300390E-06 (-0.4799432E-09)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7365484 magnetization 0.0542718

Broyden mixing:

rms(total) = 0.17653E-05 rms(broyden)= 0.17643E-05

rms(prec) = 0.29277E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8619

7.5273 3.9547 2.6997 2.4377 1.8278 1.7183 1.1054 1.1054 0.9713 0.9713

0.8373 0.8373 0.6781 0.6254 0.6317

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.80883160

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78985259

PAW double counting = 52175.16850552 -52238.08605033

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.90256178

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76994028 eV

energy without entropy = -1202.76994028 energy(sigma->0) = -1202.76994028

-- Iteration 3(17) --

POTLOK: cpu time 0.1746: real time 0.1908

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9237: real time 1.9307

RMM-DIIS: cpu time 4.2319: real time 4.2455

ORTHCH: cpu time 0.3528: real time 0.3539

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5304: real time 0.5323

MIXING: cpu time 0.0092: real time 0.0092

LOOP: cpu time 7.2330: real time 7.2729

eigenvalue-minimisations : 1036

total energy-change (2. order) :-0.1350418E-06 (-0.2214318E-09)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7365484 magnetization 0.0542718

Broyden mixing:

rms(total) = 0.10326E-05 rms(broyden)= 0.10318E-05

rms(prec) = 0.16962E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8842

7.8906 4.4945 2.7448 2.5285 2.0167 1.6994 1.1126 1.1126 1.0924 1.0924

0.8401 0.8401 0.7649 0.6641 0.6264 0.6264

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.80875122

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78985406

PAW double counting = 52175.16900206 -52238.08654685

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.90264379

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76994042 eV

energy without entropy = -1202.76994042 energy(sigma->0) = -1202.76994042

---------- Iteration 3(18) ----------

POTLOK: cpu time 0.1665: real time 0.1675

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9218: real time 1.9282

RMM-DIIS: cpu time 4.0494: real time 4.0626

ORTHCH: cpu time 0.3533: real time 0.3544

DOS: cpu time 0.0003: real time 0.0003

LOOP: cpu time 6.5012: real time 6.5229

eigenvalue-minimisations : 926

total energy-change (2. order) :-0.3149034E-07 (-0.4978062E-10)

number of electron 518.9999724 magnetization 0.9999998

augmentation part 11.7365484 magnetization 0.0542718

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.23845853

-Hartree energ DENC = -107335.80875806

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78985529

PAW double counting = 52175.16910445 -52238.08664948

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.90263798

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76994045 eV

energy without entropy = -1202.76994045 energy(sigma->0) = -1202.76994045

---

average (electrostatic) potential at core

the test charge radii are 0.5201 0.6991 1.0621 0.7215

(the norm of the test charge is 1.0000)

1 -40.7532	2 -40.7511	3 -40.7525	4 -40.7512	5 -40.7532
6 -40.7554	7 -40.7529	8 -40.7607	9 -40.7525	10 -40.7600
11 -40.7539	12 -40.7559	13 -40.6509	14 -40.6965	15 -40.7709
16 -40.6988	17 -40.6927	18 -40.8552	19 -40.6799	20 -40.6675
21 -40.6891	22 -40.6623	23 -40.0880	24 -40.1314	25 -57.4593
26 -57.6705	27 -57.6573	28 -57.4693	29 -57.6641	30 -57.4593
31 -57.6703	32 -57.6569	33 -57.4672	34 -57.6690	35 -57.4601
36 -57.6721	37 -57.6570	38 -57.4694	39 -57.6748	40 -57.4592
41 -57.6761	42 -57.6572	43 -57.4744	44 -57.6893	45 -57.4592
46 -57.6750	47 -57.6580	48 -57.4743	49 -57.6804	50 -57.4603
51 -57.6718	52 -57.6577	53 -57.4722	54 -57.6668	55 -57.6372
56 -57.6633	57 -57.6876	58 -57.6840	59 -57.6670	60 -57.6698
61 -57.6908	62 -57.6755	63 -57.6375	64 -57.6627	65 -57.6897
66 -57.6953	67 -57.6652	68 -57.6696	69 -57.6944	70 -57.7018

71 -57.6369	72 -57.6641	73 -57.6973	74 -57.7220	75 -57.6661
76 -57.6702	77 -57.7065	78 -57.7511	79 -57.6371	80 -57.6667
81 -57.7111	82 -57.7527	83 -57.6694	84 -57.6717	85 -57.7383
86 -57.8420	87 -57.6396	88 -57.6674	89 -57.7129	90 -57.7179
91 -57.6741	92 -57.6719	93 -57.7423	94 -57.7609	95 -57.6379
96 -57.6656	97 -57.6967	98 -57.6914	99 -57.6713	100 -57.6707
101 -57.7087	102 -57.6866	103 -57.6608	104 -57.6315	105 -57.6464
106 -57.2910	107 -57.3886	108 -57.6318	109 -57.5984	110 -57.6597
111 -57.6315	112 -57.6428	113 -57.3101	114 -57.3944	115 -57.6310
116 -57.6002	117 -57.6590	118 -57.6233	119 -57.6983	120 -57.6837
121 -57.3881	122 -57.6298	123 -57.7101	124 -57.6600	125 -57.6260
126 -57.8314	127 -58.3281	128 -57.3614	129 -57.6351	130 -58.1405
131 -57.6679	132 -57.6352	133 -57.8036	134 -57.4167	135 -57.3726
136 -57.6390	137 -58.0808	138 -57.6643	139 -57.6309	140 -57.6722
141 -57.3004	142 -57.3787	143 -57.6344	144 -57.6482	145 -60.8389
146 -57.3168	147 -81.2567			

E-fermi : -2.3393 XC(G=0): -2.7341 alpha+bet : -2.2521

spin component 1

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-26.9550	1.00000
2	-21.5691	1.00000
3	-21.4722	1.00000
4	-21.1001	1.00000
5	-21.0693	1.00000
6	-21.0153	1.00000
7	-20.9794	1.00000
8	-20.9774	1.00000
9	-20.8917	1.00000
10	-20.5582	1.00000
11	-20.5040	1.00000
12	-20.4123	1.00000
13	-20.3987	1.00000
14	-20.1269	1.00000
15	-19.9765	1.00000
16	-19.7038	1.00000
17	-19.6282	1.00000
18	-19.6002	1.00000

19	-19.5846	1.00000
20	-19.5293	1.00000
21	-19.5275	1.00000
22	-19.4993	1.00000
23	-19.4818	1.00000
24	-19.1125	1.00000
25	-19.0761	1.00000
26	-18.9792	1.00000
27	-18.9656	1.00000
28	-18.9012	1.00000
29	-18.7342	1.00000
30	-18.5054	1.00000
31	-18.3597	1.00000
32	-18.2760	1.00000
33	-18.2528	1.00000
34	-18.1840	1.00000
35	-18.1825	1.00000
36	-18.0805	1.00000
37	-18.0767	1.00000
38	-17.5625	1.00000
39	-17.3140	1.00000
40	-17.2883	1.00000

41	-17.2834	1.00000
42	-17.2106	1.00000
43	-17.2042	1.00000
44	-17.1774	1.00000
45	-17.0236	1.00000
46	-16.9509	1.00000
47	-16.9333	1.00000
48	-16.8939	1.00000
49	-16.8920	1.00000
50	-16.8508	1.00000
51	-16.8424	1.00000
52	-16.8218	1.00000
53	-16.8196	1.00000
54	-16.7301	1.00000
55	-16.7269	1.00000
56	-16.1788	1.00000
57	-15.7302	1.00000
58	-15.6929	1.00000
59	-15.6615	1.00000
60	-15.6378	1.00000
61	-15.6168	1.00000
62	-15.5544	1.00000

63	-15.5505	1.00000
64	-15.1759	1.00000
65	-14.8115	1.00000
66	-14.6091	1.00000
67	-14.5788	1.00000
68	-14.5356	1.00000
69	-14.4991	1.00000
70	-14.4692	1.00000
71	-14.4431	1.00000
72	-14.3347	1.00000
73	-14.3061	1.00000
74	-14.2804	1.00000
75	-14.2727	1.00000
76	-14.1832	1.00000
77	-14.1793	1.00000
78	-13.8920	1.00000
79	-13.7602	1.00000
80	-13.5945	1.00000
81	-13.5491	1.00000
82	-13.5302	1.00000
83	-13.4985	1.00000
84	-13.4467	1.00000

85	-13.3648	1.00000
86	-13.3462	1.00000
87	-13.1893	1.00000
88	-12.7870	1.00000
89	-12.7602	1.00000
90	-12.7274	1.00000
91	-12.6967	1.00000
92	-12.6867	1.00000
93	-12.6249	1.00000
94	-12.4618	1.00000
95	-12.4471	1.00000
96	-12.3824	1.00000
97	-12.3252	1.00000
98	-12.2138	1.00000
99	-12.2041	1.00000
100	-12.1658	1.00000
101	-11.9483	1.00000
102	-11.6854	1.00000
103	-11.6282	1.00000
104	-11.6118	1.00000
105	-11.5777	1.00000
106	-11.1005	1.00000

107	-11.0699	1.00000
108	-10.8994	1.00000
109	-10.8882	1.00000
110	-10.8327	1.00000
111	-10.7113	1.00000
112	-10.6797	1.00000
113	-10.6623	1.00000
114	-10.6473	1.00000
115	-10.5900	1.00000
116	-10.5816	1.00000
117	-10.5723	1.00000
118	-10.5685	1.00000
119	-10.5269	1.00000
120	-10.5260	1.00000
121	-10.5112	1.00000
122	-10.5035	1.00000
123	-10.3793	1.00000
124	-10.2939	1.00000
125	-10.2568	1.00000
126	-10.1883	1.00000
127	-10.1871	1.00000
128	-10.0639	1.00000

129	-10.0244	1.00000
130	-9.8912	1.00000
131	-9.8654	1.00000
132	-9.7942	1.00000
133	-9.7868	1.00000
134	-9.7541	1.00000
135	-9.6922	1.00000
136	-9.4493	1.00000
137	-9.4261	1.00000
138	-9.3956	1.00000
139	-9.3886	1.00000
140	-9.3803	1.00000
141	-9.3698	1.00000
142	-9.3107	1.00000
143	-9.3039	1.00000
144	-9.2979	1.00000
145	-9.2845	1.00000
146	-9.2703	1.00000
147	-9.0914	1.00000
148	-9.0044	1.00000
149	-8.9858	1.00000
150	-8.9577	1.00000

151	-8.9557	1.00000
152	-8.7925	1.00000
153	-8.7462	1.00000
154	-8.7349	1.00000
155	-8.7184	1.00000
156	-8.7093	1.00000
157	-8.6877	1.00000
158	-8.6784	1.00000
159	-8.6691	1.00000
160	-8.6543	1.00000
161	-8.5949	1.00000
162	-8.5835	1.00000
163	-8.5767	1.00000
164	-8.5683	1.00000
165	-8.4883	1.00000
166	-8.4572	1.00000
167	-8.4365	1.00000
168	-8.3460	1.00000
169	-8.2978	1.00000
170	-8.2744	1.00000
171	-8.2644	1.00000
172	-8.2338	1.00000

173	-8.2327	1.00000
174	-8.1522	1.00000
175	-8.1457	1.00000
176	-8.0782	1.00000
177	-8.0443	1.00000
178	-8.0265	1.00000
179	-8.0220	1.00000
180	-7.9733	1.00000
181	-7.9648	1.00000
182	-7.9254	1.00000
183	-7.9010	1.00000
184	-7.8855	1.00000
185	-7.8728	1.00000
186	-7.8012	1.00000
187	-7.7978	1.00000
188	-7.7479	1.00000
189	-7.7109	1.00000
190	-7.6664	1.00000
191	-7.6003	1.00000
192	-7.5852	1.00000
193	-7.5760	1.00000
194	-7.5479	1.00000

195	-7.4811	1.00000
196	-7.4805	1.00000
197	-7.4297	1.00000
198	-7.3249	1.00000
199	-7.2498	1.00000
200	-7.1582	1.00000
201	-7.0670	1.00000
202	-7.0420	1.00000
203	-7.0285	1.00000
204	-7.0137	1.00000
205	-6.9970	1.00000
206	-6.9902	1.00000
207	-6.9758	1.00000
208	-6.8663	1.00000
209	-6.8211	1.00000
210	-6.8020	1.00000
211	-6.7937	1.00000
212	-6.7325	1.00000
213	-6.6881	1.00000
214	-6.4712	1.00000
215	-6.4256	1.00000
216	-6.3962	1.00000

217	-6.3916	1.00000
218	-6.3745	1.00000
219	-6.3727	1.00000
220	-6.3176	1.00000
221	-6.3078	1.00000
222	-6.2371	1.00000
223	-6.2302	1.00000
224	-6.2297	1.00000
225	-6.0779	1.00000
226	-6.0380	1.00000
227	-5.7932	1.00000
228	-5.7523	1.00000
229	-5.6943	1.00000
230	-5.6416	1.00000
231	-5.6379	1.00000
232	-5.5593	1.00000
233	-5.5308	1.00000
234	-5.4680	1.00000
235	-5.4397	1.00000
236	-5.1663	1.00000
237	-5.0591	1.00000
238	-5.0508	1.00000

239	-5.0187	1.00000
240	-4.9894	1.00000
241	-4.9111	1.00000
242	-4.8540	1.00000
243	-4.8230	1.00000
244	-4.7902	1.00000
245	-4.6819	1.00000
246	-4.5730	1.00000
247	-4.5717	1.00000
248	-4.5061	1.00000
249	-4.4462	1.00000
250	-4.3842	1.00000
251	-4.2932	1.00000
252	-4.2663	1.00000
253	-4.2131	1.00000
254	-3.5600	1.00000
255	-3.3550	1.00000
256	-3.2018	1.00000
257	-2.9397	1.00000
258	-2.8488	1.00000
259	-2.8242	1.00000
260	-2.6076	1.00000

261	-1.9090	0.00000
262	-1.7686	0.00000
263	-1.7195	0.00000
264	-1.3474	0.00000
265	-1.3191	0.00000
266	-1.1976	0.00000
267	-0.7447	0.00000
268	-0.5850	0.00000
269	-0.5032	0.00000
270	-0.3083	0.00000
271	-0.3061	0.00000
272	-0.2905	0.00000
273	-0.1836	0.00000
274	-0.0583	0.00000
275	-0.0509	0.00000
276	-0.0108	0.00000
277	0.0346	0.00000
278	0.0835	0.00000
279	0.1727	0.00000
280	0.2203	0.00000
281	0.2475	0.00000
282	0.4198	0.00000

283	0.4466	0.00000
284	0.4815	0.00000
285	0.5972	0.00000
286	0.6740	0.00000
287	0.8185	0.00000
288	0.8751	0.00000
289	1.0488	0.00000
290	1.0913	0.00000
291	1.1207	0.00000
292	1.1623	0.00000
293	1.2232	0.00000
294	1.2445	0.00000
295	1.2876	0.00000
296	1.3138	0.00000
297	1.3472	0.00000
298	1.4119	0.00000
299	1.4665	0.00000
300	1.4821	0.00000
301	1.5537	0.00000
302	1.5865	0.00000
303	1.6238	0.00000
304	1.6778	0.00000

305	1.7506	0.00000
306	1.7628	0.00000
307	1.8746	0.00000
308	1.8942	0.00000
309	1.9047	0.00000
310	1.9142	0.00000
311	2.1223	0.00000
312	2.1874	0.00000
313	2.2081	0.00000
314	2.2345	0.00000
315	2.2752	0.00000
316	2.2920	0.00000
317	2.3315	0.00000
318	2.3533	0.00000
319	2.3716	0.00000
320	2.3981	0.00000
321	2.4201	0.00000
322	2.4301	0.00000
323	2.4407	0.00000
324	2.4527	0.00000
325	2.4618	0.00000
326	2.5247	0.00000

327	2.5397	0.00000
328	2.7014	0.00000
329	2.7287	0.00000
330	2.7529	0.00000
331	2.7565	0.00000
332	2.7656	0.00000
333	2.8150	0.00000
334	2.8334	0.00000
335	2.8596	0.00000
336	2.8909	0.00000
337	2.9238	0.00000
338	2.9463	0.00000
339	2.9787	0.00000
340	3.0053	0.00000
341	3.0340	0.00000
342	3.0440	0.00000
343	3.0658	0.00000
344	3.0847	0.00000
345	3.1503	0.00000
346	3.1624	0.00000
347	3.1799	0.00000
348	3.1916	0.00000

349	3.3024	0.00000
350	3.3229	0.00000
351	3.3531	0.00000
352	3.3676	0.00000
353	3.3900	0.00000
354	3.4329	0.00000
355	3.4764	0.00000
356	3.4839	0.00000
357	3.4859	0.00000
358	3.4983	0.00000
359	3.6344	0.00000
360	3.6731	0.00000
361	3.6875	0.00000
362	3.7323	0.00000
363	3.7511	0.00000
364	3.7585	0.00000
365	3.7725	0.00000
366	3.7938	0.00000
367	3.8115	0.00000
368	3.8333	0.00000
369	3.8379	0.00000
370	3.8516	0.00000

371	3.8763	0.00000
372	3.8836	0.00000
373	3.9097	0.00000
374	3.9235	0.00000
375	3.9340	0.00000
376	3.9574	0.00000
377	3.9726	0.00000
378	3.9839	0.00000
379	4.0161	0.00000
380	4.0689	0.00000
381	4.1644	0.00000
382	4.2464	0.00000
383	4.2578	0.00000
384	4.2589	0.00000
385	4.2854	0.00000
386	4.3138	0.00000
387	4.3282	0.00000
388	4.3417	0.00000
389	4.3710	0.00000
390	4.3809	0.00000
391	4.4173	0.00000
392	4.4452	0.00000

393	4.4694	0.00000
394	4.4805	0.00000
395	4.4861	0.00000
396	4.4965	0.00000
397	4.5171	0.00000
398	4.5509	0.00000
399	4.5900	0.00000
400	4.6081	0.00000
401	4.6269	0.00000
402	4.6423	0.00000
403	4.6567	0.00000
404	4.6795	0.00000
405	4.7040	0.00000
406	4.7314	0.00000
407	4.7464	0.00000
408	4.7671	0.00000
409	4.7831	0.00000
410	4.7839	0.00000
411	4.7974	0.00000
412	4.8277	0.00000
413	4.8634	0.00000
414	4.8722	0.00000

415	4.8984	0.00000
416	4.9315	0.00000
417	4.9837	0.00000
418	5.0043	0.00000
419	5.0108	0.00000
420	5.0350	0.00000
421	5.0389	0.00000
422	5.0643	0.00000
423	5.0814	0.00000
424	5.1142	0.00000
425	5.1178	0.00000
426	5.1373	0.00000
427	5.1407	0.00000
428	5.1535	0.00000
429	5.1750	0.00000
430	5.1850	0.00000
431	5.1883	0.00000
432	5.2164	0.00000
433	5.2354	0.00000
434	5.2413	0.00000
435	5.2559	0.00000
436	5.2892	0.00000

437	5.2953	0.00000
438	5.3088	0.00000
439	5.3320	0.00000
440	5.3491	0.00000
441	5.3668	0.00000
442	5.3742	0.00000
443	5.3922	0.00000
444	5.4209	0.00000
445	5.4531	0.00000
446	5.4632	0.00000
447	5.4816	0.00000
448	5.4945	0.00000
449	5.5190	0.00000
450	5.5495	0.00000
451	5.5667	0.00000
452	5.5749	0.00000
453	5.5954	0.00000
454	5.6150	0.00000
455	5.6588	0.00000
456	5.6811	0.00000
457	5.7106	0.00000
458	5.7247	0.00000

459	5.7473	0.00000
460	5.7653	0.00000
461	5.7850	0.00000
462	5.7902	0.00000
463	5.7968	0.00000
464	5.8028	0.00000
465	5.8099	0.00000
466	5.8322	0.00000
467	5.8459	0.00000
468	5.8696	0.00000
469	5.8818	0.00000
470	5.8853	0.00000
471	5.9014	0.00000
472	5.9142	0.00000
473	5.9293	0.00000
474	5.9471	0.00000
475	5.9805	0.00000
476	5.9875	0.00000
477	6.0208	0.00000
478	6.0315	0.00000
479	6.0553	0.00000
480	6.1993	0.00000

spin component 2

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-26.9483	1.00000
2	-21.5679	1.00000
3	-21.4706	1.00000
4	-21.0982	1.00000
5	-21.0684	1.00000
6	-21.0126	1.00000
7	-20.9779	1.00000
8	-20.9756	1.00000
9	-20.8812	1.00000
10	-20.5553	1.00000
11	-20.5006	1.00000
12	-20.4012	1.00000
13	-20.3891	1.00000
14	-20.1228	1.00000
15	-19.9533	1.00000
16	-19.7011	1.00000
17	-19.6269	1.00000

18	-19.5981	1.00000
19	-19.5782	1.00000
20	-19.5280	1.00000
21	-19.5258	1.00000
22	-19.4767	1.00000
23	-19.4623	1.00000
24	-19.1100	1.00000
25	-19.0737	1.00000
26	-18.9692	1.00000
27	-18.9560	1.00000
28	-18.8965	1.00000
29	-18.7046	1.00000
30	-18.5023	1.00000
31	-18.3527	1.00000
32	-18.2479	1.00000
33	-18.2277	1.00000
34	-18.1787	1.00000
35	-18.1770	1.00000
36	-18.0604	1.00000
37	-18.0571	1.00000
38	-17.5591	1.00000
39	-17.2977	1.00000

40	-17.2877	1.00000
41	-17.2740	1.00000
42	-17.2083	1.00000
43	-17.2073	1.00000
44	-17.1744	1.00000
45	-17.0197	1.00000
46	-16.9420	1.00000
47	-16.9229	1.00000
48	-16.8713	1.00000
49	-16.8702	1.00000
50	-16.8299	1.00000
51	-16.8236	1.00000
52	-16.8185	1.00000
53	-16.8160	1.00000
54	-16.7318	1.00000
55	-16.7257	1.00000
56	-16.1761	1.00000
57	-15.7295	1.00000
58	-15.6589	1.00000
59	-15.6440	1.00000
60	-15.6216	1.00000
61	-15.5673	1.00000

62	-15.5286	1.00000
63	-15.5258	1.00000
64	-15.1722	1.00000
65	-14.8093	1.00000
66	-14.6070	1.00000
67	-14.5613	1.00000
68	-14.5011	1.00000
69	-14.4991	1.00000
70	-14.4653	1.00000
71	-14.4388	1.00000
72	-14.3313	1.00000
73	-14.2984	1.00000
74	-14.2687	1.00000
75	-14.2644	1.00000
76	-14.1651	1.00000
77	-14.1617	1.00000
78	-13.8911	1.00000
79	-13.7578	1.00000
80	-13.5918	1.00000
81	-13.5386	1.00000
82	-13.5191	1.00000
83	-13.4949	1.00000

84	-13.4449	1.00000
85	-13.3443	1.00000
86	-13.3417	1.00000
87	-13.1878	1.00000
88	-12.7806	1.00000
89	-12.7507	1.00000
90	-12.7184	1.00000
91	-12.6782	1.00000
92	-12.6712	1.00000
93	-12.6227	1.00000
94	-12.4491	1.00000
95	-12.4322	1.00000
96	-12.3788	1.00000
97	-12.3243	1.00000
98	-12.2092	1.00000
99	-12.1989	1.00000
100	-12.1643	1.00000
101	-11.9455	1.00000
102	-11.6825	1.00000
103	-11.6116	1.00000
104	-11.5926	1.00000
105	-11.5707	1.00000

106	-11.0983	1.00000
107	-11.0673	1.00000
108	-10.8902	1.00000
109	-10.8777	1.00000
110	-10.8298	1.00000
111	-10.7052	1.00000
112	-10.6786	1.00000
113	-10.6593	1.00000
114	-10.6424	1.00000
115	-10.5821	1.00000
116	-10.5746	1.00000
117	-10.5696	1.00000
118	-10.5656	1.00000
119	-10.5163	1.00000
120	-10.5154	1.00000
121	-10.5021	1.00000
122	-10.4974	1.00000
123	-10.3784	1.00000
124	-10.2929	1.00000
125	-10.2559	1.00000
126	-10.1848	1.00000
127	-10.1837	1.00000

128	-10.0541	1.00000
129	-10.0171	1.00000
130	-9.8884	1.00000
131	-9.8630	1.00000
132	-9.7860	1.00000
133	-9.7777	1.00000
134	-9.7516	1.00000
135	-9.6898	1.00000
136	-9.4476	1.00000
137	-9.4226	1.00000
138	-9.3847	1.00000
139	-9.3797	1.00000
140	-9.3725	1.00000
141	-9.3601	1.00000
142	-9.3084	1.00000
143	-9.3011	1.00000
144	-9.2972	1.00000
145	-9.2831	1.00000
146	-9.2482	1.00000
147	-9.0902	1.00000
148	-9.0009	1.00000
149	-8.9800	1.00000

150	-8.9440	1.00000
151	-8.9430	1.00000
152	-8.7899	1.00000
153	-8.7382	1.00000
154	-8.7326	1.00000
155	-8.7128	1.00000
156	-8.7062	1.00000
157	-8.6706	1.00000
158	-8.6643	1.00000
159	-8.6566	1.00000
160	-8.6536	1.00000
161	-8.5776	1.00000
162	-8.5715	1.00000
163	-8.5668	1.00000
164	-8.5498	1.00000
165	-8.4879	1.00000
166	-8.4566	1.00000
167	-8.4349	1.00000
168	-8.3432	1.00000
169	-8.2946	1.00000
170	-8.2731	1.00000
171	-8.2335	1.00000

172	-8.2300	1.00000
173	-8.2280	1.00000
174	-8.1421	1.00000
175	-8.1344	1.00000
176	-8.0750	1.00000
177	-8.0422	1.00000
178	-8.0138	1.00000
179	-8.0074	1.00000
180	-7.9686	1.00000
181	-7.9599	1.00000
182	-7.9214	1.00000
183	-7.8913	1.00000
184	-7.8717	1.00000
185	-7.8640	1.00000
186	-7.7924	1.00000
187	-7.7885	1.00000
188	-7.7383	1.00000
189	-7.6795	1.00000
190	-7.6363	1.00000
191	-7.5981	1.00000
192	-7.5774	1.00000
193	-7.5550	1.00000

194	-7.5405	1.00000
195	-7.4731	1.00000
196	-7.4729	1.00000
197	-7.4286	1.00000
198	-7.3240	1.00000
199	-7.2365	1.00000
200	-7.1551	1.00000
201	-7.0562	1.00000
202	-7.0367	1.00000
203	-7.0162	1.00000
204	-6.9856	1.00000
205	-6.9779	1.00000
206	-6.9728	1.00000
207	-6.9414	1.00000
208	-6.8626	1.00000
209	-6.8168	1.00000
210	-6.7959	1.00000
211	-6.7885	1.00000
212	-6.7257	1.00000
213	-6.6787	1.00000
214	-6.4680	1.00000
215	-6.3956	1.00000

216	-6.3832	1.00000
217	-6.3789	1.00000
218	-6.3634	1.00000
219	-6.3389	1.00000
220	-6.3039	1.00000
221	-6.2762	1.00000
222	-6.2299	1.00000
223	-6.2286	1.00000
224	-6.2227	1.00000
225	-6.0473	1.00000
226	-6.0094	1.00000
227	-5.7569	1.00000
228	-5.7116	1.00000
229	-5.6926	1.00000
230	-5.6362	1.00000
231	-5.6235	1.00000
232	-5.5445	1.00000
233	-5.5237	1.00000
234	-5.4415	1.00000
235	-5.4123	1.00000
236	-5.1442	1.00000
237	-5.0605	1.00000

238	-5.0264	1.00000
239	-5.0230	1.00000
240	-4.9598	1.00000
241	-4.8783	1.00000
242	-4.8548	1.00000
243	-4.8033	1.00000
244	-4.7782	1.00000
245	-4.6515	1.00000
246	-4.5792	1.00000
247	-4.5761	1.00000
248	-4.4761	1.00000
249	-4.4218	1.00000
250	-4.3954	1.00000
251	-4.2970	1.00000
252	-4.2275	1.00000
253	-4.1757	1.00000
254	-3.5337	1.00000
255	-3.3096	1.00000
256	-3.1425	1.00000
257	-2.9446	1.00000
258	-2.7997	1.00000
259	-2.7406	1.00000

260	-2.0614	0.00000
261	-1.9150	0.00000
262	-1.7234	0.00000
263	-1.6797	0.00000
264	-1.3082	0.00000
265	-1.2825	0.00000
266	-1.1613	0.00000
267	-0.7233	0.00000
268	-0.5843	0.00000
269	-0.5108	0.00000
270	-0.2811	0.00000
271	-0.2781	0.00000
272	-0.2604	0.00000
273	-0.1570	0.00000
274	-0.0590	0.00000
275	-0.0486	0.00000
276	0.0128	0.00000
277	0.0396	0.00000
278	0.0783	0.00000
279	0.2078	0.00000
280	0.2554	0.00000
281	0.2791	0.00000

282	0.4332	0.00000
283	0.4511	0.00000
284	0.4827	0.00000
285	0.6019	0.00000
286	0.6945	0.00000
287	0.8212	0.00000
288	0.8818	0.00000
289	1.0593	0.00000
290	1.1090	0.00000
291	1.1416	0.00000
292	1.1769	0.00000
293	1.2322	0.00000
294	1.2502	0.00000
295	1.3090	0.00000
296	1.3193	0.00000
297	1.3607	0.00000
298	1.4310	0.00000
299	1.4786	0.00000
300	1.4997	0.00000
301	1.5781	0.00000
302	1.6026	0.00000
303	1.6524	0.00000

304	1.6866	0.00000
305	1.7581	0.00000
306	1.7730	0.00000
307	1.8786	0.00000
308	1.8995	0.00000
309	1.9077	0.00000
310	1.9222	0.00000
311	2.1386	0.00000
312	2.1985	0.00000
313	2.2199	0.00000
314	2.2530	0.00000
315	2.2892	0.00000
316	2.2965	0.00000
317	2.3368	0.00000
318	2.3610	0.00000
319	2.3824	0.00000
320	2.4080	0.00000
321	2.4284	0.00000
322	2.4354	0.00000
323	2.4518	0.00000
324	2.4573	0.00000
325	2.4676	0.00000

326	2.5272	0.00000
327	2.5454	0.00000
328	2.7065	0.00000
329	2.7348	0.00000
330	2.7530	0.00000
331	2.7590	0.00000
332	2.7744	0.00000
333	2.8296	0.00000
334	2.8464	0.00000
335	2.8725	0.00000
336	2.9022	0.00000
337	2.9324	0.00000
338	2.9557	0.00000
339	2.9835	0.00000
340	3.0069	0.00000
341	3.0381	0.00000
342	3.0507	0.00000
343	3.0715	0.00000
344	3.0922	0.00000
345	3.1528	0.00000
346	3.1712	0.00000
347	3.1885	0.00000

348	3.1998	0.00000
349	3.3080	0.00000
350	3.3275	0.00000
351	3.3616	0.00000
352	3.3711	0.00000
353	3.3932	0.00000
354	3.4384	0.00000
355	3.4817	0.00000
356	3.4913	0.00000
357	3.4939	0.00000
358	3.5047	0.00000
359	3.6394	0.00000
360	3.6769	0.00000
361	3.6999	0.00000
362	3.7381	0.00000
363	3.7550	0.00000
364	3.7603	0.00000
365	3.7774	0.00000
366	3.7985	0.00000
367	3.8144	0.00000
368	3.8406	0.00000
369	3.8472	0.00000

370	3.8659	0.00000
371	3.8801	0.00000
372	3.8929	0.00000
373	3.9208	0.00000
374	3.9353	0.00000
375	3.9484	0.00000
376	3.9593	0.00000
377	3.9829	0.00000
378	3.9864	0.00000
379	4.0219	0.00000
380	4.0783	0.00000
381	4.1708	0.00000
382	4.2588	0.00000
383	4.2626	0.00000
384	4.2698	0.00000
385	4.2931	0.00000
386	4.3219	0.00000
387	4.3349	0.00000
388	4.3509	0.00000
389	4.3808	0.00000
390	4.3857	0.00000
391	4.4231	0.00000

392	4.4492	0.00000
393	4.4745	0.00000
394	4.4831	0.00000
395	4.4927	0.00000
396	4.4996	0.00000
397	4.5205	0.00000
398	4.5553	0.00000
399	4.5931	0.00000
400	4.6108	0.00000
401	4.6287	0.00000
402	4.6458	0.00000
403	4.6597	0.00000
404	4.6854	0.00000
405	4.7087	0.00000
406	4.7371	0.00000
407	4.7515	0.00000
408	4.7705	0.00000
409	4.7867	0.00000
410	4.7895	0.00000
411	4.8031	0.00000
412	4.8326	0.00000
413	4.8690	0.00000

414	4.8846	0.00000
415	4.9037	0.00000
416	4.9423	0.00000
417	4.9935	0.00000
418	5.0096	0.00000
419	5.0132	0.00000
420	5.0383	0.00000
421	5.0441	0.00000
422	5.0686	0.00000
423	5.0857	0.00000
424	5.1176	0.00000
425	5.1220	0.00000
426	5.1412	0.00000
427	5.1442	0.00000
428	5.1700	0.00000
429	5.1796	0.00000
430	5.1887	0.00000
431	5.1931	0.00000
432	5.2213	0.00000
433	5.2378	0.00000
434	5.2447	0.00000
435	5.2615	0.00000

436	5.2979	0.00000
437	5.3026	0.00000
438	5.3119	0.00000
439	5.3363	0.00000
440	5.3530	0.00000
441	5.3708	0.00000
442	5.3818	0.00000
443	5.3950	0.00000
444	5.4294	0.00000
445	5.4594	0.00000
446	5.4697	0.00000
447	5.4871	0.00000
448	5.4988	0.00000
449	5.5258	0.00000
450	5.5677	0.00000
451	5.5726	0.00000
452	5.5943	0.00000
453	5.6074	0.00000
454	5.6246	0.00000
455	5.6711	0.00000
456	5.6917	0.00000
457	5.7187	0.00000

458	5.7280	0.00000
459	5.7493	0.00000
460	5.7643	0.00000
461	5.7906	0.00000
462	5.7934	0.00000
463	5.7991	0.00000
464	5.8054	0.00000
465	5.8218	0.00000
466	5.8280	0.00000
467	5.8602	0.00000
468	5.8668	0.00000
469	5.8843	0.00000
470	5.8928	0.00000
471	5.8943	0.00000
472	5.9093	0.00000
473	5.9371	0.00000
474	5.9533	0.00000
475	5.9678	0.00000
476	5.9933	0.00000
477	6.0151	0.00000
478	6.0618	0.00000
479	6.0848	0.00000

480 6.1509 0.00000

---

soft charge-density along one line, spin component 1

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

soft charge-density along one line, spin component 2

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

pseudopotential strength for first ion, spin component: 1

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

pseudopotential strength for first ion, spin component: 2

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

total augmentation occupancy for first ion, spin component: 1

3.579 -0.646 0.444 -0.034 -0.000

-0.646 0.130 -0.082 0.006 0.000

0.444 -0.082 0.056 -0.003 -0.000

-0.034 0.006 -0.003 0.011 0.000

-0.000 0.000 -0.000 0.000 0.007

total augmentation occupancy for first ion, spin component: 2

-0.000 0.000 -0.000 0.000 0.000

0.000 -0.000 0.000 -0.000 -0.000

-0.000 0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

---------- aborting loop because EDIFF is reached ----------

total charge

# of ion	s	p	d	tot
1	0.646	0.043	0.000	0.690
2	0.646	0.043	0.000	0.690
3	0.646	0.043	0.000	0.690
4	0.646	0.043	0.000	0.690
5	0.646	0.043	0.000	0.690
6	0.646	0.043	0.000	0.690
7	0.646	0.043	0.000	0.690
8	0.646	0.043	0.000	0.690
9	0.646	0.043	0.000	0.690
10	0.646	0.043	0.000	0.690
11	0.646	0.043	0.000	0.690
12	0.646	0.043	0.000	0.690
13	0.646	0.043	0.000	0.689
14	0.646	0.043	0.000	0.689

15	0.648	0.045	0.000	0.693
16	0.646	0.043	0.000	0.689
17	0.646	0.043	0.000	0.689
18	0.646	0.043	0.000	0.689
19	0.646	0.043	0.000	0.689
20	0.646	0.043	0.000	0.689
21	0.646	0.043	0.000	0.689
22	0.646	0.044	0.000	0.690
23	0.541	0.015	0.000	0.557
24	0.541	0.015	0.000	0.556
25	0.870	1.763	0.000	2.633
26	0.867	1.785	0.000	2.653
27	0.867	1.786	0.000	2.653
28	0.870	1.762	0.000	2.632
29	0.865	1.783	0.000	2.648
30	0.870	1.763	0.000	2.633
31	0.867	1.786	0.000	2.653
32	0.867	1.786	0.000	2.653
33	0.870	1.762	0.000	2.632
34	0.865	1.783	0.000	2.648
35	0.870	1.763	0.000	2.633
36	0.868	1.787	0.000	2.654

37	0.867	1.786	0.000	2.653
38	0.870	1.763	0.000	2.633
39	0.865	1.784	0.000	2.649
40	0.870	1.763	0.000	2.633
41	0.868	1.787	0.000	2.655
42	0.867	1.786	0.000	2.653
43	0.871	1.764	0.000	2.634
44	0.865	1.783	0.000	2.648
45	0.870	1.763	0.000	2.633
46	0.867	1.786	0.000	2.653
47	0.867	1.786	0.000	2.653
48	0.871	1.763	0.000	2.634
49	0.865	1.783	0.000	2.648
50	0.870	1.763	0.000	2.633
51	0.867	1.786	0.000	2.653
52	0.867	1.786	0.000	2.653
53	0.870	1.762	0.000	2.632
54	0.865	1.784	0.000	2.648
55	0.865	1.784	0.000	2.649
56	0.865	1.786	0.000	2.651
57	0.866	1.787	0.000	2.653
58	0.866	1.790	0.000	2.656

59	0.865	1.786	0.000	2.651
60	0.866	1.786	0.000	2.651
61	0.866	1.788	0.000	2.654
62	0.867	1.791	0.000	2.658
63	0.865	1.784	0.000	2.649
64	0.865	1.786	0.000	2.651
65	0.866	1.787	0.000	2.652
66	0.865	1.788	0.000	2.653
67	0.865	1.786	0.000	2.651
68	0.866	1.785	0.000	2.651
69	0.865	1.787	0.000	2.652
70	0.866	1.787	0.000	2.653
71	0.865	1.784	0.000	2.649
72	0.865	1.786	0.000	2.651
73	0.866	1.786	0.000	2.652
74	0.864	1.785	0.000	2.649
75	0.865	1.786	0.000	2.651
76	0.866	1.786	0.000	2.651
77	0.865	1.786	0.000	2.651
78	0.865	1.784	0.000	2.649
79	0.865	1.784	0.000	2.649
80	0.865	1.786	0.000	2.651

81	0.865	1.785	0.000	2.650
82	0.863	1.782	0.000	2.645
83	0.865	1.786	0.000	2.651
84	0.866	1.786	0.000	2.651
85	0.865	1.784	0.000	2.648
86	0.862	1.774	0.000	2.636
87	0.865	1.784	0.000	2.649
88	0.865	1.787	0.000	2.652
89	0.865	1.785	0.000	2.650
90	0.865	1.788	0.000	2.653
91	0.865	1.786	0.000	2.651
92	0.866	1.786	0.000	2.651
93	0.864	1.783	0.000	2.647
94	0.866	1.785	0.000	2.651
95	0.865	1.784	0.000	2.649
96	0.865	1.786	0.000	2.651
97	0.866	1.787	0.000	2.653
98	0.866	1.789	0.000	2.655
99	0.865	1.786	0.000	2.651
100	0.866	1.786	0.000	2.651
101	0.865	1.787	0.000	2.652
102	0.867	1.790	0.000	2.657

103	0.865	1.786	0.000	2.651
104	0.867	1.785	0.000	2.653
105	0.866	1.786	0.000	2.652
106	0.870	1.778	0.000	2.648
107	0.869	1.765	0.000	2.635
108	0.865	1.783	0.000	2.648
109	0.869	1.789	0.000	2.658
110	0.865	1.786	0.000	2.651
111	0.867	1.785	0.000	2.653
112	0.867	1.789	0.000	2.655
113	0.871	1.782	0.000	2.653
114	0.869	1.765	0.000	2.634
115	0.865	1.783	0.000	2.648
116	0.870	1.791	0.000	2.661
117	0.865	1.786	0.000	2.651
118	0.867	1.786	0.000	2.653
119	0.865	1.782	0.000	2.647
120	0.857	1.707	0.000	2.564
121	0.869	1.765	0.000	2.634
122	0.865	1.783	0.000	2.648
123	0.866	1.778	0.000	2.644
124	0.866	1.786	0.000	2.652

125	0.868	1.785	0.000	2.653
126	0.862	1.776	0.000	2.638
127	0.849	1.831	0.000	2.680
128	0.870	1.767	0.000	2.637
129	0.865	1.783	0.000	2.648
130	0.861	1.757	0.000	2.618
131	0.866	1.786	0.000	2.652
132	0.867	1.784	0.000	2.652
133	0.864	1.787	0.000	2.651
134	0.869	1.789	0.000	2.659
135	0.869	1.767	0.000	2.636
136	0.865	1.783	0.000	2.648
137	0.866	1.772	0.000	2.637
138	0.866	1.786	0.000	2.652
139	0.867	1.785	0.000	2.652
140	0.866	1.788	0.000	2.653
141	0.870	1.779	0.000	2.649
142	0.869	1.766	0.000	2.635
143	0.865	1.783	0.000	2.648
144	0.869	1.790	0.000	2.659
145	0.941	1.717	0.000	2.658
146	1.240	1.546	0.075	2.860

147	1.633	3.524	0.000	5.157
tot	123.062	221.545	0.075	344.681

magnetization (x)

# of ion	s	p	d	tot
1	0.000	-0.000	0.000	0.000
2	-0.000	0.000	0.000	-0.000
3	0.000	-0.000	0.000	0.000
4	-0.000	0.000	0.000	-0.000
5	0.000	-0.000	0.000	0.000
6	-0.000	0.000	0.000	-0.000
7	0.000	-0.000	0.000	0.000
8	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	0.000
10	-0.000	0.000	0.000	-0.000
11	0.000	-0.000	0.000	0.000
12	-0.000	0.000	0.000	-0.000

13	0.000	-0.000	0.000	0.000
14	-0.004	0.002	0.000	-0.002
15	0.000	-0.000	0.000	0.000
16	-0.004	0.002	0.000	-0.002
17	-0.004	0.002	0.000	-0.002
18	0.000	-0.000	0.000	0.000
19	-0.003	0.001	0.000	-0.002
20	0.000	-0.000	0.000	0.000
21	-0.003	0.002	0.000	-0.002
22	-0.003	0.002	0.000	-0.002
23	-0.000	0.000	0.000	-0.000
24	-0.000	0.000	0.000	-0.000
25	-0.000	-0.007	0.000	-0.008
26	-0.000	-0.002	0.000	-0.002
27	0.000	0.003	0.000	0.003
28	0.000	0.005	0.000	0.005
29	0.000	0.003	0.000	0.003
30	-0.000	-0.007	0.000	-0.008
31	-0.000	-0.002	0.000	-0.002
32	0.000	0.003	0.000	0.003
33	0.000	0.005	0.000	0.005
34	0.000	0.002	0.000	0.002

35	-0.000	-0.007	0.000	-0.008
36	-0.000	-0.002	0.000	-0.002
37	0.000	0.003	0.000	0.003
38	0.000	0.006	0.000	0.007
39	0.000	0.002	0.000	0.002
40	-0.000	-0.007	0.000	-0.008
41	-0.000	-0.002	0.000	-0.002
42	0.000	0.002	0.000	0.003
43	0.000	0.005	0.000	0.006
44	0.000	0.004	0.000	0.004
45	-0.000	-0.007	0.000	-0.008
46	-0.000	-0.002	0.000	-0.002
47	0.000	0.003	0.000	0.003
48	0.000	0.005	0.000	0.006
49	0.000	0.001	0.000	0.002
50	-0.000	-0.007	0.000	-0.008
51	-0.000	-0.002	0.000	-0.002
52	0.000	0.002	0.000	0.003
53	0.000	0.006	0.000	0.007
54	0.000	0.002	0.000	0.002
55	-0.000	-0.005	0.000	-0.006
56	-0.000	-0.007	0.000	-0.007

57	-0.000	-0.001	0.000	-0.001
58	-0.000	-0.001	0.000	-0.001
59	0.000	0.006	0.000	0.007
60	0.000	0.003	0.000	0.003
61	0.000	0.001	0.000	0.001
62	0.000	0.003	0.000	0.003
63	-0.000	-0.005	0.000	-0.006
64	-0.000	-0.007	0.000	-0.007
65	-0.000	-0.001	0.000	-0.001
66	-0.000	-0.001	0.000	-0.001
67	0.000	0.006	0.000	0.006
68	0.000	0.003	0.000	0.003
69	0.000	0.001	0.000	0.001
70	0.000	0.002	0.000	0.002
71	-0.000	-0.005	0.000	-0.006
72	-0.000	-0.007	0.000	-0.007
73	-0.000	-0.001	0.000	-0.001
74	-0.000	-0.002	0.000	-0.002
75	0.000	0.006	0.000	0.007
76	0.000	0.003	0.000	0.004
77	0.000	0.003	0.000	0.003
78	0.000	0.001	0.000	0.001

79	-0.000	-0.005	0.000	-0.006
80	-0.000	-0.007	0.000	-0.007
81	-0.000	-0.001	0.000	-0.002
82	-0.000	-0.002	0.000	-0.002
83	0.001	0.007	0.000	0.008
84	0.000	0.003	0.000	0.003
85	0.000	0.002	0.000	0.002
86	0.000	0.005	0.000	0.006
87	-0.000	-0.005	0.000	-0.005
88	-0.000	-0.007	0.000	-0.007
89	-0.000	-0.001	0.000	-0.002
90	-0.000	-0.002	0.000	-0.002
91	0.001	0.008	0.000	0.008
92	0.000	0.003	0.000	0.003
93	0.000	0.002	0.000	0.003
94	0.000	0.001	0.000	0.001
95	-0.000	-0.005	0.000	-0.006
96	-0.000	-0.007	0.000	-0.007
97	-0.000	-0.001	0.000	-0.001
98	-0.000	-0.001	0.000	-0.001
99	0.001	0.007	0.000	0.007
100	0.000	0.003	0.000	0.004

101	0.000	0.003	0.000	0.003
102	0.000	0.002	0.000	0.002
103	-0.001	-0.010	0.000	-0.011
104	-0.003	-0.028	0.000	-0.031
105	-0.000	-0.001	0.000	-0.002
106	-0.000	-0.004	0.000	-0.005
107	0.007	0.116	0.000	0.122
108	0.001	0.010	0.000	0.011
109	0.000	0.001	0.000	0.001
110	-0.001	-0.010	0.000	-0.011
111	-0.003	-0.028	0.000	-0.031
112	-0.000	-0.001	0.000	-0.002
113	-0.000	-0.003	0.000	-0.004
114	0.007	0.120	0.000	0.127
115	0.001	0.010	0.000	0.011
116	0.000	0.001	0.000	0.002
117	-0.001	-0.010	0.000	-0.011
118	-0.003	-0.026	0.000	-0.029
119	-0.000	-0.002	0.000	-0.002
120	-0.000	-0.002	0.000	-0.002
121	0.007	0.115	0.000	0.122
122	0.001	0.010	0.000	0.010

123	0.000	0.003	0.000	0.003
124	-0.001	-0.010	0.000	-0.011
125	-0.003	-0.024	0.000	-0.027
126	-0.000	-0.002	0.000	-0.002
127	-0.000	0.001	0.000	0.001
128	0.006	0.105	0.000	0.111
129	0.001	0.009	0.000	0.010
130	0.000	0.004	0.000	0.004
131	-0.001	-0.009	0.000	-0.010
132	-0.003	-0.024	0.000	-0.027
133	-0.000	-0.002	0.000	-0.002
134	-0.000	-0.002	0.000	-0.002
135	0.006	0.097	0.000	0.102
136	0.001	0.009	0.000	0.010
137	0.000	0.004	0.000	0.005
138	-0.001	-0.010	0.000	-0.011
139	-0.003	-0.026	0.000	-0.029
140	-0.000	-0.002	0.000	-0.002
141	-0.000	-0.003	0.000	-0.004
142	0.006	0.105	0.000	0.111
143	0.001	0.010	0.000	0.010
144	0.000	0.002	0.000	0.003

145	0.000	0.005	0.000	0.006
146	-0.000	0.000	-0.000	0.000
147	0.000	0.004	0.000	0.004
tot	0.001	0.513	-0.000	0.514

CHARGE: cpu time 0.5301: real time 0.5318

FORLOC: cpu time 0.0199: real time 0.0199

FORNL : cpu time 2.0332: real time 2.0409

STRESS: cpu time 6.0849: real time 6.1062

FORCOR: cpu time 0.1393: real time 0.1409

FORHAR: cpu time 0.0334: real time 0.0334

MIXING: cpu time 0.0103: real time 0.0103

OFIELD: cpu time 0.0001: real time 0.0001

DFTD3 V3.0 Rev 1

Edisp (eV) -6.61769

E6 (eV) : -3.9313

E8 (eV) : -2.6864

% E8 : 40.59

FORVDW: cpu time 1.7839: real time 1.8254

FORCE on cell =-STRESS in cart. coord. units (eV):

Direction	XX	YY	ZZ	XY	YZ	ZX
Alpha Z	233.50077	233.50077	233.50077			
Ewald	107580.16656	23476.48833	-39727.54653	11.67711	3454.27700	130.54156
Hartree	106097.57444	25032.54912	-23794.31468	-5.92948	2947.06020	94.14605
E(xc)	-1914.22774	-1916.58352	-1979.89108	0.13644	1.81998	0.13693
Local	**********	-53957.63407	57015.63390	-2.12362	-6359.44743	-221.12070
n-local	-472.64970	-482.44081	-439.52204	-0.74750	-0.68688	-0.36888
augment	-38.29507	-38.58606	-34.30583	-0.00929	-0.97764	-0.00724
Kinetic	7635.01611	7638.84747	8713.95669	-3.15905	-41.56418	-3.23410
Fock	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
vdW	-2.64276	-1.49206	-6.59296	0.00183	-0.07458	0.01212
Total	-17.74921	-15.35083	-19.08177	-0.15356	0.40647	0.10575
in kB	-4.89444	-4.23308	-5.26190	-0.04234	0.11209	0.02916

external pressure = -4.80 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

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energy-cutoff : 400.00

volume of cell : 5810.14

direct lattice vectors reciprocal lattice vectors

14.780600000 0.000000000 0.000000000 0.067656252 0.000000000 0.000000000

0.000000000 21.333900000 0.000000000 0.000000000 0.046873755 0.000000000

0.000000000 0.000000000 18.425700000 0.000000000 0.000000000 0.054272022

length of vectors

14.780600000 21.333900000 18.425700000 0.067656252 0.046873755 0.054272022

FORCES acting on ions

electron-ion (+dipol) ewald-force non-local-force convergence-correction

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0.493E-02 0.154E+03 0.361E+02 -.343E-02 -.160E+03 -.357E+02 -.180E-02 0.566E+01 -.438E+00 0.170E-06 -.416E-06 -.154E-06

-.181E-01 0.155E+03 -.340E+02 0.157E-01 -.160E+03 0.335E+02 0.116E-02 0.565E+01 0.541E+00 0.108E-05 0.442E-06 0.159E-06

0.185E+00 0.154E+03 0.360E+02 -.185E+00 -.160E+03 -.356E+02 0.888E-05 0.565E+01 -

.443E+00 0.137E-06 -.820E-06 0.555E-06

0.113E+00 0.155E+03 -.341E+02 -.993E-01 -.160E+03 0.336E+02 -.175E-01 0.565E+01 0.535E+00 0.535E-06 -.628E-06 0.639E-06

0.171E+00 0.154E+03 0.362E+02 -.173E+00 -.160E+03 -.357E+02 0.116E-02 0.566E+01 -.440E+00 -.438E-07 -.844E-06 0.508E-06

0.126E+00 0.154E+03 -.340E+02 -.108E+00 -.160E+03 0.334E+02 -.211E-01 0.565E+01 0.541E+00 -.542E-06 -.698E-06 0.543E-06

-.196E-01 0.154E+03 0.363E+02 0.184E-01 -.160E+03 -.359E+02 0.159E-02 0.566E+01 -.431E+00 -.127E-06 -.511E-06 -.213E-06

-.133E-01 0.154E+03 -.338E+02 0.202E-01 -.160E+03 0.332E+02 -.721E-02 0.565E+01 0.555E+00 -.984E-06 0.199E-06 0.155E-07

-.182E+00 0.154E+03 0.363E+02 0.182E+00 -.160E+03 -.359E+02 0.255E-03 0.566E+01 -.429E+00 -.142E-06 -.170E-06 -.901E-06

-.128E+00 0.155E+03 -.337E+02 0.115E+00 -.160E+03 0.331E+02 0.109E-01 0.565E+01 0.561E+00 -.541E-06 0.117E-05 -.423E-06

-.174E+00 0.154E+03 0.362E+02 0.176E+00 -.160E+03 -.358E+02 -.177E-02 0.566E+01 -.432E+00 0.182E-08 -.666E-07 -.869E-06

-.115E+00 0.155E+03 -.338E+02 0.958E-01 -.160E+03 0.332E+02 0.192E-01 0.565E+01 0.555E+00 0.458E-06 0.133E-05 -.381E-06

0.229E+01 -.150E+03 -.386E+02 -.228E+01 0.156E+03 0.386E+02 -.103E-01 -.566E+01 0.767E-01 -.456E-06 0.276E-07 0.129E-06

-.413E+00 -.151E+03 0.388E+02 0.414E+00 0.157E+03 -.386E+02 -.128E-02 -.567E+01 -

.269E+00 -.274E-06 0.262E-06 0.143E-06

0.136E+02 -.146E+03 -.413E+02 -.139E+02 0.151E+03 0.413E+02 0.257E+00 -.567E+01 -.347E-01 0.667E-06 0.339E-06 0.611E-08

0.163E+01 -.151E+03 0.402E+02 -.163E+01 0.156E+03 -.400E+02 -.998E-03 -.567E+01 -.229E+00 -.218E-06 -.109E-06 -.265E-06

0.353E+01 -.149E+03 0.443E+02 -.352E+01 0.155E+03 -.441E+02 -.198E-02 -.567E+01 -.180E+00 0.203E-06 -.101E-06 -.122E-06

-.148E+02 -.146E+03 -.330E+02 0.149E+02 0.151E+03 0.330E+02 -.937E-01 -.566E+01 0.478E-01 0.126E-05 0.152E-06 -.503E-06

-.298E+01 -.149E+03 0.432E+02 0.297E+01 0.155E+03 -.430E+02 0.114E-01 -.567E+01 -.241E+00 0.343E-07 0.361E-06 0.345E-06

-.378E+01 -.150E+03 -.385E+02 0.378E+01 0.156E+03 0.385E+02 -.606E-02 -.566E+01 0.239E-01 -.983E-07 0.351E-06 0.349E-06

-.208E+01 -.151E+03 0.395E+02 0.207E+01 0.156E+03 -.392E+02 0.151E-02 -.566E+01 -.282E+00 0.861E-07 0.513E-06 0.218E-06

0.708E-03 -.148E+03 0.486E+02 0.690E-02 0.154E+03 -.484E+02 -.554E-02 -.569E+01 -.158E+00 0.145E-06 0.816E-07 0.399E-06

0.196E+02 -.103E+03 0.222E+02 -.212E+02 0.103E+03 -.246E+02 0.153E+01 0.138E+00 0.238E+01 0.401E-06 0.162E-06 0.317E-06

-.192E+02 -.103E+03 0.154E+02 0.216E+02 0.103E+03 -.169E+02 -.241E+01 -.119E+00 0.152E+01 -.324E-06 0.468E-06 -.286E-06

0.725E-01 0.461E+03 0.202E+03 -.757E-01 -.462E+03 -.201E+03 0.383E-02 0.102E+01 -

.219E+00 -.181E-06 -.152E-06 -.704E-07

0.214E+00 0.353E+03 -.234E+03 -.214E+00 -.353E+03 0.234E+03 0.255E-02 0.443E+00 -.370E-01 0.108E-05 -.194E-05 0.158E-05

-.241E-01 0.351E+03 0.240E+03 0.228E-01 -.351E+03 -.241E+03 0.315E-02 0.408E+00 0.564E-01 -.495E-06 0.119E-05 -.991E-06

-.171E+00 0.462E+03 -.195E+03 0.178E+00 -.463E+03 0.195E+03 -.663E-02 0.105E+01 0.233E+00 0.242E-05 0.232E-06 0.107E-05

-.590E-01 0.210E+03 -.272E+03 0.630E-01 -.210E+03 0.272E+03 -.446E-02 0.937E-01 0.560E-01 0.170E-06 -.116E-05 0.104E-05

0.563E+00 0.461E+03 0.202E+03 -.566E+00 -.462E+03 -.201E+03 0.202E-02 0.102E+01 -.214E+00 0.951E-07 -.123E-05 0.206E-05

0.106E+01 0.352E+03 -.234E+03 -.107E+01 -.353E+03 0.234E+03 0.160E-01 0.448E+00 -.425E-01 -.799E-07 -.327E-05 0.181E-05

0.414E+00 0.351E+03 0.240E+03 -.416E+00 -.351E+03 -.240E+03 0.303E-02 0.408E+00 0.491E-01 -.284E-06 0.538E-06 0.104E-05

0.580E+00 0.462E+03 -.195E+03 -.585E+00 -.463E+03 0.195E+03 0.478E-02 0.105E+01 0.235E+00 0.109E-05 -.317E-05 0.226E-05

0.691E+00 0.210E+03 -.272E+03 -.697E+00 -.210E+03 0.272E+03 0.594E-02 0.913E-01 0.616E-01 -.870E-07 -.184E-05 0.110E-05

0.426E+00 0.461E+03 0.202E+03 -.428E+00 -.462E+03 -.202E+03 0.384E-02 0.102E+01 -.214E+00 0.164E-06 -.143E-05 0.185E-05

0.938E+00 0.352E+03 -.233E+03 -.954E+00 -.352E+03 0.233E+03 0.152E-01 0.441E+00 -

.377E-01 -.115E-05 -.190E-05 0.101E-05

0.479E+00 0.351E+03 0.241E+03 -.481E+00 -.351E+03 -.241E+03 0.250E-02 0.406E+00 0.512E-01 0.799E-07 0.796E-07 0.190E-05

0.705E+00 0.462E+03 -.194E+03 -.715E+00 -.463E+03 0.194E+03 0.789E-02 0.106E+01 0.242E+00 -.130E-05 -.313E-05 0.180E-05

0.723E+00 0.210E+03 -.271E+03 -.732E+00 -.210E+03 0.271E+03 0.654E-02 0.911E-01 0.592E-01 -.276E-06 -.116E-05 0.635E-06

-.183E+00 0.461E+03 0.202E+03 0.179E+00 -.462E+03 -.202E+03 0.448E-02 0.102E+01 -.218E+00 0.222E-06 -.567E-06 -.400E-06

-.296E+00 0.352E+03 -.233E+03 0.301E+00 -.352E+03 0.233E+03 -.233E-02 0.440E+00 -.300E-01 -.971E-06 0.584E-06 -.631E-07

0.397E-01 0.351E+03 0.241E+03 -.387E-01 -.351E+03 -.241E+03 0.223E-02 0.409E+00 0.558E-01 0.512E-06 0.263E-06 0.754E-06

0.485E-01 0.462E+03 -.194E+03 -.546E-01 -.463E+03 0.194E+03 0.390E-02 0.106E+01 0.232E+00 -.219E-05 -.910E-07 0.357E-06

-.512E-01 0.210E+03 -.271E+03 0.496E-01 -.210E+03 0.271E+03 -.306E-03 0.933E-01 0.324E-01 -.159E-06 0.220E-06 0.151E-06

-.553E+00 0.461E+03 0.202E+03 0.551E+00 -.462E+03 -.202E+03 0.762E-03 0.102E+01 -.220E+00 -.997E-07 0.382E-06 -.252E-05

-.119E+01 0.352E+03 -.233E+03 0.120E+01 -.353E+03 0.233E+03 -.161E-01 0.447E+00 -.330E-01 -.128E-07 0.197E-05 -.310E-06

-.354E+00 0.351E+03 0.241E+03 0.351E+00 -.351E+03 -.241E+03 0.206E-02 0.413E+00

0.624E-01 0.276E-06 0.844E-06 -.128E-05

-.413E+00 0.462E+03 -.194E+03 0.427E+00 -.463E+03 0.194E+03 -.115E-01 0.106E+01 0.230E+00 -.114E-05 0.305E-05 -.714E-06

-.563E+00 0.210E+03 -.271E+03 0.567E+00 -.210E+03 0.271E+03 -.930E-02 0.915E-01 0.525E-01 0.161E-06 0.973E-06 0.131E-06

-.475E+00 0.461E+03 0.202E+03 0.474E+00 -.462E+03 -.202E+03 0.307E-02 0.102E+01 -.220E+00 -.211E-06 0.681E-06 -.226E-05

-.804E+00 0.353E+03 -.234E+03 0.819E+00 -.353E+03 0.234E+03 -.149E-01 0.447E+00 -.393E-01 0.109E-05 0.796E-06 0.453E-06

-.374E+00 0.351E+03 0.241E+03 0.369E+00 -.351E+03 -.241E+03 0.964E-03 0.411E+00 0.626E-01 -.980E-07 0.128E-05 -.216E-05

-.594E+00 0.462E+03 -.194E+03 0.607E+00 -.463E+03 0.194E+03 -.169E-01 0.105E+01 0.234E+00 0.121E-05 0.331E-05 -.479E-06

-.586E+00 0.210E+03 -.272E+03 0.597E+00 -.210E+03 0.272E+03 -.102E-01 0.993E-01 0.567E-01 0.161E-06 0.252E-06 0.492E-06

-.777E-02 0.206E+03 0.279E+03 0.111E-01 -.206E+03 -.279E+03 -.360E-02 0.688E-01 -.412E-01 -.553E-06 0.874E-06 -.467E-06

0.672E+00 0.303E+02 0.296E+03 -.667E+00 -.302E+02 -.296E+03 -.467E-02 -.409E-01 0.755E-02 -.471E-06 0.592E-06 -.146E-06

-.842E+00 0.144E+03 -.282E+03 0.844E+00 -.144E+03 0.282E+03 -.311E-02 0.137E+00 0.286E-01 -.993E-07 -.197E-06 0.563E-06

0.544E+00 -.215E+02 -.285E+03 -.544E+00 0.214E+02 0.285E+03 -.919E-03 0.388E-01

0.185E-01 -.684E-06 -.113E-06 0.133E-06

0.502E+00 -.294E+02 0.293E+03 -.499E+00 0.294E+02 -.293E+03 -.552E-02 0.255E-01 -.303E-01 -.193E-06 0.291E-06 -.172E-07

0.526E+00 0.139E+03 0.289E+03 -.527E+00 -.139E+03 -.289E+03 0.179E-02 0.104E+00 -.248E-01 -.693E-06 0.778E-06 0.541E-07

-.126E+01 0.364E+02 -.287E+03 0.126E+01 -.364E+02 0.287E+03 -.766E-04 -.739E-02 0.136E-01 -.505E-06 0.152E-06 0.141E-06

0.169E+01 -.130E+03 -.271E+03 -.170E+01 0.130E+03 0.271E+03 0.105E-01 -.877E-01 0.371E-01 -.115E-05 0.266E-06 -.621E-07

0.399E+00 0.207E+03 0.280E+03 -.397E+00 -.207E+03 -.280E+03 0.706E-03 0.696E-01 -.370E-01 -.593E-06 0.951E-06 0.661E-06

0.923E+00 0.312E+02 0.296E+03 -.927E+00 -.311E+02 -.296E+03 0.225E-02 -.409E-01 0.122E-01 -.305E-06 0.908E-06 -.173E-06

0.133E+01 0.144E+03 -.282E+03 -.134E+01 -.144E+03 0.282E+03 0.503E-02 0.126E+00 0.279E-01 -.172E-06 -.101E-05 0.922E-06

0.342E+01 -.199E+02 -.285E+03 -.344E+01 0.199E+02 0.285E+03 0.133E-01 0.416E-01 0.136E-01 -.202E-06 -.176E-06 0.185E-06

0.140E+01 -.287E+02 0.294E+03 -.139E+01 0.287E+02 -.294E+03 -.348E-02 0.253E-01 -.307E-01 -.317E-06 0.762E-06 -.447E-06

0.680E+00 0.139E+03 0.290E+03 -.680E+00 -.139E+03 -.290E+03 0.617E-03 0.103E+00 -.295E-01 -.257E-06 0.925E-06 0.675E-06

0.161E+01 0.367E+02 -.287E+03 -.160E+01 -.367E+02 0.287E+03 -.130E-01 -.205E-01

0.129E-01 -.487E-06 -.439E-06 0.458E-06

0.613E+01 -.125E+03 -.271E+03 -.615E+01 0.125E+03 0.271E+03 0.215E-01 -.893E-01 0.143E-01 0.611E-07 0.501E-07 -.251E-06

0.368E+00 0.207E+03 0.280E+03 -.373E+00 -.207E+03 -.280E+03 0.106E-03 0.685E-01 -.365E-01 0.543E-07 0.899E-06 0.113E-05

-.375E-01 0.319E+02 0.296E+03 0.288E-01 -.318E+02 -.296E+03 0.105E-01 -.361E-01 0.139E-01 0.217E-06 0.724E-06 -.205E-06

0.210E+01 0.144E+03 -.281E+03 -.211E+01 -.144E+03 0.281E+03 0.119E-01 0.120E+00 0.240E-01 -.785E-07 -.118E-05 0.688E-06

0.303E+01 -.171E+02 -.283E+03 -.305E+01 0.171E+02 0.283E+03 0.241E-01 0.852E-01 0.609E-01 0.489E-06 0.215E-06 0.991E-08

0.106E+01 -.272E+02 0.294E+03 -.106E+01 0.272E+02 -.294E+03 0.289E-02 0.244E-01 -.376E-01 -.141E-06 0.844E-06 -.593E-06

0.965E-01 0.140E+03 0.290E+03 -.981E-01 -.140E+03 -.290E+03 0.131E-02 0.107E+00 -.232E-01 0.323E-06 0.787E-06 0.581E-06

0.277E+01 0.387E+02 -.286E+03 -.277E+01 -.387E+02 0.286E+03 0.632E-03 -.114E-01 0.290E-01 0.704E-07 -.470E-06 0.273E-06

0.596E+01 -.115E+03 -.267E+03 -.611E+01 0.115E+03 0.267E+03 0.149E+00 -.269E-02 0.131E+00 0.802E-06 0.101E-05 -.972E-07

-.243E+00 0.207E+03 0.280E+03 0.241E+00 -.207E+03 -.280E+03 0.438E-02 0.717E-01 -.387E-01 0.652E-06 0.812E-06 0.462E-06

-.115E+01 0.314E+02 0.294E+03 0.114E+01 -.314E+02 -.294E+03 0.917E-02 -.311E-01

0.546E-02 0.451E-06 0.304E-06 -.171E-06

0.590E+00 0.144E+03 -.281E+03 -.607E+00 -.144E+03 0.281E+03 0.177E-01 0.126E+00 0.437E-01 0.136E-06 -.338E-06 0.253E-06

-.956E+00 -.159E+02 -.286E+03 0.949E+00 0.158E+02 0.285E+03 0.583E-02 0.906E-01 0.802E-01 0.119E-05 0.363E-06 0.263E-06

-.646E+00 -.265E+02 0.293E+03 0.642E+00 0.265E+02 -.293E+03 0.491E-02 0.235E-01 -.270E-01 0.243E-06 0.524E-06 -.372E-06

-.537E+00 0.139E+03 0.289E+03 0.532E+00 -.139E+03 -.289E+03 0.654E-02 0.114E+00 -.213E-01 0.648E-06 0.527E-06 -.129E-06

0.769E+00 0.408E+02 -.287E+03 -.781E+00 -.408E+02 0.287E+03 0.534E-02 0.183E-02 -.192E-01 0.672E-06 -.536E-08 0.733E-07

-.511E+00 -.113E+03 -.276E+03 0.472E+00 0.113E+03 0.276E+03 0.386E-01 0.599E-01 -.269E+00 0.499E-06 -.985E-07 0.515E-06

-.574E+00 0.206E+03 0.279E+03 0.572E+00 -.206E+03 -.279E+03 0.113E-02 0.721E-01 -.455E-01 0.479E-06 0.698E-06 -.666E-06

-.787E+00 0.304E+02 0.294E+03 0.791E+00 -.304E+02 -.294E+03 -.755E-02 -.308E-01 -.138E-02 0.266E-06 0.484E-07 -.134E-06

-.123E+01 0.144E+03 -.281E+03 0.125E+01 -.145E+03 0.281E+03 -.158E-01 0.122E+00 0.504E-01 0.161E-06 0.847E-06 0.905E-07

-.366E+01 -.174E+02 -.283E+03 0.369E+01 0.173E+02 0.283E+03 -.310E-01 0.118E+00 0.583E-01 0.553E-07 0.912E-06 0.430E-06

-.130E+01 -.277E+02 0.291E+03 0.130E+01 0.277E+02 -.291E+03 -.132E-02 0.341E-01 -

.219E-01 0.290E-06 0.134E-07 -.179E-07

-.350E+00 0.139E+03 0.289E+03 0.349E+00 -.139E+03 -.289E+03 0.117E-04 0.112E+00 -.146E-01 0.294E-06 0.417E-06 -.701E-06

-.838E+00 0.400E+02 -.287E+03 0.830E+00 -.400E+02 0.287E+03 0.129E-01 -.735E-02 -.183E-01 0.327E-06 0.764E-06 0.283E-06

-.785E+01 -.119E+03 -.267E+03 0.805E+01 0.119E+03 0.267E+03 -.194E+00 0.726E-02 0.339E-01 0.438E-06 0.845E-06 0.109E-05

-.410E+00 0.206E+03 0.279E+03 0.411E+00 -.206E+03 -.279E+03 -.279E-02 0.716E-01 -.464E-01 -.538E-07 0.768E-06 -.115E-05

-.627E-01 0.300E+02 0.294E+03 0.725E-01 -.299E+02 -.294E+03 -.948E-02 -.347E-01 0.125E-02 -.143E-06 0.186E-06 -.635E-07

-.206E+01 0.145E+03 -.282E+03 0.208E+01 -.145E+03 0.282E+03 -.189E-01 0.132E+00 0.257E-01 0.619E-07 0.761E-06 0.209E-06

-.256E+01 -.209E+02 -.285E+03 0.258E+01 0.208E+02 0.285E+03 -.291E-01 0.409E-01 0.317E-01 -.791E-06 0.621E-06 0.133E-06

-.554E+00 -.290E+02 0.291E+03 0.559E+00 0.290E+02 -.291E+03 -.284E-02 0.293E-01 -.250E-01 0.113E-06 -.105E-06 0.212E-06

0.591E-01 0.139E+03 0.289E+03 -.593E-01 -.139E+03 -.289E+03 -.327E-03 0.109E+00 -.208E-01 -.297E-06 0.544E-06 -.612E-06

-.289E+01 0.377E+02 -.286E+03 0.291E+01 -.377E+02 0.286E+03 -.150E-01 -.307E-02 0.211E-01 -.117E-06 0.659E-06 0.160E-06

-.512E+01 -.128E+03 -.271E+03 0.517E+01 0.128E+03 0.271E+03 -.463E-01 -.862E-01

0.382E-01 -.814E-06 0.962E-06 0.641E-06

0.405E+00 -.137E+03 0.280E+03 -.397E+00 0.137E+03 -.280E+03 -.968E-02 -.127E+00 -.156E-01 0.240E-07 0.988E-07 0.151E-06

0.195E+01 -.343E+03 0.233E+03 -.195E+01 0.344E+03 -.233E+03 0.916E-02 -.460E+00 -.545E-01 -.282E-06 -.726E-07 -.368E-06

-.251E+01 -.197E+03 -.259E+03 0.252E+01 0.197E+03 0.259E+03 -.962E-02 -.197E+00 0.371E-01 -.152E-05 0.697E-06 0.439E-06

0.695E+01 -.447E+03 -.198E+03 -.696E+01 0.448E+03 0.198E+03 0.974E-02 -.112E+01 0.879E-01 -.146E-05 0.561E-07 0.252E-06

-.453E+00 -.451E+03 0.204E+03 0.454E+00 0.452E+03 -.204E+03 -.202E-02 -.108E+01 -.112E+00 -.333E-06 0.729E-06 0.349E-06

0.172E+01 -.203E+03 0.269E+03 -.171E+01 0.203E+03 -.269E+03 -.479E-02 -.926E-01 -.319E-01 -.316E-07 0.545E-07 -.334E-06

-.207E+01 -.338E+03 -.222E+03 0.212E+01 0.338E+03 0.222E+03 -.444E-01 -.604E+00 0.536E-01 -.148E-05 0.479E-06 0.101E-05

0.219E+01 -.136E+03 0.282E+03 -.219E+01 0.136E+03 -.282E+03 -.636E-02 -.126E+00 -.938E-02 -.161E-06 0.377E-06 -.840E-06

0.673E+01 -.339E+03 0.238E+03 -.671E+01 0.340E+03 -.238E+03 -.127E-01 -.461E+00 -.459E-01 -.101E-06 -.546E-06 -.141E-05

0.680E+01 -.193E+03 -.258E+03 -.682E+01 0.193E+03 0.258E+03 0.109E-01 -.145E+00 0.633E-01 -.603E-06 0.392E-06 -.350E-06

0.313E+02 -.427E+03 -.198E+03 -.314E+02 0.428E+03 0.197E+03 0.726E-01 -.969E+00

0.135E+00 0.151E-05 0.150E-05 -.387E-06

0.546E+01 -.449E+03 0.209E+03 -.546E+01 0.450E+03 -.209E+03 0.634E-03 -.108E+01 -.798E-01 -.447E-06 -.601E-06 -.105E-05

0.369E+01 -.201E+03 0.272E+03 -.369E+01 0.201E+03 -.272E+03 -.733E-03 -.975E-01 -.305E-01 -.152E-06 0.157E-06 -.135E-05

0.124E+02 -.332E+03 -.223E+03 -.125E+02 0.332E+03 0.223E+03 0.120E+00 -.534E+00 0.314E-01 -.457E-06 0.566E-06 -.477E-06

0.219E+01 -.133E+03 0.283E+03 -.220E+01 0.133E+03 -.283E+03 0.543E-03 -.128E+00 -.441E-02 -.146E-06 0.574E-06 -.118E-05

0.493E+01 -.332E+03 0.245E+03 -.490E+01 0.332E+03 -.245E+03 -.319E-01 -.476E+00 -.375E-01 0.186E-06 0.695E-07 -.539E-06

0.112E+02 -.182E+03 -.258E+03 -.113E+02 0.182E+03 0.258E+03 0.462E-01 -.979E-01 -.104E+00 0.109E-05 0.976E-06 -.215E-06

0.319E+02 -.399E+03 -.175E+03 -.322E+02 0.400E+03 0.174E+03 0.294E+00 -.141E+01 0.133E+01 -.664E-06 0.258E-05 0.662E-06

0.931E+01 -.443E+03 0.219E+03 -.931E+01 0.444E+03 -.219E+03 -.558E-02 -.109E+01 -.484E-01 0.400E-06 -.465E-06 -.890E-06

0.169E+01 -.196E+03 0.273E+03 -.170E+01 0.197E+03 -.273E+03 0.551E-02 -.109E+00 -.511E-01 -.753E-07 0.319E-06 -.963E-06

0.173E+02 -.310E+03 -.216E+03 -.176E+02 0.310E+03 0.216E+03 0.324E+00 -.217E+00 0.124E+00 0.212E-05 0.242E-05 -.642E-07

-.104E+01 -.132E+03 0.281E+03 0.103E+01 0.132E+03 -.281E+03 0.103E-01 -.127E+00

0.129E-03 -.339E-07 0.379E-06 -.553E-06

-.514E+01 -.332E+03 0.239E+03 0.513E+01 0.332E+03 -.239E+03 0.878E-02 -.494E+00 -.418E-01 -.243E-06 0.513E-06 0.442E-06

0.153E+01 -.169E+03 -.261E+03 -.166E+01 0.169E+03 0.261E+03 0.114E+00 0.361E+00 -.929E-01 0.213E-07 -.953E-07 0.268E-06

-.789E+01 -.301E+03 -.189E+03 0.750E+01 0.296E+03 0.185E+03 0.274E+00 0.502E+01 0.403E+01 -.485E-05 -.345E-05 -.907E-06

-.627E+00 -.436E+03 0.227E+03 0.624E+00 0.437E+03 -.227E+03 0.162E-02 -.120E+01 -.477E-01 0.185E-06 0.535E-06 0.720E-06

-.303E+01 -.197E+03 0.268E+03 0.302E+01 0.197E+03 -.268E+03 0.146E-01 -.111E+00 -.429E-01 -.144E-06 0.209E-06 -.616E-07

0.335E+01 -.280E+03 -.215E+03 -.523E+01 0.280E+03 0.214E+03 0.188E+01 0.610E+00 0.819E+00 -.242E-05 0.157E-05 0.126E-05

-.275E+01 -.134E+03 0.277E+03 0.275E+01 0.134E+03 -.277E+03 0.244E-02 -.123E+00 -.185E-01 0.565E-07 -.954E-07 0.241E-06

-.603E+01 -.338E+03 0.230E+03 0.602E+01 0.339E+03 -.230E+03 0.112E-01 -.494E+00 -.460E-01 0.137E-06 0.609E-06 0.658E-06

-.655E+01 -.171E+03 -.257E+03 0.662E+01 0.170E+03 0.257E+03 -.817E-01 0.495E+00 0.177E-01 0.218E-05 0.624E-06 0.110E-05

-.440E+02 -.422E+03 -.184E+03 0.446E+02 0.424E+03 0.183E+03 -.564E+00 -.111E+01 0.607E+00 0.211E-05 -.495E-05 -.393E-06

-.870E+01 -.441E+03 0.211E+03 0.869E+01 0.442E+03 -.211E+03 0.143E-01 -.111E+01 -

.751E-01 -.135E-06 0.123E-05 0.773E-06

-.294E+01 -.201E+03 0.265E+03 0.295E+01 0.201E+03 -.265E+03 -.917E-02 -.110E+00 -.203E-01 0.141E-06 -.173E-06 0.672E-06

-.145E+02 -.290E+03 -.209E+03 0.165E+02 0.289E+03 0.209E+03 -.201E+01 0.633E+00 0.776E+00 0.454E-05 -.488E-05 -.106E-05

-.139E+01 -.136E+03 0.277E+03 0.140E+01 0.136E+03 -.277E+03 -.102E-01 -.125E+00 -.239E-01 0.259E-06 -.195E-06 0.681E-06

-.278E+01 -.343E+03 0.230E+03 0.276E+01 0.343E+03 -.230E+03 0.235E-01 -.473E+00 -.591E-01 0.271E-06 0.557E-06 0.667E-06

-.104E+02 -.189E+03 -.258E+03 0.104E+02 0.189E+03 0.258E+03 -.774E-01 -.141E+00 -.518E-01 -.307E-06 0.389E-06 0.136E-05

-.149E+02 -.446E+03 -.196E+03 0.150E+02 0.447E+03 0.196E+03 -.684E-01 -.113E+01 0.986E-01 -.418E-06 0.558E-06 0.193E-05

-.550E+01 -.448E+03 0.204E+03 0.550E+01 0.449E+03 -.203E+03 -.486E-02 -.109E+01 -.125E+00 0.308E-06 0.145E-05 0.635E-06

-.909E+00 -.203E+03 0.267E+03 0.918E+00 0.203E+03 -.267E+03 -.909E-02 -.102E+00 -.316E-01 0.277E-06 -.719E-07 0.579E-06

-.162E+02 -.329E+03 -.218E+03 0.166E+02 0.329E+03 0.218E+03 -.359E+00 -.482E+00 0.412E-01 0.610E-06 -.446E-06 0.199E-05

0.433E+00 -.257E+03 -.195E+03 -.126E+01 0.249E+03 0.190E+03 0.103E+01 0.781E+01 0.488E+01 -.745E-05 0.115E-06 0.124E-05

0.533E+02 -.518E+03 -.136E+03 -.543E+02 0.522E+03 0.140E+03 0.105E+01 -.396E+01 -

.382E+01 -.464E-06 0.190E-05 0.116E-05

-.489E+02 -.585E+03 -.446E+03 0.555E+02 0.636E+03 0.480E+03 -.675E+01 -.508E+02 -.342E+02 -.732E-05 0.653E-05 0.534E-05

0.547E+01 0.276E+02 0.223E+02 -.334E-12 -.182E-11 0.148E-11 -.551E+01 -.276E+02 -.223E+02 -.140E-04 0.288E-04 0.265E-04

POSITION			TOTAL-FORCE (eV/Angst)		
1.24575	4.02870	5.43979	0.000044	0.001036	-0.000408
1.21024	4.07581	8.43726	-0.000984	0.002629	-0.001135
3.70862	4.02890	5.43965	0.000311	0.001908	-0.001092
3.67998	4.07733	8.43690	-0.004033	-0.000402	-0.002880
6.17157	4.02854	5.43942	-0.000003	-0.000120	-0.001750
6.14482	4.08292	8.43295	-0.002830	-0.003285	-0.003177
8.63513	4.02801	5.43869	0.000783	-0.000425	-0.002001
8.60339	4.08732	8.43089	-0.000128	-0.001166	-0.002198
11.09928	4.02784	5.43885	0.000877	0.001993	-0.002705
11.06021	4.08619	8.43099	-0.001741	0.000724	-0.000620
13.56311	4.02807	5.43972	0.000334	0.001640	-0.001616
13.52141	4.08047	8.43349	0.000405	-0.002241	0.000316

2.44241	15.48073	8.85224	-0.000642	-0.005269	0.002334
0.01714	15.44624	5.32469	0.000343	0.001539	-0.001190
4.86040	15.47728	8.86623	0.001055	0.000295	-0.000080
2.48016	15.44854	5.27562	0.000361	-0.001194	-0.000511
4.94382	15.44925	5.24869	0.001772	-0.002992	0.000320
12.31531	15.48242	9.00211	-0.005339	-0.000994	0.009336
9.86772	15.44556	5.34176	0.000452	-0.001078	0.000884
14.76279	15.48245	8.89951	-0.006261	-0.000543	0.005514
12.33384	15.44510	5.36128	0.001368	-0.003218	-0.001265
7.40743	15.44616	5.26463	0.002356	0.001621	0.001325
6.44846	16.34427	7.40648	-0.004521	-0.001594	0.000726
8.60064	16.47644	7.89249	0.004020	0.002759	0.004062
1.24544	5.11881	5.35500	0.000937	0.000160	-0.002437
2.44348	5.83889	8.62292	0.002464	-0.004417	0.001229
0.01380	5.79530	5.28573	0.002086	-0.002445	0.000475
1.21063	5.16420	8.54151	0.000250	-0.000501	-0.001906
2.44351	7.27931	8.74832	-0.000119	-0.001247	-0.000122
3.70866	5.11896	5.35390	-0.000436	-0.001624	0.000344
4.90800	5.84315	8.62123	-0.001106	0.003818	-0.000758
2.47701	5.79561	5.28397	0.001466	-0.000590	-0.002603
3.67679	5.16572	8.54000	-0.000139	0.001636	-0.000041
4.90764	7.28398	8.74777	0.000709	-0.000681	0.001018

6.17184	5.11860	5.35433	0.001476	0.000399	0.000900
7.37096	5.84929	8.62094	-0.000704	0.007166	-0.002432
4.94029	5.79548	5.28340	0.000619	-0.002675	-0.001169
6.14080	5.17108	8.53715	-0.002473	0.002531	0.002466
7.37071	7.28983	8.75132	-0.002082	0.001615	0.000151
8.63543	5.11820	5.35521	0.001242	0.001347	-0.001048
9.83233	5.85166	8.62337	0.002922	0.000697	-0.001082
7.40374	5.79498	5.28512	0.003460	-0.002681	-0.001333
8.60194	5.17528	8.53759	-0.001883	-0.000370	-0.000227
9.83204	7.29110	8.75719	-0.001547	-0.002639	-0.002429
11.09930	5.11814	5.35578	-0.000871	-0.003343	-0.001353
12.29449	5.84673	8.62385	-0.000044	0.005768	-0.002205
9.86750	5.79468	5.28678	-0.000740	-0.000706	0.001557
11.06261	5.17409	8.53894	0.002662	0.002566	-0.000400
12.29428	7.28729	8.75533	-0.004592	0.001113	-0.001530
13.56278	5.11829	5.35605	0.002660	0.000529	-0.001966
14.75895	5.83988	8.62434	-0.000261	-0.002596	-0.002171
12.33118	5.79480	5.28692	-0.004502	-0.001444	0.002599
13.52535	5.16844	8.54022	-0.003485	0.003789	-0.001439
14.75917	7.28012	8.75179	0.000951	0.002614	-0.000683
0.01434	7.23830	5.19017	0.000076	-0.000200	0.000083
1.24689	9.38061	5.13160	0.000539	-0.001858	0.000009

1.21085	7.98059	8.79588	-0.000936	-0.000516	0.001518
2.44214	10.12243	8.87141	-0.000960	0.003357	-0.005001
0.01532	10.08686	5.14049	-0.002031	-0.000134	-0.002391
1.24606	7.94244	5.15775	0.002020	-0.002586	0.000834
1.21082	9.41592	8.85782	-0.000725	0.004344	0.000175
2.44072	11.55513	8.88414	-0.005688	-0.002854	0.001639
2.47747	7.23842	5.18585	0.002801	0.002884	0.001319
3.70997	9.38055	5.12566	-0.001096	-0.003002	0.000052
3.67534	7.98360	8.79349	-0.000596	0.001136	0.000981
4.90487	10.12925	8.87518	0.000252	-0.000219	-0.000045
2.47867	10.08713	5.12695	-0.002248	0.001504	0.000770
3.70939	7.94242	5.15441	0.000830	-0.004006	-0.001692
3.67589	9.41970	8.85445	-0.001452	0.001919	-0.000145
4.90263	11.56506	8.89086	0.000221	0.001614	0.000787
4.94085	7.23830	5.18552	-0.004712	0.002253	0.000840
6.17318	9.38002	5.13173	0.002011	0.002106	0.001839
6.13864	7.99044	8.79647	0.002426	-0.000222	-0.001703
7.36780	10.13760	8.89473	-0.001881	0.003523	0.000859
4.94196	10.08682	5.12700	0.004158	0.001485	-0.001149
6.17284	7.94199	5.15766	-0.000041	0.000563	0.003037
6.13939	9.42660	8.86164	0.000892	-0.000765	-0.002149
7.36410	11.57721	8.92935	0.000056	-0.004432	0.003831

7.40426	7.23794	5.19012	0.002122	0.001767	0.001085
8.63700	9.37970	5.14543	-0.000557	0.002941	0.000971
8.60086	7.99568	8.80617	0.001052	-0.000349	-0.001067
9.83068	10.14286	8.92842	-0.001530	0.002698	-0.000611
7.40553	10.08627	5.14064	0.001218	-0.003547	0.003156
8.63637	7.94166	5.16555	0.002633	0.001808	-0.001401
8.60077	9.43254	8.88532	-0.006035	0.002228	-0.001315
9.82927	11.58244	9.00096	0.000462	0.002813	0.000962
9.86805	7.23787	5.19489	-0.000360	0.000111	-0.000207
11.10106	9.37979	5.15156	-0.003847	-0.001022	0.000661
11.06331	7.99411	8.80818	-0.000299	-0.001632	0.000111
12.29815	10.12943	8.90340	-0.002140	-0.001250	0.001163
9.86930	10.08593	5.15631	-0.005427	-0.001443	0.001416
11.10021	7.94175	5.16862	-0.000589	-0.003071	0.001396
11.06206	9.43062	8.88839	0.004667	0.001742	0.002129
12.30255	11.56557	8.94694	0.004574	0.001262	-0.000940
12.33169	7.23799	5.19447	-0.001046	0.000250	-0.001742
13.56437	9.38021	5.14435	0.000738	0.001647	-0.000567
13.52754	7.98555	8.80171	-0.000842	-0.002613	-0.003062
14.76233	10.12320	8.88285	-0.005224	0.001010	-0.001513
12.33257	10.08637	5.15511	0.002644	0.000558	-0.001532
13.56350	7.94214	5.16485	-0.000072	-0.000884	-0.000365

13.52731	9.42040	8.86925	-0.000046	0.003477	-0.000607
14.76430	11.55727	8.90646	-0.001960	-0.001082	0.002078
0.01611	11.52516	5.16621	-0.001082	-0.002568	0.000398
1.24770	13.67535	5.22209	0.001812	-0.002380	-0.002478
1.21217	12.26335	8.89409	0.000040	-0.000199	0.001138
2.43998	14.38728	8.86748	-0.002118	0.001034	0.000851
0.01699	14.35408	5.27295	-0.000416	-0.000571	-0.001966
1.24794	12.22963	5.17275	0.001074	0.000851	-0.001353
1.21434	13.70818	8.88771	0.001773	0.001992	0.003888
2.47958	11.52580	5.14547	-0.001607	-0.000192	-0.001469
3.71218	13.67636	5.19535	0.004665	0.000553	0.001053
3.66932	12.26248	8.88184	-0.002757	0.000127	-0.000551
4.89370	14.38589	8.86075	0.004573	-0.000877	-0.003031
2.48000	14.35596	5.23149	0.001287	-0.001095	0.001686
3.71150	12.23022	5.15602	0.000927	-0.004559	0.001018
3.66212	13.70366	8.87117	-0.006118	0.003968	-0.000790
4.94290	11.52542	5.14351	-0.000095	-0.001760	-0.001594
6.17627	13.67505	5.20032	0.000822	0.000549	0.000079
6.13145	12.27911	8.90591	0.005329	0.005761	0.004731
7.36614	14.42967	8.88203	-0.000894	-0.003535	-0.001633
4.94347	14.35627	5.21375	0.000074	-0.001924	0.001016
6.17493	12.22917	5.16623	-0.001403	-0.001028	0.001542

6.11879	13.72336	8.87765	0.005549	0.003078	0.001986
7.40625	11.52413	5.16368	0.000885	-0.003358	0.000365
8.63876	13.67323	5.24377	0.001869	0.002000	-0.001252
8.58939	12.29067	9.00208	-0.008958	0.000297	-0.002288
9.83855	14.39048	9.30305	-0.113514	-0.030467	-0.012385
7.40672	14.35386	5.23530	-0.001179	-0.000315	-0.000653
8.63820	12.22778	5.19800	0.000325	-0.001203	0.001023
8.55571	13.73596	9.04598	0.006366	-0.043743	-0.012066
9.86985	11.52338	5.18893	0.001745	-0.001977	-0.000108
11.10099	13.67352	5.27669	0.003198	-0.000883	-0.001034
11.07378	12.27333	9.00891	-0.012550	0.005295	-0.002331
12.30694	14.38896	9.00333	-0.006341	0.003702	0.003586
9.86934	14.35300	5.29564	0.002992	0.000068	0.000039
11.10161	12.22804	5.21650	-0.001106	-0.002704	0.001085
11.11464	13.70636	9.07877	0.011165	0.037591	0.015457
12.33326	11.52411	5.18815	-0.000934	0.000269	0.000540
13.56430	13.67399	5.25995	0.001543	-0.000090	0.000077
13.53626	12.26601	8.93587	-0.002461	0.004529	0.002207
14.76266	14.38906	8.90426	-0.003692	0.001927	0.003778
12.33397	14.35288	5.30710	0.002775	-0.001782	-0.001759
13.56505	12.22870	5.20105	0.000130	0.000102	-0.001123
13.54921	13.70690	8.94399	-0.001553	-0.006004	-0.002796

9.89626	15.53185	9.99472	0.218535	0.135959	0.091603
7.28864	16.40884	8.69813	-0.001930	-0.001374	-0.004380
10.02526	16.50365	10.64498	-0.079717	-0.107794	-0.070196

---

total drift:	-0.044843	0.023791	-0.023949

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

---

free energy TOTEN = -1209.38763079 eV

energy without entropy= -1209.38763079 energy(sigma->0) = -1209.38763079

d Force =-0.1011019E-03[-0.656E-02, 0.635E-02] d Energy =-0.6371352E-04-0.374E-04

d Force =-0.7125961E-01[0.377E-01,-0.180E+00] d Ewald =-0.7098629E-01-0.273E-03

POTLOK: cpu time 0.1823: real time 0.1829

---

stress matrix after NEB project (eV)

-17.74921 -0.15356 0.10575

-0.15356 -15.35083 0.40647

0.10575 0.40647 -19.08177

FORCES: max atom, RMS 0.273191 0.025759

FORCE total and by dimension 0.312307 0.218535

Stress total and by dimension 30.252210 19.081768

Finite differences progress:

Degree of freedom: 1/ 6

Displacement: 2/ 2

Total: 2/ 12

LATTYP: Found a simple orthorhombic cell.

ALAT = 14.7806000000

B/A-ratio = 1.2466138046

C/A-ratio = 1.4433717170

Lattice vectors:

A1 = (-14.7806000000, 0.0000000000, 0.0000000000)

A2 = (0.0000000000, 0.0000000000, -18.4257000000)

A3 = (0.0000000000, -21.3339000000, 0.0000000000)

Analysis of symmetry for initial positions (statically):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The static configuration has the point symmetry C_1 .

Analysis of symmetry for dynamics (positions and initial velocities):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The dynamic configuration has the point symmetry C_1 .

Analysis of constrained symmetry for selective dynamics:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The constrained configuration has the point symmetry C_1 .

Analysis of structural, dynamic, and magnetic symmetry:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a
simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations
(whereof 1 operations were pure point group operations)
out of a pool of 8 trial point group operations.

The magnetic configuration has the point symmetry C_1 .

Subroutine INISYM returns: Found 1 space group operations
(whereof 1 operations are pure point group operations),
and found 1 'primitive' translations

KPOINTS: KPT-Resolved Value to Generate K-Mesh: 0

Automatic generation of k-mesh.

Space group operators:

irot	det(A)	alpha	n_x	n_y	n_z	tau_x	tau_y	tau_z
1	1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Subroutine IBZKPT returns following result:

==========

Found 1 irreducible k-points:

Following reciprocal coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

Following cartesian coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

WAVPRE: cpu time 0.1202: real time 0.1449

FEWALD: cpu time 0.0026: real time 0.0027

ORTHCH: cpu time 1.0121: real time 1.0155

LOOP+: cpu time 167.1332: real time 168.0651

---------- Iteration 4(1) ----------

POTLOK: cpu time 0.1700: real time 0.1814

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9294: real time 1.9350

RMM-DIIS: cpu time 7.2835: real time 7.3196

ORTHCH: cpu time 0.3517: real time 0.3528

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5054: real time 0.5280

MIXING: cpu time 0.0041: real time 0.0041

LOOP: cpu time 10.2545: real time 10.3313

eigenvalue-minimisations : 1952

total energy-change (2. order) : 0.7938770E-02 (-0.9857791E-01)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7409647 magnetization 0.0543255

Broyden mixing:

rms(total) = 0.35379E-01 rms(broyden)= 0.35220E-01

rms(prec) = 0.37109E-01

weight for this iteration 100.00

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107331.40412186

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80660088

PAW double counting = 52175.16913140 -52238.08667671

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.62505209

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76200165 eV

energy without entropy = -1202.76200165 energy(sigma->0) = -1202.76200165

---------- Iteration 4(2) ----------

POTLOK: cpu time 0.1671: real time 0.1873

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9183: real time 1.9247

RMM-DIIS: cpu time 7.1104: real time 7.1457

ORTHCH: cpu time 0.3523: real time 0.3536

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5250: real time 0.5268

MIXING: cpu time 0.0046: real time 0.0046

LOOP: cpu time 10.0883: real time 10.1533

eigenvalue-minimisations : 1920

total energy-change (2. order) : 0.1013455E-02 (-0.9421488E-03)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7402902 magnetization 0.0543220

Broyden mixing:

rms(total) = 0.21257E-01 rms(broyden)= 0.21235E-01

rms(prec) = 0.22081E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5527

1.5527

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107332.03161384

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81370709

PAW double counting = 52178.83975866 -52241.76108857

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.99986827

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76098819 eV

energy without entropy = -1202.76098819 energy(sigma->0) = -1202.76098819

---------- Iteration 4(3) ----------

POTLOK: cpu time 0.1710: real time 0.1827

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9221: real time 1.9283

RMM-DIIS: cpu time 7.3015: real time 7.3400

ORTHCH: cpu time 0.3523: real time 0.3532

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5244: real time 0.5258

MIXING: cpu time 0.0051: real time 0.0051

LOOP: cpu time 10.2870: real time 10.3457

eigenvalue-minimisations : 1956

total energy-change (2. order) : 0.5675717E-03 (-0.1043139E-03)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7410103 magnetization 0.0543085

Broyden mixing:

rms(total) = 0.93161E-02 rms(broyden)= 0.93138E-02

rms(prec) = 0.96874E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5807

0.8304 2.3310

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107332.57738147

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81435307

PAW double counting = 52182.06060545 -52244.98454088

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.45157353

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76042062 eV

energy without entropy = -1202.76042062 energy(sigma->0) = -1202.76042062

---------- Iteration 4(4) ----------

POTLOK: cpu time 0.1670: real time 0.1864

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9318: real time 1.9382

RMM-DIIS: cpu time 7.1617: real time 7.1846

ORTHCH: cpu time 0.3517: real time 0.3527

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5261: real time 0.5278

MIXING: cpu time 0.0054: real time 0.0054

LOOP: cpu time 10.1542: real time 10.2055

eigenvalue-minimisations : 1927

total energy-change (2. order) : 0.9431443E-04 (-0.2702808E-04)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7407435 magnetization 0.0543011

Broyden mixing:

rms(total) = 0.25886E-02 rms(broyden)= 0.25873E-02

rms(prec) = 0.28853E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4753

2.2677 0.8673 1.2908

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107332.98036334

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81897260

PAW double counting = 52183.86235388 -52246.78904882

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.05035736

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76032631 eV

energy without entropy = -1202.76032631 energy(sigma->0) = -1202.76032631

---------- Iteration 4(5) ----------

POTLOK: cpu time 0.1689: real time 0.1870

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9189: real time 1.9255

RMM-DIIS: cpu time 7.3064: real time 7.3387

ORTHCH: cpu time 0.3510: real time 0.3523

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5238: real time 0.5256

MIXING: cpu time 0.0055: real time 0.0055

LOOP: cpu time 10.2850: real time 10.3450

eigenvalue-minimisations : 1942

total energy-change (2. order) : 0.7268485E-05 (-0.2508181E-05)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7407829 magnetization 0.0543027

Broyden mixing:

rms(total) = 0.12630E-02 rms(broyden)= 0.12620E-02

rms(prec) = 0.14793E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4321

2.2773 1.8391 0.8061 0.8061

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.09020002

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81884363

PAW double counting = 52183.75838935 -52246.68503252

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.94043621

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76031904 eV

energy without entropy = -1202.76031904 energy(sigma->0) = -1202.76031904

---------- Iteration 4(6) ----------

POTLOK: cpu time 0.1674: real time 0.1698

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9266: real time 1.9333

RMM-DIIS: cpu time 7.0498: real time 7.0822

ORTHCH: cpu time 0.3520: real time 0.3533

DOS: cpu time 0.0004: real time 0.0003

CHARGE: cpu time 0.5237: real time 0.5255

MIXING: cpu time 0.0059: real time 0.0059

LOOP: cpu time 10.0358: real time 10.0803

eigenvalue-minimisations : 1901

total energy-change (2. order) :-0.1025132E-04 (-0.6387607E-06)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7407626 magnetization 0.0543031

Broyden mixing:

rms(total) = 0.65067E-03 rms(broyden)= 0.65036E-03

rms(prec) = 0.86656E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3857

2.4271 1.9196 0.9171 0.9171 0.7476

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.19602290

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81938030

PAW double counting = 52183.59078586 -52246.51762029

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.83496900

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76032929 eV

energy without entropy = -1202.76032929 energy(sigma->0) = -1202.76032929

---------- Iteration 4(7) ----------

POTLOK: cpu time 0.1679: real time 0.1824

SETDIJ: cpu time 0.0102: real time 0.0103

EDDIAG: cpu time 1.9214: real time 1.9273

RMM-DIIS: cpu time 6.6770: real time 6.7118

ORTHCH: cpu time 0.3515: real time 0.3524

DOS: cpu time 0.0003: real time 0.0003

CHARGE: cpu time 0.5243: real time 0.5260

MIXING: cpu time 0.0060: real time 0.0060

LOOP: cpu time 9.6586: real time 9.7165

eigenvalue-minimisations : 1812

total energy-change (2. order) :-0.1620913E-04 (-0.2229325E-06)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7407733 magnetization 0.0543017

Broyden mixing:

rms(total) = 0.33385E-03 rms(broyden)= 0.33367E-03

rms(prec) = 0.53408E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4502

2.7493 2.0898 1.4984 0.8740 0.8740 0.6160

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.29010950

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81981190

PAW double counting = 52183.43130258 -52246.35826771

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.74119950

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76034550 eV

energy without entropy = -1202.76034550 energy(sigma->0) = -1202.76034550

---------- Iteration 4(8) ----------

POTLOK: cpu time 0.1666: real time 0.1854

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9209: real time 1.9270

RMM-DIIS: cpu time 6.3493: real time 6.3698

ORTHCH: cpu time 0.3509: real time 0.3521

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5246: real time 0.5262

MIXING: cpu time 0.0065: real time 0.0065

LOOP: cpu time 9.3292: real time 9.3776

eigenvalue-minimisations : 1731

total energy-change (2. order) :-0.1900066E-04 (-0.1236404E-06)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7407910 magnetization 0.0543010

Broyden mixing:

rms(total) = 0.22768E-03 rms(broyden)= 0.22757E-03

rms(prec) = 0.37579E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4018

2.7812 2.3235 1.3717 0.9766 0.9766 0.7711 0.6120

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.37605285

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.82015537

PAW double counting = 52183.27871392 -52246.20574592

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.65555176

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76036450 eV

energy without entropy = -1202.76036450 energy(sigma->0) = -1202.76036450

---------- Iteration 4(9) ----------

POTLOK: cpu time 0.1652: real time 0.1656

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9214: real time 1.9274

RMM-DIIS: cpu time 5.9933: real time 6.0134

ORTHCH: cpu time 0.3515: real time 0.3525

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5239: real time 0.5254

MIXING: cpu time 0.0067: real time 0.0067

LOOP: cpu time 8.9725: real time 9.0017

eigenvalue-minimisations : 1610

total energy-change (2. order) :-0.1888505E-04 (-0.5562337E-07)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7407912 magnetization 0.0543010

Broyden mixing:

rms(total) = 0.12933E-03 rms(broyden)= 0.12921E-03

rms(prec) = 0.24920E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5125

3.1863 2.5965 1.6383 1.4857 0.8875 0.8875 0.8076 0.6111

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.43575016

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.82042689

PAW double counting = 52183.20542577 -52246.13248970

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.59611292

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76038339 eV

energy without entropy = -1202.76038339 energy(sigma->0) = -1202.76038339

---------- Iteration 4(10) ----------

POTLOK: cpu time 0.1653: real time 0.1726

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9177: real time 1.9240

RMM-DIIS: cpu time 6.1666: real time 6.1877

ORTHCH: cpu time 0.3516: real time 0.3527

DOS: cpu time 0.0004: real time 0.0003

CHARGE: cpu time 0.5263: real time 0.5281

MIXING: cpu time 0.0069: real time 0.0069

LOOP: cpu time 9.1449: real time 9.1824

eigenvalue-minimisations : 1688

total energy-change (2. order) :-0.2908654E-04 (-0.1255691E-06)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7407924 magnetization 0.0543007

Broyden mixing:

rms(total) = 0.11439E-03 rms(broyden)= 0.11427E-03

rms(prec) = 0.15685E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5673

4.0552 2.5966 2.0872 1.1511 1.0406 1.0406 0.8158 0.7035 0.6155

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.53177087

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.82087566

PAW double counting = 52183.13824468 -52246.06537445

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.50050423

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76041247 eV

energy without entropy = -1202.76041247 energy(sigma->0) = -1202.76041247

---------- Iteration 4(11) ----------

POTLOK: cpu time 0.1667: real time 0.1846

SETDIJ: cpu time 0.0102: real time 0.0103

EDDIAG: cpu time 1.9178: real time 1.9242

RMM-DIIS: cpu time 5.5531: real time 5.5692

ORTHCH: cpu time 0.3539: real time 0.3547

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5238: real time 0.5255

MIXING: cpu time 0.0074: real time 0.0074

LOOP: cpu time 8.5334: real time 8.5763

eigenvalue-minimisations : 1510

total energy-change (2. order) :-0.9993615E-05 (-0.2593714E-07)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7407959 magnetization 0.0543005

Broyden mixing:

rms(total) = 0.57094E-04 rms(broyden)= 0.57047E-04

rms(prec) = 0.91153E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6435

4.7448 2.5693 2.1703 1.4449 1.4449 0.9748 0.9748 0.8168 0.6768 0.6180

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.55947933

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.82097219

PAW double counting = 52183.13945335 -52246.06659376

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.47289165

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76042247 eV

energy without entropy = -1202.76042247 energy(sigma->0) = -1202.76042247

---------- Iteration 4(12) ----------

POTLOK: cpu time 0.1686: real time 0.1834

SETDIJ: cpu time 0.0099: real time 0.0100

EDDIAG: cpu time 1.9246: real time 1.9311

RMM-DIIS: cpu time 5.5294: real time 5.5606

ORTHCH: cpu time 0.3515: real time 0.3526

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5240: real time 0.5256

MIXING: cpu time 0.0078: real time 0.0078

LOOP: cpu time 8.5161: real time 8.5715

eigenvalue-minimisations : 1507

total energy-change (2. order) :-0.1259484E-04 (-0.2244830E-07)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7408009 magnetization 0.0543004

Broyden mixing:

rms(total) = 0.44971E-04 rms(broyden)= 0.44927E-04

rms(prec) = 0.62623E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7769

6.1781 2.7325 2.4748 2.0067 1.0608 1.0608 1.0902 0.8309 0.8309 0.6604

0.6201

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.58047267

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.82098575

PAW double counting = 52183.16358045 -52246.09071019

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.45193514

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76043506 eV

energy without entropy = -1202.76043506 energy(sigma->0) = -1202.76043506

---------- Iteration 4(13) ----------

POTLOK: cpu time 0.1661: real time 0.1695

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9187: real time 1.9252

RMM-DIIS: cpu time 5.0822: real time 5.1081

ORTHCH: cpu time 0.3512: real time 0.3523

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5245: real time 0.5260

MIXING: cpu time 0.0079: real time 0.0080

LOOP: cpu time 8.0610: real time 8.0996

eigenvalue-minimisations : 1403

total energy-change (2. order) :-0.6715527E-05 (-0.8363735E-08)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7408004 magnetization 0.0543004

Broyden mixing:

rms(total) = 0.20320E-04 rms(broyden)= 0.20308E-04

rms(prec) = 0.33005E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7381

6.4459 2.7925 2.5286 2.0022 1.0969 1.0969 1.0254 0.8985 0.8985 0.7954

0.6549 0.6210

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.59083388

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.82100891

PAW double counting = 52183.17516026 -52246.10229038

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.44160343

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76044178 eV

energy without entropy = -1202.76044178 energy(sigma->0) = -1202.76044178

---------- Iteration 4(14) ----------

POTLOK: cpu time 0.1647: real time 0.1650

SETDIJ: cpu time 0.0217: real time 0.0219

EDDIAG: cpu time 1.9237: real time 1.9301

RMM-DIIS: cpu time 4.8904: real time 4.9282

ORTHCH: cpu time 0.3509: real time 0.3520

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5274: real time 0.5290

MIXING: cpu time 0.0082: real time 0.0082

LOOP: cpu time 7.8874: real time 7.9349

eigenvalue-minimisations : 1365

total energy-change (2. order) :-0.4569294E-05 (-0.3786505E-08)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7407995 magnetization 0.0543004

Broyden mixing:

rms(total) = 0.14748E-04 rms(broyden)= 0.14740E-04

rms(prec) = 0.22264E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8728

7.0355 3.4707 2.7263 2.2019 2.0008 1.1062 1.1062 1.0205 0.8675 0.8675

0.6872 0.6278 0.6278

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.59349426

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.82101435

PAW double counting = 52183.17267333 -52246.09980913

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.43894737

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76044635 eV

energy without entropy = -1202.76044635 energy(sigma->0) = -1202.76044635

---------- Iteration 4(15) ----------

POTLOK: cpu time 0.1664: real time 0.1865

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9183: real time 1.9246

RMM-DIIS: cpu time 4.8483: real time 4.8719

ORTHCH: cpu time 0.3514: real time 0.3526

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5241: real time 0.5258

MIXING: cpu time 0.0088: real time 0.0088

LOOP: cpu time 7.8277: real time 7.8806

eigenvalue-minimisations : 1342

total energy-change (2. order) :-0.3483539E-05 (-0.3187058E-08)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7407995 magnetization 0.0543005

Broyden mixing:

rms(total) = 0.10857E-04 rms(broyden)= 0.10854E-04

rms(prec) = 0.13993E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8989

7.5268 4.1895 2.6410 2.3733 1.9662 1.1085 1.1085 0.9737 0.9737 0.9348

0.8647 0.6757 0.6239 0.6239

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.59528041

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.82100771

PAW double counting = 52183.16830003 -52246.09543851

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.43715540

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76044983 eV

energy without entropy = -1202.76044983 energy(sigma->0) = -1202.76044983

---------- Iteration 4(16) ----------

POTLOK: cpu time 0.1665: real time 0.1796

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9212: real time 1.9277

RMM-DIIS: cpu time 4.4339: real time 4.4611

ORTHCH: cpu time 0.3516: real time 0.3527

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5246: real time 0.5265

MIXING: cpu time 0.0096: real time 0.0097

LOOP: cpu time 7.4179: real time 7.4677

eigenvalue-minimisations : 1123

total energy-change (2. order) :-0.6995033E-06 (-0.7275087E-09)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7407998 magnetization 0.0543005

Broyden mixing:

rms(total) = 0.50698E-05 rms(broyden)= 0.50672E-05

rms(prec) = 0.78509E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9031

7.7426 4.5093 2.5436 2.5436 1.9299 1.3732 1.1874 1.1874 0.9632 0.9632

0.8414 0.8414 0.6742 0.6227 0.6227

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.59537553

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.82099749

PAW double counting = 52183.16710924 -52246.09424547

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.43705299

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76045053 eV

energy without entropy = -1202.76045053 energy(sigma->0) = -1202.76045053

---------- Iteration 4(17) ----------

POTLOK: cpu time 0.1670: real time 0.1688

SETDIJ: cpu time 0.0099: real time 0.0099

EDDIAG: cpu time 1.9175: real time 1.9238

RMM-DIIS: cpu time 4.5022: real time 4.5280

ORTHCH: cpu time 0.3523: real time 0.3534

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5243: real time 0.5259

MIXING: cpu time 0.0099: real time 0.0099

LOOP: cpu time 7.4834: real time 7.5201

eigenvalue-minimisations : 1167

total energy-change (2. order) :-0.4972680E-06 (-0.4231362E-09)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7408001 magnetization 0.0543004

Broyden mixing:

rms(total) = 0.33072E-05 rms(broyden)= 0.33040E-05

rms(prec) = 0.49441E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9678

8.0359 5.0508 2.8370 2.6691 1.9991 1.9991 1.1792 1.1792 1.0671 1.0671

0.8754 0.8754 0.7324 0.6726 0.6224 0.6224

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.59526579

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.82098806

PAW double counting = 52183.16592073 -52246.09305530

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.43715546

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76045103 eV

energy without entropy = -1202.76045103 energy(sigma->0) = -1202.76045103

---------- Iteration 4(18) ----------

POTLOK: cpu time 0.1658: real time 0.1815

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9190: real time 1.9251

RMM-DIIS: cpu time 4.2278: real time 4.2537

ORTHCH: cpu time 0.3526: real time 0.3536

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5241: real time 0.5258

MIXING: cpu time 0.0098: real time 0.0099

LOOP: cpu time 7.2096: real time 7.2599

eigenvalue-minimisations : 1036

total energy-change (2. order) :-0.2024608E-06 (-0.2362848E-09)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7408002 magnetization 0.0543004

Broyden mixing:

rms(total) = 0.23556E-05 rms(broyden)= 0.23551E-05

rms(prec) = 0.31734E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9637

8.2303 5.3749 3.1352 2.5726 2.2659 1.9164 1.2117 1.2117 1.1003 1.1003

0.9399 0.8616 0.8616 0.6915 0.6654 0.6220 0.6220

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.59523949

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.82098439

PAW double counting = 52183.16578470 -52246.09291955

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.43717803

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76045123 eV

energy without entropy = -1202.76045123 energy(sigma->0) = -1202.76045123

---------- Iteration 4(19) ----------

POTLOK: cpu time 0.1669: real time 0.1819

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9190: real time 1.9257

RMM-DIIS: cpu time 4.0459: real time 4.0727

ORTHCH: cpu time 0.3508: real time 0.3538

DOS: cpu time 0.0004: real time 0.0004

LOOP: cpu time 6.4929: real time 6.5444

eigenvalue-minimisations : 914

total energy-change (2. order) :-0.5442416E-07 (-0.6418865E-10)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7408002 magnetization 0.0543004

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91325.54742994

-Hartree energ DENC = -107333.59524903

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.82098395

PAW double counting = 52183.16652543 -52246.09366077

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.43716760

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76045128 eV

energy without entropy = -1202.76045128 energy(sigma->0) = -1202.76045128

---

average (electrostatic) potential at core

the test charge radii are 0.5201 0.6991 1.0621 0.7215

(the norm of the test charge is 1.0000)

1 -40.7490	2 -40.7468	3 -40.7482	4 -40.7468	5 -40.7490
6 -40.7511	7 -40.7488	8 -40.7566	9 -40.7484	10 -40.7561
11 -40.7498	12 -40.7517	13 -40.6433	14 -40.6913	15 -40.7639
16 -40.6933	17 -40.6876	18 -40.8607	19 -40.6751	20 -40.6606
21 -40.6843	22 -40.6579	23 -40.0910	24 -40.1354	25 -57.4547
26 -57.6654	27 -57.6527	28 -57.4643	29 -57.6583	30 -57.4547
31 -57.6653	32 -57.6523	33 -57.4623	34 -57.6633	35 -57.4555
36 -57.6672	37 -57.6523	38 -57.4646	39 -57.6693	40 -57.4546
41 -57.6713	42 -57.6525	43 -57.4696	44 -57.6839	45 -57.4546
46 -57.6702	47 -57.6533	48 -57.4698	49 -57.6749	50 -57.4557
51 -57.6668	52 -57.6530	53 -57.4673	54 -57.6611	55 -57.6323
56 -57.6581	57 -57.6820	58 -57.6773	59 -57.6618	60 -57.6648
61 -57.6843	62 -57.6685	63 -57.6325	64 -57.6576	65 -57.6840
66 -57.6890	67 -57.6601	68 -57.6646	69 -57.6881	70 -57.6950
71 -57.6320	72 -57.6590	73 -57.6918	74 -57.7166	75 -57.6610
76 -57.6653	77 -57.7006	78 -57.7456	79 -57.6323	80 -57.6616
81 -57.7057	82 -57.7471	83 -57.6643	84 -57.6668	85 -57.7324
86 -57.8363	87 -57.6347	88 -57.6623	89 -57.7075	90 -57.7118
91 -57.6689	92 -57.6670	93 -57.7370	94 -57.7537	95 -57.6330
96 -57.6604	97 -57.6911	98 -57.6849	99 -57.6662	100 -57.6658
101 -57.7024	102 -57.6798	103 -57.6554	104 -57.6257	105 -57.6390
106 -57.2813	107 -57.3826	108 -57.6263	109 -57.5899	110 -57.6543

111 -57.6257	112 -57.6357	113 -57.3000	114 -57.3882	115 -57.6256
116 -57.5920	117 -57.6536	118 -57.6177	119 -57.6920	120 -57.6729
121 -57.3821	122 -57.6245	123 -57.7023	124 -57.6547	125 -57.6204
126 -57.8284	127 -58.3345	128 -57.3557	129 -57.6298	130 -58.1358
131 -57.6625	132 -57.6296	133 -57.7954	134 -57.4063	135 -57.3667
136 -57.6337	137 -58.0689	138 -57.6590	139 -57.6252	140 -57.6650
141 -57.2898	142 -57.3729	143 -57.6290	144 -57.6405	145 -60.9166
146 -57.3187	147 -81.4108			

E-fermi : -2.3362 XC(G=0): -2.7343 alpha+bet : -2.2521

spin component 1

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-27.2538	1.00000
2	-21.5626	1.00000
3	-21.4667	1.00000
4	-21.0915	1.00000

5	-21.0633	1.00000
6	-21.0084	1.00000
7	-20.9740	1.00000
8	-20.9719	1.00000
9	-20.8860	1.00000
10	-20.5480	1.00000
11	-20.4979	1.00000
12	-20.4064	1.00000
13	-20.3933	1.00000
14	-20.1165	1.00000
15	-19.9704	1.00000
16	-19.6906	1.00000
17	-19.6219	1.00000
18	-19.5943	1.00000
19	-19.5786	1.00000
20	-19.5240	1.00000
21	-19.5221	1.00000
22	-19.4935	1.00000
23	-19.4763	1.00000
24	-19.1008	1.00000
25	-19.0697	1.00000
26	-18.9725	1.00000

27	-18.9602	1.00000
28	-18.8923	1.00000
29	-18.7283	1.00000
30	-18.4926	1.00000
31	-18.3536	1.00000
32	-18.2702	1.00000
33	-18.2474	1.00000
34	-18.1777	1.00000
35	-18.1755	1.00000
36	-18.0748	1.00000
37	-18.0713	1.00000
38	-17.5472	1.00000
39	-17.3078	1.00000
40	-17.2819	1.00000
41	-17.2775	1.00000
42	-17.2047	1.00000
43	-17.1989	1.00000
44	-17.1680	1.00000
45	-17.0170	1.00000
46	-16.9451	1.00000
47	-16.9276	1.00000
48	-16.8883	1.00000

49	-16.8866	1.00000
50	-16.8454	1.00000
51	-16.8370	1.00000
52	-16.8153	1.00000
53	-16.8137	1.00000
54	-16.7248	1.00000
55	-16.7215	1.00000
56	-16.1601	1.00000
57	-15.7248	1.00000
58	-15.6871	1.00000
59	-15.6552	1.00000
60	-15.6313	1.00000
61	-15.6118	1.00000
62	-15.5490	1.00000
63	-15.5453	1.00000
64	-15.1683	1.00000
65	-14.8045	1.00000
66	-14.6018	1.00000
67	-14.5737	1.00000
68	-14.5304	1.00000
69	-14.4936	1.00000
70	-14.4641	1.00000

71	-14.4366	1.00000
72	-14.3287	1.00000
73	-14.3007	1.00000
74	-14.2750	1.00000
75	-14.2671	1.00000
76	-14.1781	1.00000
77	-14.1742	1.00000
78	-13.8870	1.00000
79	-13.7531	1.00000
80	-13.5880	1.00000
81	-13.5437	1.00000
82	-13.5247	1.00000
83	-13.4924	1.00000
84	-13.4397	1.00000
85	-13.3597	1.00000
86	-13.3409	1.00000
87	-13.1839	1.00000
88	-12.7813	1.00000
89	-12.7542	1.00000
90	-12.7225	1.00000
91	-12.6915	1.00000
92	-12.6814	1.00000

93	-12.6191	1.00000
94	-12.4568	1.00000
95	-12.4421	1.00000
96	-12.3770	1.00000
97	-12.3189	1.00000
98	-12.2086	1.00000
99	-12.1990	1.00000
100	-12.1602	1.00000
101	-11.9562	1.00000
102	-11.6801	1.00000
103	-11.6318	1.00000
104	-11.6066	1.00000
105	-11.5927	1.00000
106	-11.1357	1.00000
107	-11.0906	1.00000
108	-10.8953	1.00000
109	-10.8837	1.00000
110	-10.8292	1.00000
111	-10.7062	1.00000
112	-10.6813	1.00000
113	-10.6602	1.00000
114	-10.6417	1.00000

115	-10.5852	1.00000
116	-10.5768	1.00000
117	-10.5664	1.00000
118	-10.5627	1.00000
119	-10.5218	1.00000
120	-10.5209	1.00000
121	-10.5062	1.00000
122	-10.4984	1.00000
123	-10.3745	1.00000
124	-10.2983	1.00000
125	-10.2563	1.00000
126	-10.1846	1.00000
127	-10.1835	1.00000
128	-10.1662	1.00000
129	-10.0846	1.00000
130	-9.8911	1.00000
131	-9.8658	1.00000
132	-9.7985	1.00000
133	-9.7819	1.00000
134	-9.7693	1.00000
135	-9.6998	1.00000
136	-9.4534	1.00000

137	-9.4229	1.00000
138	-9.3912	1.00000
139	-9.3842	1.00000
140	-9.3780	1.00000
141	-9.3653	1.00000
142	-9.3104	1.00000
143	-9.3040	1.00000
144	-9.2973	1.00000
145	-9.2847	1.00000
146	-9.2679	1.00000
147	-9.0886	1.00000
148	-9.0048	1.00000
149	-8.9965	1.00000
150	-8.9567	1.00000
151	-8.9526	1.00000
152	-8.7891	1.00000
153	-8.7413	1.00000
154	-8.7296	1.00000
155	-8.7134	1.00000
156	-8.7048	1.00000
157	-8.6824	1.00000
158	-8.6752	1.00000

159	-8.6634	1.00000
160	-8.6499	1.00000
161	-8.5909	1.00000
162	-8.5783	1.00000
163	-8.5719	1.00000
164	-8.5636	1.00000
165	-8.4825	1.00000
166	-8.4523	1.00000
167	-8.4314	1.00000
168	-8.3404	1.00000
169	-8.2929	1.00000
170	-8.2710	1.00000
171	-8.2594	1.00000
172	-8.2286	1.00000
173	-8.2277	1.00000
174	-8.1472	1.00000
175	-8.1407	1.00000
176	-8.0737	1.00000
177	-8.0399	1.00000
178	-8.0221	1.00000
179	-8.0172	1.00000
180	-7.9686	1.00000

181	-7.9599	1.00000
182	-7.9200	1.00000
183	-7.8958	1.00000
184	-7.8807	1.00000
185	-7.8675	1.00000
186	-7.7964	1.00000
187	-7.7928	1.00000
188	-7.7438	1.00000
189	-7.7061	1.00000
190	-7.6620	1.00000
191	-7.5945	1.00000
192	-7.5798	1.00000
193	-7.5715	1.00000
194	-7.5420	1.00000
195	-7.4760	1.00000
196	-7.4754	1.00000
197	-7.4237	1.00000
198	-7.3191	1.00000
199	-7.2446	1.00000
200	-7.1641	1.00000
201	-7.0629	1.00000
202	-7.0377	1.00000

203	-7.0230	1.00000
204	-7.0084	1.00000
205	-6.9915	1.00000
206	-6.9846	1.00000
207	-6.9706	1.00000
208	-6.8629	1.00000
209	-6.8161	1.00000
210	-6.7971	1.00000
211	-6.7887	1.00000
212	-6.7274	1.00000
213	-6.6844	1.00000
214	-6.4650	1.00000
215	-6.4203	1.00000
216	-6.3908	1.00000
217	-6.3864	1.00000
218	-6.3688	1.00000
219	-6.3670	1.00000
220	-6.3121	1.00000
221	-6.3023	1.00000
222	-6.2323	1.00000
223	-6.2252	1.00000
224	-6.2246	1.00000

225	-6.0725	1.00000
226	-6.0324	1.00000
227	-5.7878	1.00000
228	-5.7469	1.00000
229	-5.6879	1.00000
230	-5.6365	1.00000
231	-5.6327	1.00000
232	-5.5543	1.00000
233	-5.5258	1.00000
234	-5.4623	1.00000
235	-5.4338	1.00000
236	-5.1635	1.00000
237	-5.0536	1.00000
238	-5.0450	1.00000
239	-5.0129	1.00000
240	-4.9832	1.00000
241	-4.9052	1.00000
242	-4.8485	1.00000
243	-4.8165	1.00000
244	-4.7839	1.00000
245	-4.6788	1.00000
246	-4.5675	1.00000

247	-4.5661	1.00000
248	-4.4991	1.00000
249	-4.4407	1.00000
250	-4.3782	1.00000
251	-4.2882	1.00000
252	-4.2591	1.00000
253	-4.2076	1.00000
254	-3.5425	1.00000
255	-3.3494	1.00000
256	-3.1909	1.00000
257	-2.9350	1.00000
258	-2.8431	1.00000
259	-2.8182	1.00000
260	-2.5990	1.00000
261	-1.9044	0.00000
262	-1.7615	0.00000
263	-1.7136	0.00000
264	-1.3376	0.00000
265	-1.2891	0.00000
266	-1.1781	0.00000
267	-0.7359	0.00000
268	-0.5796	0.00000

269	-0.4966	0.00000
270	-0.3028	0.00000
271	-0.3006	0.00000
272	-0.2850	0.00000
273	-0.1782	0.00000
274	-0.0528	0.00000
275	-0.0448	0.00000
276	-0.0052	0.00000
277	0.0400	0.00000
278	0.0895	0.00000
279	0.1779	0.00000
280	0.2257	0.00000
281	0.2530	0.00000
282	0.4253	0.00000
283	0.4527	0.00000
284	0.4863	0.00000
285	0.5949	0.00000
286	0.6741	0.00000
287	0.8190	0.00000
288	0.8685	0.00000
289	1.0494	0.00000
290	1.0890	0.00000

291	1.1220	0.00000
292	1.1639	0.00000
293	1.2242	0.00000
294	1.2451	0.00000
295	1.2897	0.00000
296	1.3148	0.00000
297	1.3489	0.00000
298	1.4127	0.00000
299	1.4648	0.00000
300	1.4834	0.00000
301	1.5565	0.00000
302	1.5871	0.00000
303	1.6258	0.00000
304	1.6787	0.00000
305	1.7526	0.00000
306	1.7656	0.00000
307	1.8693	0.00000
308	1.8892	0.00000
309	1.9070	0.00000
310	1.9142	0.00000
311	2.1244	0.00000
312	2.1852	0.00000

313	2.2103	0.00000
314	2.2358	0.00000
315	2.2761	0.00000
316	2.2930	0.00000
317	2.3321	0.00000
318	2.3562	0.00000
319	2.3749	0.00000
320	2.4004	0.00000
321	2.4180	0.00000
322	2.4316	0.00000
323	2.4357	0.00000
324	2.4538	0.00000
325	2.4608	0.00000
326	2.5215	0.00000
327	2.5362	0.00000
328	2.7002	0.00000
329	2.7274	0.00000
330	2.7550	0.00000
331	2.7581	0.00000
332	2.7651	0.00000
333	2.8146	0.00000
334	2.8361	0.00000

335	2.8613	0.00000
336	2.8911	0.00000
337	2.9236	0.00000
338	2.9464	0.00000
339	2.9794	0.00000
340	3.0065	0.00000
341	3.0347	0.00000
342	3.0431	0.00000
343	3.0664	0.00000
344	3.0862	0.00000
345	3.1486	0.00000
346	3.1617	0.00000
347	3.1789	0.00000
348	3.1924	0.00000
349	3.3000	0.00000
350	3.3210	0.00000
351	3.3512	0.00000
352	3.3666	0.00000
353	3.3876	0.00000
354	3.4306	0.00000
355	3.4750	0.00000
356	3.4856	0.00000

357	3.4892	0.00000
358	3.5023	0.00000
359	3.6330	0.00000
360	3.6727	0.00000
361	3.6843	0.00000
362	3.7336	0.00000
363	3.7530	0.00000
364	3.7604	0.00000
365	3.7718	0.00000
366	3.7940	0.00000
367	3.8127	0.00000
368	3.8365	0.00000
369	3.8405	0.00000
370	3.8532	0.00000
371	3.8780	0.00000
372	3.8860	0.00000
373	3.9106	0.00000
374	3.9267	0.00000
375	3.9343	0.00000
376	3.9582	0.00000
377	3.9737	0.00000
378	3.9835	0.00000

379	4.0158	0.00000
380	4.0670	0.00000
381	4.1646	0.00000
382	4.2470	0.00000
383	4.2581	0.00000
384	4.2588	0.00000
385	4.2861	0.00000
386	4.3136	0.00000
387	4.3282	0.00000
388	4.3410	0.00000
389	4.3728	0.00000
390	4.3828	0.00000
391	4.4170	0.00000
392	4.4446	0.00000
393	4.4676	0.00000
394	4.4802	0.00000
395	4.4881	0.00000
396	4.4966	0.00000
397	4.5170	0.00000
398	4.5521	0.00000
399	4.5921	0.00000
400	4.6084	0.00000

401	4.6281	0.00000
402	4.6436	0.00000
403	4.6571	0.00000
404	4.6803	0.00000
405	4.7044	0.00000
406	4.7322	0.00000
407	4.7454	0.00000
408	4.7666	0.00000
409	4.7835	0.00000
410	4.7841	0.00000
411	4.7970	0.00000
412	4.8289	0.00000
413	4.8657	0.00000
414	4.8722	0.00000
415	4.8981	0.00000
416	4.9308	0.00000
417	4.9842	0.00000
418	5.0047	0.00000
419	5.0113	0.00000
420	5.0357	0.00000
421	5.0400	0.00000
422	5.0649	0.00000

423	5.0819	0.00000
424	5.1139	0.00000
425	5.1177	0.00000
426	5.1372	0.00000
427	5.1411	0.00000
428	5.1564	0.00000
429	5.1756	0.00000
430	5.1856	0.00000
431	5.1890	0.00000
432	5.2151	0.00000
433	5.2363	0.00000
434	5.2406	0.00000
435	5.2560	0.00000
436	5.2917	0.00000
437	5.2973	0.00000
438	5.3102	0.00000
439	5.3307	0.00000
440	5.3505	0.00000
441	5.3685	0.00000
442	5.3752	0.00000
443	5.3955	0.00000
444	5.4207	0.00000

445	5.4538	0.00000
446	5.4629	0.00000
447	5.4821	0.00000
448	5.4944	0.00000
449	5.5215	0.00000
450	5.5506	0.00000
451	5.5691	0.00000
452	5.5762	0.00000
453	5.5953	0.00000
454	5.6186	0.00000
455	5.6603	0.00000
456	5.6820	0.00000
457	5.7113	0.00000
458	5.7234	0.00000
459	5.7442	0.00000
460	5.7594	0.00000
461	5.7830	0.00000
462	5.7916	0.00000
463	5.7968	0.00000
464	5.8036	0.00000
465	5.8083	0.00000
466	5.8270	0.00000

467	5.8460	0.00000
468	5.8614	0.00000
469	5.8804	0.00000
470	5.8861	0.00000
471	5.8940	0.00000
472	5.9145	0.00000
473	5.9239	0.00000
474	5.9481	0.00000
475	5.9666	0.00000
476	5.9801	0.00000
477	6.0126	0.00000
478	6.0215	0.00000
479	6.0344	0.00000
480	6.1422	0.00000

spin component 2

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-27.2470	1.00000
2	-21.5614	1.00000
3	-21.4651	1.00000

4	-21.0897	1.00000
5	-21.0624	1.00000
6	-21.0056	1.00000
7	-20.9726	1.00000
8	-20.9700	1.00000
9	-20.8755	1.00000
10	-20.5450	1.00000
11	-20.4944	1.00000
12	-20.3954	1.00000
13	-20.3837	1.00000
14	-20.1122	1.00000
15	-19.9474	1.00000
16	-19.6878	1.00000
17	-19.6207	1.00000
18	-19.5922	1.00000
19	-19.5721	1.00000
20	-19.5227	1.00000
21	-19.5204	1.00000
22	-19.4710	1.00000
23	-19.4569	1.00000
24	-19.0983	1.00000
25	-19.0673	1.00000

26	-18.9625	1.00000
27	-18.9507	1.00000
28	-18.8875	1.00000
29	-18.6988	1.00000
30	-18.4895	1.00000
31	-18.3465	1.00000
32	-18.2420	1.00000
33	-18.2223	1.00000
34	-18.1725	1.00000
35	-18.1700	1.00000
36	-18.0548	1.00000
37	-18.0518	1.00000
38	-17.5438	1.00000
39	-17.2911	1.00000
40	-17.2814	1.00000
41	-17.2685	1.00000
42	-17.2025	1.00000
43	-17.2019	1.00000
44	-17.1650	1.00000
45	-17.0130	1.00000
46	-16.9361	1.00000
47	-16.9170	1.00000

48	-16.8658	1.00000
49	-16.8648	1.00000
50	-16.8245	1.00000
51	-16.8178	1.00000
52	-16.8123	1.00000
53	-16.8104	1.00000
54	-16.7264	1.00000
55	-16.7205	1.00000
56	-16.1574	1.00000
57	-15.7241	1.00000
58	-15.6525	1.00000
59	-15.6374	1.00000
60	-15.6164	1.00000
61	-15.5618	1.00000
62	-15.5232	1.00000
63	-15.5206	1.00000
64	-15.1646	1.00000
65	-14.8023	1.00000
66	-14.5996	1.00000
67	-14.5562	1.00000
68	-14.4956	1.00000
69	-14.4940	1.00000

70	-14.4600	1.00000
71	-14.4324	1.00000
72	-14.3252	1.00000
73	-14.2929	1.00000
74	-14.2634	1.00000
75	-14.2590	1.00000
76	-14.1600	1.00000
77	-14.1566	1.00000
78	-13.8861	1.00000
79	-13.7507	1.00000
80	-13.5853	1.00000
81	-13.5331	1.00000
82	-13.5137	1.00000
83	-13.4889	1.00000
84	-13.4380	1.00000
85	-13.3390	1.00000
86	-13.3365	1.00000
87	-13.1823	1.00000
88	-12.7747	1.00000
89	-12.7449	1.00000
90	-12.7135	1.00000
91	-12.6730	1.00000

92	-12.6659	1.00000
93	-12.6169	1.00000
94	-12.4442	1.00000
95	-12.4272	1.00000
96	-12.3735	1.00000
97	-12.3181	1.00000
98	-12.2040	1.00000
99	-12.1938	1.00000
100	-12.1587	1.00000
101	-11.9533	1.00000
102	-11.6771	1.00000
103	-11.6209	1.00000
104	-11.5875	1.00000
105	-11.5799	1.00000
106	-11.1327	1.00000
107	-11.0888	1.00000
108	-10.8863	1.00000
109	-10.8732	1.00000
110	-10.8262	1.00000
111	-10.7002	1.00000
112	-10.6802	1.00000
113	-10.6570	1.00000

114	-10.6369	1.00000
115	-10.5771	1.00000
116	-10.5695	1.00000
117	-10.5638	1.00000
118	-10.5598	1.00000
119	-10.5113	1.00000
120	-10.5103	1.00000
121	-10.4970	1.00000
122	-10.4924	1.00000
123	-10.3736	1.00000
124	-10.2970	1.00000
125	-10.2543	1.00000
126	-10.1804	1.00000
127	-10.1797	1.00000
128	-10.1517	1.00000
129	-10.0825	1.00000
130	-9.8883	1.00000
131	-9.8641	1.00000
132	-9.7936	1.00000
133	-9.7728	1.00000
134	-9.7635	1.00000
135	-9.6981	1.00000

136	-9.4520	1.00000
137	-9.4194	1.00000
138	-9.3795	1.00000
139	-9.3759	1.00000
140	-9.3713	1.00000
141	-9.3554	1.00000
142	-9.3080	1.00000
143	-9.3016	1.00000
144	-9.2952	1.00000
145	-9.2853	1.00000
146	-9.2447	1.00000
147	-9.0874	1.00000
148	-9.0016	1.00000
149	-8.9932	1.00000
150	-8.9417	1.00000
151	-8.9383	1.00000
152	-8.7866	1.00000
153	-8.7332	1.00000
154	-8.7274	1.00000
155	-8.7081	1.00000
156	-8.7020	1.00000
157	-8.6654	1.00000

158	-8.6591	1.00000
159	-8.6523	1.00000
160	-8.6491	1.00000
161	-8.5739	1.00000
162	-8.5669	1.00000
163	-8.5621	1.00000
164	-8.5445	1.00000
165	-8.4820	1.00000
166	-8.4517	1.00000
167	-8.4298	1.00000
168	-8.3376	1.00000
169	-8.2892	1.00000
170	-8.2695	1.00000
171	-8.2290	1.00000
172	-8.2249	1.00000
173	-8.2230	1.00000
174	-8.1371	1.00000
175	-8.1295	1.00000
176	-8.0705	1.00000
177	-8.0377	1.00000
178	-8.0087	1.00000
179	-8.0037	1.00000

180	-7.9641	1.00000
181	-7.9548	1.00000
182	-7.9159	1.00000
183	-7.8860	1.00000
184	-7.8669	1.00000
185	-7.8587	1.00000
186	-7.7876	1.00000
187	-7.7835	1.00000
188	-7.7342	1.00000
189	-7.6743	1.00000
190	-7.6321	1.00000
191	-7.5923	1.00000
192	-7.5720	1.00000
193	-7.5498	1.00000
194	-7.5352	1.00000
195	-7.4679	1.00000
196	-7.4678	1.00000
197	-7.4226	1.00000
198	-7.3182	1.00000
199	-7.2314	1.00000
200	-7.1613	1.00000
201	-7.0506	1.00000

202	-7.0319	1.00000
203	-7.0120	1.00000
204	-6.9806	1.00000
205	-6.9724	1.00000
206	-6.9672	1.00000
207	-6.9362	1.00000
208	-6.8591	1.00000
209	-6.8118	1.00000
210	-6.7910	1.00000
211	-6.7835	1.00000
212	-6.7206	1.00000
213	-6.6750	1.00000
214	-6.4617	1.00000
215	-6.3902	1.00000
216	-6.3776	1.00000
217	-6.3736	1.00000
218	-6.3577	1.00000
219	-6.3333	1.00000
220	-6.2987	1.00000
221	-6.2706	1.00000
222	-6.2249	1.00000
223	-6.2235	1.00000

224	-6.2180	1.00000
225	-6.0419	1.00000
226	-6.0039	1.00000
227	-5.7517	1.00000
228	-5.7062	1.00000
229	-5.6863	1.00000
230	-5.6310	1.00000
231	-5.6184	1.00000
232	-5.5394	1.00000
233	-5.5186	1.00000
234	-5.4358	1.00000
235	-5.4063	1.00000
236	-5.1415	1.00000
237	-5.0552	1.00000
238	-5.0206	1.00000
239	-5.0171	1.00000
240	-4.9535	1.00000
241	-4.8723	1.00000
242	-4.8494	1.00000
243	-4.7968	1.00000
244	-4.7719	1.00000
245	-4.6483	1.00000

246	-4.5736	1.00000
247	-4.5706	1.00000
248	-4.4692	1.00000
249	-4.4164	1.00000
250	-4.3894	1.00000
251	-4.2920	1.00000
252	-4.2201	1.00000
253	-4.1702	1.00000
254	-3.5154	1.00000
255	-3.3039	1.00000
256	-3.1312	1.00000
257	-2.9400	1.00000
258	-2.7941	1.00000
259	-2.7340	1.00000
260	-2.0541	0.00000
261	-1.9104	0.00000
262	-1.7164	0.00000
263	-1.6736	0.00000
264	-1.2805	0.00000
265	-1.2650	0.00000
266	-1.1476	0.00000
267	-0.7145	0.00000

268	-0.5789	0.00000
269	-0.5042	0.00000
270	-0.2757	0.00000
271	-0.2725	0.00000
272	-0.2548	0.00000
273	-0.1515	0.00000
274	-0.0528	0.00000
275	-0.0432	0.00000
276	0.0184	0.00000
277	0.0451	0.00000
278	0.0844	0.00000
279	0.2130	0.00000
280	0.2607	0.00000
281	0.2846	0.00000
282	0.4390	0.00000
283	0.4568	0.00000
284	0.4876	0.00000
285	0.5995	0.00000
286	0.6944	0.00000
287	0.8218	0.00000
288	0.8751	0.00000
289	1.0568	0.00000

290	1.1081	0.00000
291	1.1447	0.00000
292	1.1779	0.00000
293	1.2329	0.00000
294	1.2510	0.00000
295	1.3108	0.00000
296	1.3210	0.00000
297	1.3622	0.00000
298	1.4320	0.00000
299	1.4752	0.00000
300	1.5033	0.00000
301	1.5797	0.00000
302	1.6047	0.00000
303	1.6538	0.00000
304	1.6876	0.00000
305	1.7599	0.00000
306	1.7759	0.00000
307	1.8741	0.00000
308	1.8968	0.00000
309	1.9099	0.00000
310	1.9192	0.00000
311	2.1405	0.00000

312	2.1965	0.00000
313	2.2214	0.00000
314	2.2547	0.00000
315	2.2897	0.00000
316	2.2981	0.00000
317	2.3373	0.00000
318	2.3636	0.00000
319	2.3854	0.00000
320	2.4109	0.00000
321	2.4292	0.00000
322	2.4370	0.00000
323	2.4444	0.00000
324	2.4590	0.00000
325	2.4659	0.00000
326	2.5241	0.00000
327	2.5419	0.00000
328	2.7051	0.00000
329	2.7338	0.00000
330	2.7552	0.00000
331	2.7609	0.00000
332	2.7734	0.00000
333	2.8287	0.00000

334	2.8495	0.00000
335	2.8747	0.00000
336	2.9023	0.00000
337	2.9323	0.00000
338	2.9558	0.00000
339	2.9842	0.00000
340	3.0081	0.00000
341	3.0384	0.00000
342	3.0500	0.00000
343	3.0720	0.00000
344	3.0938	0.00000
345	3.1512	0.00000
346	3.1696	0.00000
347	3.1881	0.00000
348	3.2007	0.00000
349	3.3059	0.00000
350	3.3254	0.00000
351	3.3598	0.00000
352	3.3701	0.00000
353	3.3908	0.00000
354	3.4360	0.00000
355	3.4803	0.00000

356	3.4919	0.00000
357	3.4984	0.00000
358	3.5088	0.00000
359	3.6380	0.00000
360	3.6766	0.00000
361	3.6967	0.00000
362	3.7394	0.00000
363	3.7569	0.00000
364	3.7622	0.00000
365	3.7767	0.00000
366	3.7990	0.00000
367	3.8158	0.00000
368	3.8435	0.00000
369	3.8495	0.00000
370	3.8673	0.00000
371	3.8820	0.00000
372	3.8955	0.00000
373	3.9205	0.00000
374	3.9383	0.00000
375	3.9498	0.00000
376	3.9598	0.00000
377	3.9829	0.00000

378	3.9870	0.00000
379	4.0220	0.00000
380	4.0764	0.00000
381	4.1711	0.00000
382	4.2599	0.00000
383	4.2620	0.00000
384	4.2699	0.00000
385	4.2936	0.00000
386	4.3216	0.00000
387	4.3349	0.00000
388	4.3503	0.00000
389	4.3829	0.00000
390	4.3878	0.00000
391	4.4228	0.00000
392	4.4486	0.00000
393	4.4727	0.00000
394	4.4834	0.00000
395	4.4948	0.00000
396	4.4995	0.00000
397	4.5202	0.00000
398	4.5565	0.00000
399	4.5952	0.00000

400	4.6112	0.00000
401	4.6298	0.00000
402	4.6469	0.00000
403	4.6601	0.00000
404	4.6862	0.00000
405	4.7093	0.00000
406	4.7375	0.00000
407	4.7508	0.00000
408	4.7699	0.00000
409	4.7872	0.00000
410	4.7893	0.00000
411	4.8028	0.00000
412	4.8337	0.00000
413	4.8707	0.00000
414	4.8859	0.00000
415	4.9028	0.00000
416	4.9414	0.00000
417	4.9939	0.00000
418	5.0101	0.00000
419	5.0138	0.00000
420	5.0395	0.00000
421	5.0449	0.00000

422	5.0692	0.00000
423	5.0861	0.00000
424	5.1174	0.00000
425	5.1217	0.00000
426	5.1413	0.00000
427	5.1444	0.00000
428	5.1724	0.00000
429	5.1804	0.00000
430	5.1896	0.00000
431	5.1939	0.00000
432	5.2201	0.00000
433	5.2387	0.00000
434	5.2438	0.00000
435	5.2617	0.00000
436	5.3001	0.00000
437	5.3045	0.00000
438	5.3135	0.00000
439	5.3349	0.00000
440	5.3546	0.00000
441	5.3726	0.00000
442	5.3826	0.00000
443	5.3980	0.00000

444	5.4292	0.00000
445	5.4599	0.00000
446	5.4693	0.00000
447	5.4879	0.00000
448	5.4985	0.00000
449	5.5287	0.00000
450	5.5680	0.00000
451	5.5754	0.00000
452	5.5960	0.00000
453	5.6070	0.00000
454	5.6284	0.00000
455	5.6729	0.00000
456	5.6927	0.00000
457	5.7204	0.00000
458	5.7275	0.00000
459	5.7477	0.00000
460	5.7628	0.00000
461	5.7906	0.00000
462	5.7949	0.00000
463	5.7996	0.00000
464	5.8058	0.00000
465	5.8215	0.00000

466	5.8265	0.00000
467	5.8584	0.00000
468	5.8639	0.00000
469	5.8866	0.00000
470	5.8922	0.00000
471	5.8952	0.00000
472	5.9122	0.00000
473	5.9344	0.00000
474	5.9555	0.00000
475	5.9640	0.00000
476	5.9862	0.00000
477	6.0039	0.00000
478	6.0375	0.00000
479	6.0494	0.00000
480	6.1074	0.00000

---

soft charge-density along one line, spin component 1

0 1 2 3 4 5 6 7

8 9

total charge-density along one line

soft charge-density along one line, spin component 2

0 1 2 3 4 5 6 7

8 9

total charge-density along one line

pseudopotential strength for first ion, spin component: 1

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

pseudopotential strength for first ion, spin component: 2

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.827 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

total augmentation occupancy for first ion, spin component: 1

3.579 -0.646 0.444 -0.034 -0.000

-0.646 0.130 -0.082 0.006 0.000

0.444 -0.082 0.056 -0.003 -0.000

-0.034 0.006 -0.003 0.011 0.000

-0.000 0.000 -0.000 0.000 0.007

total augmentation occupancy for first ion, spin component: 2

-0.000 0.000 -0.000 0.000 0.000

0.000 -0.000 0.000 -0.000 -0.000

-0.000 0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

---------- aborting loop because EDIFF is reached ----------

total charge

# of ion	s	p	d	tot

1	0.646	0.043	0.000	0.690
2	0.646	0.043	0.000	0.690
3	0.646	0.043	0.000	0.690
4	0.646	0.043	0.000	0.690
5	0.646	0.043	0.000	0.690
6	0.646	0.043	0.000	0.690
7	0.646	0.043	0.000	0.690
8	0.646	0.043	0.000	0.690
9	0.646	0.043	0.000	0.690
10	0.646	0.043	0.000	0.690
11	0.646	0.043	0.000	0.690
12	0.646	0.043	0.000	0.690
13	0.646	0.043	0.000	0.689
14	0.646	0.043	0.000	0.689
15	0.649	0.045	0.000	0.693
16	0.646	0.043	0.000	0.689
17	0.646	0.043	0.000	0.689
18	0.646	0.043	0.000	0.689
19	0.646	0.043	0.000	0.689
20	0.646	0.043	0.000	0.689
21	0.646	0.043	0.000	0.689
22	0.646	0.044	0.000	0.690

23	0.541	0.015	0.000	0.556
24	0.541	0.015	0.000	0.556
25	0.870	1.763	0.000	2.633
26	0.867	1.785	0.000	2.653
27	0.867	1.786	0.000	2.653
28	0.870	1.762	0.000	2.632
29	0.865	1.783	0.000	2.648
30	0.870	1.763	0.000	2.633
31	0.867	1.786	0.000	2.653
32	0.867	1.786	0.000	2.653
33	0.870	1.762	0.000	2.632
34	0.865	1.783	0.000	2.648
35	0.870	1.763	0.000	2.633
36	0.868	1.787	0.000	2.654
37	0.867	1.786	0.000	2.653
38	0.870	1.763	0.000	2.633
39	0.865	1.784	0.000	2.649
40	0.870	1.763	0.000	2.633
41	0.868	1.787	0.000	2.655
42	0.867	1.786	0.000	2.653
43	0.871	1.764	0.000	2.634
44	0.865	1.783	0.000	2.648

45	0.870	1.763	0.000	2.633
46	0.867	1.786	0.000	2.653
47	0.867	1.786	0.000	2.653
48	0.871	1.763	0.000	2.634
49	0.865	1.783	0.000	2.648
50	0.870	1.763	0.000	2.633
51	0.867	1.786	0.000	2.653
52	0.867	1.786	0.000	2.653
53	0.870	1.762	0.000	2.632
54	0.865	1.784	0.000	2.648
55	0.865	1.784	0.000	2.649
56	0.865	1.786	0.000	2.651
57	0.866	1.787	0.000	2.653
58	0.866	1.790	0.000	2.656
59	0.865	1.786	0.000	2.651
60	0.866	1.786	0.000	2.651
61	0.866	1.788	0.000	2.654
62	0.867	1.791	0.000	2.658
63	0.865	1.784	0.000	2.649
64	0.865	1.786	0.000	2.651
65	0.866	1.787	0.000	2.652
66	0.865	1.788	0.000	2.653

67	0.865	1.786	0.000	2.651
68	0.866	1.785	0.000	2.651
69	0.865	1.787	0.000	2.652
70	0.866	1.787	0.000	2.653
71	0.865	1.784	0.000	2.649
72	0.865	1.786	0.000	2.651
73	0.866	1.786	0.000	2.652
74	0.864	1.785	0.000	2.649
75	0.865	1.786	0.000	2.651
76	0.866	1.786	0.000	2.651
77	0.865	1.786	0.000	2.651
78	0.865	1.784	0.000	2.649
79	0.865	1.784	0.000	2.649
80	0.865	1.786	0.000	2.651
81	0.865	1.785	0.000	2.650
82	0.863	1.782	0.000	2.645
83	0.865	1.786	0.000	2.651
84	0.866	1.786	0.000	2.651
85	0.865	1.784	0.000	2.648
86	0.862	1.774	0.000	2.636
87	0.865	1.784	0.000	2.649
88	0.865	1.787	0.000	2.652

89	0.865	1.785	0.000	2.650
90	0.865	1.788	0.000	2.653
91	0.865	1.786	0.000	2.651
92	0.866	1.786	0.000	2.651
93	0.864	1.783	0.000	2.647
94	0.866	1.785	0.000	2.651
95	0.865	1.784	0.000	2.649
96	0.865	1.786	0.000	2.651
97	0.866	1.787	0.000	2.653
98	0.866	1.789	0.000	2.655
99	0.865	1.786	0.000	2.651
100	0.866	1.786	0.000	2.651
101	0.865	1.787	0.000	2.652
102	0.867	1.790	0.000	2.657
103	0.865	1.786	0.000	2.651
104	0.867	1.785	0.000	2.653
105	0.866	1.786	0.000	2.652
106	0.870	1.778	0.000	2.648
107	0.869	1.765	0.000	2.635
108	0.865	1.783	0.000	2.648
109	0.869	1.789	0.000	2.658
110	0.865	1.786	0.000	2.651

111	0.867	1.785	0.000	2.653
112	0.867	1.789	0.000	2.655
113	0.871	1.782	0.000	2.653
114	0.869	1.765	0.000	2.634
115	0.865	1.783	0.000	2.648
116	0.870	1.791	0.000	2.661
117	0.865	1.786	0.000	2.651
118	0.867	1.785	0.000	2.653
119	0.865	1.782	0.000	2.647
120	0.857	1.707	0.000	2.564
121	0.869	1.765	0.000	2.634
122	0.865	1.783	0.000	2.648
123	0.866	1.778	0.000	2.644
124	0.866	1.786	0.000	2.652
125	0.867	1.785	0.000	2.653
126	0.862	1.776	0.000	2.638
127	0.846	1.820	0.000	2.666
128	0.870	1.767	0.000	2.637
129	0.865	1.783	0.000	2.648
130	0.860	1.757	0.000	2.617
131	0.866	1.786	0.000	2.652
132	0.867	1.784	0.000	2.652

133	0.864	1.787	0.000	2.651
134	0.869	1.790	0.000	2.659
135	0.869	1.767	0.000	2.636
136	0.865	1.783	0.000	2.648
137	0.866	1.772	0.000	2.638
138	0.866	1.786	0.000	2.652
139	0.867	1.785	0.000	2.652
140	0.866	1.788	0.000	2.653
141	0.870	1.779	0.000	2.649
142	0.869	1.766	0.000	2.635
143	0.865	1.783	0.000	2.648
144	0.869	1.790	0.000	2.659
145	0.945	1.726	0.000	2.671
146	1.240	1.546	0.074	2.860
147	1.636	3.543	0.000	5.179
---	---	---	---	---
tot	123.064	221.564	0.074	344.702

magnetization (x)

# of ion	s	p	d	tot
1	0.000	-0.000	0.000	0.000
2	-0.000	0.000	0.000	-0.000
3	0.000	-0.000	0.000	0.000
4	-0.000	0.000	0.000	-0.000
5	0.000	-0.000	0.000	0.000
6	-0.000	0.000	0.000	-0.000
7	0.000	-0.000	0.000	0.000
8	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	0.000
10	-0.000	0.000	0.000	-0.000
11	0.000	-0.000	0.000	0.000
12	-0.000	0.000	0.000	-0.000
13	0.000	-0.000	0.000	0.000
14	-0.004	0.002	0.000	-0.002
15	0.000	-0.000	0.000	0.000
16	-0.004	0.002	0.000	-0.002
17	-0.004	0.002	0.000	-0.002
18	0.000	-0.000	0.000	0.000
19	-0.003	0.001	0.000	-0.002
20	0.000	-0.000	0.000	0.000

21	-0.003	0.002	0.000	-0.002
22	-0.003	0.002	0.000	-0.002
23	-0.000	0.000	0.000	-0.000
24	-0.000	0.000	0.000	-0.000
25	-0.000	-0.007	0.000	-0.008
26	-0.000	-0.002	0.000	-0.002
27	0.000	0.003	0.000	0.003
28	0.000	0.005	0.000	0.005
29	0.000	0.003	0.000	0.003
30	-0.000	-0.007	0.000	-0.008
31	-0.000	-0.002	0.000	-0.002
32	0.000	0.003	0.000	0.003
33	0.000	0.005	0.000	0.005
34	0.000	0.002	0.000	0.002
35	-0.000	-0.007	0.000	-0.008
36	-0.000	-0.002	0.000	-0.002
37	0.000	0.003	0.000	0.003
38	0.000	0.006	0.000	0.007
39	0.000	0.002	0.000	0.002
40	-0.000	-0.007	0.000	-0.008
41	-0.000	-0.002	0.000	-0.002
42	0.000	0.002	0.000	0.003

43	0.000	0.005	0.000	0.005
44	0.000	0.004	0.000	0.004
45	-0.000	-0.007	0.000	-0.008
46	-0.000	-0.002	0.000	-0.002
47	0.000	0.002	0.000	0.003
48	0.000	0.005	0.000	0.006
49	0.000	0.001	0.000	0.001
50	-0.000	-0.007	0.000	-0.008
51	-0.000	-0.002	0.000	-0.002
52	0.000	0.002	0.000	0.003
53	0.000	0.006	0.000	0.007
54	0.000	0.002	0.000	0.002
55	-0.000	-0.005	0.000	-0.006
56	-0.000	-0.007	0.000	-0.007
57	-0.000	-0.001	0.000	-0.001
58	-0.000	-0.001	0.000	-0.001
59	0.000	0.006	0.000	0.007
60	0.000	0.003	0.000	0.003
61	0.000	0.001	0.000	0.001
62	0.000	0.002	0.000	0.003
63	-0.000	-0.005	0.000	-0.006
64	-0.000	-0.007	0.000	-0.007

65	-0.000	-0.001	0.000	-0.001
66	-0.000	-0.001	0.000	-0.001
67	0.000	0.006	0.000	0.006
68	0.000	0.003	0.000	0.003
69	0.000	0.001	0.000	0.001
70	0.000	0.002	0.000	0.002
71	-0.000	-0.005	0.000	-0.006
72	-0.000	-0.007	0.000	-0.007
73	-0.000	-0.001	0.000	-0.001
74	-0.000	-0.002	0.000	-0.002
75	0.000	0.006	0.000	0.007
76	0.000	0.003	0.000	0.004
77	0.000	0.003	0.000	0.003
78	0.000	0.001	0.000	0.001
79	-0.000	-0.005	0.000	-0.006
80	-0.000	-0.007	0.000	-0.007
81	-0.000	-0.001	0.000	-0.002
82	-0.000	-0.002	0.000	-0.002
83	0.001	0.007	0.000	0.007
84	0.000	0.003	0.000	0.003
85	0.000	0.002	0.000	0.002
86	0.000	0.005	0.000	0.006

87	-0.000	-0.005	0.000	-0.005
88	-0.000	-0.007	0.000	-0.007
89	-0.000	-0.001	0.000	-0.002
90	-0.000	-0.002	0.000	-0.002
91	0.001	0.008	0.000	0.008
92	0.000	0.003	0.000	0.003
93	0.000	0.002	0.000	0.003
94	0.000	0.001	0.000	0.001
95	-0.000	-0.005	0.000	-0.006
96	-0.000	-0.007	0.000	-0.007
97	-0.000	-0.001	0.000	-0.001
98	-0.000	-0.001	0.000	-0.001
99	0.001	0.007	0.000	0.007
100	0.000	0.003	0.000	0.004
101	0.000	0.003	0.000	0.003
102	0.000	0.002	0.000	0.002
103	-0.001	-0.010	0.000	-0.011
104	-0.003	-0.028	0.000	-0.031
105	-0.000	-0.001	0.000	-0.002
106	-0.000	-0.004	0.000	-0.004
107	0.007	0.115	0.000	0.122
108	0.001	0.010	0.000	0.011

109	0.000	0.001	0.000	0.001
110	-0.001	-0.010	0.000	-0.011
111	-0.003	-0.028	0.000	-0.031
112	-0.000	-0.001	0.000	-0.002
113	-0.000	-0.003	0.000	-0.003
114	0.007	0.120	0.000	0.127
115	0.001	0.010	0.000	0.011
116	0.000	0.001	0.000	0.002
117	-0.001	-0.010	0.000	-0.011
118	-0.003	-0.026	0.000	-0.029
119	-0.000	-0.002	0.000	-0.002
120	-0.000	-0.002	0.000	-0.002
121	0.007	0.115	0.000	0.122
122	0.001	0.010	0.000	0.010
123	0.000	0.003	0.000	0.003
124	-0.001	-0.010	0.000	-0.011
125	-0.003	-0.024	0.000	-0.027
126	-0.000	-0.002	0.000	-0.002
127	-0.000	0.001	0.000	0.001
128	0.006	0.104	0.000	0.110
129	0.001	0.009	0.000	0.010
130	0.000	0.004	0.000	0.004

131	-0.001	-0.009	0.000	-0.010
132	-0.003	-0.024	0.000	-0.027
133	-0.000	-0.002	0.000	-0.002
134	-0.000	-0.002	0.000	-0.002
135	0.006	0.097	0.000	0.102
136	0.001	0.009	0.000	0.010
137	0.000	0.004	0.000	0.004
138	-0.001	-0.010	0.000	-0.011
139	-0.003	-0.026	0.000	-0.029
140	-0.000	-0.002	0.000	-0.002
141	-0.000	-0.003	0.000	-0.003
142	0.006	0.105	0.000	0.111
143	0.001	0.010	0.000	0.010
144	0.000	0.002	0.000	0.003
145	0.000	0.005	0.000	0.006
146	-0.000	0.000	-0.000	0.000
147	0.000	0.004	0.000	0.004
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tot	0.001	0.513	-0.000	0.514

CHARGE: cpu time 0.5224: real time 0.5242

FORLOC: cpu time 0.0199: real time 0.0199

FORNL : cpu time 2.0696: real time 2.0840

STRESS: cpu time 6.2301: real time 6.2532

FORCOR: cpu time 0.1415: real time 0.1423

FORHAR: cpu time 0.0328: real time 0.0329

MIXING: cpu time 0.0105: real time 0.0106

OFIELD: cpu time 0.0002: real time 0.0002

DFTD3 V3.0 Rev 1

Edisp (eV) -6.61770

E6 (eV) : -3.9313

E8 (eV) : -2.6864

% E8 : 40.59

FORVDW: cpu time 1.7852: real time 1.8215

FORCE on cell =-STRESS in cart. coord. units (eV):

Direction	XX	YY	ZZ	XY	YZ	ZX
Alpha Z	233.50077	233.50077	233.50077			
Ewald	107573.96327	23480.77830	-39729.32422	10.26183	3455.09611	129.11670

Hartree	106094.90783	25035.71845	-23797.03112	-6.56260	2945.88593	93.32398
E(xc)	-1914.26306	-1916.61568	-1979.91715	0.13246	1.82458	0.13166
Local	**********	-53964.61555	57020.49303	-0.21976	-6358.71617	-218.93046
n-local	-472.70442	-482.52188	-439.65613	-0.69807	-0.83007	-0.32950
augment	-38.25994	-38.58114	-34.31782	0.00653	-0.99147	-0.00354
Kinetic	7635.37254	7638.80451	8714.00360	-3.09641	-41.48820	-3.20399
Fock	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
vdW	-2.64369	-1.49410	-6.59320	0.00169	-0.07496	0.01176
Total	-17.73482	-15.02632	-18.84224	-0.17432	0.70574	0.11662
in kB	-4.89047	-4.14359	-5.19585	-0.04807	0.19461	0.03216

external pressure = -4.74 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

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energy-cutoff : 400.00

volume of cell : 5810.14

direct lattice vectors			reciprocal lattice vectors		
14.780600000	0.000000000	0.000000000	0.067656252	0.000000000	0.000000000
0.000000000	21.333900000	0.000000000	0.000000000	0.046873755	0.000000000
0.000000000	0.000000000	18.425700000	0.000000000	0.000000000	0.054272022

length of vectors

14.780600000 21.333900000 18.425700000 0.067656252 0.046873755 0.054272022

FORCES acting on ions

electron-ion (+dipol) ewald-force non-local-force convergence-correction

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0.455E-02 0.154E+03 0.361E+02 -.304E-02 -.160E+03 -.357E+02 -.180E-02 0.566E+01 -.438E+00 -.788E-07 0.488E-06 0.547E-06

-.186E-01 0.155E+03 -.340E+02 0.162E-01 -.160E+03 0.335E+02 0.114E-02 0.565E+01 0.541E+00 -.118E-05 -.556E-06 -.310E-06

0.184E+00 0.154E+03 0.360E+02 -.184E+00 -.160E+03 -.356E+02 0.127E-04 0.565E+01 -.443E+00 -.124E-06 0.804E-06 0.688E-07

0.112E+00 0.155E+03 -.341E+02 -.989E-01 -.160E+03 0.336E+02 -.174E-01 0.565E+01 0.535E+00 0.194E-07 0.127E-06 -.706E-06

0.172E+00 0.154E+03 0.362E+02 -.173E+00 -.160E+03 -.357E+02 0.117E-02 0.566E+01 -.440E+00 -.512E-07 0.651E-06 0.610E-06

0.126E+00 0.154E+03 -.340E+02 -.108E+00 -.160E+03 0.334E+02 -.211E-01 0.565E+01 0.541E+00 0.114E-05 -.956E-07 0.436E-07

-.192E-01 0.154E+03 0.363E+02 0.180E-01 -.160E+03 -.359E+02 0.159E-02 0.566E+01 -

.431E+00 -.579E-08 0.275E-06 0.156E-05

-.128E-01 0.154E+03 -.338E+02 0.196E-01 -.160E+03 0.332E+02 -.719E-02 0.565E+01 0.555E+00 0.981E-06 -.970E-06 0.118E-05

-.182E+00 0.154E+03 0.363E+02 0.182E+00 -.160E+03 -.359E+02 0.251E-03 0.565E+01 -.429E+00 0.147E-06 0.686E-07 0.201E-05

-.128E+00 0.155E+03 -.337E+02 0.115E+00 -.160E+03 0.331E+02 0.109E-01 0.565E+01 0.561E+00 0.611E-07 -.160E-05 0.156E-05

-.174E+00 0.154E+03 0.362E+02 0.176E+00 -.160E+03 -.358E+02 -.178E-02 0.566E+01 -.432E+00 0.110E-06 0.119E-06 0.153E-05

-.115E+00 0.155E+03 -.338E+02 0.960E-01 -.160E+03 0.332E+02 0.192E-01 0.565E+01 0.555E+00 -.102E-05 -.140E-05 0.849E-06

0.228E+01 -.150E+03 -.386E+02 -.227E+01 0.156E+03 0.386E+02 -.103E-01 -.566E+01 0.768E-01 0.577E-06 -.351E-06 0.866E-08

-.415E+00 -.151E+03 0.388E+02 0.417E+00 0.157E+03 -.386E+02 -.132E-02 -.567E+01 -.269E+00 0.106E-06 -.434E-06 -.351E-07

0.136E+02 -.146E+03 -.413E+02 -.138E+02 0.151E+03 0.413E+02 0.257E+00 -.567E+01 -.346E-01 -.414E-07 -.845E-07 -.344E-06

0.162E+01 -.151E+03 0.402E+02 -.162E+01 0.156E+03 -.400E+02 -.993E-03 -.567E+01 -.229E+00 0.257E-06 -.412E-07 0.750E-06

0.352E+01 -.149E+03 0.443E+02 -.352E+01 0.155E+03 -.441E+02 -.189E-02 -.567E+01 -.180E+00 0.348E-06 -.119E-06 0.710E-06

-.148E+02 -.146E+03 -.330E+02 0.149E+02 0.151E+03 0.329E+02 -.980E-01 -.566E+01

0.502E-01 -.115E-05 0.643E-06 0.951E-06

-.297E+01 -.149E+03 0.432E+02 0.296E+01 0.155E+03 -.430E+02 0.114E-01 -.567E+01 -.241E+00 -.371E-06 -.634E-06 -.512E-06

-.379E+01 -.150E+03 -.385E+02 0.379E+01 0.155E+03 0.385E+02 -.649E-02 -.566E+01 0.242E-01 0.165E-06 -.304E-06 0.247E-06

-.207E+01 -.151E+03 0.395E+02 0.207E+01 0.156E+03 -.392E+02 0.146E-02 -.566E+01 -.282E+00 -.338E-06 -.755E-06 -.572E-06

0.150E-02 -.148E+03 0.486E+02 0.614E-02 0.154E+03 -.484E+02 -.556E-02 -.569E+01 -.158E+00 0.271E-07 -.401E-06 -.420E-07

0.196E+02 -.103E+03 0.222E+02 -.212E+02 0.103E+03 -.246E+02 0.153E+01 0.140E+00 0.238E+01 -.559E-07 -.754E-06 0.542E-06

-.191E+02 -.103E+03 0.154E+02 0.215E+02 0.103E+03 -.169E+02 -.241E+01 -.118E+00 0.152E+01 0.133E-06 -.121E-05 0.149E-05

0.714E-01 0.461E+03 0.202E+03 -.746E-01 -.462E+03 -.201E+03 0.381E-02 0.102E+01 -.219E+00 0.483E-06 0.266E-06 0.453E-06

0.212E+00 0.353E+03 -.234E+03 -.212E+00 -.353E+03 0.234E+03 0.260E-02 0.441E+00 -.370E-01 -.989E-06 0.899E-06 -.329E-05

-.244E-01 0.351E+03 0.240E+03 0.231E-01 -.351E+03 -.241E+03 0.311E-02 0.407E+00 0.562E-01 0.111E-05 -.110E-05 0.119E-05

-.173E+00 0.462E+03 -.195E+03 0.180E+00 -.463E+03 0.195E+03 -.669E-02 0.105E+01 0.233E+00 -.303E-05 -.124E-05 -.225E-05

-.622E-01 0.210E+03 -.272E+03 0.662E-01 -.210E+03 0.272E+03 -.448E-02 0.925E-01

0.561E-01 -.283E-06 0.121E-05 -.214E-05

0.562E+00 0.461E+03 0.202E+03 -.565E+00 -.462E+03 -.201E+03 0.204E-02 0.102E+01 -.214E+00 -.449E-06 0.961E-06 -.100E-05

0.106E+01 0.352E+03 -.234E+03 -.107E+01 -.353E+03 0.234E+03 0.161E-01 0.447E+00 -.424E-01 0.158E-05 0.531E-06 -.239E-05

0.413E+00 0.351E+03 0.240E+03 -.415E+00 -.351E+03 -.240E+03 0.303E-02 0.407E+00 0.490E-01 0.248E-06 -.556E-06 -.133E-05

0.578E+00 0.462E+03 -.195E+03 -.583E+00 -.463E+03 0.195E+03 0.484E-02 0.105E+01 0.235E+00 0.328E-06 0.119E-05 -.337E-05

0.687E+00 0.210E+03 -.272E+03 -.693E+00 -.210E+03 0.272E+03 0.622E-02 0.902E-01 0.616E-01 0.625E-06 0.103E-05 -.144E-05

0.426E+00 0.461E+03 0.202E+03 -.428E+00 -.462E+03 -.202E+03 0.390E-02 0.102E+01 -.214E+00 -.888E-06 0.384E-06 0.123E-05

0.938E+00 0.352E+03 -.233E+03 -.954E+00 -.352E+03 0.233E+03 0.152E-01 0.440E+00 -.376E-01 0.219E-05 -.252E-05 0.693E-06

0.478E+00 0.351E+03 0.241E+03 -.480E+00 -.351E+03 -.241E+03 0.254E-02 0.405E+00 0.510E-01 -.928E-06 -.545E-06 -.864E-06

0.704E+00 0.462E+03 -.194E+03 -.715E+00 -.463E+03 0.194E+03 0.800E-02 0.106E+01 0.242E+00 0.318E-05 -.110E-05 -.705E-06

0.722E+00 0.210E+03 -.271E+03 -.731E+00 -.210E+03 0.271E+03 0.676E-02 0.901E-01 0.593E-01 0.700E-06 -.103E-05 0.272E-06

-.182E+00 0.461E+03 0.202E+03 0.178E+00 -.462E+03 -.202E+03 0.451E-02 0.102E+01 -

.218E+00 -.643E-06 -.556E-06 0.472E-05

-.294E+00 0.352E+03 -.233E+03 0.298E+00 -.352E+03 0.233E+03 -.209E-02 0.439E+00 -.298E-01 0.662E-06 -.505E-05 0.293E-05

0.398E-01 0.351E+03 0.241E+03 -.389E-01 -.351E+03 -.241E+03 0.228E-02 0.409E+00 0.556E-01 -.120E-05 -.103E-05 0.227E-05

0.501E-01 0.462E+03 -.194E+03 -.562E-01 -.463E+03 0.194E+03 0.408E-02 0.106E+01 0.232E+00 0.236E-05 -.518E-05 0.306E-05

-.479E-01 0.210E+03 -.271E+03 0.459E-01 -.210E+03 0.271E+03 -.293E-03 0.925E-01 0.325E-01 0.128E-06 -.292E-05 0.133E-05

-.551E+00 0.461E+03 0.202E+03 0.550E+00 -.462E+03 -.202E+03 0.740E-03 0.101E+01 -.220E+00 0.465E-06 -.110E-05 0.613E-05

-.119E+01 0.352E+03 -.233E+03 0.120E+01 -.353E+03 0.233E+03 -.163E-01 0.446E+00 -.329E-01 -.117E-05 -.538E-05 0.217E-05

-.352E+00 0.351E+03 0.241E+03 0.349E+00 -.351E+03 -.241E+03 0.206E-02 0.413E+00 0.622E-01 -.211E-06 -.144E-05 0.479E-05

-.411E+00 0.462E+03 -.194E+03 0.425E+00 -.463E+03 0.194E+03 -.116E-01 0.106E+01 0.231E+00 -.409E-07 -.741E-05 0.417E-05

-.557E+00 0.210E+03 -.271E+03 0.562E+00 -.210E+03 0.271E+03 -.963E-02 0.905E-01 0.526E-01 -.607E-06 -.263E-05 0.818E-06

-.475E+00 0.461E+03 0.202E+03 0.474E+00 -.462E+03 -.202E+03 0.301E-02 0.102E+01 -.221E+00 0.101E-05 -.742E-06 0.406E-05

-.804E+00 0.353E+03 -.234E+03 0.819E+00 -.353E+03 0.234E+03 -.150E-01 0.446E+00 -

.392E-01 -.225E-05 -.240E-05 -.909E-06

-.373E+00 0.351E+03 0.241E+03 0.368E+00 -.351E+03 -.241E+03 0.906E-03 0.410E+00 0.624E-01 0.993E-06 -.153E-05 0.428E-05

-.594E+00 0.462E+03 -.194E+03 0.607E+00 -.463E+03 0.194E+03 -.172E-01 0.105E+01 0.234E+00 -.284E-05 -.564E-05 0.164E-05

-.585E+00 0.210E+03 -.272E+03 0.596E+00 -.210E+03 0.272E+03 -.103E-01 0.981E-01 0.566E-01 -.623E-06 -.773E-06 -.986E-06

-.757E-02 0.206E+03 0.279E+03 0.109E-01 -.206E+03 -.279E+03 -.363E-02 0.682E-01 -.414E-01 0.133E-05 -.141E-05 -.845E-07

0.670E+00 0.303E+02 0.296E+03 -.665E+00 -.302E+02 -.296E+03 -.469E-02 -.413E-01 0.723E-02 0.466E-06 -.149E-05 -.152E-06

-.844E+00 0.144E+03 -.282E+03 0.846E+00 -.144E+03 0.282E+03 -.322E-02 0.136E+00 0.287E-01 0.861E-07 0.542E-06 -.105E-05

0.534E+00 -.215E+02 -.285E+03 -.535E+00 0.214E+02 0.285E+03 -.789E-03 0.375E-01 0.186E-01 0.663E-06 0.162E-05 0.119E-05

0.503E+00 -.294E+02 0.293E+03 -.500E+00 0.294E+02 -.293E+03 -.555E-02 0.251E-01 -.306E-01 0.170E-06 -.787E-06 0.218E-06

0.525E+00 0.139E+03 0.289E+03 -.525E+00 -.139E+03 -.289E+03 0.177E-02 0.103E+00 -.250E-01 0.858E-06 -.169E-05 -.102E-05

-.126E+01 0.364E+02 -.287E+03 0.126E+01 -.364E+02 0.287E+03 -.180E-03 -.870E-02 0.140E-01 0.584E-06 0.112E-05 0.483E-06

0.167E+01 -.130E+03 -.271E+03 -.169E+01 0.130E+03 0.271E+03 0.107E-01 -.887E-01

0.373E-01 0.875E-06 0.853E-06 0.193E-05

0.397E+00 0.207E+03 0.280E+03 -.395E+00 -.207E+03 -.280E+03 0.719E-03 0.691E-01 -.373E-01 0.372E-06 -.164E-05 -.176E-05

0.918E+00 0.312E+02 0.296E+03 -.922E+00 -.311E+02 -.296E+03 0.231E-02 -.413E-01 0.119E-01 -.202E-07 -.171E-05 -.334E-06

0.132E+01 0.144E+03 -.282E+03 -.133E+01 -.144E+03 0.282E+03 0.509E-02 0.125E+00 0.280E-01 0.108E-06 0.141E-05 -.119E-05

0.341E+01 -.199E+02 -.285E+03 -.342E+01 0.199E+02 0.285E+03 0.140E-01 0.403E-01 0.137E-01 -.471E-06 0.150E-05 0.110E-05

0.139E+01 -.287E+02 0.294E+03 -.139E+01 0.287E+02 -.294E+03 -.346E-02 0.249E-01 -.310E-01 0.194E-06 -.151E-05 0.466E-06

0.677E+00 0.139E+03 0.290E+03 -.677E+00 -.139E+03 -.290E+03 0.657E-03 0.103E+00 -.297E-01 -.269E-06 -.178E-05 -.158E-05

0.160E+01 0.367E+02 -.287E+03 -.158E+01 -.366E+02 0.287E+03 -.125E-01 -.217E-01 0.130E-01 0.996E-07 0.161E-05 0.526E-06

0.610E+01 -.125E+03 -.271E+03 -.612E+01 0.125E+03 0.271E+03 0.226E-01 -.901E-01 0.146E-01 -.110E-05 0.719E-06 0.123E-05

0.366E+00 0.207E+03 0.280E+03 -.371E+00 -.207E+03 -.280E+03 0.152E-03 0.680E-01 -.367E-01 -.104E-05 -.137E-05 -.137E-05

-.415E-01 0.319E+02 0.296E+03 0.328E-01 -.318E+02 -.296E+03 0.106E-01 -.365E-01 0.136E-01 -.551E-06 -.674E-06 -.199E-06

0.209E+01 0.144E+03 -.281E+03 -.210E+01 -.144E+03 0.281E+03 0.123E-01 0.119E+00

0.241E-01 0.404E-06 0.525E-06 -.121E-06

0.302E+01 -.172E+02 -.283E+03 -.304E+01 0.171E+02 0.283E+03 0.249E-01 0.866E-01 0.616E-01 -.856E-06 0.220E-06 0.780E-06

0.105E+01 -.272E+02 0.294E+03 -.105E+01 0.272E+02 -.294E+03 0.295E-02 0.240E-01 -.378E-01 -.152E-07 -.103E-05 0.233E-06

0.943E-01 0.140E+03 0.290E+03 -.959E-01 -.140E+03 -.290E+03 0.135E-02 0.107E+00 -.234E-01 -.120E-05 -.109E-05 -.449E-06

0.276E+01 0.387E+02 -.286E+03 -.276E+01 -.387E+02 0.286E+03 0.162E-02 -.116E-01 0.294E-01 -.283E-06 0.772E-06 0.758E-06

0.591E+01 -.115E+03 -.267E+03 -.607E+01 0.115E+03 0.267E+03 0.154E+00 0.133E-02 0.132E+00 -.350E-06 0.232E-05 0.765E-07

-.244E+00 0.207E+03 0.280E+03 0.241E+00 -.207E+03 -.280E+03 0.441E-02 0.712E-01 -.389E-01 -.127E-05 -.969E-06 0.890E-06

-.115E+01 0.314E+02 0.294E+03 0.114E+01 -.314E+02 -.294E+03 0.917E-02 -.314E-01 0.519E-02 -.503E-06 0.463E-06 0.158E-06

0.591E+00 0.144E+03 -.281E+03 -.609E+00 -.144E+03 0.281E+03 0.180E-01 0.125E+00 0.438E-01 -.154E-06 -.119E-05 0.892E-06

-.941E+00 -.159E+02 -.286E+03 0.932E+00 0.158E+02 0.286E+03 0.591E-02 0.900E-01 0.807E-01 -.969E-06 0.153E-05 0.616E-06

-.648E+00 -.265E+02 0.293E+03 0.645E+00 0.265E+02 -.293E+03 0.491E-02 0.232E-01 -.273E-01 -.230E-06 0.302E-06 -.153E-06

-.535E+00 0.139E+03 0.289E+03 0.531E+00 -.139E+03 -.289E+03 0.653E-02 0.113E+00 -

.215E-01 -.875E-06 -.400E-06 0.127E-05

0.770E+00 0.407E+02 -.287E+03 -.782E+00 -.407E+02 0.287E+03 0.539E-02 0.174E-02 -.188E-01 -.976E-06 -.169E-06 0.804E-06

-.462E+00 -.113E+03 -.276E+03 0.428E+00 0.113E+03 0.277E+03 0.343E-01 0.598E-01 -.268E+00 -.198E-05 -.465E-05 -.558E-07

-.572E+00 0.206E+03 0.279E+03 0.570E+00 -.206E+03 -.279E+03 0.114E-02 0.716E-01 -.457E-01 -.361E-06 -.659E-06 0.260E-05

-.781E+00 0.304E+02 0.294E+03 0.785E+00 -.304E+02 -.294E+03 -.759E-02 -.312E-01 -.162E-02 0.118E-06 0.634E-06 0.288E-06

-.123E+01 0.144E+03 -.281E+03 0.124E+01 -.144E+03 0.281E+03 -.160E-01 0.122E+00 0.505E-01 -.194E-06 -.193E-05 0.106E-05

-.364E+01 -.174E+02 -.283E+03 0.367E+01 0.173E+02 0.283E+03 -.311E-01 0.116E+00 0.595E-01 0.481E-06 -.423E-06 0.754E-06

-.130E+01 -.277E+02 0.291E+03 0.129E+01 0.277E+02 -.291E+03 -.136E-02 0.338E-01 -.221E-01 -.118E-06 0.107E-05 -.381E-06

-.346E+00 0.139E+03 0.289E+03 0.345E+00 -.139E+03 -.289E+03 -.315E-05 0.111E+00 -.148E-01 0.371E-06 -.207E-06 0.173E-05

-.822E+00 0.400E+02 -.287E+03 0.814E+00 -.400E+02 0.287E+03 0.121E-01 -.793E-02 -.180E-01 0.306E-06 -.798E-06 0.801E-06

-.782E+01 -.119E+03 -.267E+03 0.801E+01 0.119E+03 0.267E+03 -.190E+00 0.210E-02 0.367E-01 0.644E-06 0.333E-05 0.630E-06

-.407E+00 0.206E+03 0.279E+03 0.409E+00 -.206E+03 -.279E+03 -.283E-02 0.711E-01 -

.466E-01 0.970E-06 -.832E-06 0.210E-05

-.595E-01 0.300E+02 0.294E+03 0.693E-01 -.299E+02 -.294E+03 -.954E-02 -.351E-01 0.938E-03 0.484E-06 -.351E-06 0.102E-06

-.206E+01 0.145E+03 -.282E+03 0.207E+01 -.145E+03 0.282E+03 -.191E-01 0.131E+00 0.257E-01 -.199E-06 -.856E-06 0.804E-07

-.256E+01 -.208E+02 -.285E+03 0.258E+01 0.208E+02 0.285E+03 -.295E-01 0.399E-01 0.321E-01 0.105E-05 0.810E-06 0.926E-06

-.548E+00 -.290E+02 0.291E+03 0.553E+00 0.290E+02 -.291E+03 -.290E-02 0.289E-01 -.253E-01 0.472E-08 0.435E-06 -.185E-06

0.611E-01 0.139E+03 0.289E+03 -.612E-01 -.139E+03 -.289E+03 -.382E-03 0.109E+00 -.210E-01 0.110E-05 -.854E-06 0.624E-06

-.288E+01 0.377E+02 -.286E+03 0.290E+01 -.377E+02 0.286E+03 -.151E-01 -.456E-02 0.212E-01 0.320E-06 -.515E-07 0.641E-06

-.512E+01 -.128E+03 -.271E+03 0.517E+01 0.128E+03 0.271E+03 -.468E-01 -.871E-01 0.380E-01 0.164E-05 0.101E-06 0.106E-05

0.405E+00 -.137E+03 0.280E+03 -.397E+00 0.137E+03 -.280E+03 -.976E-02 -.128E+00 -.160E-01 -.401E-06 -.482E-06 0.723E-06

0.194E+01 -.343E+03 0.233E+03 -.195E+01 0.344E+03 -.233E+03 0.905E-02 -.461E+00 -.553E-01 -.198E-06 -.518E-07 0.214E-05

-.252E+01 -.197E+03 -.259E+03 0.253E+01 0.197E+03 0.259E+03 -.936E-02 -.199E+00 0.370E-01 0.160E-05 -.160E-07 0.153E-05

0.691E+01 -.447E+03 -.198E+03 -.693E+01 0.448E+03 0.198E+03 0.100E-01 -.112E+01

0.885E-01 0.156E-05 -.192E-05 0.724E-06

-.460E+00 -.451E+03 0.204E+03 0.461E+00 0.452E+03 -.204E+03 -.230E-02 -.108E+01 -.113E+00 -.389E-06 -.112E-05 0.387E-06

0.171E+01 -.203E+03 0.269E+03 -.171E+01 0.203E+03 -.269E+03 -.484E-02 -.931E-01 -.324E-01 -.234E-06 -.551E-06 0.185E-05

-.210E+01 -.338E+03 -.222E+03 0.214E+01 0.338E+03 0.222E+03 -.441E-01 -.606E+00 0.543E-01 0.175E-05 -.216E-05 0.896E-06

0.218E+01 -.136E+03 0.282E+03 -.218E+01 0.136E+03 -.282E+03 -.631E-02 -.126E+00 -.985E-02 0.228E-06 -.933E-06 0.190E-05

0.672E+01 -.339E+03 0.238E+03 -.670E+01 0.340E+03 -.238E+03 -.124E-01 -.462E+00 -.466E-01 0.106E-05 0.418E-06 0.308E-05

0.678E+01 -.193E+03 -.259E+03 -.679E+01 0.193E+03 0.258E+03 0.112E-01 -.147E+00 0.636E-01 0.436E-07 0.252E-06 0.167E-05

0.312E+02 -.427E+03 -.198E+03 -.313E+02 0.428E+03 0.197E+03 0.726E-01 -.965E+00 0.130E+00 -.710E-06 -.104E-05 -.722E-06

0.544E+01 -.449E+03 0.209E+03 -.544E+01 0.450E+03 -.209E+03 0.689E-03 -.108E+01 -.803E-01 0.646E-06 0.105E-06 0.311E-05

0.368E+01 -.201E+03 0.272E+03 -.368E+01 0.201E+03 -.272E+03 -.623E-03 -.979E-01 -.310E-01 0.608E-06 -.300E-06 0.237E-05

0.124E+02 -.332E+03 -.223E+03 -.125E+02 0.332E+03 0.223E+03 0.120E+00 -.536E+00 0.316E-01 0.339E-06 -.139E-05 0.781E-06

0.219E+01 -.133E+03 0.283E+03 -.219E+01 0.133E+03 -.283E+03 0.681E-03 -.128E+00 -

.482E-02 0.631E-06 -.291E-06 0.131E-05

0.492E+01 -.332E+03 0.245E+03 -.488E+01 0.332E+03 -.245E+03 -.316E-01 -.476E+00 -.380E-01 0.136E-05 0.968E-06 0.844E-06

0.112E+02 -.182E+03 -.258E+03 -.112E+02 0.182E+03 0.258E+03 0.478E-01 -.993E-01 -.104E+00 0.827E-07 0.172E-05 0.970E-07

0.316E+02 -.399E+03 -.175E+03 -.319E+02 0.401E+03 0.174E+03 0.291E+00 -.139E+01 0.133E+01 0.394E-05 -.329E-06 0.191E-05

0.930E+01 -.443E+03 0.219E+03 -.929E+01 0.444E+03 -.219E+03 -.510E-02 -.109E+01 -.484E-01 0.149E-05 0.683E-06 0.252E-05

0.168E+01 -.196E+03 0.273E+03 -.169E+01 0.197E+03 -.273E+03 0.563E-02 -.109E+00 -.516E-01 0.946E-06 0.730E-06 0.676E-06

0.172E+02 -.310E+03 -.216E+03 -.175E+02 0.310E+03 0.216E+03 0.325E+00 -.219E+00 0.124E+00 -.538E-06 -.296E-05 -.505E-06

-.104E+01 -.132E+03 0.281E+03 0.103E+01 0.132E+03 -.281E+03 0.103E-01 -.127E+00 -.216E-03 0.337E-06 0.819E-06 -.403E-06

-.513E+01 -.331E+03 0.239E+03 0.512E+01 0.332E+03 -.239E+03 0.862E-02 -.494E+00 -.425E-01 0.157E-07 0.106E-05 -.233E-05

0.151E+01 -.170E+03 -.261E+03 -.163E+01 0.169E+03 0.261E+03 0.117E+00 0.376E+00 -.981E-01 -.582E-05 -.239E-05 -.125E-06

-.670E+01 -.303E+03 -.190E+03 0.626E+01 0.298E+03 0.187E+03 0.466E+00 0.534E+01 0.398E+01 -.367E-05 0.132E-04 0.205E-05

-.629E+00 -.436E+03 0.227E+03 0.626E+00 0.437E+03 -.227E+03 0.163E-02 -.119E+01 -

.478E-01 0.570E-06 0.458E-06 -.718E-06

-.303E+01 -.197E+03 0.268E+03 0.302E+01 0.197E+03 -.268E+03 0.145E-01 -.112E+00 -.432E-01 0.185E-06 0.118E-05 -.173E-05

0.309E+01 -.281E+03 -.215E+03 -.496E+01 0.280E+03 0.214E+03 0.191E+01 0.653E+00 0.826E+00 -.939E-05 0.408E-05 0.188E-05

-.274E+01 -.134E+03 0.277E+03 0.274E+01 0.134E+03 -.277E+03 0.240E-02 -.124E+00 -.189E-01 -.827E-07 0.119E-05 -.173E-05

-.600E+01 -.338E+03 0.230E+03 0.600E+01 0.339E+03 -.230E+03 0.112E-01 -.494E+00 -.467E-01 -.854E-06 0.103E-06 -.304E-05

-.644E+01 -.171E+03 -.257E+03 0.651E+01 0.170E+03 0.257E+03 -.762E-01 0.488E+00 0.133E-01 0.622E-05 0.988E-06 0.565E-06

-.440E+02 -.422E+03 -.184E+03 0.446E+02 0.423E+03 0.183E+03 -.558E+00 -.108E+01 0.641E+00 -.442E-05 -.515E-05 0.292E-05

-.867E+01 -.441E+03 0.211E+03 0.866E+01 0.442E+03 -.211E+03 0.142E-01 -.111E+01 -.762E-01 -.933E-06 -.514E-06 -.294E-05

-.292E+01 -.201E+03 0.265E+03 0.293E+01 0.201E+03 -.265E+03 -.922E-02 -.110E+00 -.208E-01 -.545E-06 0.898E-06 -.216E-05

-.142E+02 -.290E+03 -.209E+03 0.162E+02 0.289E+03 0.209E+03 -.198E+01 0.610E+00 0.781E+00 0.122E-04 -.966E-06 0.116E-05

-.138E+01 -.136E+03 0.277E+03 0.139E+01 0.136E+03 -.277E+03 -.103E-01 -.125E+00 -.243E-01 -.670E-06 0.687E-06 -.930E-06

-.278E+01 -.343E+03 0.230E+03 0.276E+01 0.343E+03 -.230E+03 0.233E-01 -.474E+00 -

.599E-01 -.129E-05 -.384E-06 -.819E-06

-.103E+02 -.189E+03 -.258E+03 0.104E+02 0.189E+03 0.258E+03 -.775E-01 -.140E+00 -.531E-01 -.165E-05 0.189E-05 0.742E-06

-.149E+02 -.446E+03 -.196E+03 0.150E+02 0.447E+03 0.196E+03 -.689E-01 -.112E+01 0.100E+00 0.167E-05 -.245E-05 0.566E-06

-.548E+01 -.448E+03 0.204E+03 0.549E+01 0.449E+03 -.203E+03 -.508E-02 -.108E+01 -.125E+00 -.128E-05 -.173E-05 -.238E-05

-.905E+00 -.203E+03 0.267E+03 0.913E+00 0.203E+03 -.267E+03 -.921E-02 -.102E+00 -.321E-01 -.940E-06 0.131E-06 -.248E-06

-.162E+02 -.329E+03 -.218E+03 0.166E+02 0.329E+03 0.218E+03 -.359E+00 -.481E+00 0.437E-01 -.217E-05 -.446E-05 0.112E-05

-.269E+01 -.252E+03 -.187E+03 0.158E+01 0.243E+03 0.181E+03 0.971E+00 0.764E+01 0.496E+01 -.299E-05 0.755E-05 0.555E-05

0.532E+02 -.518E+03 -.137E+03 -.543E+02 0.522E+03 0.140E+03 0.104E+01 -.395E+01 -.382E+01 0.361E-05 -.331E-05 0.198E-05

-.471E+02 -.587E+03 -.449E+03 0.532E+02 0.640E+03 0.485E+03 -.602E+01 -.514E+02 -.352E+02 -.769E-05 -.197E-04 -.406E-05

0.454E+01 0.280E+02 0.232E+02 -.291E-12 0.136E-11 0.159E-11 -.459E+01 -.280E+02 -.232E+02 -.648E-05 -.761E-04 0.768E-04

POSITION			TOTAL-FORCE (eV/Angst)		
1.24575	4.02870	5.43979	0.000046	0.000985	-0.000365
1.21024	4.07581	8.43726	-0.000976	0.002533	-0.001203
3.70862	4.02890	5.43965	0.000305	0.001857	-0.001050
3.67998	4.07733	8.43690	-0.004039	-0.000497	-0.002956
6.17157	4.02854	5.43942	-0.000016	-0.000174	-0.001709
6.14482	4.08292	8.43295	-0.002848	-0.003379	-0.003264
8.63513	4.02801	5.43869	0.000770	-0.000483	-0.001964
8.60339	4.08732	8.43089	-0.000142	-0.001250	-0.002306
11.09928	4.02784	5.43885	0.000876	0.001931	-0.002677
11.06021	4.08619	8.43099	-0.001744	0.000630	-0.000739
13.56311	4.02807	5.43972	0.000340	0.001585	-0.001579
13.52141	4.08047	8.43349	0.000414	-0.002333	0.000215
2.44241	15.48073	8.85224	-0.000619	-0.005149	0.002153
0.01714	15.44624	5.32469	0.000378	0.001559	-0.001129
4.86040	15.47728	8.86623	0.000614	0.000422	0.000382
2.48016	15.44854	5.27562	0.000355	-0.001188	-0.000421
4.94382	15.44925	5.24869	0.001690	-0.002903	0.000246
12.31531	15.48242	9.00211	-0.002753	0.002877	0.000562
9.86772	15.44556	5.34176	0.000454	-0.001029	0.000880
14.76279	15.48245	8.89951	-0.005830	-0.000253	0.005411

12.33384	15.44510	5.36128	0.001408	-0.003148	-0.001291
7.40743	15.44616	5.26463	0.002356	0.001804	0.001243
6.44846	16.34427	7.40648	-0.003986	0.001707	0.004050
8.60064	16.47644	7.89249	0.009111	0.001354	0.003307
1.24544	5.11881	5.35500	0.000972	0.000330	-0.002524
2.44348	5.83889	8.62292	0.002419	-0.004499	0.001214
0.01380	5.79530	5.28573	0.002061	-0.002567	0.000488
1.21063	5.16420	8.54151	0.000286	-0.000490	-0.001789
2.44351	7.27931	8.74832	-0.000141	-0.001173	-0.000088
3.70866	5.11896	5.35390	-0.000440	-0.001465	0.000276
4.90800	5.84315	8.62123	-0.001024	0.003787	-0.000788
2.47701	5.79561	5.28397	0.001439	-0.000715	-0.002592
3.67679	5.16572	8.54000	-0.000173	0.001650	0.000051
4.90764	7.28398	8.74777	0.000922	-0.000566	0.001076
6.17184	5.11860	5.35433	0.001459	0.000594	0.000808
7.37096	5.84929	8.62094	-0.000715	0.007016	-0.002445
4.94029	5.79548	5.28340	0.000615	-0.002809	-0.001157
6.14080	5.17108	8.53715	-0.002527	0.002645	0.002602
7.37071	7.28983	8.75132	-0.001969	0.001660	0.000159
8.63543	5.11820	5.35521	0.001259	0.001585	-0.001157
9.83233	5.85166	8.62337	0.002747	0.000087	-0.001117
7.40374	5.79498	5.28512	0.003442	-0.002825	-0.001320

8.60194	5.17528	8.53759	-0.001715	-0.000188	-0.000064
9.83204	7.29110	8.75719	-0.001907	-0.001922	-0.002344
11.09930	5.11814	5.35578	-0.000879	-0.003112	-0.001439
12.29449	5.84673	8.62385	0.000139	0.005606	-0.002202
9.86750	5.79468	5.28678	-0.000761	-0.000878	0.001563
11.06261	5.17409	8.53894	0.002534	0.002898	-0.000257
12.29428	7.28729	8.75533	-0.004460	0.001305	-0.001491
13.56278	5.11829	5.35605	0.002666	0.000739	-0.002072
14.75895	5.83988	8.62434	-0.000232	-0.002686	-0.002223
12.33118	5.79480	5.28692	-0.004487	-0.001604	0.002610
13.52535	5.16844	8.54022	-0.003563	0.003919	-0.001284
14.75917	7.28012	8.75179	0.000750	0.002546	-0.000666
0.01434	7.23830	5.19017	0.000076	-0.000195	0.000076
1.24689	9.38061	5.13160	0.000519	-0.001830	-0.000006
1.21085	7.98059	8.79588	-0.000800	-0.000497	0.001545
2.44214	10.12243	8.87141	-0.001115	0.002218	-0.005036
0.01532	10.08686	5.14049	-0.002014	-0.000129	-0.002382
1.24606	7.94244	5.15775	0.002030	-0.002602	0.000845
1.21082	9.41592	8.85782	-0.000201	0.004588	0.000219
2.44072	11.55513	8.88414	-0.006273	-0.001499	0.001851
2.47747	7.23842	5.18585	0.002789	0.002913	0.001301
3.70997	9.38055	5.12566	-0.001086	-0.002988	0.000043

3.67534	7.98360	8.79349	-0.000625	0.001120	0.000948
4.90487	10.12925	8.87518	0.000732	-0.001259	-0.000051
2.47867	10.08713	5.12695	-0.002263	0.001529	0.000774
3.70939	7.94242	5.15441	0.000805	-0.004007	-0.001682
3.67589	9.41970	8.85445	-0.001624	0.002031	-0.000122
4.90263	11.56506	8.89086	0.000410	0.003071	0.000826
4.94085	7.23830	5.18552	-0.004693	0.002282	0.000823
6.17318	9.38002	5.13173	0.002063	0.002151	0.001823
6.13864	7.99044	8.79647	0.002368	-0.000626	-0.001667
7.36780	10.13760	8.89473	-0.000255	0.002778	0.000996
4.94196	10.08682	5.12700	0.004118	0.001494	-0.001137
6.17284	7.94199	5.15766	-0.000074	0.000530	0.003041
6.13939	9.42660	8.86164	0.000133	0.000004	-0.002049
7.36410	11.57721	8.92935	0.000097	-0.000131	0.003111
7.40426	7.23794	5.19012	0.002135	0.001784	0.001072
8.63700	9.37970	5.14543	-0.000467	0.003003	0.000935
8.60086	7.99568	8.80617	0.001347	-0.001282	-0.001222
9.83068	10.14286	8.92842	-0.002236	0.000276	-0.000208
7.40553	10.08627	5.14064	0.001154	-0.003612	0.003169
8.63637	7.94166	5.16555	0.002639	0.001754	-0.001394
8.60077	9.43254	8.88532	-0.005984	0.003364	-0.001258
9.82927	11.58244	9.00096	0.000636	0.007799	0.001040

9.86805	7.23787	5.19489	-0.000371	0.000137	-0.000246
11.10106	9.37979	5.15156	-0.003859	-0.000994	0.000649
11.06331	7.99411	8.80818	-0.000470	-0.002147	-0.000014
12.29815	10.12943	8.90340	-0.000774	-0.001155	0.001788
9.86930	10.08593	5.15631	-0.005481	-0.001548	0.001414
11.10021	7.94175	5.16862	-0.000631	-0.003093	0.001407
11.06206	9.43062	8.88839	0.004283	0.002550	0.002070
12.30255	11.56557	8.94694	0.002560	0.000362	-0.001221
12.33169	7.23799	5.19447	-0.001007	0.000257	-0.001760
13.56437	9.38021	5.14435	0.000670	0.001693	-0.000587
13.52754	7.98555	8.80171	-0.000760	-0.002906	-0.003112
14.76233	10.12320	8.88285	-0.005744	0.000340	-0.001659
12.33257	10.08637	5.15511	0.002689	0.000482	-0.001526
13.56350	7.94214	5.16485	-0.000089	-0.000911	-0.000360
13.52731	9.42040	8.86925	0.000288	0.003534	-0.000417
14.76430	11.55727	8.90646	-0.002813	0.000301	0.001471
0.01611	11.52516	5.16621	-0.001067	-0.002500	0.000389
1.24770	13.67535	5.22209	0.002047	-0.001767	-0.002455
1.21217	12.26335	8.89409	0.001486	-0.000416	0.001141
2.43998	14.38728	8.86748	-0.001685	-0.001381	0.000830
0.01699	14.35408	5.27295	-0.000651	-0.001325	-0.001940
1.24794	12.22963	5.17275	0.001026	0.000934	-0.001339

1.21434	13.70818	8.88771	-0.000131	0.004666	0.003684
2.47958	11.52580	5.14547	-0.001617	-0.000161	-0.001494
3.71218	13.67636	5.19535	0.004470	0.001202	0.001124
3.66932	12.26248	8.88184	-0.002767	0.000190	-0.000607
4.89370	14.38589	8.86075	0.001987	-0.003159	-0.003050
2.48000	14.35596	5.23149	0.001218	-0.001824	0.001689
3.71150	12.23022	5.15602	0.000909	-0.004455	0.001029
3.66212	13.70366	8.87117	-0.005652	0.006319	-0.001573
4.94290	11.52542	5.14351	-0.000082	-0.001693	-0.001604
6.17627	13.67505	5.20032	0.000639	0.001332	0.000141
6.13145	12.27911	8.90591	0.004040	0.005220	0.004516
7.36614	14.42967	8.88203	-0.018037	-0.003435	-0.000131
4.94347	14.35627	5.21375	0.000215	-0.002665	0.001185
6.17493	12.22917	5.16623	-0.001379	-0.001015	0.001520
6.11879	13.72336	8.87765	0.010228	0.009494	0.001897
7.40625	11.52413	5.16368	0.000896	-0.003209	0.000357
8.63876	13.67323	5.24377	0.002006	0.003002	-0.001243
8.58939	12.29067	9.00208	0.002496	-0.007022	-0.005660
9.83855	14.39048	9.30305	0.033192	0.413797	0.237461
7.40672	14.35386	5.23530	-0.001049	-0.001430	-0.000429
8.63820	12.22778	5.19800	0.000371	-0.001233	0.001035
8.55571	13.73596	9.04598	0.049708	0.050446	0.030588

9.86985	11.52338	5.18893	0.001737	-0.001777	-0.000124
11.10099	13.67352	5.27669	0.003007	-0.000061	-0.000938
11.07378	12.27333	9.00891	-0.004888	-0.001855	-0.007941
12.30694	14.38896	9.00333	0.015377	-0.008463	0.003289
9.86934	14.35300	5.29564	0.002978	-0.001005	-0.000368
11.10161	12.22804	5.21650	-0.001153	-0.002666	0.001068
11.11464	13.70636	9.07877	-0.049159	0.055941	0.028204
12.33326	11.52411	5.18815	-0.000896	0.000413	0.000540
13.56430	13.67399	5.25995	0.001821	0.000621	0.000119
13.53626	12.26601	8.93587	-0.001352	0.003136	0.001735
14.76266	14.38906	8.90426	0.000508	-0.001504	0.003412
12.33397	14.35288	5.30710	0.002668	-0.002715	-0.001638
13.56505	12.22870	5.20105	0.000042	0.000163	-0.001123
13.54921	13.70690	8.94399	-0.006102	0.003567	0.004239
9.91126	15.54685	9.99472	-0.131556	-1.492130	-0.905437
7.28864	16.40884	8.69813	-0.009333	-0.012874	-0.007165
10.02526	16.50365	10.64498	0.115771	0.976037	0.633326

---

total drift:	-0.044234	0.023294	-0.023658

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

---

free energy TOTEN = -1209.37815505 eV

energy without entropy= -1209.37815505 energy(sigma->0) = -1209.37815505

d Force =-0.9518943E-02[-0.244E-01, 0.532E-02] d Energy =-0.9475737E-02-0.432E-04

d Force = 0.3691188E+01[0.366E+01, 0.372E+01] d Ewald = 0.3691029E+01 0.160E-03

POTLOK: cpu time 0.1989: real time 0.1996

---

stress matrix after NEB project (eV)

-17.73482 -0.17432 0.11662

-0.17432 -15.02632 0.70574

0.11662 0.70574 -18.84224

FORCES: max atom, RMS 1.750308 0.173612

FORCE total and by dimension 2.104930 1.492130

Stress total and by dimension 29.940409 18.842242

Finite differences progress:

Degree of freedom: 2/ 6

Displacement: 1/ 2

Total: 3/ 12

LATTYP: Found a simple orthorhombic cell.

ALAT = 14.7806000000

B/A-ratio = 1.2466138046

C/A-ratio = 1.4433717170

Lattice vectors:

A1 = (-14.7806000000, 0.0000000000, 0.0000000000)

A2 = (0.0000000000, 0.0000000000, -18.4257000000)

A3 = (0.0000000000, -21.3339000000, 0.0000000000)

Analysis of symmetry for initial positions (statically):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The static configuration has the point symmetry C_1 .

Analysis of symmetry for dynamics (positions and initial velocities):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The dynamic configuration has the point symmetry C_1 .

Analysis of constrained symmetry for selective dynamics:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The constrained configuration has the point symmetry C_1 .

Analysis of structural, dynamic, and magnetic symmetry:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The magnetic configuration has the point symmetry C_1 .

Subroutine INISYM returns: Found 1 space group operations

(whereof 1 operations are pure point group operations),

and found 1 'primitive' translations

KPOINTS: KPT-Resolved Value to Generate K-Mesh: 0

Automatic generation of k-mesh.

Space group operators:

irot	det(A)	alpha	n_x	n_y	n_z	tau_x	tau_y	tau_z
1	1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Subroutine IBZKPT returns following result:

==========

Found 1 irreducible k-points:

Following reciprocal coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

Following cartesian coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

WAVPRE: cpu time 0.1206: real time 0.1330

FEWALD: cpu time 0.0027: real time 0.0027

ORTHCH: cpu time 0.9982: real time 1.0013

LOOP+: cpu time 179.8284: real time 180.8808

---------- Iteration 5(1) ----------

POTLOK: cpu time 0.1684: real time 0.1797

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9254: real time 1.9317

RMM-DIIS: cpu time 7.2725: real time 7.3149

ORTHCH: cpu time 0.3556: real time 0.3567

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5267: real time 0.5285

MIXING: cpu time 0.0043: real time 0.0044

LOOP: cpu time 10.2634: real time 10.3265

eigenvalue-minimisations : 1956

total energy-change (2. order) :-0.6961632E-02 (-0.2175637E+00)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7333105 magnetization 0.0541906

Broyden mixing:

rms(total) = 0.58102E-01 rms(broyden)= 0.57904E-01

rms(prec) = 0.60607E-01

weight for this iteration 100.00

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107342.18780223

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79514203

PAW double counting = 52183.16710294 -52246.09423871

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5812.27908553

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76741286 eV

energy without entropy = -1202.76741286 energy(sigma->0) = -1202.76741286

---------- Iteration 5(2) ----------

POTLOK: cpu time 0.1715: real time 0.1826

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9271: real time 1.9341

RMM-DIIS: cpu time 7.0911: real time 7.1172

ORTHCH: cpu time 0.3551: real time 0.3562

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5245: real time 0.5261

MIXING: cpu time 0.0049: real time 0.0049

LOOP: cpu time 10.0848: real time 10.1316

eigenvalue-minimisations : 1920

total energy-change (2. order) : 0.5270256E-02 (-0.2068401E-02)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7336497 magnetization 0.0541972

Broyden mixing:

rms(total) = 0.35720E-01 rms(broyden)= 0.35697E-01

rms(prec) = 0.37267E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.2657

2.2657

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107341.12148652

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78433281

PAW double counting = 52176.80514563 -52239.72554719

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.33605597

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76214260 eV

energy without entropy = -1202.76214260 energy(sigma->0) = -1202.76214260

---------- Iteration 5(3) ----------

POTLOK: cpu time 0.1658: real time 0.1907

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9245: real time 1.9315

RMM-DIIS: cpu time 7.2338: real time 7.2568

ORTHCH: cpu time 0.3520: real time 0.3531

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5253: real time 0.5270

MIXING: cpu time 0.0051: real time 0.0051

LOOP: cpu time 10.2170: real time 10.2747

eigenvalue-minimisations : 1946

total energy-change (2. order) : 0.2164327E-02 (-0.6395618E-03)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7341954 magnetization 0.0542518

Broyden mixing:

rms(total) = 0.89841E-02 rms(broyden)= 0.89739E-02

rms(prec) = 0.98567E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5968

1.0795 2.1140

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107339.50883606

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77807275

PAW double counting = 52168.95584349 -52231.86807555

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.94845154

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.75997828 eV

energy without entropy = -1202.75997828 energy(sigma->0) = -1202.75997828

---------- Iteration 5(4) ----------

POTLOK: cpu time 0.1659: real time 0.1842

SETDIJ: cpu time 0.0102: real time 0.0103

EDDIAG: cpu time 1.9265: real time 1.9328

RMM-DIIS: cpu time 7.1611: real time 7.1818

ORTHCH: cpu time 0.3522: real time 0.3532

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5246: real time 0.5261

MIXING: cpu time 0.0052: real time 0.0053

LOOP: cpu time 10.1461: real time 10.1940

eigenvalue-minimisations : 1927

total energy-change (2. order) : 0.1225504E-03 (-0.3856869E-04)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7335594 magnetization 0.0542400

Broyden mixing:

rms(total) = 0.49018E-02 rms(broyden)= 0.48991E-02

rms(prec) = 0.52936E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5160

2.1981 1.5724 0.7776

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107339.43945424

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78025351

PAW double counting = 52169.89013286 -52232.80328641

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.01897009

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.75985573 eV

energy without entropy = -1202.75985573 energy(sigma->0) = -1202.75985573

---------- Iteration 5(5) ----------

POTLOK: cpu time 0.1642: real time 0.1648

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9278: real time 1.9336

RMM-DIIS: cpu time 7.3516: real time 7.3741

ORTHCH: cpu time 0.3543: real time 0.3552

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5254: real time 0.5271

MIXING: cpu time 0.0055: real time 0.0055

LOOP: cpu time 10.3391: real time 10.3707

eigenvalue-minimisations : 1953

total energy-change (2. order) :-0.4141794E-04 (-0.8578577E-05)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7336830 magnetization 0.0542410

Broyden mixing:

rms(total) = 0.20331E-02 rms(broyden)= 0.20325E-02

rms(prec) = 0.24605E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4703

2.4399 1.6513 0.9516 0.8384

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107339.19070649

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77821329

PAW double counting = 52170.30798454 -52233.22030920

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.26654792

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.75989714 eV

energy without entropy = -1202.75989714 energy(sigma->0) = -1202.75989714

---------- Iteration 5(6) ----------

POTLOK: cpu time 0.1658: real time 0.1845

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9276: real time 1.9340

RMM-DIIS: cpu time 7.1404: real time 7.1668

ORTHCH: cpu time 0.3519: real time 0.3531

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5255: real time 0.5269

MIXING: cpu time 0.0058: real time 0.0058

LOOP: cpu time 10.1276: real time 10.1817

eigenvalue-minimisations : 1913

total energy-change (2. order) :-0.6337096E-04 (-0.1297635E-05)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7337157 magnetization 0.0542410

Broyden mixing:

rms(total) = 0.10116E-02 rms(broyden)= 0.10112E-02

rms(prec) = 0.14010E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4056

2.5080 1.8333 1.1508 0.8327 0.7031

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.98224196

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77732959

PAW double counting = 52170.85015434 -52233.76212387

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.47454725

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.75996052 eV

energy without entropy = -1202.75996052 energy(sigma->0) = -1202.75996052

---------- Iteration 5(7) ----------

POTLOK: cpu time 0.1731: real time 0.1768

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9378: real time 1.9434

RMM-DIIS: cpu time 7.0011: real time 7.0435

ORTHCH: cpu time 0.3541: real time 0.3550

DOS: cpu time 0.0003: real time 0.0003

CHARGE: cpu time 0.5290: real time 0.5304

MIXING: cpu time 0.0056: real time 0.0056

LOOP: cpu time 10.0113: real time 10.0651

eigenvalue-minimisations : 1877

total energy-change (2. order) :-0.7092879E-04 (-0.5514477E-06)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7337058 magnetization 0.0542426

Broyden mixing:

rms(total) = 0.59948E-03 rms(broyden)= 0.59934E-03

rms(prec) = 0.94404E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4507

2.7038 2.2060 1.3481 0.9189 0.9189 0.6085

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.82846681

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77672448

PAW double counting = 52171.29917962 -52234.21101324

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.62792413

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76003144 eV

energy without entropy = -1202.76003144 energy(sigma->0) = -1202.76003144

---------- Iteration 5(8) ----------

POTLOK: cpu time 0.1644: real time 0.1660

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9233: real time 1.9296

RMM-DIIS: cpu time 6.5759: real time 6.5966

ORTHCH: cpu time 0.3514: real time 0.3523

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5271: real time 0.5289

MIXING: cpu time 0.0056: real time 0.0056

LOOP: cpu time 9.5582: real time 9.5896

eigenvalue-minimisations : 1785

total energy-change (2. order) :-0.6803446E-04 (-0.4161448E-06)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7336893 magnetization 0.0542437

Broyden mixing:

rms(total) = 0.31218E-03 rms(broyden)= 0.31208E-03

rms(prec) = 0.61397E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4604

2.8270 2.3090 1.4734 1.0720 1.0720 0.8620 0.6078

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.68231889

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77606381

PAW double counting = 52171.63545621 -52234.54716916

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.77360009

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76009948 eV

energy without entropy = -1202.76009948 energy(sigma->0) = -1202.76009948

---------- Iteration 5(9) ----------

POTLOK: cpu time 0.1652: real time 0.1781

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9317: real time 1.9381

RMM-DIIS: cpu time 6.4455: real time 6.4764

ORTHCH: cpu time 0.3511: real time 0.3523

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5266: real time 0.5284

MIXING: cpu time 0.0064: real time 0.0065

LOOP: cpu time 9.4370: real time 9.4903

eigenvalue-minimisations : 1773

total energy-change (2. order) :-0.8120634E-04 (-0.5495803E-06)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7336694 magnetization 0.0542440

Broyden mixing:

rms(total) = 0.19541E-03 rms(broyden)= 0.19526E-03

rms(prec) = 0.38205E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5582

3.4083 2.5527 1.9778 1.1879 0.9949 0.9949 0.7336 0.6151

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.52170678

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77525533

PAW double counting = 52171.79569983 -52234.70730989

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.93358781

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76018069 eV

energy without entropy = -1202.76018069 energy(sigma->0) = -1202.76018069

---------- Iteration 5(10) ----------

POTLOK: cpu time 0.1646: real time 0.1811

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9286: real time 1.9353

RMM-DIIS: cpu time 6.3194: real time 6.3418

ORTHCH: cpu time 0.3514: real time 0.3522

DOS: cpu time 0.0004: real time 0.0003

CHARGE: cpu time 0.5282: real time 0.5298

MIXING: cpu time 0.0068: real time 0.0067

LOOP: cpu time 9.3094: real time 9.3574

eigenvalue-minimisations : 1738

total energy-change (2. order) :-0.6628858E-04 (-0.5378547E-06)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7336630 magnetization 0.0542448

Broyden mixing:

rms(total) = 0.12594E-03 rms(broyden)= 0.12579E-03

rms(prec) = 0.21315E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6241

4.2817 2.5662 2.1288 1.2412 1.2412 0.9212 0.9212 0.6977 0.6177

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.38130320

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77453694

PAW double counting = 52171.84807916 -52234.75960404

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.07342447

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76024697 eV

energy without entropy = -1202.76024697 energy(sigma->0) = -1202.76024697

---------- Iteration 5(11) ----------

POTLOK: cpu time 0.1668: real time 0.1841

```
      SETDIJ:    cpu time       0.0101: real time       0.0101
      EDDIAG:    cpu time       1.9277: real time       1.9345
    RMM-DIIS:    cpu time       6.0769: real time       6.1047
      ORTHCH:    cpu time       0.3510: real time       0.3521
         DOS:    cpu time       0.0004: real time       0.0004
      CHARGE:    cpu time       0.5267: real time       0.5285
      MIXING:    cpu time       0.0070: real time       0.0070
      ----------------------------------------
        LOOP:    cpu time       9.0664: real time       9.1212

eigenvalue-minimisations    :    1657
total energy-change (2. order) :-0.2986547E-04    (-0.1735327E-06)
number of electron          518.9999729 magnetization             0.9999998
augmentation part             11.7336630 magnetization             0.0542449

Broyden mixing:
  rms(total) = 0.80347E-04        rms(broyden)= 0.80281E-04
  rms(prec ) = 0.13536E-03
  weight for this iteration         100.00

eigenvalues of (default mixing * dielectric matrix)
  average eigenvalue GAMMA=      1.7729
```

5.5502 2.6565 2.2482 1.9149 1.1336 1.1336 0.9032 0.9032 0.6221 0.6631

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.32254338

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77427601

PAW double counting = 52171.81632837 -52234.72783662

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.13196985

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76027684 eV

energy without entropy = -1202.76027684 energy(sigma->0) = -1202.76027684

---------- Iteration 5(12) ----------

POTLOK: cpu time 0.1648: real time 0.1669

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9252: real time 1.9320

RMM-DIIS: cpu time 5.9365: real time 5.9613

ORTHCH: cpu time 0.3523: real time 0.3535

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5276: real time 0.5295

MIXING: cpu time 0.0074: real time 0.0075

LOOP: cpu time 8.9243: real time 8.9610

eigenvalue-minimisations : 1614

total energy-change (2. order) :-0.2038423E-04 (-0.9111422E-07)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7336581 magnetization 0.0542449

Broyden mixing:

rms(total) = 0.43614E-04 rms(broyden)= 0.43575E-04

rms(prec) = 0.77171E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8098

6.2479 2.7548 2.4148 1.9967 1.2461 1.2461 0.9576 0.9576 0.8090 0.6238

0.6529

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.28880503

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77419275

PAW double counting = 52171.77034573 -52234.68186976

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.16562955

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76029722 eV

energy without entropy = -1202.76029722 energy(sigma->0) = -1202.76029722

---------- Iteration 5(13) ----------

POTLOK: cpu time 0.1683: real time 0.1703

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9216: real time 1.9281

RMM-DIIS: cpu time 5.5372: real time 5.5534

ORTHCH: cpu time 0.3528: real time 0.3537

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5280: real time 0.5298

MIXING: cpu time 0.0078: real time 0.0078

LOOP: cpu time 8.5261: real time 8.5536

eigenvalue-minimisations : 1495

total energy-change (2. order) :-0.9471638E-05 (-0.2989513E-07)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7336588 magnetization 0.0542449

Broyden mixing:

rms(total) = 0.29171E-04 rms(broyden)= 0.29163E-04

rms(prec) = 0.49484E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8549

6.7288 2.9375 2.6649 1.9830 1.8072 1.1424 1.1424 0.9254 0.9254 0.7324

0.6256 0.6433

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.27672075

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77416621

PAW double counting = 52171.76334561 -52234.67486727

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.17769914

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76030670 eV

energy without entropy = -1202.76030670 energy(sigma->0) = -1202.76030670

---------- Iteration 5(14) ----------

POTLOK: cpu time 0.1672: real time 0.1862

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9264: real time 1.9322

RMM-DIIS: cpu time 5.2624: real time 5.3364

ORTHCH: cpu time 0.3508: real time 0.3518

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5271: real time 0.5287

MIXING: cpu time 0.0080: real time 0.0080

LOOP: cpu time 8.2523: real time 8.3539

eigenvalue-minimisations : 1449

total energy-change (2. order) :-0.5957125E-05 (-0.1714253E-07)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7336581 magnetization 0.0542449

Broyden mixing:

rms(total) = 0.18140E-04 rms(broyden)= 0.18132E-04

rms(prec) = 0.29320E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9301

7.1739 3.8343 2.6631 2.3105 1.8488 1.2480 1.2480 0.9825 0.9825 0.8438

0.6946 0.6310 0.6310

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.27083600

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77416503

PAW double counting = 52171.77280933 -52234.68432980

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.18358985

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76031265 eV

energy without entropy = -1202.76031265 energy(sigma->0) = -1202.76031265

---------- Iteration 5(15) ----------

POTLOK: cpu time 0.1664: real time 0.1789

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9256: real time 1.9322

RMM-DIIS: cpu time 4.9807: real time 5.0043

ORTHCH: cpu time 0.3524: real time 0.3533

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5275: real time 0.5290

MIXING: cpu time 0.0087: real time 0.0088

LOOP: cpu time 7.9718: real time 8.0170

eigenvalue-minimisations : 1378

total energy-change (2. order) :-0.2751207E-05 (-0.6660790E-08)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7336576 magnetization 0.0542448

Broyden mixing:

rms(total) = 0.10555E-04 rms(broyden)= 0.10548E-04

rms(prec) = 0.16934E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9682

7.6829 4.4920 2.5896 2.5177 1.8771 1.5030 1.1239 1.1239 0.9618 0.9618

0.7922 0.6743 0.6277 0.6277

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.26822594

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77416491

PAW double counting = 52171.78264361 -52234.69416397

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.18620266

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76031540 eV

energy without entropy = -1202.76031540 energy(sigma->0) = -1202.76031540

---------- Iteration 5(16) ----------

POTLOK: cpu time 0.1680: real time 0.1805

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9244: real time 1.9308

RMM-DIIS: cpu time 4.7641: real time 4.7823

ORTHCH: cpu time 0.3514: real time 0.3524

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5274: real time 0.5290

MIXING: cpu time 0.0092: real time 0.0092

LOOP: cpu time 7.7549: real time 7.7946

eigenvalue-minimisations : 1283

total energy-change (2. order) :-0.1252163E-05 (-0.1880261E-08)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7336580 magnetization 0.0542448

Broyden mixing:

rms(total) = 0.60868E-05 rms(broyden)= 0.60822E-05

rms(prec) = 0.10769E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9720

7.9355 4.8104 2.6620 2.5485 2.0323 1.5440 1.2307 1.2307 0.9858 0.9858

0.9317 0.7640 0.6679 0.6256 0.6256

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.26732957

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77416300

PAW double counting = 52171.78616762 -52234.69768715

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.18709919

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76031666 eV

energy without entropy = -1202.76031666 energy(sigma->0) = -1202.76031666

---------- Iteration 5(17) ----------

POTLOK: cpu time 0.1725: real time 0.1730

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9282: real time 1.9335

RMM-DIIS: cpu time 4.7358: real time 4.7588

ORTHCH: cpu time 0.3522: real time 0.3531

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5276: real time 0.5291

MIXING: cpu time 0.0094: real time 0.0094

LOOP: cpu time 7.7362: real time 7.7675

eigenvalue-minimisations : 1280

total energy-change (2. order) :-0.1180255E-05 (-0.9748833E-09)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7336579 magnetization 0.0542448

Broyden mixing:

rms(total) = 0.42278E-05 rms(broyden)= 0.42256E-05

rms(prec) = 0.68691E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9992

8.1497 5.1564 2.9213 2.5432 2.2380 1.7642 1.5362 1.1325 1.1325 0.9702

0.9702 0.8391 0.7223 0.6633 0.6243 0.6243

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.26682937

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77417064

PAW double counting = 52171.78593159 -52234.69745218

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.18760714

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76031784 eV

energy without entropy = -1202.76031784 energy(sigma->0) = -1202.76031784

---------- Iteration 5(18) ----------

POTLOK: cpu time 0.1667: real time 0.1835

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9246: real time 1.9310

RMM-DIIS: cpu time 4.7563: real time 4.7732

ORTHCH: cpu time 0.3535: real time 0.3545

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5275: real time 0.5292

MIXING: cpu time 0.0102: real time 0.0102

LOOP: cpu time 7.7493: real time 7.7921

eigenvalue-minimisations : 1276

total energy-change (2. order) :-0.1013832E-05 (-0.5644667E-09)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7336577 magnetization 0.0542448

Broyden mixing:

rms(total) = 0.25572E-05 rms(broyden)= 0.25561E-05

rms(prec) = 0.39363E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0421

8.4456 5.5119 3.5764 2.5549 2.4657 1.9781 1.4710 1.2010 1.2010 0.9867

0.9867 0.9665 0.7846 0.6887 0.6494 0.6224 0.6253

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.26656626

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77417820

PAW double counting = 52171.78435804 -52234.69587989

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.18787758

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76031885 eV

energy without entropy = -1202.76031885 energy(sigma->0) = -1202.76031885

---------- Iteration 5(19) ----------

POTLOK: cpu time 0.1684: real time 0.1817

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9277: real time 1.9344

RMM-DIIS: cpu time 4.3655: real time 4.3794

ORTHCH: cpu time 0.3508: real time 0.3519

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5268: real time 0.5285

MIXING: cpu time 0.0101: real time 0.0101

LOOP: cpu time 7.3599: real time 7.3964

eigenvalue-minimisations : 1096

total energy-change (2. order) :-0.2101879E-06 (-0.1725633E-09)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7336578 magnetization 0.0542448

Broyden mixing:

rms(total) = 0.14886E-05 rms(broyden)= 0.14880E-05

rms(prec) = 0.24400E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0536

8.5261 5.9064 3.8680 2.5468 2.5468 1.9458 1.5620 1.4105 1.1429 1.1429

1.1412 0.9348 0.9348 0.7827 0.6832 0.6389 0.6211 0.6287

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.26643855

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77417947

PAW double counting = 52171.78339280 -52234.69491455

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.18800687

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76031906 eV

energy without entropy = -1202.76031906 energy(sigma->0) = -1202.76031906

---------- Iteration 5(20) ----------

POTLOK: cpu time 0.1653: real time 0.1657

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9268: real time 1.9329

RMM-DIIS: cpu time 4.1620: real time 4.1738

ORTHCH: cpu time 0.3504: real time 0.3515

DOS: cpu time 0.0003: real time 0.0003

LOOP: cpu time 6.6148: real time 6.6343

eigenvalue-minimisations : 973

total energy-change (2. order) :-0.6263872E-07 (-0.7295142E-10)

number of electron 518.9999729 magnetization 0.9999998

augmentation part 11.7336578 magnetization 0.0542448

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91333.00078184

-Hartree energ DENC = -107338.26631824

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77417752

PAW double counting = 52171.78311498 -52234.69463584

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.18812617

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76031912 eV

energy without entropy = -1202.76031912 energy(sigma->0) = -1202.76031912

---

average (electrostatic) potential at core

the test charge radii are 0.5201 0.6991 1.0621 0.7215

(the norm of the test charge is 1.0000)

1 -40.7566	2 -40.7547	3 -40.7559	4 -40.7547	5 -40.7566
6 -40.7588	7 -40.7562	8 -40.7639	9 -40.7558	10 -40.7634
11 -40.7573	12 -40.7593	13 -40.6570	14 -40.7008	15 -40.7759
16 -40.7031	17 -40.6964	18 -40.8605	19 -40.6833	20 -40.6735
21 -40.6929	22 -40.6652	23 -40.0792	24 -40.1206	25 -57.4631
26 -57.6745	27 -57.6611	28 -57.4732	29 -57.6688	30 -57.4631
31 -57.6743	32 -57.6607	33 -57.4712	34 -57.6736	35 -57.4639
36 -57.6761	37 -57.6607	38 -57.4733	39 -57.6793	40 -57.4629
41 -57.6801	42 -57.6609	43 -57.4781	44 -57.6938	45 -57.4629
46 -57.6791	47 -57.6617	48 -57.4784	49 -57.6850	50 -57.4641
51 -57.6758	52 -57.6614	53 -57.4761	54 -57.6715	55 -57.6411
56 -57.6674	57 -57.6922	58 -57.6895	59 -57.6711	60 -57.6737
61 -57.6960	62 -57.6812	63 -57.6414	64 -57.6668	65 -57.6943
66 -57.7006	67 -57.6694	68 -57.6735	69 -57.6997	70 -57.7074
71 -57.6409	72 -57.6682	73 -57.7019	74 -57.7272	75 -57.6702
76 -57.6741	77 -57.7117	78 -57.7575	79 -57.6410	80 -57.6708
81 -57.7155	82 -57.7575	83 -57.6735	84 -57.6756	85 -57.7429
86 -57.8472	87 -57.6435	88 -57.6715	89 -57.7174	90 -57.7227
91 -57.6782	92 -57.6758	93 -57.7476	94 -57.7661	95 -57.6418
96 -57.6697	97 -57.7013	98 -57.6966	99 -57.6755	100 -57.6746
101 -57.7136	102 -57.6923	103 -57.6651	104 -57.6361	105 -57.6523
106 -57.2987	107 -57.3934	108 -57.6361	109 -57.6052	110 -57.6640

111 -57.6360	112 -57.6488	113 -57.3181	114 -57.3992	115 -57.6353
116 -57.6070	117 -57.6632	118 -57.6275	119 -57.7045	120 -57.6936
121 -57.3927	122 -57.6340	123 -57.7166	124 -57.6641	125 -57.6302
126 -57.8388	127 -58.3243	128 -57.3657	129 -57.6393	130 -58.1521
131 -57.6721	132 -57.6396	133 -57.8066	134 -57.4268	135 -57.3772
136 -57.6432	137 -58.0883	138 -57.6686	139 -57.6354	140 -57.6778
141 -57.3086	142 -57.3833	143 -57.6387	144 -57.6551	145 -60.7792
146 -57.3103	147 -81.1350			

E-fermi : -2.3506 XC(G=0): -2.7341 alpha+bet : -2.2521

spin component 1

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-26.7220	1.00000
2	-21.5748	1.00000
3	-21.4767	1.00000
4	-21.1085	1.00000

5	-21.0742	1.00000
6	-21.0214	1.00000
7	-20.9837	1.00000
8	-20.9818	1.00000
9	-20.8965	1.00000
10	-20.5683	1.00000
11	-20.5091	1.00000
12	-20.4172	1.00000
13	-20.4031	1.00000
14	-20.1370	1.00000
15	-19.9816	1.00000
16	-19.7166	1.00000
17	-19.6334	1.00000
18	-19.6052	1.00000
19	-19.5896	1.00000
20	-19.5336	1.00000
21	-19.5319	1.00000
22	-19.5041	1.00000
23	-19.4862	1.00000
24	-19.1239	1.00000
25	-19.0813	1.00000
26	-18.9849	1.00000

27	-18.9699	1.00000
28	-18.9091	1.00000
29	-18.7391	1.00000
30	-18.5171	1.00000
31	-18.3650	1.00000
32	-18.2808	1.00000
33	-18.2573	1.00000
34	-18.1898	1.00000
35	-18.1877	1.00000
36	-18.0851	1.00000
37	-18.0811	1.00000
38	-17.5766	1.00000
39	-17.3193	1.00000
40	-17.2937	1.00000
41	-17.2882	1.00000
42	-17.2157	1.00000
43	-17.2085	1.00000
44	-17.1856	1.00000
45	-17.0290	1.00000
46	-16.9558	1.00000
47	-16.9381	1.00000
48	-16.8984	1.00000

49	-16.8965	1.00000
50	-16.8552	1.00000
51	-16.8468	1.00000
52	-16.8275	1.00000
53	-16.8244	1.00000
54	-16.7343	1.00000
55	-16.7313	1.00000
56	-16.1949	1.00000
57	-15.7348	1.00000
58	-15.6974	1.00000
59	-15.6659	1.00000
60	-15.6432	1.00000
61	-15.6210	1.00000
62	-15.5587	1.00000
63	-15.5547	1.00000
64	-15.1825	1.00000
65	-14.8155	1.00000
66	-14.6156	1.00000
67	-14.5828	1.00000
68	-14.5397	1.00000
69	-14.5034	1.00000
70	-14.4735	1.00000

71	-14.4485	1.00000
72	-14.3395	1.00000
73	-14.3109	1.00000
74	-14.2847	1.00000
75	-14.2774	1.00000
76	-14.1872	1.00000
77	-14.1834	1.00000
78	-13.8940	1.00000
79	-13.7670	1.00000
80	-13.5996	1.00000
81	-13.5535	1.00000
82	-13.5346	1.00000
83	-13.5035	1.00000
84	-13.4525	1.00000
85	-13.3689	1.00000
86	-13.3505	1.00000
87	-13.1945	1.00000
88	-12.7920	1.00000
89	-12.7651	1.00000
90	-12.7326	1.00000
91	-12.7010	1.00000
92	-12.6916	1.00000

93	-12.6293	1.00000
94	-12.4659	1.00000
95	-12.4510	1.00000
96	-12.3873	1.00000
97	-12.3297	1.00000
98	-12.2178	1.00000
99	-12.2082	1.00000
100	-12.1704	1.00000
101	-11.9447	1.00000
102	-11.6905	1.00000
103	-11.6295	1.00000
104	-11.6160	1.00000
105	-11.5641	1.00000
106	-11.0915	1.00000
107	-11.0364	1.00000
108	-10.9019	1.00000
109	-10.8920	1.00000
110	-10.8346	1.00000
111	-10.7157	1.00000
112	-10.6811	1.00000
113	-10.6654	1.00000
114	-10.6518	1.00000

115	-10.5941	1.00000
116	-10.5855	1.00000
117	-10.5774	1.00000
118	-10.5734	1.00000
119	-10.5310	1.00000
120	-10.5302	1.00000
121	-10.5153	1.00000
122	-10.5076	1.00000
123	-10.3833	1.00000
124	-10.2952	1.00000
125	-10.2608	1.00000
126	-10.1922	1.00000
127	-10.1911	1.00000
128	-10.0256	1.00000
129	-9.9708	1.00000
130	-9.8886	1.00000
131	-9.8567	1.00000
132	-9.7959	1.00000
133	-9.7907	1.00000
134	-9.7408	1.00000
135	-9.6726	1.00000
136	-9.4473	1.00000

137	-9.4274	1.00000
138	-9.3991	1.00000
139	-9.3924	1.00000
140	-9.3818	1.00000
141	-9.3731	1.00000
142	-9.3151	1.00000
143	-9.3079	1.00000
144	-9.2917	1.00000
145	-9.2824	1.00000
146	-9.2695	1.00000
147	-9.0948	1.00000
148	-9.0074	1.00000
149	-8.9776	1.00000
150	-8.9618	1.00000
151	-8.9387	1.00000
152	-8.7963	1.00000
153	-8.7502	1.00000
154	-8.7395	1.00000
155	-8.7224	1.00000
156	-8.7127	1.00000
157	-8.6921	1.00000
158	-8.6804	1.00000

159	-8.6737	1.00000
160	-8.6575	1.00000
161	-8.5978	1.00000
162	-8.5876	1.00000
163	-8.5805	1.00000
164	-8.5719	1.00000
165	-8.4932	1.00000
166	-8.4619	1.00000
167	-8.4407	1.00000
168	-8.3505	1.00000
169	-8.3019	1.00000
170	-8.2778	1.00000
171	-8.2677	1.00000
172	-8.2379	1.00000
173	-8.2367	1.00000
174	-8.1560	1.00000
175	-8.1496	1.00000
176	-8.0807	1.00000
177	-8.0485	1.00000
178	-8.0306	1.00000
179	-8.0252	1.00000
180	-7.9774	1.00000

181	-7.9690	1.00000
182	-7.9287	1.00000
183	-7.9052	1.00000
184	-7.8893	1.00000
185	-7.8771	1.00000
186	-7.8050	1.00000
187	-7.8018	1.00000
188	-7.7513	1.00000
189	-7.7148	1.00000
190	-7.6701	1.00000
191	-7.6050	1.00000
192	-7.5896	1.00000
193	-7.5798	1.00000
194	-7.5524	1.00000
195	-7.4851	1.00000
196	-7.4846	1.00000
197	-7.4335	1.00000
198	-7.3298	1.00000
199	-7.2539	1.00000
200	-7.1501	1.00000
201	-7.0695	1.00000
202	-7.0453	1.00000

203	-7.0331	1.00000
204	-7.0183	1.00000
205	-7.0015	1.00000
206	-6.9947	1.00000
207	-6.9800	1.00000
208	-6.8699	1.00000
209	-6.8251	1.00000
210	-6.8059	1.00000
211	-6.7974	1.00000
212	-6.7365	1.00000
213	-6.6892	1.00000
214	-6.4767	1.00000
215	-6.4295	1.00000
216	-6.4009	1.00000
217	-6.3957	1.00000
218	-6.3791	1.00000
219	-6.3777	1.00000
220	-6.3221	1.00000
221	-6.3121	1.00000
222	-6.2412	1.00000
223	-6.2341	1.00000
224	-6.2338	1.00000

225	-6.0826	1.00000
226	-6.0426	1.00000
227	-5.7972	1.00000
228	-5.7572	1.00000
229	-5.6998	1.00000
230	-5.6458	1.00000
231	-5.6417	1.00000
232	-5.5634	1.00000
233	-5.5349	1.00000
234	-5.4731	1.00000
235	-5.4445	1.00000
236	-5.1677	1.00000
237	-5.0637	1.00000
238	-5.0559	1.00000
239	-5.0234	1.00000
240	-4.9946	1.00000
241	-4.9158	1.00000
242	-4.8585	1.00000
243	-4.8282	1.00000
244	-4.7955	1.00000
245	-4.6832	1.00000
246	-4.5776	1.00000

247	-4.5764	1.00000
248	-4.5120	1.00000
249	-4.4504	1.00000
250	-4.3892	1.00000
251	-4.2973	1.00000
252	-4.2722	1.00000
253	-4.2177	1.00000
254	-3.5752	1.00000
255	-3.3596	1.00000
256	-3.2104	1.00000
257	-2.9435	1.00000
258	-2.8534	1.00000
259	-2.8290	1.00000
260	-2.6144	1.00000
261	-1.9128	0.00000
262	-1.7740	0.00000
263	-1.7240	0.00000
264	-1.3521	0.00000
265	-1.3201	0.00000
266	-1.2013	0.00000
267	-0.7529	0.00000
268	-0.5895	0.00000

269	-0.5070	0.00000
270	-0.3128	0.00000
271	-0.3108	0.00000
272	-0.2950	0.00000
273	-0.1879	0.00000
274	-0.0629	0.00000
275	-0.0545	0.00000
276	-0.0153	0.00000
277	0.0301	0.00000
278	0.0794	0.00000
279	0.1681	0.00000
280	0.2154	0.00000
281	0.2431	0.00000
282	0.4153	0.00000
283	0.4431	0.00000
284	0.4772	0.00000
285	0.5999	0.00000
286	0.6751	0.00000
287	0.8186	0.00000
288	0.8774	0.00000
289	1.0445	0.00000
290	1.0842	0.00000

291	1.1199	0.00000
292	1.1609	0.00000
293	1.2221	0.00000
294	1.2437	0.00000
295	1.2853	0.00000
296	1.3135	0.00000
297	1.3439	0.00000
298	1.4106	0.00000
299	1.4660	0.00000
300	1.4835	0.00000
301	1.5495	0.00000
302	1.5866	0.00000
303	1.6232	0.00000
304	1.6767	0.00000
305	1.7488	0.00000
306	1.7606	0.00000
307	1.8776	0.00000
308	1.8964	0.00000
309	1.9033	0.00000
310	1.9161	0.00000
311	2.1220	0.00000
312	2.1887	0.00000

313	2.2063	0.00000
314	2.2339	0.00000
315	2.2744	0.00000
316	2.2909	0.00000
317	2.3306	0.00000
318	2.3506	0.00000
319	2.3692	0.00000
320	2.3954	0.00000
321	2.4206	0.00000
322	2.4284	0.00000
323	2.4452	0.00000
324	2.4532	0.00000
325	2.4630	0.00000
326	2.5266	0.00000
327	2.5408	0.00000
328	2.7018	0.00000
329	2.7297	0.00000
330	2.7512	0.00000
331	2.7546	0.00000
332	2.7647	0.00000
333	2.8139	0.00000
334	2.8323	0.00000

335	2.8569	0.00000
336	2.8911	0.00000
337	2.9243	0.00000
338	2.9463	0.00000
339	2.9777	0.00000
340	3.0038	0.00000
341	3.0334	0.00000
342	3.0453	0.00000
343	3.0657	0.00000
344	3.0836	0.00000
345	3.1515	0.00000
346	3.1630	0.00000
347	3.1809	0.00000
348	3.1912	0.00000
349	3.3023	0.00000
350	3.3247	0.00000
351	3.3534	0.00000
352	3.3684	0.00000
353	3.3914	0.00000
354	3.4347	0.00000
355	3.4775	0.00000
356	3.4805	0.00000

357	3.4851	0.00000
358	3.4949	0.00000
359	3.6355	0.00000
360	3.6731	0.00000
361	3.6893	0.00000
362	3.7308	0.00000
363	3.7493	0.00000
364	3.7570	0.00000
365	3.7728	0.00000
366	3.7932	0.00000
367	3.8105	0.00000
368	3.8307	0.00000
369	3.8364	0.00000
370	3.8503	0.00000
371	3.8749	0.00000
372	3.8815	0.00000
373	3.9092	0.00000
374	3.9210	0.00000
375	3.9334	0.00000
376	3.9570	0.00000
377	3.9713	0.00000
378	3.9847	0.00000

379	4.0165	0.00000
380	4.0713	0.00000
381	4.1645	0.00000
382	4.2457	0.00000
383	4.2569	0.00000
384	4.2583	0.00000
385	4.2846	0.00000
386	4.3130	0.00000
387	4.3273	0.00000
388	4.3413	0.00000
389	4.3694	0.00000
390	4.3792	0.00000
391	4.4177	0.00000
392	4.4447	0.00000
393	4.4702	0.00000
394	4.4802	0.00000
395	4.4842	0.00000
396	4.4963	0.00000
397	4.5181	0.00000
398	4.5490	0.00000
399	4.5885	0.00000
400	4.6073	0.00000

401	4.6261	0.00000
402	4.6416	0.00000
403	4.6563	0.00000
404	4.6787	0.00000
405	4.7034	0.00000
406	4.7308	0.00000
407	4.7472	0.00000
408	4.7674	0.00000
409	4.7825	0.00000
410	4.7833	0.00000
411	4.7973	0.00000
412	4.8276	0.00000
413	4.8605	0.00000
414	4.8715	0.00000
415	4.8976	0.00000
416	4.9318	0.00000
417	4.9829	0.00000
418	5.0039	0.00000
419	5.0101	0.00000
420	5.0341	0.00000
421	5.0383	0.00000
422	5.0642	0.00000

423	5.0816	0.00000
424	5.1144	0.00000
425	5.1173	0.00000
426	5.1366	0.00000
427	5.1405	0.00000
428	5.1510	0.00000
429	5.1744	0.00000
430	5.1844	0.00000
431	5.1873	0.00000
432	5.2165	0.00000
433	5.2343	0.00000
434	5.2413	0.00000
435	5.2556	0.00000
436	5.2871	0.00000
437	5.2936	0.00000
438	5.3076	0.00000
439	5.3326	0.00000
440	5.3476	0.00000
441	5.3654	0.00000
442	5.3721	0.00000
443	5.3896	0.00000
444	5.4209	0.00000

445	5.4527	0.00000
446	5.4639	0.00000
447	5.4808	0.00000
448	5.4944	0.00000
449	5.5163	0.00000
450	5.5486	0.00000
451	5.5663	0.00000
452	5.5743	0.00000
453	5.5955	0.00000
454	5.6118	0.00000
455	5.6551	0.00000
456	5.6806	0.00000
457	5.7078	0.00000
458	5.7228	0.00000
459	5.7443	0.00000
460	5.7581	0.00000
461	5.7810	0.00000
462	5.7873	0.00000
463	5.7939	0.00000
464	5.7989	0.00000
465	5.8072	0.00000
466	5.8243	0.00000

467	5.8413	0.00000
468	5.8564	0.00000
469	5.8727	0.00000
470	5.8797	0.00000
471	5.8860	0.00000
472	5.9068	0.00000
473	5.9159	0.00000
474	5.9395	0.00000
475	5.9576	0.00000
476	5.9746	0.00000
477	5.9960	0.00000
478	6.0103	0.00000
479	6.0195	0.00000
480	6.1033	0.00000

spin component 2

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-26.7154	1.00000
2	-21.5736	1.00000
3	-21.4751	1.00000

4	-21.1066	1.00000
5	-21.0734	1.00000
6	-21.0187	1.00000
7	-20.9823	1.00000
8	-20.9800	1.00000
9	-20.8858	1.00000
10	-20.5654	1.00000
11	-20.5057	1.00000
12	-20.4060	1.00000
13	-20.3934	1.00000
14	-20.1330	1.00000
15	-19.9583	1.00000
16	-19.7139	1.00000
17	-19.6321	1.00000
18	-19.6031	1.00000
19	-19.5833	1.00000
20	-19.5323	1.00000
21	-19.5301	1.00000
22	-19.4814	1.00000
23	-19.4666	1.00000
24	-19.1215	1.00000
25	-19.0789	1.00000

26	-18.9750	1.00000
27	-18.9603	1.00000
28	-18.9044	1.00000
29	-18.7094	1.00000
30	-18.5141	1.00000
31	-18.3581	1.00000
32	-18.2527	1.00000
33	-18.2320	1.00000
34	-18.1845	1.00000
35	-18.1824	1.00000
36	-18.0649	1.00000
37	-18.0614	1.00000
38	-17.5733	1.00000
39	-17.3034	1.00000
40	-17.2931	1.00000
41	-17.2786	1.00000
42	-17.2132	1.00000
43	-17.2116	1.00000
44	-17.1827	1.00000
45	-17.0251	1.00000
46	-16.9471	1.00000
47	-16.9279	1.00000

48	-16.8757	1.00000
49	-16.8746	1.00000
50	-16.8344	1.00000
51	-16.8284	1.00000
52	-16.8235	1.00000
53	-16.8207	1.00000
54	-16.7362	1.00000
55	-16.7300	1.00000
56	-16.1923	1.00000
57	-15.7339	1.00000
58	-15.6633	1.00000
59	-15.6498	1.00000
60	-15.6258	1.00000
61	-15.5717	1.00000
62	-15.5328	1.00000
63	-15.5299	1.00000
64	-15.1789	1.00000
65	-14.8133	1.00000
66	-14.6134	1.00000
67	-14.5652	1.00000
68	-14.5054	1.00000
69	-14.5034	1.00000

70	-14.4696	1.00000
71	-14.4440	1.00000
72	-14.3362	1.00000
73	-14.3034	1.00000
74	-14.2729	1.00000
75	-14.2690	1.00000
76	-14.1691	1.00000
77	-14.1658	1.00000
78	-13.8931	1.00000
79	-13.7646	1.00000
80	-13.5970	1.00000
81	-13.5430	1.00000
82	-13.5234	1.00000
83	-13.4998	1.00000
84	-13.4508	1.00000
85	-13.3486	1.00000
86	-13.3458	1.00000
87	-13.1930	1.00000
88	-12.7860	1.00000
89	-12.7555	1.00000
90	-12.7238	1.00000
91	-12.6824	1.00000

92	-12.6757	1.00000
93	-12.6271	1.00000
94	-12.4533	1.00000
95	-12.4361	1.00000
96	-12.3837	1.00000
97	-12.3288	1.00000
98	-12.2132	1.00000
99	-12.2030	1.00000
100	-12.1688	1.00000
101	-11.9421	1.00000
102	-11.6876	1.00000
103	-11.6108	1.00000
104	-11.5968	1.00000
105	-11.5594	1.00000
106	-11.0899	1.00000
107	-11.0331	1.00000
108	-10.8926	1.00000
109	-10.8815	1.00000
110	-10.8318	1.00000
111	-10.7098	1.00000
112	-10.6799	1.00000
113	-10.6625	1.00000

114	-10.6468	1.00000
115	-10.5862	1.00000
116	-10.5789	1.00000
117	-10.5743	1.00000
118	-10.5704	1.00000
119	-10.5203	1.00000
120	-10.5195	1.00000
121	-10.5062	1.00000
122	-10.5015	1.00000
123	-10.3825	1.00000
124	-10.2944	1.00000
125	-10.2600	1.00000
126	-10.1888	1.00000
127	-10.1877	1.00000
128	-10.0219	1.00000
129	-9.9614	1.00000
130	-9.8860	1.00000
131	-9.8521	1.00000
132	-9.7870	1.00000
133	-9.7816	1.00000
134	-9.7392	1.00000
135	-9.6688	1.00000

136	-9.4453	1.00000
137	-9.4241	1.00000
138	-9.3887	1.00000
139	-9.3833	1.00000
140	-9.3732	1.00000
141	-9.3638	1.00000
142	-9.3128	1.00000
143	-9.3057	1.00000
144	-9.2904	1.00000
145	-9.2786	1.00000
146	-9.2500	1.00000
147	-9.0935	1.00000
148	-9.0038	1.00000
149	-8.9643	1.00000
150	-8.9476	1.00000
151	-8.9337	1.00000
152	-8.7938	1.00000
153	-8.7424	1.00000
154	-8.7369	1.00000
155	-8.7167	1.00000
156	-8.7089	1.00000
157	-8.6748	1.00000

158	-8.6686	1.00000
159	-8.6600	1.00000
160	-8.6567	1.00000
161	-8.5803	1.00000
162	-8.5752	1.00000
163	-8.5704	1.00000
164	-8.5538	1.00000
165	-8.4928	1.00000
166	-8.4613	1.00000
167	-8.4390	1.00000
168	-8.3479	1.00000
169	-8.2992	1.00000
170	-8.2760	1.00000
171	-8.2372	1.00000
172	-8.2341	1.00000
173	-8.2318	1.00000
174	-8.1458	1.00000
175	-8.1383	1.00000
176	-8.0775	1.00000
177	-8.0464	1.00000
178	-8.0182	1.00000
179	-8.0098	1.00000

180	-7.9727	1.00000
181	-7.9641	1.00000
182	-7.9246	1.00000
183	-7.8957	1.00000
184	-7.8755	1.00000
185	-7.8682	1.00000
186	-7.7962	1.00000
187	-7.7925	1.00000
188	-7.7418	1.00000
189	-7.6836	1.00000
190	-7.6399	1.00000
191	-7.6027	1.00000
192	-7.5818	1.00000
193	-7.5595	1.00000
194	-7.5441	1.00000
195	-7.4771	1.00000
196	-7.4770	1.00000
197	-7.4324	1.00000
198	-7.3289	1.00000
199	-7.2406	1.00000
200	-7.1464	1.00000
201	-7.0606	1.00000

202	-7.0405	1.00000
203	-7.0190	1.00000
204	-6.9899	1.00000
205	-6.9825	1.00000
206	-6.9773	1.00000
207	-6.9455	1.00000
208	-6.8662	1.00000
209	-6.8208	1.00000
210	-6.7998	1.00000
211	-6.7923	1.00000
212	-6.7297	1.00000
213	-6.6798	1.00000
214	-6.4735	1.00000
215	-6.3998	1.00000
216	-6.3879	1.00000
217	-6.3830	1.00000
218	-6.3683	1.00000
219	-6.3436	1.00000
220	-6.3080	1.00000
221	-6.2807	1.00000
222	-6.2340	1.00000
223	-6.2326	1.00000

224	-6.2268	1.00000
225	-6.0519	1.00000
226	-6.0140	1.00000
227	-5.7609	1.00000
228	-5.7165	1.00000
229	-5.6981	1.00000
230	-5.6403	1.00000
231	-5.6273	1.00000
232	-5.5485	1.00000
233	-5.5279	1.00000
234	-5.4466	1.00000
235	-5.4171	1.00000
236	-5.1455	1.00000
237	-5.0649	1.00000
238	-5.0316	1.00000
239	-5.0276	1.00000
240	-4.9653	1.00000
241	-4.8830	1.00000
242	-4.8593	1.00000
243	-4.8086	1.00000
244	-4.7835	1.00000
245	-4.6530	1.00000

246	-4.5839	1.00000
247	-4.5807	1.00000
248	-4.4820	1.00000
249	-4.4261	1.00000
250	-4.4004	1.00000
251	-4.3011	1.00000
252	-4.2335	1.00000
253	-4.1802	1.00000
254	-3.5495	1.00000
255	-3.3143	1.00000
256	-3.1512	1.00000
257	-2.9484	1.00000
258	-2.8043	1.00000
259	-2.7460	1.00000
260	-2.0671	0.00000
261	-1.9187	0.00000
262	-1.7287	0.00000
263	-1.6842	0.00000
264	-1.3075	0.00000
265	-1.2883	0.00000
266	-1.1655	0.00000
267	-0.7315	0.00000

268	-0.5889	0.00000
269	-0.5146	0.00000
270	-0.2857	0.00000
271	-0.2828	0.00000
272	-0.2649	0.00000
273	-0.1612	0.00000
274	-0.0626	0.00000
275	-0.0531	0.00000
276	0.0085	0.00000
277	0.0351	0.00000
278	0.0743	0.00000
279	0.2034	0.00000
280	0.2506	0.00000
281	0.2748	0.00000
282	0.4292	0.00000
283	0.4473	0.00000
284	0.4784	0.00000
285	0.6047	0.00000
286	0.6954	0.00000
287	0.8214	0.00000
288	0.8844	0.00000
289	1.0545	0.00000

290	1.1026	0.00000
291	1.1401	0.00000
292	1.1759	0.00000
293	1.2310	0.00000
294	1.2498	0.00000
295	1.3064	0.00000
296	1.3187	0.00000
297	1.3579	0.00000
298	1.4294	0.00000
299	1.4812	0.00000
300	1.4982	0.00000
301	1.5747	0.00000
302	1.6017	0.00000
303	1.6521	0.00000
304	1.6854	0.00000
305	1.7564	0.00000
306	1.7706	0.00000
307	1.8811	0.00000
308	1.8996	0.00000
309	1.9062	0.00000
310	1.9270	0.00000
311	2.1384	0.00000

312	2.1995	0.00000
313	2.2187	0.00000
314	2.2522	0.00000
315	2.2883	0.00000
316	2.2953	0.00000
317	2.3360	0.00000
318	2.3585	0.00000
319	2.3802	0.00000
320	2.4050	0.00000
321	2.4275	0.00000
322	2.4336	0.00000
323	2.4562	0.00000
324	2.4578	0.00000
325	2.4700	0.00000
326	2.5291	0.00000
327	2.5466	0.00000
328	2.7071	0.00000
329	2.7355	0.00000
330	2.7513	0.00000
331	2.7576	0.00000
332	2.7734	0.00000
333	2.8287	0.00000

334	2.8452	0.00000
335	2.8693	0.00000
336	2.9024	0.00000
337	2.9328	0.00000
338	2.9558	0.00000
339	2.9826	0.00000
340	3.0054	0.00000
341	3.0375	0.00000
342	3.0520	0.00000
343	3.0714	0.00000
344	3.0910	0.00000
345	3.1540	0.00000
346	3.1724	0.00000
347	3.1892	0.00000
348	3.1992	0.00000
349	3.3078	0.00000
350	3.3296	0.00000
351	3.3616	0.00000
352	3.3720	0.00000
353	3.3946	0.00000
354	3.4402	0.00000
355	3.4829	0.00000

356	3.4894	0.00000
357	3.4916	0.00000
358	3.5013	0.00000
359	3.6404	0.00000
360	3.6770	0.00000
361	3.7017	0.00000
362	3.7366	0.00000
363	3.7530	0.00000
364	3.7590	0.00000
365	3.7776	0.00000
366	3.7978	0.00000
367	3.8133	0.00000
368	3.8382	0.00000
369	3.8459	0.00000
370	3.8648	0.00000
371	3.8786	0.00000
372	3.8907	0.00000
373	3.9209	0.00000
374	3.9328	0.00000
375	3.9470	0.00000
376	3.9592	0.00000
377	3.9822	0.00000

378	3.9869	0.00000
379	4.0221	0.00000
380	4.0806	0.00000
381	4.1708	0.00000
382	4.2581	0.00000
383	4.2623	0.00000
384	4.2686	0.00000
385	4.2923	0.00000
386	4.3211	0.00000
387	4.3340	0.00000
388	4.3505	0.00000
389	4.3791	0.00000
390	4.3838	0.00000
391	4.4236	0.00000
392	4.4487	0.00000
393	4.4754	0.00000
394	4.4827	0.00000
395	4.4904	0.00000
396	4.4992	0.00000
397	4.5217	0.00000
398	4.5535	0.00000
399	4.5916	0.00000

400	4.6099	0.00000
401	4.6278	0.00000
402	4.6453	0.00000
403	4.6593	0.00000
404	4.6846	0.00000
405	4.7082	0.00000
406	4.7368	0.00000
407	4.7520	0.00000
408	4.7710	0.00000
409	4.7863	0.00000
410	4.7887	0.00000
411	4.8030	0.00000
412	4.8326	0.00000
413	4.8655	0.00000
414	4.8840	0.00000
415	4.9031	0.00000
416	4.9425	0.00000
417	4.9927	0.00000
418	5.0093	0.00000
419	5.0124	0.00000
420	5.0370	0.00000
421	5.0436	0.00000

422	5.0685	0.00000
423	5.0858	0.00000
424	5.1178	0.00000
425	5.1214	0.00000
426	5.1406	0.00000
427	5.1440	0.00000
428	5.1678	0.00000
429	5.1789	0.00000
430	5.1878	0.00000
431	5.1921	0.00000
432	5.2214	0.00000
433	5.2368	0.00000
434	5.2447	0.00000
435	5.2613	0.00000
436	5.2959	0.00000
437	5.3009	0.00000
438	5.3106	0.00000
439	5.3370	0.00000
440	5.3515	0.00000
441	5.3691	0.00000
442	5.3797	0.00000
443	5.3927	0.00000

444	5.4292	0.00000
445	5.4590	0.00000
446	5.4705	0.00000
447	5.4862	0.00000
448	5.4992	0.00000
449	5.5229	0.00000
450	5.5674	0.00000
451	5.5720	0.00000
452	5.5932	0.00000
453	5.6080	0.00000
454	5.6216	0.00000
455	5.6671	0.00000
456	5.6914	0.00000
457	5.7168	0.00000
458	5.7271	0.00000
459	5.7486	0.00000
460	5.7628	0.00000
461	5.7885	0.00000
462	5.7900	0.00000
463	5.7969	0.00000
464	5.8029	0.00000
465	5.8198	0.00000

466	5.8255	0.00000
467	5.8543	0.00000
468	5.8613	0.00000
469	5.8792	0.00000
470	5.8861	0.00000
471	5.8895	0.00000
472	5.9047	0.00000
473	5.9253	0.00000
474	5.9480	0.00000
475	5.9600	0.00000
476	5.9784	0.00000
477	5.9878	0.00000
478	6.0131	0.00000
479	6.0297	0.00000
480	6.0751	0.00000

---

soft charge-density along one line, spin component 1

0 1 2 3 4 5 6 7

8 9

total charge-density along one line

soft charge-density along one line, spin component 2

0 1 2 3 4 5 6 7

8 9

total charge-density along one line

pseudopotential strength for first ion, spin component: 1

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

pseudopotential strength for first ion, spin component: 2

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

total augmentation occupancy for first ion, spin component: 1

3.579 -0.646 0.444 -0.034 -0.000

-0.646 0.130 -0.082 0.006 0.000

0.444 -0.082 0.056 -0.003 -0.000

-0.034 0.006 -0.003 0.011 0.000

-0.000 0.000 -0.000 0.000 0.007

total augmentation occupancy for first ion, spin component: 2

-0.000 0.000 -0.000 0.000 0.000

0.000 -0.000 0.000 -0.000 -0.000

-0.000 0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

---------- aborting loop because EDIFF is reached ----------

total charge

# of ion	s	p	d	tot

1	0.646	0.043	0.000	0.690
2	0.646	0.043	0.000	0.690
3	0.646	0.043	0.000	0.690
4	0.646	0.043	0.000	0.690
5	0.646	0.043	0.000	0.690
6	0.646	0.043	0.000	0.690
7	0.646	0.043	0.000	0.690
8	0.646	0.043	0.000	0.690
9	0.646	0.043	0.000	0.690
10	0.646	0.043	0.000	0.690
11	0.646	0.043	0.000	0.690
12	0.646	0.043	0.000	0.690
13	0.646	0.043	0.000	0.689
14	0.646	0.043	0.000	0.689
15	0.648	0.045	0.000	0.693
16	0.646	0.043	0.000	0.689
17	0.646	0.043	0.000	0.689
18	0.646	0.043	0.000	0.689
19	0.646	0.043	0.000	0.689
20	0.646	0.043	0.000	0.689
21	0.646	0.043	0.000	0.689
22	0.646	0.044	0.000	0.690

23	0.542	0.015	0.000	0.557
24	0.541	0.015	0.000	0.556
25	0.870	1.763	0.000	2.633
26	0.867	1.785	0.000	2.653
27	0.867	1.786	0.000	2.653
28	0.870	1.762	0.000	2.632
29	0.865	1.783	0.000	2.648
30	0.870	1.763	0.000	2.633
31	0.867	1.786	0.000	2.653
32	0.867	1.786	0.000	2.653
33	0.870	1.762	0.000	2.632
34	0.865	1.783	0.000	2.648
35	0.870	1.763	0.000	2.633
36	0.868	1.787	0.000	2.654
37	0.867	1.786	0.000	2.653
38	0.870	1.763	0.000	2.633
39	0.865	1.784	0.000	2.649
40	0.870	1.763	0.000	2.633
41	0.868	1.787	0.000	2.655
42	0.867	1.786	0.000	2.653
43	0.871	1.764	0.000	2.634
44	0.865	1.783	0.000	2.648

45	0.870	1.763	0.000	2.633
46	0.867	1.786	0.000	2.653
47	0.867	1.786	0.000	2.653
48	0.871	1.763	0.000	2.634
49	0.865	1.783	0.000	2.648
50	0.870	1.763	0.000	2.633
51	0.867	1.786	0.000	2.653
52	0.867	1.786	0.000	2.653
53	0.870	1.762	0.000	2.632
54	0.865	1.784	0.000	2.648
55	0.865	1.784	0.000	2.649
56	0.865	1.786	0.000	2.651
57	0.866	1.787	0.000	2.653
58	0.866	1.790	0.000	2.656
59	0.865	1.786	0.000	2.651
60	0.866	1.786	0.000	2.651
61	0.866	1.788	0.000	2.654
62	0.867	1.791	0.000	2.658
63	0.865	1.784	0.000	2.649
64	0.865	1.786	0.000	2.651
65	0.866	1.787	0.000	2.652
66	0.865	1.788	0.000	2.653

67	0.865	1.786	0.000	2.651
68	0.866	1.785	0.000	2.651
69	0.865	1.787	0.000	2.652
70	0.866	1.787	0.000	2.653
71	0.865	1.784	0.000	2.649
72	0.865	1.786	0.000	2.651
73	0.866	1.786	0.000	2.652
74	0.864	1.785	0.000	2.649
75	0.865	1.786	0.000	2.651
76	0.866	1.786	0.000	2.651
77	0.865	1.786	0.000	2.651
78	0.865	1.784	0.000	2.649
79	0.865	1.784	0.000	2.649
80	0.865	1.786	0.000	2.651
81	0.865	1.785	0.000	2.650
82	0.863	1.782	0.000	2.645
83	0.865	1.786	0.000	2.651
84	0.866	1.786	0.000	2.651
85	0.865	1.784	0.000	2.648
86	0.862	1.774	0.000	2.636
87	0.865	1.784	0.000	2.649
88	0.865	1.787	0.000	2.652

89	0.865	1.785	0.000	2.650
90	0.865	1.788	0.000	2.653
91	0.865	1.786	0.000	2.651
92	0.866	1.786	0.000	2.651
93	0.864	1.783	0.000	2.647
94	0.866	1.785	0.000	2.651
95	0.865	1.784	0.000	2.649
96	0.865	1.786	0.000	2.651
97	0.866	1.787	0.000	2.653
98	0.866	1.789	0.000	2.655
99	0.865	1.786	0.000	2.651
100	0.866	1.786	0.000	2.651
101	0.865	1.787	0.000	2.652
102	0.867	1.790	0.000	2.657
103	0.865	1.786	0.000	2.651
104	0.867	1.785	0.000	2.653
105	0.866	1.786	0.000	2.652
106	0.870	1.778	0.000	2.648
107	0.869	1.765	0.000	2.635
108	0.865	1.783	0.000	2.648
109	0.869	1.789	0.000	2.658
110	0.865	1.786	0.000	2.651

111	0.867	1.785	0.000	2.653
112	0.867	1.789	0.000	2.655
113	0.871	1.782	0.000	2.653
114	0.869	1.765	0.000	2.634
115	0.865	1.783	0.000	2.648
116	0.870	1.791	0.000	2.661
117	0.865	1.786	0.000	2.651
118	0.867	1.786	0.000	2.653
119	0.865	1.782	0.000	2.647
120	0.858	1.706	0.000	2.564
121	0.869	1.765	0.000	2.634
122	0.865	1.783	0.000	2.648
123	0.866	1.778	0.000	2.644
124	0.866	1.786	0.000	2.652
125	0.868	1.785	0.000	2.653
126	0.862	1.776	0.000	2.638
127	0.852	1.842	0.000	2.694
128	0.870	1.767	0.000	2.637
129	0.865	1.783	0.000	2.648
130	0.860	1.757	0.000	2.617
131	0.866	1.786	0.000	2.652
132	0.867	1.784	0.000	2.652

133	0.864	1.787	0.000	2.651
134	0.869	1.789	0.000	2.659
135	0.869	1.767	0.000	2.636
136	0.865	1.783	0.000	2.648
137	0.866	1.772	0.000	2.638
138	0.866	1.786	0.000	2.652
139	0.867	1.785	0.000	2.652
140	0.866	1.788	0.000	2.654
141	0.870	1.779	0.000	2.649
142	0.869	1.766	0.000	2.635
143	0.865	1.783	0.000	2.648
144	0.869	1.790	0.000	2.659
145	0.940	1.711	0.000	2.651
146	1.240	1.545	0.075	2.860
147	1.631	3.510	0.000	5.141
---	---	---	---	---
tot	123.061	221.535	0.075	344.670

magnetization (x)

# of ion	s	p	d	tot
1	0.000	-0.000	0.000	0.000
2	-0.000	0.000	0.000	-0.000
3	0.000	-0.000	0.000	0.000
4	-0.000	0.000	0.000	-0.000
5	0.000	-0.000	0.000	0.000
6	-0.000	0.000	0.000	-0.000
7	0.000	-0.000	0.000	0.000
8	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	0.000
10	-0.000	0.000	0.000	-0.000
11	0.000	-0.000	0.000	0.000
12	-0.000	0.000	0.000	-0.000
13	0.000	-0.000	0.000	0.000
14	-0.004	0.002	0.000	-0.002
15	0.000	-0.000	0.000	0.000
16	-0.004	0.002	0.000	-0.002
17	-0.004	0.002	0.000	-0.002
18	0.000	-0.000	0.000	0.000
19	-0.003	0.001	0.000	-0.002
20	0.000	-0.000	0.000	0.000

21	-0.003	0.002	0.000	-0.002
22	-0.003	0.002	0.000	-0.002
23	-0.000	0.000	0.000	-0.000
24	-0.000	0.000	0.000	-0.000
25	-0.000	-0.007	0.000	-0.008
26	-0.000	-0.002	0.000	-0.002
27	0.000	0.003	0.000	0.003
28	0.000	0.005	0.000	0.005
29	0.000	0.003	0.000	0.003
30	-0.000	-0.007	0.000	-0.008
31	-0.000	-0.002	0.000	-0.002
32	0.000	0.003	0.000	0.003
33	0.000	0.005	0.000	0.005
34	0.000	0.002	0.000	0.002
35	-0.000	-0.007	0.000	-0.008
36	-0.000	-0.002	0.000	-0.002
37	0.000	0.003	0.000	0.003
38	0.000	0.006	0.000	0.007
39	0.000	0.002	0.000	0.002
40	-0.000	-0.007	0.000	-0.008
41	-0.000	-0.002	0.000	-0.002
42	0.000	0.002	0.000	0.003

43	0.000	0.005	0.000	0.006
44	0.000	0.004	0.000	0.004
45	-0.000	-0.007	0.000	-0.008
46	-0.000	-0.002	0.000	-0.002
47	0.000	0.003	0.000	0.003
48	0.000	0.005	0.000	0.006
49	0.000	0.001	0.000	0.002
50	-0.000	-0.007	0.000	-0.008
51	-0.000	-0.002	0.000	-0.002
52	0.000	0.003	0.000	0.003
53	0.000	0.006	0.000	0.007
54	0.000	0.002	0.000	0.002
55	-0.000	-0.005	0.000	-0.006
56	-0.000	-0.007	0.000	-0.007
57	-0.000	-0.001	0.000	-0.001
58	-0.000	-0.001	0.000	-0.001
59	0.000	0.006	0.000	0.007
60	0.000	0.003	0.000	0.003
61	0.000	0.001	0.000	0.001
62	0.000	0.003	0.000	0.003
63	-0.000	-0.005	0.000	-0.006
64	-0.000	-0.007	0.000	-0.007

65	-0.000	-0.001	0.000	-0.001
66	-0.000	-0.001	0.000	-0.001
67	0.000	0.006	0.000	0.006
68	0.000	0.003	0.000	0.003
69	0.000	0.001	0.000	0.001
70	0.000	0.002	0.000	0.002
71	-0.000	-0.005	0.000	-0.006
72	-0.000	-0.007	0.000	-0.007
73	-0.000	-0.001	0.000	-0.001
74	-0.000	-0.002	0.000	-0.002
75	0.000	0.006	0.000	0.007
76	0.000	0.003	0.000	0.004
77	0.000	0.003	0.000	0.003
78	0.000	0.001	0.000	0.001
79	-0.000	-0.005	0.000	-0.006
80	-0.000	-0.007	0.000	-0.007
81	-0.000	-0.001	0.000	-0.002
82	-0.000	-0.002	0.000	-0.002
83	0.001	0.007	0.000	0.008
84	0.000	0.003	0.000	0.003
85	0.000	0.002	0.000	0.002
86	0.000	0.005	0.000	0.006

87	-0.000	-0.005	0.000	-0.005
88	-0.000	-0.007	0.000	-0.007
89	-0.000	-0.001	0.000	-0.002
90	-0.000	-0.002	0.000	-0.002
91	0.001	0.008	0.000	0.008
92	0.000	0.003	0.000	0.003
93	0.000	0.002	0.000	0.003
94	0.000	0.001	0.000	0.001
95	-0.000	-0.005	0.000	-0.006
96	-0.000	-0.007	0.000	-0.007
97	-0.000	-0.001	0.000	-0.001
98	-0.000	-0.001	0.000	-0.001
99	0.001	0.007	0.000	0.007
100	0.000	0.003	0.000	0.004
101	0.000	0.003	0.000	0.003
102	0.000	0.002	0.000	0.002
103	-0.001	-0.010	0.000	-0.011
104	-0.003	-0.028	0.000	-0.031
105	-0.000	-0.001	0.000	-0.002
106	-0.000	-0.004	0.000	-0.005
107	0.007	0.116	0.000	0.122
108	0.001	0.010	0.000	0.011

109	0.000	0.001	0.000	0.001
110	-0.001	-0.010	0.000	-0.011
111	-0.003	-0.028	0.000	-0.031
112	-0.000	-0.001	0.000	-0.002
113	-0.000	-0.004	0.000	-0.004
114	0.007	0.120	0.000	0.127
115	0.001	0.010	0.000	0.011
116	0.000	0.001	0.000	0.002
117	-0.001	-0.010	0.000	-0.011
118	-0.003	-0.026	0.000	-0.029
119	-0.000	-0.002	0.000	-0.002
120	-0.000	-0.002	0.000	-0.002
121	0.007	0.115	0.000	0.122
122	0.001	0.010	0.000	0.010
123	0.000	0.003	0.000	0.003
124	-0.001	-0.010	0.000	-0.011
125	-0.003	-0.024	0.000	-0.027
126	-0.000	-0.002	0.000	-0.002
127	-0.000	0.001	0.000	0.001
128	0.006	0.105	0.000	0.111
129	0.001	0.009	0.000	0.010
130	0.000	0.004	0.000	0.004

131	-0.001	-0.009	0.000	-0.010
132	-0.003	-0.024	0.000	-0.027
133	-0.000	-0.002	0.000	-0.002
134	-0.000	-0.002	0.000	-0.002
135	0.006	0.097	0.000	0.102
136	0.001	0.009	0.000	0.010
137	0.000	0.004	0.000	0.005
138	-0.001	-0.010	0.000	-0.011
139	-0.003	-0.026	0.000	-0.029
140	-0.000	-0.002	0.000	-0.002
141	-0.000	-0.004	0.000	-0.004
142	0.006	0.105	0.000	0.111
143	0.001	0.010	0.000	0.010
144	0.000	0.002	0.000	0.003
145	0.000	0.005	0.000	0.006
146	-0.000	0.000	-0.000	0.000
147	0.000	0.004	0.000	0.004
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tot	0.001	0.513	-0.000	0.514

CHARGE: cpu time 0.5247: real time 0.5264

FORLOC: cpu time 0.0201: real time 0.0202

FORNL : cpu time 2.0355: real time 2.0424

STRESS: cpu time 6.0931: real time 6.1112

FORCOR: cpu time 0.1397: real time 0.1411

FORHAR: cpu time 0.0330: real time 0.0331

MIXING: cpu time 0.0110: real time 0.0110

OFIELD: cpu time 0.0001: real time 0.0001

DFTD3 V3.0 Rev 1

Edisp (eV) -6.61787

E6 (eV) : -3.9313

E8 (eV) : -2.6866

% E8 : 40.60

FORVDW: cpu time 1.8081: real time 1.8617

FORCE on cell =-STRESS in cart. coord. units (eV):

Direction	XX	YY	ZZ	XY	YZ	ZX
Alpha Z	233.50077	233.50077	233.50077			
Ewald	107585.35095	23473.21104	-39725.69125	9.21379	3454.78175	127.91527

Hartree	106100.65844	25029.44834	-23791.84042	-6.89135	2948.41163	93.05998
E(xc)	-1914.21418	-1916.56476	-1979.88100	0.13125	1.81975	0.12858
Local	**********	-53951.37111	57011.06869	0.96144	-6361.41937	-217.63314
n-local	-472.60200	-482.40630	-439.44480	-0.66324	-0.57896	-0.30682
augment	-38.31184	-38.60666	-34.29964	0.01205	-0.97420	0.00359
Kinetic	7634.95511	7638.80904	8713.98116	-3.07602	-41.68506	-3.17520
Fock	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
vdW	-2.64013	-1.48994	-6.59298	0.00104	-0.07386	0.01157
Total	-17.74616	-15.46958	-19.19948	-0.31103	0.28168	0.00384
in kB	-4.89360	-4.26582	-5.29436	-0.08577	0.07768	0.00106

external pressure = -4.82 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

energy-cutoff : 400.00

volume of cell : 5810.14

direct lattice vectors			reciprocal lattice vectors		
14.780600000	0.000000000	0.000000000	0.067656252	0.000000000	0.000000000
0.000000000	21.333900000	0.000000000	0.000000000	0.046873755	0.000000000
0.000000000	0.000000000	18.425700000	0.000000000	0.000000000	0.054272022

length of vectors

14.780600000 21.333900000 18.425700000 0.067656252 0.046873755 0.054272022

FORCES acting on ions

electron-ion (+dipol) ewald-force non-local-force convergence-correction

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0.465E-02 0.154E+03 0.361E+02 -.316E-02 -.160E+03 -.357E+02 -.179E-02 0.566E+01 -.438E+00 -.100E-06 -.446E-06 -.925E-06

-.185E-01 0.155E+03 -.340E+02 0.160E-01 -.160E+03 0.335E+02 0.116E-02 0.565E+01 0.541E+00 0.533E-06 0.337E-06 0.580E-07

0.184E+00 0.154E+03 0.360E+02 -.184E+00 -.160E+03 -.356E+02 0.393E-05 0.565E+01 -.443E+00 0.285E-06 -.638E-06 -.666E-06

0.112E+00 0.155E+03 -.341E+02 -.987E-01 -.160E+03 0.336E+02 -.175E-01 0.565E+01 0.535E+00 0.175E-06 0.329E-07 0.298E-06

0.171E+00 0.154E+03 0.362E+02 -.173E+00 -.160E+03 -.357E+02 0.115E-02 0.566E+01 -.440E+00 0.383E-06 -.816E-06 -.822E-06

0.126E+00 0.154E+03 -.340E+02 -.108E+00 -.160E+03 0.334E+02 -.211E-01 0.565E+01 0.541E+00 -.385E-06 -.256E-06 -.409E-06

-.193E-01 0.154E+03 0.363E+02 0.182E-01 -.160E+03 -.359E+02 0.158E-02 0.566E+01 -

.431E+00 0.142E-06 -.807E-06 -.126E-05

-.129E-01 0.154E+03 -.338E+02 0.198E-01 -.160E+03 0.332E+02 -.721E-02 0.565E+01 0.555E+00 -.493E-06 -.191E-06 -.137E-05

-.182E+00 0.154E+03 0.363E+02 0.182E+00 -.160E+03 -.359E+02 0.259E-03 0.566E+01 -.429E+00 -.273E-06 -.611E-06 -.148E-05

-.128E+00 0.155E+03 -.337E+02 0.115E+00 -.160E+03 0.331E+02 0.109E-01 0.565E+01 0.561E+00 -.114E-06 0.253E-06 -.162E-05

-.174E+00 0.154E+03 0.362E+02 0.176E+00 -.160E+03 -.358E+02 -.176E-02 0.566E+01 -.432E+00 -.437E-06 -.444E-06 -.131E-05

-.115E+00 0.155E+03 -.338E+02 0.956E-01 -.160E+03 0.332E+02 0.192E-01 0.565E+01 0.555E+00 0.283E-06 0.454E-06 -.893E-06

0.228E+01 -.150E+03 -.386E+02 -.227E+01 0.156E+03 0.386E+02 -.103E-01 -.566E+01 0.766E-01 -.405E-06 0.570E-06 -.182E-06

-.416E+00 -.151E+03 0.388E+02 0.417E+00 0.157E+03 -.386E+02 -.125E-02 -.567E+01 -.269E+00 0.317E-06 0.875E-06 -.130E-07

0.136E+02 -.146E+03 -.413E+02 -.138E+02 0.151E+03 0.413E+02 0.256E+00 -.567E+01 -.350E-01 0.294E-06 0.400E-06 -.205E-06

0.162E+01 -.151E+03 0.402E+02 -.162E+01 0.156E+03 -.400E+02 -.102E-02 -.567E+01 -.229E+00 -.284E-06 0.560E-06 -.677E-06

0.352E+01 -.149E+03 0.443E+02 -.352E+01 0.155E+03 -.441E+02 -.210E-02 -.567E+01 -.180E+00 -.413E-06 0.417E-06 -.310E-06

-.148E+02 -.146E+03 -.330E+02 0.149E+02 0.151E+03 0.329E+02 -.936E-01 -.566E+01

0.472E-01 -.542E-06 0.603E-06 -.288E-06

-.297E+01 -.149E+03 0.432E+02 0.296E+01 0.155E+03 -.430E+02 0.115E-01 -.567E+01 -.241E+00 0.723E-07 0.694E-06 0.106E-05

-.379E+01 -.150E+03 -.385E+02 0.379E+01 0.156E+03 0.385E+02 -.592E-02 -.566E+01 0.237E-01 0.214E-06 0.556E-06 -.464E-06

-.207E+01 -.151E+03 0.395E+02 0.207E+01 0.156E+03 -.392E+02 0.156E-02 -.566E+01 -.282E+00 0.696E-06 0.862E-06 0.664E-06

0.173E-02 -.148E+03 0.486E+02 0.589E-02 0.154E+03 -.484E+02 -.551E-02 -.570E+01 -.158E+00 -.446E-06 0.583E-06 0.812E-06

0.196E+02 -.103E+03 0.222E+02 -.212E+02 0.103E+03 -.246E+02 0.153E+01 0.137E+00 0.238E+01 0.491E-06 0.646E-06 -.155E-06

-.192E+02 -.103E+03 0.153E+02 0.216E+02 0.103E+03 -.168E+02 -.242E+01 -.121E+00 0.151E+01 -.529E-07 0.574E-06 0.214E-06

0.711E-01 0.461E+03 0.202E+03 -.744E-01 -.462E+03 -.201E+03 0.385E-02 0.102E+01 -.219E+00 -.687E-06 -.273E-06 -.238E-05

0.212E+00 0.353E+03 -.234E+03 -.212E+00 -.353E+03 0.234E+03 0.260E-02 0.444E+00 -.371E-01 0.836E-06 0.167E-06 0.266E-05

-.254E-01 0.351E+03 0.240E+03 0.240E-01 -.351E+03 -.241E+03 0.319E-02 0.408E+00 0.565E-01 -.134E-05 0.179E-06 -.265E-05

-.173E+00 0.462E+03 -.195E+03 0.180E+00 -.463E+03 0.195E+03 -.659E-02 0.105E+01 0.233E+00 0.162E-05 0.206E-05 0.153E-05

-.622E-01 0.210E+03 -.272E+03 0.664E-01 -.210E+03 0.272E+03 -.449E-02 0.947E-01

0.560E-01 0.403E-06 -.616E-06 0.218E-05

0.562E+00 0.461E+03 0.202E+03 -.565E+00 -.462E+03 -.201E+03 0.199E-02 0.102E+01 -.214E+00 0.798E-06 -.850E-06 -.151E-05

0.106E+01 0.352E+03 -.234E+03 -.107E+01 -.353E+03 0.234E+03 0.159E-01 0.449E+00 -.425E-01 -.683E-06 0.317E-08 0.161E-05

0.413E+00 0.351E+03 0.240E+03 -.415E+00 -.351E+03 -.240E+03 0.302E-02 0.408E+00 0.493E-01 -.512E-07 0.161E-07 -.105E-05

0.579E+00 0.462E+03 -.195E+03 -.584E+00 -.463E+03 0.195E+03 0.475E-02 0.105E+01 0.235E+00 0.178E-06 0.758E-06 0.229E-05

0.692E+00 0.210E+03 -.272E+03 -.698E+00 -.210E+03 0.272E+03 0.586E-02 0.923E-01 0.616E-01 -.389E-06 -.249E-06 0.152E-05

0.426E+00 0.461E+03 0.202E+03 -.429E+00 -.462E+03 -.202E+03 0.380E-02 0.102E+01 -.213E+00 0.143E-05 -.135E-05 -.274E-05

0.940E+00 0.352E+03 -.233E+03 -.956E+00 -.352E+03 0.233E+03 0.150E-01 0.442E+00 -.378E-01 -.167E-05 0.103E-05 -.151E-05

0.479E+00 0.351E+03 0.241E+03 -.481E+00 -.351E+03 -.241E+03 0.246E-02 0.406E+00 0.514E-01 0.123E-05 -.456E-06 -.135E-05

0.705E+00 0.462E+03 -.194E+03 -.716E+00 -.463E+03 0.194E+03 0.773E-02 0.106E+01 0.242E+00 -.177E-05 0.924E-06 -.423E-06

0.728E+00 0.210E+03 -.271E+03 -.737E+00 -.210E+03 0.271E+03 0.634E-02 0.920E-01 0.592E-01 -.945E-06 0.138E-05 -.289E-06

-.181E+00 0.461E+03 0.202E+03 0.178E+00 -.462E+03 -.202E+03 0.447E-02 0.102E+01 -

.218E+00 0.766E-06 -.150E-05 -.483E-05

-.294E+00 0.352E+03 -.233E+03 0.298E+00 -.352E+03 0.233E+03 -.205E-02 0.441E+00 -.300E-01 -.281E-06 0.270E-05 -.354E-05

0.409E-01 0.351E+03 0.241E+03 -.399E-01 -.351E+03 -.241E+03 0.219E-02 0.410E+00 0.559E-01 0.125E-05 -.835E-06 -.348E-05

0.503E-01 0.462E+03 -.194E+03 -.565E-01 -.463E+03 0.194E+03 0.387E-02 0.106E+01 0.232E+00 -.136E-05 0.218E-05 -.386E-05

-.476E-01 0.210E+03 -.271E+03 0.456E-01 -.210E+03 0.271E+03 -.194E-03 0.941E-01 0.323E-01 -.406E-07 0.245E-05 -.139E-05

-.552E+00 0.461E+03 0.202E+03 0.550E+00 -.462E+03 -.202E+03 0.793E-03 0.102E+01 -.219E+00 -.722E-06 -.960E-06 -.557E-05

-.119E+01 0.352E+03 -.233E+03 0.120E+01 -.353E+03 0.233E+03 -.161E-01 0.449E+00 -.331E-01 0.647E-06 0.226E-05 -.268E-05

-.352E+00 0.351E+03 0.241E+03 0.349E+00 -.351E+03 -.241E+03 0.207E-02 0.414E+00 0.625E-01 0.234E-06 -.807E-06 -.505E-05

-.412E+00 0.462E+03 -.194E+03 0.426E+00 -.463E+03 0.194E+03 -.114E-01 0.106E+01 0.230E+00 0.456E-07 0.335E-05 -.470E-05

-.564E+00 0.210E+03 -.271E+03 0.568E+00 -.210E+03 0.271E+03 -.922E-02 0.925E-01 0.525E-01 0.421E-06 0.241E-05 -.825E-06

-.475E+00 0.461E+03 0.202E+03 0.474E+00 -.462E+03 -.202E+03 0.312E-02 0.102E+01 -.220E+00 -.159E-05 -.335E-06 -.438E-05

-.806E+00 0.353E+03 -.234E+03 0.821E+00 -.353E+03 0.234E+03 -.149E-01 0.448E+00 -

.393E-01 0.113E-05 0.141E-05 0.441E-06

-.374E+00 0.351E+03 0.241E+03 0.368E+00 -.351E+03 -.241E+03 0.101E-02 0.411E+00 0.628E-01 -.131E-05 -.299E-06 -.465E-05

-.595E+00 0.462E+03 -.194E+03 0.608E+00 -.463E+03 0.194E+03 -.169E-01 0.106E+01 0.234E+00 0.131E-05 0.334E-05 -.200E-05

-.590E+00 0.210E+03 -.272E+03 0.601E+00 -.210E+03 0.272E+03 -.101E-01 0.100E+00 0.567E-01 0.525E-06 0.718E-06 0.909E-06

-.101E-01 0.206E+03 0.279E+03 0.134E-01 -.206E+03 -.279E+03 -.358E-02 0.692E-01 -.410E-01 -.114E-05 0.377E-06 -.163E-05

0.667E+00 0.303E+02 0.296E+03 -.662E+00 -.302E+02 -.296E+03 -.467E-02 -.406E-01 0.781E-02 -.421E-06 0.128E-05 -.106E-05

-.848E+00 0.144E+03 -.282E+03 0.850E+00 -.144E+03 0.282E+03 -.314E-02 0.138E+00 0.286E-01 0.218E-06 -.280E-06 0.130E-05

0.534E+00 -.215E+02 -.285E+03 -.534E+00 0.214E+02 0.285E+03 -.786E-03 0.399E-01 0.186E-01 0.317E-07 0.576E-06 -.544E-06

0.496E+00 -.294E+02 0.293E+03 -.493E+00 0.294E+02 -.293E+03 -.551E-02 0.258E-01 -.301E-01 -.558E-07 0.105E-05 -.111E-05

0.523E+00 0.139E+03 0.289E+03 -.523E+00 -.139E+03 -.289E+03 0.180E-02 0.104E+00 -.246E-01 -.724E-06 0.823E-06 -.750E-06

-.127E+01 0.364E+02 -.287E+03 0.127E+01 -.364E+02 0.287E+03 0.695E-04 -.640E-02 0.136E-01 -.719E-06 0.256E-06 0.926E-07

0.167E+01 -.130E+03 -.271E+03 -.169E+01 0.130E+03 0.271E+03 0.105E-01 -.870E-01

0.370E-01 -.165E-06 0.115E-05 -.117E-05

0.397E+00 0.207E+03 0.280E+03 -.395E+00 -.207E+03 -.280E+03 0.697E-03 0.700E-01 -.368E-01 -.284E-06 0.679E-06 -.385E-06

0.921E+00 0.312E+02 0.296E+03 -.924E+00 -.311E+02 -.296E+03 0.219E-02 -.407E-01 0.125E-01 0.301E-08 0.138E-05 -.745E-06

0.133E+01 0.144E+03 -.282E+03 -.133E+01 -.144E+03 0.282E+03 0.491E-02 0.127E+00 0.279E-01 0.272E-06 -.716E-06 0.152E-05

0.343E+01 -.199E+02 -.285E+03 -.344E+01 0.199E+02 0.285E+03 0.131E-01 0.424E-01 0.135E-01 0.123E-05 0.767E-06 -.171E-06

0.139E+01 -.287E+02 0.294E+03 -.139E+01 0.287E+02 -.294E+03 -.351E-02 0.256E-01 -.304E-01 -.226E-06 0.176E-05 -.137E-05

0.679E+00 0.139E+03 0.290E+03 -.679E+00 -.139E+03 -.290E+03 0.579E-03 0.104E+00 -.293E-01 0.251E-06 0.843E-06 -.241E-06

0.160E+01 0.367E+02 -.287E+03 -.159E+01 -.367E+02 0.287E+03 -.131E-01 -.194E-01 0.127E-01 0.768E-06 0.129E-07 0.737E-07

0.613E+01 -.125E+03 -.271E+03 -.615E+01 0.125E+03 0.271E+03 0.213E-01 -.886E-01 0.147E-01 0.108E-05 0.915E-06 -.462E-06

0.368E+00 0.207E+03 0.280E+03 -.373E+00 -.207E+03 -.280E+03 0.607E-04 0.689E-01 -.363E-01 0.980E-06 0.209E-06 -.658E-06

-.344E-01 0.319E+02 0.296E+03 0.258E-01 -.319E+02 -.296E+03 0.105E-01 -.359E-01 0.142E-01 0.386E-06 0.355E-06 -.538E-06

0.210E+01 0.144E+03 -.281E+03 -.211E+01 -.144E+03 0.281E+03 0.119E-01 0.121E+00

0.239E-01 -.389E-06 0.101E-05 0.622E-06

0.305E+01 -.171E+02 -.283E+03 -.307E+01 0.170E+02 0.283E+03 0.240E-01 0.878E-01 0.600E-01 0.953E-06 0.196E-05 0.541E-06

0.106E+01 -.272E+02 0.294E+03 -.106E+01 0.272E+02 -.294E+03 0.281E-02 0.246E-01 -.373E-01 -.150E-06 0.118E-05 -.780E-06

0.985E-01 0.140E+03 0.290E+03 -.100E+00 -.140E+03 -.290E+03 0.125E-02 0.108E+00 -.230E-01 0.966E-06 0.623E-07 -.107E-05

0.278E+01 0.387E+02 -.286E+03 -.278E+01 -.387E+02 0.286E+03 0.777E-03 -.101E-01 0.291E-01 0.552E-06 0.102E-05 0.293E-06

0.599E+01 -.115E+03 -.267E+03 -.615E+01 0.115E+03 0.267E+03 0.153E+00 0.195E-02 0.128E+00 0.196E-05 -.942E-06 0.689E-06

-.241E+00 0.207E+03 0.280E+03 0.239E+00 -.207E+03 -.280E+03 0.436E-02 0.722E-01 -.385E-01 0.109E-05 -.472E-06 -.243E-05

-.114E+01 0.314E+02 0.294E+03 0.113E+01 -.314E+02 -.294E+03 0.920E-02 -.308E-01 0.569E-02 0.401E-06 -.690E-06 -.688E-06

0.597E+00 0.144E+03 -.281E+03 -.615E+00 -.144E+03 0.281E+03 0.176E-01 0.127E+00 0.437E-01 0.289E-06 0.191E-05 -.389E-06

-.939E+00 -.158E+02 -.286E+03 0.931E+00 0.158E+02 0.285E+03 0.609E-02 0.918E-01 0.798E-01 0.672E-06 0.443E-05 0.100E-05

-.639E+00 -.265E+02 0.293E+03 0.636E+00 0.265E+02 -.293E+03 0.490E-02 0.237E-01 -.268E-01 0.478E-08 -.210E-06 -.438E-07

-.533E+00 0.139E+03 0.289E+03 0.529E+00 -.139E+03 -.289E+03 0.657E-02 0.114E+00 -

.211E-01 0.730E-06 -.693E-06 -.246E-05

0.785E+00 0.408E+02 -.287E+03 -.797E+00 -.408E+02 0.287E+03 0.494E-02 0.253E-02 -.193E-01 0.673E-06 0.310E-05 0.563E-06

-.457E+00 -.113E+03 -.276E+03 0.423E+00 0.113E+03 0.276E+03 0.354E-01 0.608E-01 -.269E+00 0.114E-06 0.116E-05 0.113E-05

-.572E+00 0.206E+03 0.279E+03 0.570E+00 -.206E+03 -.279E+03 0.117E-02 0.726E-01 -.453E-01 0.301E-06 -.784E-06 -.368E-05

-.785E+00 0.304E+02 0.294E+03 0.789E+00 -.304E+02 -.294E+03 -.751E-02 -.305E-01 -.113E-02 0.332E-07 -.770E-06 -.918E-06

-.123E+01 0.144E+03 -.281E+03 0.125E+01 -.145E+03 0.281E+03 -.155E-01 0.123E+00 0.504E-01 -.299E-06 0.277E-05 -.542E-06

-.367E+01 -.174E+02 -.283E+03 0.370E+01 0.173E+02 0.283E+03 -.306E-01 0.118E+00 0.579E-01 -.133E-05 0.235E-05 0.575E-06

-.130E+01 -.277E+02 0.291E+03 0.129E+01 0.277E+02 -.291E+03 -.128E-02 0.344E-01 -.216E-01 0.241E-06 -.928E-06 0.213E-06

-.349E+00 0.139E+03 0.289E+03 0.348E+00 -.139E+03 -.289E+03 0.350E-04 0.112E+00 -.144E-01 -.228E-06 -.727E-06 -.285E-05

-.836E+00 0.400E+02 -.287E+03 0.828E+00 -.400E+02 0.287E+03 0.130E-01 -.696E-02 -.185E-01 -.339E-06 0.332E-05 0.515E-06

-.790E+01 -.119E+03 -.267E+03 0.809E+01 0.119E+03 0.267E+03 -.190E+00 0.470E-02 0.324E-01 -.151E-05 -.112E-05 0.496E-06

-.410E+00 0.206E+03 0.279E+03 0.412E+00 -.206E+03 -.279E+03 -.276E-02 0.721E-01 -

.462E-01 -.924E-06 -.410E-06 -.331E-05

-.667E-01 0.300E+02 0.294E+03 0.764E-01 -.299E+02 -.294E+03 -.943E-02 -.344E-01 0.151E-02 -.409E-06 0.252E-06 -.106E-05

-.206E+01 0.145E+03 -.282E+03 0.208E+01 -.145E+03 0.282E+03 -.188E-01 0.133E+00 0.256E-01 -.690E-07 0.193E-05 0.298E-06

-.258E+01 -.208E+02 -.285E+03 0.260E+01 0.208E+02 0.285E+03 -.287E-01 0.420E-01 0.315E-01 -.160E-05 0.119E-05 -.158E-06

-.556E+00 -.290E+02 0.291E+03 0.561E+00 0.290E+02 -.291E+03 -.281E-02 0.295E-01 -.248E-01 0.176E-06 -.385E-06 -.343E-06

0.569E-01 0.139E+03 0.289E+03 -.571E-01 -.139E+03 -.289E+03 -.302E-03 0.109E+00 -.206E-01 -.101E-05 0.342E-07 -.198E-05

-.291E+01 0.378E+02 -.286E+03 0.292E+01 -.378E+02 0.286E+03 -.145E-01 -.276E-02 0.207E-01 -.917E-06 0.156E-05 0.287E-06

-.515E+01 -.128E+03 -.271E+03 0.520E+01 0.128E+03 0.271E+03 -.460E-01 -.852E-01 0.377E-01 -.155E-05 0.114E-05 -.438E-06

0.395E+00 -.137E+03 0.280E+03 -.387E+00 0.137E+03 -.280E+03 -.963E-02 -.127E+00 -.152E-01 0.620E-06 0.862E-06 -.116E-05

0.193E+01 -.343E+03 0.233E+03 -.194E+01 0.344E+03 -.233E+03 0.916E-02 -.460E+00 -.540E-01 0.699E-06 0.147E-05 -.224E-05

-.254E+01 -.197E+03 -.259E+03 0.255E+01 0.197E+03 0.259E+03 -.962E-02 -.196E+00 0.368E-01 -.118E-05 0.984E-06 -.993E-06

0.691E+01 -.447E+03 -.198E+03 -.693E+01 0.448E+03 0.198E+03 0.926E-02 -.112E+01

0.878E-01 -.104E-05 0.493E-06 -.674E-06

-.467E+00 -.451E+03 0.204E+03 0.468E+00 0.452E+03 -.204E+03 -.185E-02 -.108E+01 -.112E+00 0.148E-05 0.245E-05 -.597E-06

0.171E+01 -.203E+03 0.269E+03 -.170E+01 0.203E+03 -.269E+03 -.478E-02 -.922E-01 -.315E-01 0.436E-06 0.143E-05 -.212E-05

-.211E+01 -.338E+03 -.222E+03 0.216E+01 0.338E+03 0.222E+03 -.444E-01 -.602E+00 0.533E-01 -.758E-06 0.366E-06 -.709E-06

0.218E+01 -.136E+03 0.282E+03 -.218E+01 0.136E+03 -.282E+03 -.641E-02 -.125E+00 -.898E-02 -.190E-06 0.158E-05 -.223E-05

0.672E+01 -.339E+03 0.238E+03 -.670E+01 0.340E+03 -.238E+03 -.130E-01 -.461E+00 -.453E-01 -.105E-05 0.107E-05 -.266E-05

0.679E+01 -.193E+03 -.258E+03 -.680E+01 0.193E+03 0.258E+03 0.111E-01 -.144E+00 0.631E-01 0.855E-06 0.637E-06 -.950E-06

0.313E+02 -.427E+03 -.198E+03 -.313E+02 0.428E+03 0.197E+03 0.727E-01 -.975E+00 0.140E+00 0.127E-05 -.606E-06 -.354E-06

0.544E+01 -.449E+03 0.209E+03 -.544E+01 0.451E+03 -.209E+03 0.514E-03 -.108E+01 -.793E-01 -.583E-06 0.186E-05 -.296E-05

0.369E+01 -.201E+03 0.272E+03 -.368E+01 0.201E+03 -.272E+03 -.845E-03 -.973E-01 -.301E-01 -.745E-06 0.140E-05 -.220E-05

0.124E+02 -.332E+03 -.223E+03 -.125E+02 0.332E+03 0.223E+03 0.121E+00 -.533E+00 0.313E-01 0.177E-06 -.434E-06 -.557E-06

0.219E+01 -.133E+03 0.283E+03 -.220E+01 0.133E+03 -.283E+03 0.410E-03 -.128E+00 -

.403E-02 -.755E-06 0.964E-06 -.111E-05

0.493E+01 -.332E+03 0.245E+03 -.490E+01 0.332E+03 -.245E+03 -.322E-01 -.476E+00 -.370E-01 -.184E-05 0.529E-06 0.502E-06

0.113E+02 -.182E+03 -.258E+03 -.113E+02 0.182E+03 0.258E+03 0.468E-01 -.985E-01 -.105E+00 -.100E-06 0.200E-06 0.360E-07

0.319E+02 -.399E+03 -.175E+03 -.322E+02 0.401E+03 0.174E+03 0.302E+00 -.144E+01 0.132E+01 -.242E-05 0.413E-05 -.804E-06

0.930E+01 -.443E+03 0.219E+03 -.930E+01 0.444E+03 -.219E+03 -.611E-02 -.110E+01 -.481E-01 -.167E-05 0.983E-06 -.139E-05

0.170E+01 -.196E+03 0.273E+03 -.170E+01 0.197E+03 -.273E+03 0.537E-02 -.109E+00 -.506E-01 -.134E-05 0.282E-06 0.907E-07

0.172E+02 -.310E+03 -.216E+03 -.176E+02 0.310E+03 0.216E+03 0.325E+00 -.219E+00 0.122E+00 -.733E-06 -.323E-06 -.420E-06

-.103E+01 -.132E+03 0.281E+03 0.102E+01 0.132E+03 -.281E+03 0.102E-01 -.127E+00 0.524E-03 -.709E-06 -.422E-06 0.967E-06

-.512E+01 -.332E+03 0.239E+03 0.511E+01 0.332E+03 -.239E+03 0.905E-02 -.495E+00 -.412E-01 -.953E-06 -.278E-06 0.343E-05

0.164E+01 -.169E+03 -.261E+03 -.177E+01 0.169E+03 0.261E+03 0.119E+00 0.369E+00 -.885E-01 0.510E-05 -.454E-05 0.107E-05

-.637E+01 -.300E+03 -.187E+03 0.586E+01 0.294E+03 0.183E+03 0.479E+00 0.472E+01 0.408E+01 0.152E-05 0.519E-05 0.249E-05

-.617E+00 -.436E+03 0.227E+03 0.615E+00 0.437E+03 -.227E+03 0.168E-02 -.120E+01 -

.483E-01 -.182E-05 0.784E-06 0.267E-05

-.302E+01 -.197E+03 0.268E+03 0.300E+01 0.197E+03 -.268E+03 0.147E-01 -.112E+00 -.424E-01 -.438E-06 -.868E-06 0.241E-05

0.357E+01 -.280E+03 -.215E+03 -.554E+01 0.280E+03 0.214E+03 0.192E+01 0.634E+00 0.816E+00 0.898E-05 0.135E-05 0.146E-05

-.274E+01 -.134E+03 0.277E+03 0.274E+01 0.134E+03 -.277E+03 0.255E-02 -.123E+00 -.181E-01 0.142E-06 -.112E-05 0.212E-05

-.601E+01 -.338E+03 0.230E+03 0.601E+01 0.339E+03 -.230E+03 0.113E-01 -.494E+00 -.452E-01 0.991E-06 -.267E-06 0.337E-05

-.656E+01 -.171E+03 -.257E+03 0.664E+01 0.170E+03 0.257E+03 -.790E-01 0.484E+00 0.232E-01 -.452E-05 -.335E-05 0.871E-06

-.444E+02 -.422E+03 -.184E+03 0.449E+02 0.424E+03 0.183E+03 -.569E+00 -.112E+01 0.613E+00 0.588E-06 0.354E-05 -.695E-06

-.867E+01 -.441E+03 0.211E+03 0.866E+01 0.443E+03 -.211E+03 0.146E-01 -.112E+01 -.743E-01 0.750E-07 0.278E-06 0.417E-05

-.293E+01 -.201E+03 0.265E+03 0.294E+01 0.201E+03 -.265E+03 -.912E-02 -.110E+00 -.200E-01 0.651E-06 -.995E-06 0.241E-05

-.147E+02 -.290E+03 -.209E+03 0.168E+02 0.289E+03 0.208E+03 -.198E+01 0.601E+00 0.787E+00 -.907E-05 0.130E-05 0.115E-05

-.139E+01 -.136E+03 0.277E+03 0.140E+01 0.136E+03 -.277E+03 -.101E-01 -.125E+00 -.235E-01 0.847E-06 -.580E-06 0.916E-06

-.280E+01 -.343E+03 0.230E+03 0.277E+01 0.343E+03 -.230E+03 0.237E-01 -.473E+00 -

.585E-01 0.201E-05 0.969E-06 0.758E-06

-.104E+02 -.189E+03 -.258E+03 0.105E+02 0.189E+03 0.258E+03 -.768E-01 -.139E+00 -.520E-01 -.169E-06 -.496E-06 -.117E-06

-.150E+02 -.446E+03 -.196E+03 0.150E+02 0.447E+03 0.196E+03 -.699E-01 -.113E+01 0.993E-01 0.172E-06 0.150E-06 -.897E-06

-.550E+01 -.448E+03 0.204E+03 0.550E+01 0.449E+03 -.203E+03 -.465E-02 -.109E+01 -.125E+00 0.236E-05 0.159E-05 0.249E-05

-.919E+00 -.203E+03 0.267E+03 0.927E+00 0.203E+03 -.267E+03 -.901E-02 -.102E+00 -.312E-01 0.138E-05 0.248E-06 0.170E-06

-.163E+02 -.329E+03 -.218E+03 0.167E+02 0.329E+03 0.218E+03 -.360E+00 -.480E+00 0.421E-01 0.129E-05 -.880E-06 -.845E-06

-.399E+01 -.261E+03 -.200E+03 0.312E+01 0.254E+03 0.196E+03 0.990E+00 0.796E+01 0.483E+01 -.891E-06 -.449E-05 -.625E-05

0.530E+02 -.518E+03 -.137E+03 -.540E+02 0.522E+03 0.141E+03 0.107E+01 -.396E+01 -.382E+01 0.169E-05 0.271E-05 -.243E-05

-.461E+02 -.583E+03 -.443E+03 0.517E+02 0.633E+03 0.476E+03 -.571E+01 -.505E+02 -.334E+02 -.424E-05 -.204E-04 -.205E-04

0.419E+01 0.275E+02 0.215E+02 -.291E-12 -.330E-11 0.284E-11 -.423E+01 -.275E+02 -.216E+02 -.409E-05 0.564E-04 -.104E-03

POSITION			TOTAL-FORCE (eV/Angst)		
1.24575	4.02870	5.43979	0.000034	0.001067	-0.000440
1.21024	4.07581	8.43726	-0.000997	0.002700	-0.001064
3.70862	4.02890	5.43965	0.000308	0.001938	-0.001126
3.67998	4.07733	8.43690	-0.004033	-0.000332	-0.002827
6.17157	4.02854	5.43942	-0.000001	-0.000089	-0.001782
6.14482	4.08292	8.43295	-0.002823	-0.003218	-0.003100
8.63513	4.02801	5.43869	0.000782	-0.000389	-0.002026
8.60339	4.08732	8.43089	-0.000128	-0.001093	-0.002101
11.09928	4.02784	5.43885	0.000868	0.002026	-0.002734
11.06021	4.08619	8.43099	-0.001749	0.000787	-0.000532
13.56311	4.02807	5.43972	0.000321	0.001672	-0.001647
13.52141	4.08047	8.43349	0.000387	-0.002168	0.000392
2.44241	15.48073	8.85224	-0.000627	-0.005386	0.002509
0.01714	15.44624	5.32469	0.000312	0.001521	-0.001250
4.86040	15.47728	8.86623	0.001566	0.000021	-0.001069
2.48016	15.44854	5.27562	0.000368	-0.001213	-0.000583
4.94382	15.44925	5.24869	0.001868	-0.003089	0.000381
12.31531	15.48242	9.00211	-0.005875	0.000346	0.007827
9.86772	15.44556	5.34176	0.000398	-0.001177	0.000944
14.76279	15.48245	8.89951	-0.006428	-0.000685	0.005640

12.33384	15.44510	5.36128	0.001312	-0.003274	-0.001259
7.40743	15.44616	5.26463	0.002384	0.001297	0.001552
6.44846	16.34427	7.40648	-0.001431	-0.004028	0.000002
8.60064	16.47644	7.89249	0.001180	0.002882	0.006861
1.24544	5.11881	5.35500	0.000918	-0.000003	-0.002375
2.44348	5.83889	8.62292	0.002418	-0.004358	0.001236
0.01380	5.79530	5.28573	0.002087	-0.002338	0.000467
1.21063	5.16420	8.54151	0.000226	-0.000532	-0.001985
2.44351	7.27931	8.74832	-0.000018	-0.001331	-0.000148
3.70866	5.11896	5.35390	-0.000414	-0.001786	0.000405
4.90800	5.84315	8.62123	-0.001135	0.003877	-0.000711
2.47701	5.79561	5.28397	0.001456	-0.000477	-0.002610
3.67679	5.16572	8.54000	-0.000076	0.001637	-0.000120
4.90764	7.28398	8.74777	0.000475	-0.000645	0.001002
6.17184	5.11860	5.35433	0.001492	0.000191	0.000996
7.37096	5.84929	8.62094	-0.000533	0.007158	-0.002446
4.94029	5.79548	5.28340	0.000587	-0.002563	-0.001179
6.14080	5.17108	8.53715	-0.002512	0.002436	0.002342
7.37071	7.28983	8.75132	-0.002015	0.001562	0.000128
8.63543	5.11820	5.35521	0.001218	0.001121	-0.000967
9.83233	5.85166	8.62337	0.002827	0.001208	-0.001062
7.40374	5.79498	5.28512	0.003467	-0.002548	-0.001342

8.60194	5.17528	8.53759	-0.002063	-0.000651	-0.000341
9.83204	7.29110	8.75719	-0.001766	-0.003252	-0.002508
11.09930	5.11814	5.35578	-0.000862	-0.003573	-0.001275
12.29449	5.84673	8.62385	-0.000085	0.005888	-0.002184
9.86750	5.79468	5.28678	-0.000739	-0.000554	0.001552
11.06261	5.17409	8.53894	0.002775	0.002493	-0.000515
12.29428	7.28729	8.75533	-0.004598	0.001083	-0.001534
13.56278	5.11829	5.35605	0.002645	0.000336	-0.001882
14.75895	5.83988	8.62434	-0.000234	-0.002631	-0.002156
12.33118	5.79480	5.28692	-0.004526	-0.001330	0.002591
13.52535	5.16844	8.54022	-0.003451	0.003682	-0.001556
14.75917	7.28012	8.75179	0.001134	0.002542	-0.000719
0.01434	7.23830	5.19017	0.000092	-0.000215	0.000092
1.24689	9.38061	5.13160	0.000565	-0.001886	0.000019
1.21085	7.98059	8.79588	-0.001067	-0.000458	0.001558
2.44214	10.12243	8.87141	-0.000695	0.004342	-0.004972
0.01532	10.08686	5.14049	-0.002070	-0.000136	-0.002399
1.24606	7.94244	5.15775	0.001985	-0.002594	0.000829
1.21082	9.41592	8.85782	-0.001316	0.004203	0.000167
2.44072	11.55513	8.88414	-0.006007	-0.004083	0.001433
2.47747	7.23842	5.18585	0.002799	0.002848	0.001335
3.70997	9.38055	5.12566	-0.001084	-0.003027	0.000061

3.67534	7.98360	8.79349	-0.000507	0.000984	0.000965
4.90487	10.12925	8.87518	-0.000220	0.000724	0.000132
2.47867	10.08713	5.12695	-0.002277	0.001481	0.000771
3.70939	7.94242	5.15441	0.000831	-0.004009	-0.001701
3.67589	9.41970	8.85445	-0.001308	0.001845	-0.000154
4.90263	11.56506	8.89086	-0.001208	-0.000157	0.001018
4.94085	7.23830	5.18552	-0.004720	0.002225	0.000851
6.17318	9.38002	5.13173	0.001988	0.002040	0.001857
6.13864	7.99044	8.79647	0.002557	-0.000002	-0.001657
7.36780	10.13760	8.89473	-0.000958	0.003547	0.000160
4.94196	10.08682	5.12700	0.004146	0.001469	-0.001158
6.17284	7.94199	5.15766	-0.000036	0.000586	0.003038
6.13939	9.42660	8.86164	0.001364	-0.000790	-0.002304
7.36410	11.57721	8.92935	-0.001527	-0.004062	0.003938
7.40426	7.23794	5.19012	0.002146	0.001747	0.001090
8.63700	9.37970	5.14543	-0.000618	0.002891	0.000981
8.60086	7.99568	8.80617	0.000865	0.000191	-0.000899
9.83068	10.14286	8.92842	-0.002270	0.004729	-0.001203
7.40553	10.08627	5.14064	0.001249	-0.003537	0.003138
8.63637	7.94166	5.16555	0.002582	0.001821	-0.001406
8.60077	9.43254	8.88532	-0.006150	0.001418	-0.001258
9.82927	11.58244	9.00096	0.001549	-0.001219	0.000961

9.86805	7.23787	5.19489	-0.000369	0.000068	-0.000169
11.10106	9.37979	5.15156	-0.003808	-0.001067	0.000689
11.06331	7.99411	8.80818	-0.000079	-0.001122	0.000268
12.29815	10.12943	8.90340	-0.000954	-0.001022	0.000971
9.86930	10.08593	5.15631	-0.005426	-0.001372	0.001419
11.10021	7.94175	5.16862	-0.000577	-0.003058	0.001390
11.06206	9.43062	8.88839	0.004949	0.001126	0.002077
12.30255	11.56557	8.94694	0.004183	-0.001869	-0.000336
12.33169	7.23799	5.19447	-0.001056	0.000234	-0.001732
13.56437	9.38021	5.14435	0.000778	0.001601	-0.000550
13.52754	7.98555	8.80171	-0.000782	-0.002224	-0.003102
14.76233	10.12320	8.88285	-0.004688	0.001455	-0.001551
12.33257	10.08637	5.15511	0.002591	0.000589	-0.001538
13.56350	7.94214	5.16485	-0.000085	-0.000869	-0.000368
13.52731	9.42040	8.86925	-0.000576	0.002786	-0.000639
14.76430	11.55727	8.90646	-0.001661	-0.001725	0.002064
0.01611	11.52516	5.16621	-0.001091	-0.002622	0.000409
1.24770	13.67535	5.22209	0.001628	-0.002856	-0.002494
1.21217	12.26335	8.89409	-0.000247	-0.000194	0.001234
2.43998	14.38728	8.86748	-0.003681	0.003091	0.000803
0.01699	14.35408	5.27295	-0.000239	-0.000012	-0.001985
1.24794	12.22963	5.17275	0.001078	0.000780	-0.001369

1.21434	13.70818	8.88771	0.004214	0.000089	0.003885
2.47958	11.52580	5.14547	-0.001617	-0.000232	-0.001455
3.71218	13.67636	5.19535	0.004783	-0.000013	0.001028
3.66932	12.26248	8.88184	-0.001470	-0.000126	-0.000623
4.89370	14.38589	8.86075	0.005964	0.000184	-0.001853
2.48000	14.35596	5.23149	0.001346	-0.000536	0.001703
3.71150	12.23022	5.15602	0.000889	-0.004599	0.001004
3.66212	13.70366	8.87117	-0.004749	0.002088	0.000272
4.94290	11.52542	5.14351	-0.000062	-0.001855	-0.001584
6.17627	13.67505	5.20032	0.001059	-0.000109	-0.000001
6.13145	12.27911	8.90591	0.006408	0.007856	0.004734
7.36614	14.42967	8.88203	0.017540	0.002672	0.000733
4.94347	14.35627	5.21375	-0.000002	-0.001135	0.000970
6.17493	12.22917	5.16623	-0.001466	-0.001069	0.001603
6.11879	13.72336	8.87765	0.000495	-0.006990	-0.001627
7.40625	11.52413	5.16368	0.000921	-0.003487	0.000365
8.63876	13.67323	5.24377	0.001688	0.001229	-0.001392
8.58939	12.29067	9.00208	-0.003013	0.008266	0.004088
9.83855	14.39048	9.30305	-0.027676	-0.458948	-0.262284
7.40672	14.35386	5.23530	-0.001236	0.000701	-0.001052
8.63820	12.22778	5.19800	0.000243	-0.001242	0.001095
8.55571	13.73596	9.04598	-0.048369	-0.059630	-0.023230

9.86985	11.52338	5.18893	0.001761	-0.002164	-0.000083
11.10099	13.67352	5.27669	0.003365	-0.001632	-0.001016
11.07378	12.27333	9.00891	-0.002632	0.009502	0.002591
12.30694	14.38896	9.00333	-0.017553	0.006350	-0.000390
9.86934	14.35300	5.29564	0.002868	0.001030	0.000310
11.10161	12.22804	5.21650	-0.001078	-0.002778	0.001060
11.11464	13.70636	9.07877	0.053726	-0.054659	-0.029168
12.33326	11.52411	5.18815	-0.000955	0.000157	0.000545
13.56430	13.67399	5.25995	0.001311	-0.000632	0.000060
13.53626	12.26601	8.93587	-0.003198	0.005345	0.002485
14.76266	14.38906	8.90426	-0.007942	0.003914	0.003859
12.33397	14.35288	5.30710	0.002875	-0.001093	-0.001870
13.56505	12.22870	5.20105	0.000158	0.000033	-0.001137
13.54921	13.70690	8.94399	0.004760	-0.010712	-0.002141
9.91126	15.51685	9.99472	0.128473	1.469900	0.880149
7.28864	16.40884	8.69813	0.009228	0.004171	0.001756
10.02526	16.50365	10.64498	-0.098323	-0.911234	-0.567831

---

total drift:	-0.044042	0.025523	-0.024340

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

---

free energy TOTEN = -1209.37819232 eV

energy without entropy= -1209.37819232 energy(sigma->0) = -1209.37819232

d Force = 0.3334634E-03[-0.441E-01, 0.448E-01] d Energy = 0.3726225E-04 0.296E-03

d Force =-0.7453164E+01[-0.763E+01,-0.728E+01] d Ewald =-0.7453352E+01 0.188E-03

POTLOK: cpu time 0.1766: real time 0.1773

---

stress matrix after NEB project (eV)

-17.74616 -0.31103 0.00384

-0.31103 -15.46958 0.28168

0.00384 0.28168 -19.19948

FORCES: max atom, RMS 1.718072 0.167296

FORCE total and by dimension 2.028354 1.469900

Stress total and by dimension 30.384309 19.199481

Finite differences progress:

Degree of freedom: 2/ 6

Displacement: 2/ 2

Total: 4/ 12

LATTYP: Found a simple orthorhombic cell.

ALAT = 14.7806000000

B/A-ratio = 1.2466138046

C/A-ratio = 1.4433717170

Lattice vectors:

A1 = (-14.7806000000, 0.0000000000, 0.0000000000)

A2 = (0.0000000000, 0.0000000000, -18.4257000000)

A3 = (0.0000000000, -21.3339000000, 0.0000000000)

Analysis of symmetry for initial positions (statically):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The static configuration has the point symmetry C_1 .

Analysis of symmetry for dynamics (positions and initial velocities):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The dynamic configuration has the point symmetry C_1 .

Analysis of constrained symmetry for selective dynamics:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The constrained configuration has the point symmetry C_1 .

Analysis of structural, dynamic, and magnetic symmetry:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The magnetic configuration has the point symmetry C_1 .

Subroutine INISYM returns: Found 1 space group operations

(whereof 1 operations are pure point group operations),

and found 1 'primitive' translations

KPOINTS: KPT-Resolved Value to Generate K-Mesh: 0

Automatic generation of k-mesh.

Space group operators:

irot	det(A)	alpha	n_x	n_y	n_z	tau_x	tau_y	tau_z
1	1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Subroutine IBZKPT returns following result:

==========

Found 1 irreducible k-points:

Following reciprocal coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

Following cartesian coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

WAVPRE: cpu time 0.1211: real time 0.1468

FEWALD: cpu time 0.0028: real time 0.0028

ORTHCH: cpu time 1.0109: real time 1.0145

LOOP+: cpu time 191.4862: real time 192.5254

---------- Iteration 6(1) ----------

POTLOK: cpu time 0.1693: real time 0.1825

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9276: real time 1.9344

RMM-DIIS: cpu time 7.2910: real time 7.3196

ORTHCH: cpu time 0.3536: real time 0.3547

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5227: real time 0.5244

MIXING: cpu time 0.0044: real time 0.0044

LOOP: cpu time 10.2790: real time 10.3305

eigenvalue-minimisations : 1956

total energy-change (2. order) :-0.1001863E-01 (-0.1100821E+00)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7398031 magnetization 0.0543081

Broyden mixing:

rms(total) = 0.47550E-01 rms(broyden)= 0.47421E-01

rms(prec) = 0.49948E-01

weight for this iteration 100.00

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107330.69646930

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79414627

PAW double counting = 52171.78321098 -52234.69473161

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5817.17277353

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77033769 eV

energy without entropy = -1202.77033769 energy(sigma->0) = -1202.77033769

---------- Iteration 6(2) ----------

POTLOK: cpu time 0.1649: real time 0.1839

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9241: real time 1.9306

RMM-DIIS: cpu time 7.1049: real time 7.1310

ORTHCH: cpu time 0.3526: real time 0.3536

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5220: real time 0.5237

MIXING: cpu time 0.0046: real time 0.0046

LOOP: cpu time 10.0833: real time 10.1379

eigenvalue-minimisations : 1920

total energy-change (2. order) : 0.2702445E-02 (-0.1194759E-02)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7391938 magnetization 0.0543051

Broyden mixing:

rms(total) = 0.28967E-01 rms(broyden)= 0.28947E-01

rms(prec) = 0.30122E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7760

1.7760

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107331.63086935

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80346232

PAW double counting = 52177.30293271 -52240.21947228

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.23996815

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76763524 eV

energy without entropy = -1202.76763524 energy(sigma->0) = -1202.76763524

---------- Iteration 6(3) ----------

POTLOK: cpu time 0.1715: real time 0.1814

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9337: real time 1.9398

RMM-DIIS: cpu time 7.2619: real time 7.2913

ORTHCH: cpu time 0.3560: real time 0.3570

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5236: real time 0.5251

MIXING: cpu time 0.0051: real time 0.0051

LOOP: cpu time 10.2624: real time 10.3103

eigenvalue-minimisations : 1951

total energy-change (2. order) : 0.1331199E-02 (-0.2327101E-03)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7398417 magnetization 0.0542807

Broyden mixing:

rms(total) = 0.10298E-01 rms(broyden)= 0.10295E-01

rms(prec) = 0.10787E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5890

0.8801 2.2980

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107332.58532328

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80705228

PAW double counting = 52182.04596580 -52244.96724008

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.28303826

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76630404 eV

energy without entropy = -1202.76630404 energy(sigma->0) = -1202.76630404

---------- Iteration 6(4) ----------

POTLOK: cpu time 0.1663: real time 0.1826

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9235: real time 1.9299

RMM-DIIS: cpu time 7.1773: real time 7.2127

ORTHCH: cpu time 0.3522: real time 0.3532

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5237: real time 0.5254

MIXING: cpu time 0.0051: real time 0.0051

LOOP: cpu time 10.1584: real time 10.2193

eigenvalue-minimisations : 1928

total energy-change (2. order) : 0.1567427E-03 (-0.3120966E-04)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7395726 magnetization 0.0542737

Broyden mixing:

rms(total) = 0.34379E-02 rms(broyden)= 0.34364E-02

rms(prec) = 0.38359E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5455

2.1910 0.8726 1.5728

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107333.06872087

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81198433

PAW double counting = 52183.26893354 -52246.19291292

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.80171088

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76614730 eV

energy without entropy = -1202.76614730 energy(sigma->0) = -1202.76614730

---------- Iteration 6(5) ----------

POTLOK: cpu time 0.1675: real time 0.1869

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9238: real time 1.9302

RMM-DIIS: cpu time 7.2366: real time 7.2621

ORTHCH: cpu time 0.3538: real time 0.3549

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5245: real time 0.5260

MIXING: cpu time 0.0057: real time 0.0057

LOOP: cpu time 10.2223: real time 10.2762

eigenvalue-minimisations : 1942

total energy-change (2. order) : 0.7849347E-05 (-0.5490326E-05)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396528 magnetization 0.0542764

Broyden mixing:

rms(total) = 0.16238E-02 rms(broyden)= 0.16225E-02

rms(prec) = 0.19470E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4412

2.2577 1.8986 0.8042 0.8042

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107333.26968438

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81210898

PAW double counting = 52182.77204465 -52245.69601456

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.60087365

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76613945 eV

energy without entropy = -1202.76613945 energy(sigma->0) = -1202.76613945

---------- Iteration 6(6) ----------

POTLOK: cpu time 0.1664: real time 0.1709

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9242: real time 1.9307

RMM-DIIS: cpu time 7.1129: real time 7.1518

ORTHCH: cpu time 0.3522: real time 0.3532

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5225: real time 0.5239

MIXING: cpu time 0.0060: real time 0.0060

LOOP: cpu time 10.0946: real time 10.1469

eigenvalue-minimisations : 1915

total energy-change (2. order) :-0.1597672E-04 (-0.7317084E-06)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396200 magnetization 0.0542762

Broyden mixing:

rms(total) = 0.87071E-03 rms(broyden)= 0.87044E-03

rms(prec) = 0.12039E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4706

2.5054 1.9658 1.0617 1.0617 0.7584

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107333.41584290

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81301085

PAW double counting = 52182.45561432 -52245.37987409

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.45534312

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76615543 eV

energy without entropy = -1202.76615543 energy(sigma->0) = -1202.76615543

---------- Iteration 6(7) ----------

POTLOK: cpu time 0.1677: real time 0.1839

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9211: real time 1.9279

RMM-DIIS: cpu time 7.0744: real time 7.1154

ORTHCH: cpu time 0.3521: real time 0.3532

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5226: real time 0.5243

MIXING: cpu time 0.0060: real time 0.0061

LOOP: cpu time 10.0543: real time 10.1212

eigenvalue-minimisations : 1915

total energy-change (2. order) :-0.3850990E-04 (-0.7349703E-06)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396365 magnetization 0.0542735

Broyden mixing:

rms(total) = 0.43019E-03 rms(broyden)= 0.42986E-03

rms(prec) = 0.70721E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4625

2.7466 2.1948 1.4468 0.8763 0.8763 0.6342

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107333.60734269

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81388009

PAW double counting = 52182.05238625 -52244.97686777

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.26452930

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76619394 eV

energy without entropy = -1202.76619394 energy(sigma->0) = -1202.76619394

---------- Iteration 6(8) ----------

POTLOK: cpu time 0.1656: real time 0.1803

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9216: real time 1.9277

RMM-DIIS: cpu time 6.3237: real time 6.3448

ORTHCH: cpu time 0.3536: real time 0.3547

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5227: real time 0.5243

MIXING: cpu time 0.0066: real time 0.0066

LOOP: cpu time 9.3043: real time 9.3489

eigenvalue-minimisations : 1726

total energy-change (2. order) :-0.2808717E-04 (-0.1158261E-06)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396544 magnetization 0.0542730

Broyden mixing:

rms(total) = 0.30015E-03 rms(broyden)= 0.30002E-03

rms(prec) = 0.52021E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4128

2.7619 2.3588 1.2523 1.0608 1.0608 0.7702 0.6250

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107333.70678129

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81426704

PAW double counting = 52181.86940472 -52244.79393771

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.16545428

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76622202 eV

energy without entropy = -1202.76622202 energy(sigma->0) = -1202.76622202

---------- Iteration 6(9) ----------

POTLOK: cpu time 0.1756: real time 0.1812

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9333: real time 1.9400

RMM-DIIS: cpu time 6.2988: real time 6.3274

ORTHCH: cpu time 0.3510: real time 0.3521

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5280: real time 0.5297

MIXING: cpu time 0.0067: real time 0.0068

LOOP: cpu time 9.3040: real time 9.3480

eigenvalue-minimisations : 1736

total energy-change (2. order) :-0.4233239E-04 (-0.1657503E-06)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396555 magnetization 0.0542729

Broyden mixing:

rms(total) = 0.19358E-03 rms(broyden)= 0.19338E-03

rms(prec) = 0.34359E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5676

3.4856 2.5739 1.8979 1.3419 0.9113 0.9113 0.8029 0.6163

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107333.81953903

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81479173

PAW double counting = 52181.76546902 -52244.69006439

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.05320119

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76626436 eV

energy without entropy = -1202.76626436 energy(sigma->0) = -1202.76626436

---------- Iteration 6(10) ----------

POTLOK: cpu time 0.1658: real time 0.1675

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9209: real time 1.9273

RMM-DIIS: cpu time 6.2383: real time 6.2556

ORTHCH: cpu time 0.3505: real time 0.3514

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5222: real time 0.5238

MIXING: cpu time 0.0071: real time 0.0071

LOOP: cpu time 9.2154: real time 9.2433

eigenvalue-minimisations : 1712

total energy-change (2. order) :-0.4665642E-04 (-0.2161806E-06)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396622 magnetization 0.0542723

Broyden mixing:

rms(total) = 0.13873E-03 rms(broyden)= 0.13861E-03

rms(prec) = 0.19686E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5907

4.1712 2.5619 2.1255 1.1272 1.1272 1.0498 0.8307 0.7059 0.6170

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107333.95896625

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81541695

PAW double counting = 52181.68441218 -52244.60908998

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.91436341

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76631101 eV

energy without entropy = -1202.76631101 energy(sigma->0) = -1202.76631101

---------- Iteration 6(11) ----------

POTLOK: cpu time 0.1680: real time 0.1822

```
      SETDIJ:    cpu time       0.0099: real time       0.0099
      EDDIAG:    cpu time       1.9204: real time       1.9273
    RMM-DIIS:    cpu time       5.9011: real time       5.9315
      ORTHCH:    cpu time       0.3507: real time       0.3518
         DOS:    cpu time       0.0004: real time       0.0004
      CHARGE:    cpu time       0.5222: real time       0.5240
      MIXING:    cpu time       0.0078: real time       0.0078
      ------------------------------------------
        LOOP:    cpu time       8.8805: real time       8.9350

eigenvalue-minimisations    :    1581
total energy-change (2. order) :-0.1588106E-04    (-0.4255913E-07)
number of electron          518.9999721 magnetization             0.9999998
augmentation part             11.7396659 magnetization             0.0542721

Broyden mixing:
  rms(total) = 0.76246E-04        rms(broyden)= 0.76184E-04
  rms(prec ) = 0.12548E-03
  weight for this iteration         100.00

eigenvalues of (default mixing * dielectric matrix)
  average eigenvalue GAMMA=      1.7205
```

5.1459 2.4493 2.4493 1.7806 1.3169 0.9753 0.9753 0.8168 0.6769 0.6181

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107333.99194078

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81551560

PAW double counting = 52181.69856150 -52244.62324442

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.88149830

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76632689 eV

energy without entropy = -1202.76632689 energy(sigma->0) = -1202.76632689

---------- Iteration 6(12) ----------

POTLOK: cpu time 0.1660: real time 0.1804

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9193: real time 1.9256

RMM-DIIS: cpu time 5.8275: real time 5.8608

ORTHCH: cpu time 0.3511: real time 0.3524

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5055: real time 0.5261

MIXING: cpu time 0.0080: real time 0.0081

LOOP: cpu time 8.7881: real time 8.8641

eigenvalue-minimisations : 1593

total energy-change (2. order) :-0.2325797E-04 (-0.4434690E-07)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396699 magnetization 0.0542720

Broyden mixing:

rms(total) = 0.55568E-04 rms(broyden)= 0.55533E-04

rms(prec) = 0.78786E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7969

6.2787 2.7955 2.4544 2.0199 1.1039 1.1039 1.0281 0.8477 0.8477 0.6680

0.6186

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107334.02696759

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81555603

PAW double counting = 52181.74510527 -52244.66977425

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.84654911

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76635015 eV

energy without entropy = -1202.76635015 energy(sigma->0) = -1202.76635015

---------- Iteration 6(13) ----------

POTLOK: cpu time 0.1657: real time 0.1675

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9201: real time 1.9269

RMM-DIIS: cpu time 5.2375: real time 5.2600

ORTHCH: cpu time 0.3530: real time 0.3542

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5229: real time 0.5247

MIXING: cpu time 0.0080: real time 0.0080

LOOP: cpu time 8.2177: real time 8.2519

eigenvalue-minimisations : 1444

total energy-change (2. order) :-0.8375973E-05 (-0.1146803E-07)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396691 magnetization 0.0542721

Broyden mixing:

rms(total) = 0.27406E-04 rms(broyden)= 0.27381E-04

rms(prec) = 0.45569E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7812

6.4961 2.8447 2.4661 2.0617 1.2692 1.2692 1.0076 1.0076 0.8344 0.8344

0.6645 0.6189

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107334.03792523

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81557829

PAW double counting = 52181.75389046 -52244.67855974

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.83562182

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76635853 eV

energy without entropy = -1202.76635853 energy(sigma->0) = -1202.76635853

---------- Iteration 6(14) ----------

POTLOK: cpu time 0.1681: real time 0.1698

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9220: real time 1.9287

RMM-DIIS: cpu time 5.1813: real time 5.2009

ORTHCH: cpu time 0.3511: real time 0.3521

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5226: real time 0.5244

MIXING: cpu time 0.0084: real time 0.0084

LOOP: cpu time 8.1640: real time 8.1949

eigenvalue-minimisations : 1442

total energy-change (2. order) :-0.8807430E-05 (-0.8813363E-08)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396691 magnetization 0.0542721

Broyden mixing:

rms(total) = 0.19557E-04 rms(broyden)= 0.19550E-04

rms(prec) = 0.28154E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8882

7.0721 3.5856 2.7161 2.2696 1.9531 1.1084 1.1084 1.0077 0.8702 0.8702

0.6202 0.6532 0.7113

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107334.04242101

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81557008

PAW double counting = 52181.74343998 -52244.66811596

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.83111994

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76636734 eV

energy without entropy = -1202.76636734 energy(sigma->0) = -1202.76636734

---------- Iteration 6(15) ----------

POTLOK: cpu time 0.1662: real time 0.1821

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9222: real time 1.9286

RMM-DIIS: cpu time 4.8156: real time 4.8475

ORTHCH: cpu time 0.3509: real time 0.3521

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5225: real time 0.5244

MIXING: cpu time 0.0087: real time 0.0087

LOOP: cpu time 7.7968: real time 7.8541

eigenvalue-minimisations : 1335

total energy-change (2. order) :-0.3679939E-05 (-0.3125490E-08)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396692 magnetization 0.0542721

Broyden mixing:

rms(total) = 0.11390E-04 rms(broyden)= 0.11385E-04

rms(prec) = 0.16582E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9059

7.5049 4.2027 2.5995 2.3688 1.9530 1.1500 1.1500 1.0126 1.0126 0.8964

0.8964 0.6765 0.6214 0.6375

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107334.04418538

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81555783

PAW double counting = 52181.74031509 -52244.66499138

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.82934667

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76637102 eV

energy without entropy = -1202.76637102 energy(sigma->0) = -1202.76637102

---------- Iteration 6(16) ----------

POTLOK: cpu time 0.1685: real time 0.1863

SETDIJ: cpu time 0.0129: real time 0.0135

EDDIAG: cpu time 1.9335: real time 1.9401

RMM-DIIS: cpu time 4.7434: real time 4.7751

ORTHCH: cpu time 0.3508: real time 0.3520

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5243: real time 0.5260

MIXING: cpu time 0.0094: real time 0.0095

LOOP: cpu time 7.7431: real time 7.8030

eigenvalue-minimisations : 1275

total energy-change (2. order) :-0.1490218E-05 (-0.9629550E-09)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396693 magnetization 0.0542721

Broyden mixing:

rms(total) = 0.59416E-05 rms(broyden)= 0.59378E-05

rms(prec) = 0.10363E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9270

7.7636 4.6199 2.5698 2.5698 1.9209 1.5233 1.1849 1.1849 0.9711 0.9711

0.8512 0.8512 0.6741 0.6242 0.6242

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107334.04451178

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81554787

PAW double counting = 52181.73956386 -52244.66423826

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.82901369

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76637251 eV

energy without entropy = -1202.76637251 energy(sigma->0) = -1202.76637251

---------- Iteration 6(17) ----------

POTLOK: cpu time 0.1665: real time 0.1675

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9208: real time 1.9271

RMM-DIIS: cpu time 4.7375: real time 4.7532

ORTHCH: cpu time 0.3511: real time 0.3521

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5237: real time 0.5253

MIXING: cpu time 0.0095: real time 0.0095

LOOP: cpu time 7.7196: real time 7.7452

eigenvalue-minimisations : 1265

total energy-change (2. order) :-0.1115535E-05 (-0.7635501E-09)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396695 magnetization 0.0542721

Broyden mixing:

rms(total) = 0.41050E-05 rms(broyden)= 0.41030E-05

rms(prec) = 0.63889E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9766

8.1112 5.1214 2.9628 2.5360 2.0549 1.8698 1.1980 1.1980 1.0674 1.0674

0.8853 0.8853 0.7523 0.6711 0.6220 0.6220

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107334.04451708

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81553701

PAW double counting = 52181.73692633 -52244.66160033

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.82899905

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76637362 eV

energy without entropy = -1202.76637362 energy(sigma->0) = -1202.76637362

---------- Iteration 6(18) ----------

POTLOK: cpu time 0.1641: real time 0.1649

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9234: real time 1.9295

RMM-DIIS: cpu time 4.3713: real time 4.3847

ORTHCH: cpu time 0.3535: real time 0.3545

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5245: real time 0.5262

MIXING: cpu time 0.0097: real time 0.0097

LOOP: cpu time 7.3569: real time 7.3799

eigenvalue-minimisations : 1086

total energy-change (2. order) :-0.3313617E-06 (-0.3225162E-09)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396696 magnetization 0.0542721

Broyden mixing:

rms(total) = 0.25719E-05 rms(broyden)= 0.25710E-05

rms(prec) = 0.39517E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9865

8.2682 5.3904 3.1904 2.4496 2.4496 1.8673 1.3809 1.2120 1.2120 0.9948

0.9948 0.8694 0.8694 0.7111 0.6683 0.6216 0.6216

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107334.04449544

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81553178

PAW double counting = 52181.73747278 -52244.66214721

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.82901537

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76637395 eV

energy without entropy = -1202.76637395 energy(sigma->0) = -1202.76637395

---------- Iteration 6(19) ----------

POTLOK: cpu time 0.1655: real time 0.1814

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9189: real time 1.9257

RMM-DIIS: cpu time 4.1754: real time 4.1893

ORTHCH: cpu time 0.3527: real time 0.3539

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5243: real time 0.5261

MIXING: cpu time 0.0104: real time 0.0105

LOOP: cpu time 7.1577: real time 7.1975

eigenvalue-minimisations : 994

total energy-change (2. order) :-0.1415465E-06 (-0.1111546E-09)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396696 magnetization 0.0542721

Broyden mixing:

rms(total) = 0.14905E-05 rms(broyden)= 0.14899E-05

rms(prec) = 0.23172E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0205

8.4209 5.8132 3.6608 2.5523 2.5523 1.9588 1.5699 1.2577 1.2577 1.0722

1.0722 0.8671 0.8671 0.8633 0.6702 0.6702 0.6218 0.6218

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107334.04446347

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81552866

PAW double counting = 52181.73931320 -52244.66398794

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.82904405

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76637409 eV

energy without entropy = -1202.76637409 energy(sigma->0) = -1202.76637409

---------- Iteration 6(20) ----------

POTLOK: cpu time 0.1669: real time 0.1808

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9281: real time 1.9344

RMM-DIIS: cpu time 4.1064: real time 4.1358

ORTHCH: cpu time 0.3528: real time 0.3538

DOS: cpu time 0.0003: real time 0.0003

LOOP: cpu time 6.5645: real time 6.6151

eigenvalue-minimisations : 954

total energy-change (2. order) :-0.4895992E-07 (-0.1283027E-09)

number of electron 518.9999721 magnetization 0.9999998

augmentation part 11.7396696 magnetization 0.0542721

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91326.38559271

-Hartree energ DENC = -107334.04442813

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81552717

PAW double counting = 52181.73957990 -52244.66425486

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.82907772

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76637414 eV

energy without entropy = -1202.76637414 energy(sigma->0) = -1202.76637414

---

average (electrostatic) potential at core

the test charge radii are 0.5201 0.6991 1.0621 0.7215

(the norm of the test charge is 1.0000)

1 -40.7503	2 -40.7482	3 -40.7496	4 -40.7482	5 -40.7503
6 -40.7525	7 -40.7501	8 -40.7578	9 -40.7497	10 -40.7573
11 -40.7511	12 -40.7531	13 -40.6463	14 -40.6932	15 -40.7661
16 -40.6953	17 -40.6894	18 -40.8581	19 -40.6761	20 -40.6637
21 -40.6858	22 -40.6589	23 -40.0866	24 -40.1245	25 -57.4562
26 -57.6671	27 -57.6542	28 -57.4659	29 -57.6603	30 -57.4562
31 -57.6669	32 -57.6538	33 -57.4639	34 -57.6651	35 -57.4570
36 -57.6688	37 -57.6538	38 -57.4661	39 -57.6710	40 -57.4561
41 -57.6728	42 -57.6540	43 -57.4710	44 -57.6855	45 -57.4561
46 -57.6718	47 -57.6548	48 -57.4713	49 -57.6767	50 -57.4572
51 -57.6684	52 -57.6546	53 -57.4689	54 -57.6631	55 -57.6339
56 -57.6599	57 -57.6839	58 -57.6797	59 -57.6636	60 -57.6665
61 -57.6866	62 -57.6711	63 -57.6342	64 -57.6593	65 -57.6859
66 -57.6912	67 -57.6618	68 -57.6663	69 -57.6903	70 -57.6973
71 -57.6337	72 -57.6607	73 -57.6935	74 -57.7180	75 -57.6627
76 -57.6669	77 -57.7025	78 -57.7468	79 -57.6339	80 -57.6633
81 -57.7073	82 -57.7485	83 -57.6660	84 -57.6684	85 -57.7338
86 -57.8369	87 -57.6363	88 -57.6640	89 -57.7092	90 -57.7134
91 -57.6706	92 -57.6686	93 -57.7386	94 -57.7553	95 -57.6346
96 -57.6622	97 -57.6929	98 -57.6871	99 -57.6679	100 -57.6674
101 -57.7044	102 -57.6823	103 -57.6573	104 -57.6278	105 -57.6419
106 -57.2853	107 -57.3849	108 -57.6282	109 -57.5933	110 -57.6562

111 -57.6278	112 -57.6384	113 -57.3039	114 -57.3905	115 -57.6275
116 -57.5952	117 -57.6555	118 -57.6196	119 -57.6941	120 -57.6763
121 -57.3843	122 -57.6263	123 -57.7046	124 -57.6564	125 -57.6222
126 -57.8276	127 -58.3255	128 -57.3576	129 -57.6315	130 -58.1346
131 -57.6643	132 -57.6314	133 -57.7950	134 -57.4103	135 -57.3687
136 -57.6354	137 -58.0695	138 -57.6608	139 -57.6273	140 -57.6674
141 -57.2944	142 -57.3749	143 -57.6308	144 -57.6434	145 -60.8855
146 -57.3135	147 -81.3569			

E-fermi : -2.3538 XC(G=0): -2.7344 alpha+bet : -2.2521

spin component 1

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-27.1578	1.00000
2	-21.5646	1.00000
3	-21.4685	1.00000
4	-21.0941	1.00000

5	-21.0652	1.00000
6	-21.0107	1.00000
7	-20.9758	1.00000
8	-20.9737	1.00000
9	-20.8879	1.00000
10	-20.5514	1.00000
11	-20.4998	1.00000
12	-20.4084	1.00000
13	-20.3951	1.00000
14	-20.1199	1.00000
15	-19.9724	1.00000
16	-19.6953	1.00000
17	-19.6237	1.00000
18	-19.5962	1.00000
19	-19.5806	1.00000
20	-19.5258	1.00000
21	-19.5239	1.00000
22	-19.4955	1.00000
23	-19.4781	1.00000
24	-19.1049	1.00000
25	-19.0715	1.00000
26	-18.9747	1.00000

27	-18.9619	1.00000
28	-18.8948	1.00000
29	-18.7302	1.00000
30	-18.4969	1.00000
31	-18.3555	1.00000
32	-18.2722	1.00000
33	-18.2491	1.00000
34	-18.1799	1.00000
35	-18.1777	1.00000
36	-18.0768	1.00000
37	-18.0731	1.00000
38	-17.5513	1.00000
39	-17.3099	1.00000
40	-17.2839	1.00000
41	-17.2794	1.00000
42	-17.2067	1.00000
43	-17.2007	1.00000
44	-17.1712	1.00000
45	-17.0186	1.00000
46	-16.9470	1.00000
47	-16.9295	1.00000
48	-16.8902	1.00000

49	-16.8884	1.00000
50	-16.8472	1.00000
51	-16.8388	1.00000
52	-16.8173	1.00000
53	-16.8156	1.00000
54	-16.7265	1.00000
55	-16.7233	1.00000
56	-16.1664	1.00000
57	-15.7265	1.00000
58	-15.6891	1.00000
59	-15.6566	1.00000
60	-15.6333	1.00000
61	-15.6134	1.00000
62	-15.5508	1.00000
63	-15.5470	1.00000
64	-15.1670	1.00000
65	-14.8059	1.00000
66	-14.6040	1.00000
67	-14.5753	1.00000
68	-14.5321	1.00000
69	-14.4955	1.00000
70	-14.4652	1.00000

71	-14.4385	1.00000
72	-14.3306	1.00000
73	-14.3025	1.00000
74	-14.2768	1.00000
75	-14.2689	1.00000
76	-14.1798	1.00000
77	-14.1759	1.00000
78	-13.8872	1.00000
79	-13.7551	1.00000
80	-13.5898	1.00000
81	-13.5454	1.00000
82	-13.5265	1.00000
83	-13.4939	1.00000
84	-13.4417	1.00000
85	-13.3614	1.00000
86	-13.3427	1.00000
87	-13.1846	1.00000
88	-12.7832	1.00000
89	-12.7562	1.00000
90	-12.7241	1.00000
91	-12.6933	1.00000
92	-12.6832	1.00000

93	-12.6206	1.00000
94	-12.4584	1.00000
95	-12.4437	1.00000
96	-12.3787	1.00000
97	-12.3203	1.00000
98	-12.2103	1.00000
99	-12.2007	1.00000
100	-12.1617	1.00000
101	-11.9523	1.00000
102	-11.6815	1.00000
103	-11.6292	1.00000
104	-11.6083	1.00000
105	-11.5875	1.00000
106	-11.1211	1.00000
107	-11.0844	1.00000
108	-10.8967	1.00000
109	-10.8852	1.00000
110	-10.8304	1.00000
111	-10.7080	1.00000
112	-10.6804	1.00000
113	-10.6604	1.00000
114	-10.6436	1.00000

115	-10.5868	1.00000
116	-10.5783	1.00000
117	-10.5683	1.00000
118	-10.5646	1.00000
119	-10.5235	1.00000
120	-10.5226	1.00000
121	-10.5078	1.00000
122	-10.5001	1.00000
123	-10.3753	1.00000
124	-10.2956	1.00000
125	-10.2552	1.00000
126	-10.1852	1.00000
127	-10.1842	1.00000
128	-10.1285	1.00000
129	-10.0662	1.00000
130	-9.8918	1.00000
131	-9.8650	1.00000
132	-9.7958	1.00000
133	-9.7836	1.00000
134	-9.7655	1.00000
135	-9.6993	1.00000
136	-9.4518	1.00000

137	-9.4240	1.00000
138	-9.3928	1.00000
139	-9.3856	1.00000
140	-9.3788	1.00000
141	-9.3668	1.00000
142	-9.3093	1.00000
143	-9.3048	1.00000
144	-9.2989	1.00000
145	-9.2844	1.00000
146	-9.2688	1.00000
147	-9.0907	1.00000
148	-9.0030	1.00000
149	-8.9939	1.00000
150	-8.9571	1.00000
151	-8.9543	1.00000
152	-8.7904	1.00000
153	-8.7430	1.00000
154	-8.7313	1.00000
155	-8.7151	1.00000
156	-8.7057	1.00000
157	-8.6842	1.00000
158	-8.6757	1.00000

159	-8.6653	1.00000
160	-8.6513	1.00000
161	-8.5918	1.00000
162	-8.5800	1.00000
163	-8.5735	1.00000
164	-8.5651	1.00000
165	-8.4843	1.00000
166	-8.4536	1.00000
167	-8.4331	1.00000
168	-8.3425	1.00000
169	-8.2943	1.00000
170	-8.2721	1.00000
171	-8.2603	1.00000
172	-8.2304	1.00000
173	-8.2294	1.00000
174	-8.1488	1.00000
175	-8.1424	1.00000
176	-8.0751	1.00000
177	-8.0413	1.00000
178	-8.0231	1.00000
179	-8.0185	1.00000
180	-7.9700	1.00000

181	-7.9613	1.00000
182	-7.9216	1.00000
183	-7.8976	1.00000
184	-7.8823	1.00000
185	-7.8692	1.00000
186	-7.7981	1.00000
187	-7.7945	1.00000
188	-7.7451	1.00000
189	-7.7074	1.00000
190	-7.6626	1.00000
191	-7.5964	1.00000
192	-7.5815	1.00000
193	-7.5724	1.00000
194	-7.5435	1.00000
195	-7.4777	1.00000
196	-7.4771	1.00000
197	-7.4251	1.00000
198	-7.3207	1.00000
199	-7.2464	1.00000
200	-7.1580	1.00000
201	-7.0633	1.00000
202	-7.0388	1.00000

203	-7.0248	1.00000
204	-7.0100	1.00000
205	-6.9934	1.00000
206	-6.9864	1.00000
207	-6.9722	1.00000
208	-6.8634	1.00000
209	-6.8177	1.00000
210	-6.7987	1.00000
211	-6.7900	1.00000
212	-6.7291	1.00000
213	-6.6842	1.00000
214	-6.4672	1.00000
215	-6.4212	1.00000
216	-6.3923	1.00000
217	-6.3881	1.00000
218	-6.3706	1.00000
219	-6.3688	1.00000
220	-6.3136	1.00000
221	-6.3034	1.00000
222	-6.2327	1.00000
223	-6.2267	1.00000
224	-6.2262	1.00000

225	-6.0742	1.00000
226	-6.0334	1.00000
227	-5.7889	1.00000
228	-5.7481	1.00000
229	-5.6899	1.00000
230	-5.6382	1.00000
231	-5.6340	1.00000
232	-5.5551	1.00000
233	-5.5274	1.00000
234	-5.4640	1.00000
235	-5.4353	1.00000
236	-5.1632	1.00000
237	-5.0553	1.00000
238	-5.0465	1.00000
239	-5.0148	1.00000
240	-4.9850	1.00000
241	-4.9068	1.00000
242	-4.8503	1.00000
243	-4.8184	1.00000
244	-4.7859	1.00000
245	-4.6788	1.00000
246	-4.5693	1.00000

247	-4.5680	1.00000
248	-4.5011	1.00000
249	-4.4424	1.00000
250	-4.3803	1.00000
251	-4.2898	1.00000
252	-4.2613	1.00000
253	-4.2094	1.00000
254	-3.5496	1.00000
255	-3.3513	1.00000
256	-3.1954	1.00000
257	-2.9365	1.00000
258	-2.8450	1.00000
259	-2.8202	1.00000
260	-2.6025	1.00000
261	-1.9059	0.00000
262	-1.7641	0.00000
263	-1.7153	0.00000
264	-1.3409	0.00000
265	-1.2887	0.00000
266	-1.1789	0.00000
267	-0.7413	0.00000
268	-0.5816	0.00000

269	-0.4968	0.00000
270	-0.3047	0.00000
271	-0.3024	0.00000
272	-0.2868	0.00000
273	-0.1801	0.00000
274	-0.0549	0.00000
275	-0.0453	0.00000
276	-0.0077	0.00000
277	0.0380	0.00000
278	0.0890	0.00000
279	0.1761	0.00000
280	0.2235	0.00000
281	0.2513	0.00000
282	0.4212	0.00000
283	0.4519	0.00000
284	0.4849	0.00000
285	0.5981	0.00000
286	0.6796	0.00000
287	0.8196	0.00000
288	0.8737	0.00000
289	1.0469	0.00000
290	1.0870	0.00000

291	1.1243	0.00000
292	1.1648	0.00000
293	1.2237	0.00000
294	1.2456	0.00000
295	1.2893	0.00000
296	1.3148	0.00000
297	1.3476	0.00000
298	1.4136	0.00000
299	1.4681	0.00000
300	1.4821	0.00000
301	1.5554	0.00000
302	1.5878	0.00000
303	1.6265	0.00000
304	1.6788	0.00000
305	1.7520	0.00000
306	1.7647	0.00000
307	1.8738	0.00000
308	1.8982	0.00000
309	1.9059	0.00000
310	1.9159	0.00000
311	2.1193	0.00000
312	2.1849	0.00000

313	2.2098	0.00000
314	2.2365	0.00000
315	2.2765	0.00000
316	2.2922	0.00000
317	2.3316	0.00000
318	2.3551	0.00000
319	2.3739	0.00000
320	2.3998	0.00000
321	2.4225	0.00000
322	2.4307	0.00000
323	2.4406	0.00000
324	2.4531	0.00000
325	2.4620	0.00000
326	2.5221	0.00000
327	2.5369	0.00000
328	2.7001	0.00000
329	2.7285	0.00000
330	2.7546	0.00000
331	2.7578	0.00000
332	2.7651	0.00000
333	2.8174	0.00000
334	2.8364	0.00000

335	2.8542	0.00000
336	2.8912	0.00000
337	2.9246	0.00000
338	2.9470	0.00000
339	2.9792	0.00000
340	3.0057	0.00000
341	3.0347	0.00000
342	3.0450	0.00000
343	3.0663	0.00000
344	3.0859	0.00000
345	3.1493	0.00000
346	3.1628	0.00000
347	3.1797	0.00000
348	3.1914	0.00000
349	3.3008	0.00000
350	3.3216	0.00000
351	3.3515	0.00000
352	3.3668	0.00000
353	3.3892	0.00000
354	3.4308	0.00000
355	3.4753	0.00000
356	3.4854	0.00000

357	3.4871	0.00000
358	3.5010	0.00000
359	3.6339	0.00000
360	3.6729	0.00000
361	3.6857	0.00000
362	3.7302	0.00000
363	3.7530	0.00000
364	3.7600	0.00000
365	3.7724	0.00000
366	3.7943	0.00000
367	3.8129	0.00000
368	3.8355	0.00000
369	3.8390	0.00000
370	3.8510	0.00000
371	3.8773	0.00000
372	3.8848	0.00000
373	3.9100	0.00000
374	3.9250	0.00000
375	3.9344	0.00000
376	3.9577	0.00000
377	3.9732	0.00000
378	3.9831	0.00000

379	4.0155	0.00000
380	4.0685	0.00000
381	4.1640	0.00000
382	4.2462	0.00000
383	4.2570	0.00000
384	4.2586	0.00000
385	4.2850	0.00000
386	4.3127	0.00000
387	4.3279	0.00000
388	4.3409	0.00000
389	4.3722	0.00000
390	4.3819	0.00000
391	4.4174	0.00000
392	4.4442	0.00000
393	4.4686	0.00000
394	4.4800	0.00000
395	4.4859	0.00000
396	4.4966	0.00000
397	4.5169	0.00000
398	4.5510	0.00000
399	4.5907	0.00000
400	4.6078	0.00000

401	4.6274	0.00000
402	4.6430	0.00000
403	4.6568	0.00000
404	4.6800	0.00000
405	4.7043	0.00000
406	4.7317	0.00000
407	4.7456	0.00000
408	4.7665	0.00000
409	4.7828	0.00000
410	4.7840	0.00000
411	4.7970	0.00000
412	4.8274	0.00000
413	4.8631	0.00000
414	4.8722	0.00000
415	4.8977	0.00000
416	4.9310	0.00000
417	4.9836	0.00000
418	5.0044	0.00000
419	5.0110	0.00000
420	5.0354	0.00000
421	5.0395	0.00000
422	5.0650	0.00000

423	5.0818	0.00000
424	5.1133	0.00000
425	5.1174	0.00000
426	5.1372	0.00000
427	5.1409	0.00000
428	5.1555	0.00000
429	5.1753	0.00000
430	5.1853	0.00000
431	5.1886	0.00000
432	5.2152	0.00000
433	5.2361	0.00000
434	5.2405	0.00000
435	5.2559	0.00000
436	5.2907	0.00000
437	5.2965	0.00000
438	5.3092	0.00000
439	5.3313	0.00000
440	5.3498	0.00000
441	5.3678	0.00000
442	5.3742	0.00000
443	5.3943	0.00000
444	5.4205	0.00000

445	5.4538	0.00000
446	5.4631	0.00000
447	5.4816	0.00000
448	5.4943	0.00000
449	5.5205	0.00000
450	5.5505	0.00000
451	5.5682	0.00000
452	5.5761	0.00000
453	5.5954	0.00000
454	5.6173	0.00000
455	5.6579	0.00000
456	5.6817	0.00000
457	5.7098	0.00000
458	5.7227	0.00000
459	5.7437	0.00000
460	5.7574	0.00000
461	5.7820	0.00000
462	5.7907	0.00000
463	5.7958	0.00000
464	5.8020	0.00000
465	5.8074	0.00000
466	5.8240	0.00000

467	5.8440	0.00000
468	5.8551	0.00000
469	5.8753	0.00000
470	5.8831	0.00000
471	5.8881	0.00000
472	5.9119	0.00000
473	5.9167	0.00000
474	5.9433	0.00000
475	5.9561	0.00000
476	5.9725	0.00000
477	5.9878	0.00000
478	6.0096	0.00000
479	6.0169	0.00000
480	6.0860	0.00000

spin component 2

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-27.1511	1.00000
2	-21.5634	1.00000
3	-21.4669	1.00000

4	-21.0922	1.00000
5	-21.0643	1.00000
6	-21.0079	1.00000
7	-20.9743	1.00000
8	-20.9719	1.00000
9	-20.8774	1.00000
10	-20.5484	1.00000
11	-20.4964	1.00000
12	-20.3973	1.00000
13	-20.3855	1.00000
14	-20.1156	1.00000
15	-19.9494	1.00000
16	-19.6925	1.00000
17	-19.6224	1.00000
18	-19.5941	1.00000
19	-19.5741	1.00000
20	-19.5245	1.00000
21	-19.5222	1.00000
22	-19.4729	1.00000
23	-19.4587	1.00000
24	-19.1024	1.00000
25	-19.0691	1.00000

26	-18.9647	1.00000
27	-18.9524	1.00000
28	-18.8900	1.00000
29	-18.7007	1.00000
30	-18.4938	1.00000
31	-18.3484	1.00000
32	-18.2440	1.00000
33	-18.2240	1.00000
34	-18.1746	1.00000
35	-18.1723	1.00000
36	-18.0568	1.00000
37	-18.0535	1.00000
38	-17.5479	1.00000
39	-17.2934	1.00000
40	-17.2833	1.00000
41	-17.2702	1.00000
42	-17.2045	1.00000
43	-17.2037	1.00000
44	-17.1682	1.00000
45	-17.0146	1.00000
46	-16.9380	1.00000
47	-16.9190	1.00000

48	-16.8676	1.00000
49	-16.8667	1.00000
50	-16.8263	1.00000
51	-16.8196	1.00000
52	-16.8144	1.00000
53	-16.8122	1.00000
54	-16.7282	1.00000
55	-16.7222	1.00000
56	-16.1637	1.00000
57	-15.7258	1.00000
58	-15.6538	1.00000
59	-15.6394	1.00000
60	-15.6181	1.00000
61	-15.5637	1.00000
62	-15.5250	1.00000
63	-15.5223	1.00000
64	-15.1633	1.00000
65	-14.8037	1.00000
66	-14.6018	1.00000
67	-14.5578	1.00000
68	-14.4974	1.00000
69	-14.4956	1.00000

70	-14.4613	1.00000
71	-14.4343	1.00000
72	-14.3271	1.00000
73	-14.2947	1.00000
74	-14.2651	1.00000
75	-14.2608	1.00000
76	-14.1617	1.00000
77	-14.1583	1.00000
78	-13.8863	1.00000
79	-13.7527	1.00000
80	-13.5870	1.00000
81	-13.5347	1.00000
82	-13.5154	1.00000
83	-13.4904	1.00000
84	-13.4399	1.00000
85	-13.3408	1.00000
86	-13.3382	1.00000
87	-13.1830	1.00000
88	-12.7766	1.00000
89	-12.7467	1.00000
90	-12.7151	1.00000
91	-12.6748	1.00000

92	-12.6677	1.00000
93	-12.6184	1.00000
94	-12.4458	1.00000
95	-12.4288	1.00000
96	-12.3752	1.00000
97	-12.3194	1.00000
98	-12.2057	1.00000
99	-12.1955	1.00000
100	-12.1602	1.00000
101	-11.9495	1.00000
102	-11.6785	1.00000
103	-11.6157	1.00000
104	-11.5892	1.00000
105	-11.5772	1.00000
106	-11.1183	1.00000
107	-11.0824	1.00000
108	-10.8876	1.00000
109	-10.8747	1.00000
110	-10.8274	1.00000
111	-10.7019	1.00000
112	-10.6793	1.00000
113	-10.6573	1.00000

114	-10.6388	1.00000
115	-10.5787	1.00000
116	-10.5712	1.00000
117	-10.5657	1.00000
118	-10.5617	1.00000
119	-10.5129	1.00000
120	-10.5120	1.00000
121	-10.4987	1.00000
122	-10.4941	1.00000
123	-10.3744	1.00000
124	-10.2945	1.00000
125	-10.2539	1.00000
126	-10.1818	1.00000
127	-10.1806	1.00000
128	-10.1130	1.00000
129	-10.0636	1.00000
130	-9.8890	1.00000
131	-9.8631	1.00000
132	-9.7895	1.00000
133	-9.7745	1.00000
134	-9.7610	1.00000
135	-9.6975	1.00000

136	-9.4503	1.00000
137	-9.4205	1.00000
138	-9.3812	1.00000
139	-9.3771	1.00000
140	-9.3718	1.00000
141	-9.3569	1.00000
142	-9.3069	1.00000
143	-9.3024	1.00000
144	-9.2972	1.00000
145	-9.2845	1.00000
146	-9.2458	1.00000
147	-9.0895	1.00000
148	-8.9995	1.00000
149	-8.9904	1.00000
150	-8.9427	1.00000
151	-8.9400	1.00000
152	-8.7879	1.00000
153	-8.7349	1.00000
154	-8.7290	1.00000
155	-8.7096	1.00000
156	-8.7027	1.00000
157	-8.6672	1.00000

158	-8.6609	1.00000
159	-8.6535	1.00000
160	-8.6505	1.00000
161	-8.5746	1.00000
162	-8.5684	1.00000
163	-8.5637	1.00000
164	-8.5463	1.00000
165	-8.4839	1.00000
166	-8.4530	1.00000
167	-8.4315	1.00000
168	-8.3397	1.00000
169	-8.2909	1.00000
170	-8.2706	1.00000
171	-8.2300	1.00000
172	-8.2266	1.00000
173	-8.2245	1.00000
174	-8.1387	1.00000
175	-8.1312	1.00000
176	-8.0718	1.00000
177	-8.0392	1.00000
178	-8.0101	1.00000
179	-8.0043	1.00000

180	-7.9653	1.00000
181	-7.9564	1.00000
182	-7.9174	1.00000
183	-7.8878	1.00000
184	-7.8685	1.00000
185	-7.8604	1.00000
186	-7.7892	1.00000
187	-7.7851	1.00000
188	-7.7356	1.00000
189	-7.6758	1.00000
190	-7.6327	1.00000
191	-7.5942	1.00000
192	-7.5737	1.00000
193	-7.5514	1.00000
194	-7.5361	1.00000
195	-7.4696	1.00000
196	-7.4695	1.00000
197	-7.4240	1.00000
198	-7.3198	1.00000
199	-7.2331	1.00000
200	-7.1550	1.00000
201	-7.0520	1.00000

202	-7.0332	1.00000
203	-7.0130	1.00000
204	-6.9821	1.00000
205	-6.9743	1.00000
206	-6.9691	1.00000
207	-6.9379	1.00000
208	-6.8595	1.00000
209	-6.8134	1.00000
210	-6.7926	1.00000
211	-6.7848	1.00000
212	-6.7223	1.00000
213	-6.6747	1.00000
214	-6.4638	1.00000
215	-6.3914	1.00000
216	-6.3795	1.00000
217	-6.3754	1.00000
218	-6.3595	1.00000
219	-6.3351	1.00000
220	-6.2991	1.00000
221	-6.2724	1.00000
222	-6.2264	1.00000
223	-6.2251	1.00000

224	-6.2182	1.00000
225	-6.0436	1.00000
226	-6.0049	1.00000
227	-5.7529	1.00000
228	-5.7074	1.00000
229	-5.6882	1.00000
230	-5.6328	1.00000
231	-5.6195	1.00000
232	-5.5406	1.00000
233	-5.5200	1.00000
234	-5.4375	1.00000
235	-5.4079	1.00000
236	-5.1412	1.00000
237	-5.0569	1.00000
238	-5.0223	1.00000
239	-5.0188	1.00000
240	-4.9553	1.00000
241	-4.8740	1.00000
242	-4.8511	1.00000
243	-4.7988	1.00000
244	-4.7738	1.00000
245	-4.6483	1.00000

246	-4.5754	1.00000
247	-4.5724	1.00000
248	-4.4713	1.00000
249	-4.4181	1.00000
250	-4.3914	1.00000
251	-4.2936	1.00000
252	-4.2225	1.00000
253	-4.1720	1.00000
254	-3.5229	1.00000
255	-3.3058	1.00000
256	-3.1359	1.00000
257	-2.9415	1.00000
258	-2.7960	1.00000
259	-2.7364	1.00000
260	-2.0570	0.00000
261	-1.9118	0.00000
262	-1.7189	0.00000
263	-1.6753	0.00000
264	-1.2835	0.00000
265	-1.2644	0.00000
266	-1.1489	0.00000
267	-0.7199	0.00000

268	-0.5809	0.00000
269	-0.5044	0.00000
270	-0.2775	0.00000
271	-0.2744	0.00000
272	-0.2566	0.00000
273	-0.1534	0.00000
274	-0.0533	0.00000
275	-0.0449	0.00000
276	0.0157	0.00000
277	0.0429	0.00000
278	0.0838	0.00000
279	0.2112	0.00000
280	0.2586	0.00000
281	0.2829	0.00000
282	0.4369	0.00000
283	0.4543	0.00000
284	0.4858	0.00000
285	0.6032	0.00000
286	0.6999	0.00000
287	0.8224	0.00000
288	0.8806	0.00000
289	1.0547	0.00000

290	1.1071	0.00000
291	1.1446	0.00000
292	1.1800	0.00000
293	1.2325	0.00000
294	1.2514	0.00000
295	1.3106	0.00000
296	1.3207	0.00000
297	1.3614	0.00000
298	1.4325	0.00000
299	1.4793	0.00000
300	1.5005	0.00000
301	1.5788	0.00000
302	1.6044	0.00000
303	1.6556	0.00000
304	1.6875	0.00000
305	1.7592	0.00000
306	1.7751	0.00000
307	1.8772	0.00000
308	1.9029	0.00000
309	1.9092	0.00000
310	1.9248	0.00000
311	2.1361	0.00000

312	2.1967	0.00000
313	2.2214	0.00000
314	2.2544	0.00000
315	2.2903	0.00000
316	2.2968	0.00000
317	2.3369	0.00000
318	2.3626	0.00000
319	2.3846	0.00000
320	2.4100	0.00000
321	2.4301	0.00000
322	2.4361	0.00000
323	2.4518	0.00000
324	2.4576	0.00000
325	2.4684	0.00000
326	2.5246	0.00000
327	2.5426	0.00000
328	2.7053	0.00000
329	2.7344	0.00000
330	2.7547	0.00000
331	2.7603	0.00000
332	2.7735	0.00000
333	2.8320	0.00000

334	2.8495	0.00000
335	2.8673	0.00000
336	2.9024	0.00000
337	2.9331	0.00000
338	2.9565	0.00000
339	2.9841	0.00000
340	3.0073	0.00000
341	3.0386	0.00000
342	3.0516	0.00000
343	3.0719	0.00000
344	3.0935	0.00000
345	3.1519	0.00000
346	3.1719	0.00000
347	3.1882	0.00000
348	3.1993	0.00000
349	3.3066	0.00000
350	3.3262	0.00000
351	3.3600	0.00000
352	3.3703	0.00000
353	3.3924	0.00000
354	3.4362	0.00000
355	3.4806	0.00000

356	3.4917	0.00000
357	3.4961	0.00000
358	3.5075	0.00000
359	3.6388	0.00000
360	3.6768	0.00000
361	3.6980	0.00000
362	3.7364	0.00000
363	3.7567	0.00000
364	3.7618	0.00000
365	3.7773	0.00000
366	3.7992	0.00000
367	3.8159	0.00000
368	3.8425	0.00000
369	3.8474	0.00000
370	3.8659	0.00000
371	3.8812	0.00000
372	3.8944	0.00000
373	3.9202	0.00000
374	3.9368	0.00000
375	3.9495	0.00000
376	3.9592	0.00000
377	3.9826	0.00000

378	3.9864	0.00000
379	4.0216	0.00000
380	4.0777	0.00000
381	4.1705	0.00000
382	4.2580	0.00000
383	4.2627	0.00000
384	4.2689	0.00000
385	4.2928	0.00000
386	4.3206	0.00000
387	4.3345	0.00000
388	4.3502	0.00000
389	4.3821	0.00000
390	4.3869	0.00000
391	4.4231	0.00000
392	4.4483	0.00000
393	4.4734	0.00000
394	4.4831	0.00000
395	4.4929	0.00000
396	4.4993	0.00000
397	4.5201	0.00000
398	4.5555	0.00000
399	4.5938	0.00000

400	4.6106	0.00000
401	4.6292	0.00000
402	4.6464	0.00000
403	4.6597	0.00000
404	4.6858	0.00000
405	4.7091	0.00000
406	4.7372	0.00000
407	4.7508	0.00000
408	4.7699	0.00000
409	4.7871	0.00000
410	4.7889	0.00000
411	4.8028	0.00000
412	4.8324	0.00000
413	4.8677	0.00000
414	4.8855	0.00000
415	4.9027	0.00000
416	4.9417	0.00000
417	4.9932	0.00000
418	5.0098	0.00000
419	5.0135	0.00000
420	5.0389	0.00000
421	5.0446	0.00000

422	5.0693	0.00000
423	5.0861	0.00000
424	5.1167	0.00000
425	5.1215	0.00000
426	5.1412	0.00000
427	5.1443	0.00000
428	5.1716	0.00000
429	5.1800	0.00000
430	5.1893	0.00000
431	5.1934	0.00000
432	5.2202	0.00000
433	5.2385	0.00000
434	5.2437	0.00000
435	5.2616	0.00000
436	5.2993	0.00000
437	5.3036	0.00000
438	5.3123	0.00000
439	5.3356	0.00000
440	5.3538	0.00000
441	5.3719	0.00000
442	5.3817	0.00000
443	5.3969	0.00000

444	5.4288	0.00000
445	5.4599	0.00000
446	5.4695	0.00000
447	5.4874	0.00000
448	5.4986	0.00000
449	5.5277	0.00000
450	5.5684	0.00000
451	5.5745	0.00000
452	5.5957	0.00000
453	5.6072	0.00000
454	5.6271	0.00000
455	5.6702	0.00000
456	5.6924	0.00000
457	5.7192	0.00000
458	5.7272	0.00000
459	5.7479	0.00000
460	5.7624	0.00000
461	5.7900	0.00000
462	5.7939	0.00000
463	5.7987	0.00000
464	5.8047	0.00000
465	5.8208	0.00000

466	5.8258	0.00000
467	5.8557	0.00000
468	5.8614	0.00000
469	5.8843	0.00000
470	5.8888	0.00000
471	5.8930	0.00000
472	5.9103	0.00000
473	5.9251	0.00000
474	5.9498	0.00000
475	5.9579	0.00000
476	5.9749	0.00000
477	5.9830	0.00000
478	6.0062	0.00000
479	6.0238	0.00000
480	6.0620	0.00000

---

soft charge-density along one line, spin component 1

0 1 2 3 4 5 6 7

8 9

total charge-density along one line

soft charge-density along one line, spin component 2

0 1 2 3 4 5 6 7

8 9

total charge-density along one line

pseudopotential strength for first ion, spin component: 1

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

pseudopotential strength for first ion, spin component: 2

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

total augmentation occupancy for first ion, spin component: 1

3.579 -0.646 0.444 -0.034 -0.000

-0.646 0.130 -0.082 0.006 0.000

0.444 -0.082 0.056 -0.003 -0.000

-0.034 0.006 -0.003 0.011 0.000

-0.000 0.000 -0.000 0.000 0.007

total augmentation occupancy for first ion, spin component: 2

-0.000 0.000 -0.000 0.000 0.000

0.000 -0.000 0.000 -0.000 -0.000

-0.000 0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

---------- aborting loop because EDIFF is reached ----------

total charge

# of ion	s	p	d	tot

1	0.646	0.043	0.000	0.690
2	0.646	0.043	0.000	0.690
3	0.646	0.043	0.000	0.690
4	0.646	0.043	0.000	0.690
5	0.646	0.043	0.000	0.690
6	0.646	0.043	0.000	0.690
7	0.646	0.043	0.000	0.690
8	0.646	0.043	0.000	0.690
9	0.646	0.043	0.000	0.690
10	0.646	0.043	0.000	0.690
11	0.646	0.043	0.000	0.690
12	0.646	0.043	0.000	0.690
13	0.646	0.043	0.000	0.689
14	0.646	0.043	0.000	0.689
15	0.648	0.045	0.000	0.693
16	0.646	0.043	0.000	0.689
17	0.646	0.043	0.000	0.689
18	0.646	0.043	0.000	0.689
19	0.646	0.043	0.000	0.689
20	0.646	0.043	0.000	0.689
21	0.646	0.043	0.000	0.689
22	0.646	0.044	0.000	0.690

23	0.541	0.015	0.000	0.557
24	0.541	0.015	0.000	0.556
25	0.870	1.763	0.000	2.633
26	0.867	1.785	0.000	2.653
27	0.867	1.786	0.000	2.653
28	0.870	1.762	0.000	2.632
29	0.865	1.783	0.000	2.648
30	0.870	1.763	0.000	2.633
31	0.867	1.786	0.000	2.653
32	0.867	1.786	0.000	2.653
33	0.870	1.762	0.000	2.632
34	0.865	1.783	0.000	2.648
35	0.870	1.763	0.000	2.633
36	0.868	1.787	0.000	2.654
37	0.867	1.786	0.000	2.653
38	0.870	1.763	0.000	2.633
39	0.865	1.784	0.000	2.649
40	0.870	1.763	0.000	2.633
41	0.868	1.787	0.000	2.655
42	0.867	1.786	0.000	2.653
43	0.871	1.764	0.000	2.634
44	0.865	1.783	0.000	2.648

45	0.870	1.763	0.000	2.633
46	0.867	1.786	0.000	2.653
47	0.867	1.786	0.000	2.653
48	0.871	1.763	0.000	2.634
49	0.865	1.783	0.000	2.648
50	0.870	1.763	0.000	2.633
51	0.867	1.786	0.000	2.653
52	0.867	1.786	0.000	2.653
53	0.870	1.762	0.000	2.632
54	0.865	1.784	0.000	2.648
55	0.865	1.784	0.000	2.649
56	0.865	1.786	0.000	2.651
57	0.866	1.787	0.000	2.653
58	0.866	1.790	0.000	2.656
59	0.865	1.786	0.000	2.651
60	0.866	1.786	0.000	2.651
61	0.866	1.788	0.000	2.654
62	0.867	1.791	0.000	2.658
63	0.865	1.784	0.000	2.649
64	0.865	1.786	0.000	2.651
65	0.866	1.787	0.000	2.652
66	0.865	1.788	0.000	2.653

67	0.865	1.786	0.000	2.651
68	0.866	1.785	0.000	2.651
69	0.865	1.787	0.000	2.652
70	0.866	1.787	0.000	2.653
71	0.865	1.784	0.000	2.649
72	0.865	1.786	0.000	2.651
73	0.866	1.786	0.000	2.652
74	0.864	1.785	0.000	2.649
75	0.865	1.786	0.000	2.651
76	0.866	1.786	0.000	2.651
77	0.865	1.786	0.000	2.651
78	0.865	1.784	0.000	2.649
79	0.865	1.784	0.000	2.649
80	0.865	1.786	0.000	2.651
81	0.865	1.785	0.000	2.650
82	0.863	1.782	0.000	2.645
83	0.865	1.786	0.000	2.651
84	0.866	1.786	0.000	2.651
85	0.865	1.784	0.000	2.648
86	0.862	1.774	0.000	2.636
87	0.865	1.784	0.000	2.649
88	0.865	1.787	0.000	2.652

89	0.865	1.785	0.000	2.650
90	0.865	1.788	0.000	2.653
91	0.865	1.786	0.000	2.651
92	0.866	1.786	0.000	2.651
93	0.864	1.783	0.000	2.647
94	0.866	1.785	0.000	2.651
95	0.865	1.784	0.000	2.649
96	0.865	1.786	0.000	2.651
97	0.866	1.787	0.000	2.653
98	0.866	1.789	0.000	2.655
99	0.865	1.786	0.000	2.651
100	0.866	1.786	0.000	2.651
101	0.865	1.787	0.000	2.652
102	0.867	1.790	0.000	2.657
103	0.865	1.786	0.000	2.651
104	0.867	1.785	0.000	2.653
105	0.866	1.786	0.000	2.652
106	0.870	1.778	0.000	2.648
107	0.869	1.765	0.000	2.635
108	0.865	1.783	0.000	2.648
109	0.869	1.789	0.000	2.658
110	0.865	1.786	0.000	2.651

111	0.867	1.785	0.000	2.653
112	0.867	1.789	0.000	2.655
113	0.871	1.782	0.000	2.653
114	0.869	1.765	0.000	2.634
115	0.865	1.783	0.000	2.648
116	0.870	1.791	0.000	2.661
117	0.865	1.786	0.000	2.651
118	0.867	1.786	0.000	2.653
119	0.865	1.782	0.000	2.647
120	0.857	1.707	0.000	2.564
121	0.869	1.765	0.000	2.634
122	0.865	1.783	0.000	2.648
123	0.866	1.778	0.000	2.644
124	0.866	1.786	0.000	2.652
125	0.867	1.785	0.000	2.653
126	0.862	1.776	0.000	2.638
127	0.847	1.824	0.000	2.671
128	0.870	1.767	0.000	2.637
129	0.865	1.783	0.000	2.648
130	0.860	1.757	0.000	2.617
131	0.866	1.786	0.000	2.652
132	0.867	1.784	0.000	2.652

133	0.864	1.787	0.000	2.651
134	0.869	1.790	0.000	2.659
135	0.869	1.767	0.000	2.636
136	0.865	1.783	0.000	2.648
137	0.866	1.772	0.000	2.638
138	0.866	1.786	0.000	2.652
139	0.867	1.785	0.000	2.652
140	0.866	1.788	0.000	2.654
141	0.870	1.779	0.000	2.649
142	0.869	1.766	0.000	2.635
143	0.865	1.783	0.000	2.648
144	0.869	1.790	0.000	2.659
145	0.944	1.724	0.000	2.668
146	1.240	1.546	0.074	2.860
147	1.635	3.537	0.000	5.173

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tot	123.064	221.559	0.074	344.697

magnetization (x)

# of ion	s	p	d	tot
1	0.000	-0.000	0.000	0.000
2	-0.000	0.000	0.000	-0.000
3	0.000	-0.000	0.000	0.000
4	-0.000	0.000	0.000	-0.000
5	0.000	-0.000	0.000	0.000
6	-0.000	0.000	0.000	-0.000
7	0.000	-0.000	0.000	0.000
8	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	0.000
10	-0.000	0.000	0.000	-0.000
11	0.000	-0.000	0.000	0.000
12	-0.000	0.000	0.000	-0.000
13	0.000	-0.000	0.000	0.000
14	-0.004	0.002	0.000	-0.002
15	0.000	-0.000	0.000	0.000
16	-0.004	0.002	0.000	-0.002
17	-0.004	0.002	0.000	-0.002
18	0.000	-0.000	0.000	0.000
19	-0.003	0.001	0.000	-0.002
20	0.000	-0.000	0.000	0.000

21	-0.003	0.002	0.000	-0.002
22	-0.003	0.002	0.000	-0.002
23	-0.000	0.000	0.000	-0.000
24	-0.000	0.000	0.000	-0.000
25	-0.000	-0.007	0.000	-0.008
26	-0.000	-0.002	0.000	-0.002
27	0.000	0.003	0.000	0.003
28	0.000	0.005	0.000	0.005
29	0.000	0.003	0.000	0.003
30	-0.000	-0.007	0.000	-0.008
31	-0.000	-0.002	0.000	-0.002
32	0.000	0.003	0.000	0.003
33	0.000	0.005	0.000	0.005
34	0.000	0.002	0.000	0.002
35	-0.000	-0.007	0.000	-0.008
36	-0.000	-0.002	0.000	-0.002
37	0.000	0.003	0.000	0.003
38	0.000	0.006	0.000	0.007
39	0.000	0.002	0.000	0.002
40	-0.000	-0.007	0.000	-0.008
41	-0.000	-0.002	0.000	-0.002
42	0.000	0.002	0.000	0.003

43	0.000	0.005	0.000	0.005
44	0.000	0.004	0.000	0.004
45	-0.000	-0.007	0.000	-0.008
46	-0.000	-0.002	0.000	-0.002
47	0.000	0.002	0.000	0.003
48	0.000	0.005	0.000	0.006
49	0.000	0.001	0.000	0.001
50	-0.000	-0.007	0.000	-0.008
51	-0.000	-0.002	0.000	-0.002
52	0.000	0.002	0.000	0.003
53	0.000	0.006	0.000	0.007
54	0.000	0.002	0.000	0.002
55	-0.000	-0.005	0.000	-0.006
56	-0.000	-0.007	0.000	-0.007
57	-0.000	-0.001	0.000	-0.001
58	-0.000	-0.001	0.000	-0.001
59	0.000	0.006	0.000	0.007
60	0.000	0.003	0.000	0.003
61	0.000	0.001	0.000	0.001
62	0.000	0.003	0.000	0.003
63	-0.000	-0.005	0.000	-0.006
64	-0.000	-0.007	0.000	-0.007

65	-0.000	-0.001	0.000	-0.001
66	-0.000	-0.001	0.000	-0.001
67	0.000	0.006	0.000	0.006
68	0.000	0.003	0.000	0.003
69	0.000	0.001	0.000	0.001
70	0.000	0.002	0.000	0.002
71	-0.000	-0.005	0.000	-0.006
72	-0.000	-0.007	0.000	-0.007
73	-0.000	-0.001	0.000	-0.001
74	-0.000	-0.002	0.000	-0.002
75	0.000	0.006	0.000	0.007
76	0.000	0.003	0.000	0.004
77	0.000	0.003	0.000	0.003
78	0.000	0.001	0.000	0.001
79	-0.000	-0.005	0.000	-0.006
80	-0.000	-0.007	0.000	-0.007
81	-0.000	-0.001	0.000	-0.002
82	-0.000	-0.002	0.000	-0.002
83	0.001	0.007	0.000	0.008
84	0.000	0.003	0.000	0.003
85	0.000	0.002	0.000	0.002
86	0.000	0.005	0.000	0.006

87	-0.000	-0.005	0.000	-0.005
88	-0.000	-0.007	0.000	-0.007
89	-0.000	-0.001	0.000	-0.002
90	-0.000	-0.002	0.000	-0.002
91	0.001	0.008	0.000	0.008
92	0.000	0.003	0.000	0.003
93	0.000	0.002	0.000	0.003
94	0.000	0.001	0.000	0.001
95	-0.000	-0.005	0.000	-0.006
96	-0.000	-0.007	0.000	-0.007
97	-0.000	-0.001	0.000	-0.001
98	-0.000	-0.001	0.000	-0.001
99	0.001	0.007	0.000	0.007
100	0.000	0.003	0.000	0.004
101	0.000	0.003	0.000	0.003
102	0.000	0.002	0.000	0.002
103	-0.001	-0.010	0.000	-0.011
104	-0.003	-0.028	0.000	-0.031
105	-0.000	-0.001	0.000	-0.002
106	-0.000	-0.004	0.000	-0.005
107	0.007	0.115	0.000	0.122
108	0.001	0.010	0.000	0.011

109	0.000	0.001	0.000	0.001
110	-0.001	-0.010	0.000	-0.011
111	-0.003	-0.028	0.000	-0.031
112	-0.000	-0.001	0.000	-0.002
113	-0.000	-0.003	0.000	-0.004
114	0.007	0.120	0.000	0.127
115	0.001	0.010	0.000	0.011
116	0.000	0.001	0.000	0.002
117	-0.001	-0.010	0.000	-0.011
118	-0.003	-0.026	0.000	-0.029
119	-0.000	-0.002	0.000	-0.002
120	-0.000	-0.002	0.000	-0.002
121	0.007	0.115	0.000	0.122
122	0.001	0.010	0.000	0.010
123	0.000	0.003	0.000	0.003
124	-0.001	-0.010	0.000	-0.011
125	-0.003	-0.024	0.000	-0.027
126	-0.000	-0.002	0.000	-0.002
127	-0.000	0.001	0.000	0.001
128	0.006	0.105	0.000	0.111
129	0.001	0.009	0.000	0.010
130	0.000	0.004	0.000	0.004

131	-0.001	-0.009	0.000	-0.010
132	-0.003	-0.024	0.000	-0.027
133	-0.000	-0.002	0.000	-0.002
134	-0.000	-0.002	0.000	-0.002
135	0.006	0.097	0.000	0.102
136	0.001	0.009	0.000	0.010
137	0.000	0.004	0.000	0.005
138	-0.001	-0.010	0.000	-0.011
139	-0.003	-0.026	0.000	-0.029
140	-0.000	-0.002	0.000	-0.002
141	-0.000	-0.003	0.000	-0.004
142	0.006	0.105	0.000	0.111
143	0.001	0.010	0.000	0.010
144	0.000	0.002	0.000	0.003
145	0.000	0.005	0.000	0.006
146	-0.000	0.000	-0.000	0.000
147	0.000	0.004	0.000	0.004
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tot	0.001	0.513	-0.000	0.514

CHARGE: cpu time 0.5221: real time 0.5239

FORLOC: cpu time 0.0200: real time 0.0201

FORNL : cpu time 2.0736: real time 2.0802

STRESS: cpu time 6.2289: real time 6.2524

FORCOR: cpu time 0.1416: real time 0.1425

FORHAR: cpu time 0.0332: real time 0.0332

MIXING: cpu time 0.0111: real time 0.0111

OFIELD: cpu time 0.0001: real time 0.0001

DFTD3 V3.0 Rev 1

Edisp (eV) -6.61788

E6 (eV) : -3.9312

E8 (eV) : -2.6867

% E8 : 40.60

FORVDW: cpu time 1.8660: real time 1.8870

FORCE on cell =-STRESS in cart. coord. units (eV):

Direction	XX	YY	ZZ	XY	YZ	ZX
Alpha Z	233.50077	233.50077	233.50077			
Ewald	107574.75723	23474.38913	-39722.89083	10.33575	3456.73956	128.46657

Hartree	106095.11356	25028.80123	-23789.87054	-6.54886	2948.09852	93.12870
E(xc)	-1914.26059	-1916.60262	-1979.91978	0.13381	1.82311	0.12901
Local	**********	-53951.14416	57006.55993	-0.30975	-6362.72245	-218.15919
n-local	-472.68663	-482.59179	-439.52821	-0.69625	-0.75328	-0.32285
augment	-38.26865	-38.61240	-34.28570	0.00591	-0.97678	0.00065
Kinetic	7635.33750	7638.72520	8714.09441	-3.10619	-41.49768	-3.16743
Fock	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
vdW	-2.64320	-1.49329	-6.59299	0.00160	-0.07448	0.01160
Total	-17.74740	-15.02793	-18.93295	-0.18399	0.63651	0.08707
in kB	-4.89394	-4.14403	-5.22087	-0.05074	0.17552	0.02401

external pressure = -4.75 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

energy-cutoff : 400.00

volume of cell : 5810.14

direct lattice vectors			reciprocal lattice vectors		
14.780600000	0.000000000	0.000000000	0.067656252	0.000000000	0.000000000
0.000000000	21.333900000	0.000000000	0.000000000	0.046873755	0.000000000
0.000000000	0.000000000	18.425700000	0.000000000	0.000000000	0.054272022

length of vectors

14.780600000 21.333900000 18.425700000 0.067656252 0.046873755 0.054272022

FORCES acting on ions

electron-ion (+dipol) ewald-force non-local-force convergence-correction

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0.468E-02 0.154E+03 0.361E+02 -.317E-02 -.160E+03 -.357E+02 -.180E-02 0.566E+01 -.438E+00 0.164E-06 0.464E-06 0.706E-06

-.185E-01 0.155E+03 -.340E+02 0.161E-01 -.160E+03 0.335E+02 0.115E-02 0.565E+01 0.541E+00 -.509E-06 -.122E-06 -.142E-06

0.184E+00 0.154E+03 0.360E+02 -.184E+00 -.160E+03 -.356E+02 0.933E-05 0.565E+01 -.443E+00 -.233E-06 0.602E-06 0.464E-06

0.112E+00 0.155E+03 -.341E+02 -.988E-01 -.160E+03 0.336E+02 -.175E-01 0.565E+01 0.535E+00 -.793E-07 0.154E-06 -.393E-06

0.171E+00 0.154E+03 0.362E+02 -.173E+00 -.160E+03 -.357E+02 0.117E-02 0.566E+01 -.440E+00 -.387E-06 0.670E-06 0.738E-06

0.126E+00 0.154E+03 -.340E+02 -.108E+00 -.160E+03 0.334E+02 -.211E-01 0.565E+01 0.541E+00 0.383E-06 0.267E-06 0.278E-06

-.193E-01 0.154E+03 0.363E+02 0.182E-01 -.160E+03 -.359E+02 0.159E-02 0.566E+01 -

.431E+00 -.173E-06 0.633E-06 0.125E-05

-.129E-01 0.154E+03 -.338E+02 0.198E-01 -.160E+03 0.332E+02 -.719E-02 0.565E+01 0.555E+00 0.475E-06 0.355E-06 0.115E-05

-.182E+00 0.154E+03 0.363E+02 0.182E+00 -.160E+03 -.359E+02 0.255E-03 0.566E+01 -.429E+00 0.218E-06 0.539E-06 0.147E-05

-.128E+00 0.155E+03 -.337E+02 0.115E+00 -.160E+03 0.331E+02 0.109E-01 0.565E+01 0.561E+00 0.684E-07 0.993E-07 0.140E-05

-.174E+00 0.154E+03 0.362E+02 0.175E+00 -.160E+03 -.358E+02 -.177E-02 0.566E+01 -.432E+00 0.415E-06 0.421E-06 0.121E-05

-.115E+00 0.155E+03 -.338E+02 0.958E-01 -.160E+03 0.332E+02 0.192E-01 0.565E+01 0.555E+00 -.340E-06 -.159E-06 0.765E-06

0.228E+01 -.150E+03 -.386E+02 -.227E+01 0.156E+03 0.386E+02 -.104E-01 -.566E+01 0.768E-01 0.380E-06 -.538E-06 0.734E-07

-.412E+00 -.151E+03 0.388E+02 0.413E+00 0.157E+03 -.386E+02 -.129E-02 -.567E+01 -.269E+00 -.206E-06 -.736E-06 -.803E-07

0.136E+02 -.146E+03 -.413E+02 -.138E+02 0.151E+03 0.413E+02 0.257E+00 -.567E+01 -.348E-01 -.120E-06 -.154E-06 0.320E-07

0.162E+01 -.151E+03 0.402E+02 -.162E+01 0.156E+03 -.400E+02 -.100E-02 -.567E+01 -.229E+00 0.279E-06 -.538E-06 0.593E-06

0.352E+01 -.149E+03 0.443E+02 -.352E+01 0.155E+03 -.441E+02 -.195E-02 -.567E+01 -.180E+00 0.431E-06 -.388E-06 0.303E-06

-.148E+02 -.146E+03 -.329E+02 0.149E+02 0.151E+03 0.329E+02 -.957E-01 -.566E+01

0.505E-01 0.183E-06 -.128E-06 0.375E-06

-.297E+01 -.149E+03 0.432E+02 0.296E+01 0.155E+03 -.430E+02 0.115E-01 -.567E+01 -.241E+00 -.179E-06 -.577E-06 -.103E-05

-.379E+01 -.150E+03 -.385E+02 0.379E+01 0.156E+03 0.385E+02 -.631E-02 -.566E+01 0.241E-01 -.120E-06 -.494E-06 0.390E-06

-.207E+01 -.151E+03 0.395E+02 0.207E+01 0.156E+03 -.392E+02 0.153E-02 -.566E+01 -.282E+00 -.594E-06 -.681E-06 -.771E-06

-.488E-02 -.148E+03 0.486E+02 0.126E-01 0.154E+03 -.484E+02 -.560E-02 -.569E+01 -.158E+00 0.315E-06 -.390E-06 -.734E-06

0.196E+02 -.103E+03 0.222E+02 -.212E+02 0.103E+03 -.246E+02 0.154E+01 0.139E+00 0.238E+01 -.523E-06 -.638E-06 0.124E-06

-.192E+02 -.103E+03 0.153E+02 0.216E+02 0.103E+03 -.168E+02 -.241E+01 -.118E+00 0.152E+01 0.702E-07 -.790E-06 -.162E-06

0.715E-01 0.461E+03 0.202E+03 -.748E-01 -.462E+03 -.201E+03 0.382E-02 0.102E+01 -.219E+00 0.859E-06 0.348E-06 0.158E-05

0.212E+00 0.353E+03 -.234E+03 -.212E+00 -.353E+03 0.234E+03 0.260E-02 0.442E+00 -.370E-01 -.477E-06 -.760E-06 -.254E-05

-.244E-01 0.351E+03 0.240E+03 0.230E-01 -.351E+03 -.241E+03 0.314E-02 0.408E+00 0.562E-01 0.147E-05 -.523E-07 0.212E-05

-.173E+00 0.462E+03 -.195E+03 0.180E+00 -.463E+03 0.195E+03 -.666E-02 0.105E+01 0.233E+00 -.163E-05 -.206E-05 -.156E-05

-.622E-01 0.210E+03 -.272E+03 0.663E-01 -.210E+03 0.272E+03 -.450E-02 0.930E-01

0.561E-01 -.890E-07 0.720E-06 -.187E-05

0.562E+00 0.461E+03 0.202E+03 -.564E+00 -.462E+03 -.201E+03 0.202E-02 0.102E+01 -.214E+00 -.714E-06 0.654E-06 0.751E-06

0.106E+01 0.352E+03 -.234E+03 -.107E+01 -.353E+03 0.234E+03 0.160E-01 0.447E+00 -.424E-01 0.543E-06 -.485E-06 -.154E-05

0.413E+00 0.351E+03 0.240E+03 -.415E+00 -.351E+03 -.240E+03 0.302E-02 0.407E+00 0.490E-01 0.161E-06 -.194E-06 0.321E-06

0.578E+00 0.462E+03 -.195E+03 -.583E+00 -.463E+03 0.195E+03 0.478E-02 0.105E+01 0.235E+00 0.357E-07 -.863E-06 -.240E-05

0.689E+00 0.210E+03 -.272E+03 -.695E+00 -.210E+03 0.272E+03 0.597E-02 0.906E-01 0.615E-01 0.539E-06 0.622E-06 -.117E-05

0.425E+00 0.461E+03 0.202E+03 -.428E+00 -.462E+03 -.202E+03 0.386E-02 0.102E+01 -.214E+00 -.156E-05 0.104E-05 0.228E-05

0.939E+00 0.352E+03 -.233E+03 -.955E+00 -.352E+03 0.233E+03 0.151E-01 0.440E+00 -.377E-01 0.195E-05 -.133E-05 0.136E-05

0.478E+00 0.351E+03 0.241E+03 -.480E+00 -.351E+03 -.241E+03 0.250E-02 0.406E+00 0.511E-01 -.131E-05 0.186E-06 0.848E-06

0.704E+00 0.462E+03 -.194E+03 -.715E+00 -.463E+03 0.194E+03 0.787E-02 0.106E+01 0.242E+00 0.165E-05 -.132E-05 0.267E-06

0.724E+00 0.210E+03 -.271E+03 -.733E+00 -.210E+03 0.271E+03 0.652E-02 0.903E-01 0.593E-01 0.118E-05 -.602E-06 0.511E-06

-.182E+00 0.461E+03 0.202E+03 0.178E+00 -.462E+03 -.202E+03 0.450E-02 0.102E+01 -

.218E+00 -.792E-06 0.123E-05 0.460E-05

-.294E+00 0.352E+03 -.233E+03 0.298E+00 -.352E+03 0.233E+03 -.202E-02 0.439E+00 -.299E-01 0.389E-06 -.251E-05 0.325E-05

0.398E-01 0.351E+03 0.241E+03 -.389E-01 -.351E+03 -.241E+03 0.225E-02 0.409E+00 0.556E-01 -.135E-05 0.786E-06 0.300E-05

0.501E-01 0.462E+03 -.194E+03 -.562E-01 -.463E+03 0.194E+03 0.400E-02 0.106E+01 0.232E+00 0.174E-05 -.221E-05 0.333E-05

-.478E-01 0.210E+03 -.271E+03 0.458E-01 -.210E+03 0.271E+03 -.220E-03 0.926E-01 0.325E-01 0.136E-06 -.184E-05 0.145E-05

-.551E+00 0.461E+03 0.202E+03 0.549E+00 -.462E+03 -.202E+03 0.766E-03 0.102E+01 -.220E+00 0.601E-06 0.997E-06 0.543E-05

-.119E+01 0.352E+03 -.233E+03 0.120E+01 -.353E+03 0.233E+03 -.162E-01 0.446E+00 -.330E-01 -.908E-06 -.263E-05 0.240E-05

-.352E+00 0.351E+03 0.241E+03 0.349E+00 -.351E+03 -.241E+03 0.207E-02 0.413E+00 0.622E-01 -.154E-06 0.913E-06 0.480E-05

-.412E+00 0.462E+03 -.194E+03 0.425E+00 -.463E+03 0.194E+03 -.115E-01 0.106E+01 0.230E+00 -.184E-06 -.328E-05 0.413E-05

-.560E+00 0.210E+03 -.271E+03 0.565E+00 -.210E+03 0.271E+03 -.939E-02 0.907E-01 0.525E-01 -.705E-06 -.165E-05 0.919E-06

-.474E+00 0.461E+03 0.202E+03 0.474E+00 -.462E+03 -.202E+03 0.305E-02 0.102E+01 -.221E+00 0.162E-05 0.463E-06 0.392E-05

-.805E+00 0.353E+03 -.234E+03 0.819E+00 -.353E+03 0.234E+03 -.150E-01 0.446E+00 -

.393E-01 -.152E-05 -.184E-05 -.393E-06

-.373E+00 0.351E+03 0.241E+03 0.368E+00 -.351E+03 -.241E+03 0.947E-03 0.410E+00 0.625E-01 0.118E-05 0.493E-06 0.426E-05

-.594E+00 0.462E+03 -.194E+03 0.607E+00 -.463E+03 0.194E+03 -.170E-01 0.105E+01 0.234E+00 -.158E-05 -.310E-05 0.178E-05

-.587E+00 0.210E+03 -.272E+03 0.598E+00 -.210E+03 0.272E+03 -.101E-01 0.985E-01 0.566E-01 -.103E-05 -.536E-06 -.723E-06

-.801E-02 0.206E+03 0.279E+03 0.114E-01 -.206E+03 -.279E+03 -.360E-02 0.684E-01 -.413E-01 0.112E-05 -.297E-06 0.127E-05

0.669E+00 0.303E+02 0.296E+03 -.664E+00 -.302E+02 -.296E+03 -.466E-02 -.411E-01 0.734E-02 0.204E-06 -.107E-05 0.952E-06

-.845E+00 0.144E+03 -.282E+03 0.847E+00 -.144E+03 0.282E+03 -.318E-02 0.136E+00 0.287E-01 -.331E-06 0.496E-06 -.111E-05

0.534E+00 -.215E+02 -.285E+03 -.534E+00 0.214E+02 0.285E+03 -.792E-03 0.383E-01 0.187E-01 0.103E-06 0.340E-06 0.544E-06

0.502E+00 -.294E+02 0.293E+03 -.499E+00 0.294E+02 -.293E+03 -.551E-02 0.253E-01 -.305E-01 -.160E-06 -.621E-06 0.994E-06

0.525E+00 0.139E+03 0.289E+03 -.525E+00 -.139E+03 -.289E+03 0.178E-02 0.103E+00 -.250E-01 0.611E-06 -.951E-06 0.489E-06

-.126E+01 0.364E+02 -.287E+03 0.126E+01 -.364E+02 0.287E+03 -.396E-04 -.812E-02 0.139E-01 0.358E-06 0.552E-06 -.740E-09

0.167E+01 -.130E+03 -.271E+03 -.169E+01 0.130E+03 0.271E+03 0.105E-01 -.881E-01

0.373E-01 0.268E-06 -.454E-06 0.113E-05

0.397E+00 0.207E+03 0.280E+03 -.395E+00 -.207E+03 -.280E+03 0.711E-03 0.693E-01 -.372E-01 0.239E-06 -.827E-06 -.352E-07

0.918E+00 0.312E+02 0.296E+03 -.922E+00 -.311E+02 -.296E+03 0.225E-02 -.411E-01 0.120E-01 0.155E-06 -.120E-05 0.687E-06

0.133E+01 0.144E+03 -.282E+03 -.133E+01 -.144E+03 0.282E+03 0.495E-02 0.126E+00 0.280E-01 0.133E-06 0.912E-06 -.118E-05

0.341E+01 -.199E+02 -.285E+03 -.343E+01 0.199E+02 0.285E+03 0.134E-01 0.408E-01 0.138E-01 -.151E-06 0.360E-06 0.217E-06

0.139E+01 -.287E+02 0.294E+03 -.139E+01 0.287E+02 -.294E+03 -.348E-02 0.251E-01 -.309E-01 0.149E-06 -.139E-05 0.125E-05

0.677E+00 0.139E+03 0.290E+03 -.677E+00 -.139E+03 -.290E+03 0.622E-03 0.103E+00 -.296E-01 -.228E-06 -.955E-06 0.523E-07

0.160E+01 0.367E+02 -.287E+03 -.159E+01 -.367E+02 0.287E+03 -.128E-01 -.211E-01 0.129E-01 -.109E-06 0.639E-06 0.530E-07

0.611E+01 -.125E+03 -.271E+03 -.613E+01 0.125E+03 0.271E+03 0.216E-01 -.899E-01 0.148E-01 -.117E-06 -.240E-06 0.482E-06

0.366E+00 0.207E+03 0.280E+03 -.371E+00 -.207E+03 -.280E+03 0.106E-03 0.682E-01 -.366E-01 -.858E-06 -.284E-06 0.363E-06

-.406E-01 0.319E+02 0.296E+03 0.320E-01 -.318E+02 -.296E+03 0.105E-01 -.364E-01 0.137E-01 -.107E-06 -.141E-07 0.504E-06

0.210E+01 0.144E+03 -.281E+03 -.211E+01 -.144E+03 0.281E+03 0.120E-01 0.120E+00

0.242E-01 0.660E-06 0.811E-07 -.335E-06

0.303E+01 -.172E+02 -.283E+03 -.305E+01 0.171E+02 0.283E+03 0.239E-01 0.852E-01 0.617E-01 0.134E-06 -.415E-06 -.275E-06

0.105E+01 -.272E+02 0.294E+03 -.105E+01 0.272E+02 -.294E+03 0.286E-02 0.242E-01 -.378E-01 0.451E-06 -.695E-06 0.740E-06

0.950E-01 0.140E+03 0.290E+03 -.966E-01 -.140E+03 -.290E+03 0.129E-02 0.107E+00 -.233E-01 -.821E-06 0.243E-07 0.901E-06

0.276E+01 0.387E+02 -.286E+03 -.277E+01 -.387E+02 0.286E+03 0.723E-03 -.117E-01 0.297E-01 0.434E-06 0.327E-06 -.139E-06

0.595E+01 -.115E+03 -.267E+03 -.610E+01 0.115E+03 0.267E+03 0.151E+00 -.151E-02 0.131E+00 0.112E-05 0.137E-05 -.308E-06

-.243E+00 0.207E+03 0.280E+03 0.241E+00 -.207E+03 -.280E+03 0.437E-02 0.714E-01 -.388E-01 -.106E-05 0.661E-06 0.199E-05

-.115E+01 0.314E+02 0.294E+03 0.114E+01 -.314E+02 -.294E+03 0.916E-02 -.313E-01 0.523E-02 -.134E-06 0.120E-05 0.597E-06

0.594E+00 0.144E+03 -.281E+03 -.611E+00 -.144E+03 0.281E+03 0.178E-01 0.125E+00 0.437E-01 0.414E-06 -.109E-05 0.650E-06

-.940E+00 -.159E+02 -.286E+03 0.932E+00 0.158E+02 0.285E+03 0.612E-02 0.887E-01 0.806E-01 -.329E-06 0.195E-06 -.460E-06

-.648E+00 -.265E+02 0.293E+03 0.644E+00 0.265E+02 -.293E+03 0.487E-02 0.233E-01 -.273E-01 0.283E-06 0.746E-06 0.647E-07

-.535E+00 0.139E+03 0.289E+03 0.531E+00 -.139E+03 -.289E+03 0.653E-02 0.114E+00 -

.215E-01 -.539E-06 0.101E-05 0.209E-05

0.776E+00 0.408E+02 -.287E+03 -.788E+00 -.408E+02 0.287E+03 0.513E-02 0.124E-02 -.190E-01 -.254E-06 -.344E-06 -.102E-06

-.460E+00 -.113E+03 -.276E+03 0.426E+00 0.113E+03 0.276E+03 0.348E-01 0.575E-01 -.269E+00 -.368E-06 -.875E-06 -.709E-06

-.572E+00 0.206E+03 0.279E+03 0.570E+00 -.206E+03 -.279E+03 0.115E-02 0.718E-01 -.457E-01 -.216E-06 0.118E-05 0.330E-05

-.782E+00 0.304E+02 0.294E+03 0.785E+00 -.304E+02 -.294E+03 -.754E-02 -.310E-01 -.158E-02 -.192E-06 0.119E-05 0.802E-06

-.123E+01 0.144E+03 -.281E+03 0.124E+01 -.145E+03 0.281E+03 -.157E-01 0.122E+00 0.504E-01 -.196E-06 -.166E-05 0.773E-06

-.365E+01 -.174E+02 -.283E+03 0.369E+01 0.173E+02 0.283E+03 -.303E-01 0.115E+00 0.598E-01 -.103E-06 -.765E-06 -.168E-06

-.130E+01 -.277E+02 0.291E+03 0.129E+01 0.277E+02 -.291E+03 -.133E-02 0.338E-01 -.221E-01 -.177E-06 0.135E-05 -.125E-06

-.347E+00 0.139E+03 0.289E+03 0.346E+00 -.139E+03 -.289E+03 0.272E-04 0.111E+00 -.148E-01 0.136E-06 0.113E-05 0.251E-05

-.828E+00 0.400E+02 -.287E+03 0.820E+00 -.400E+02 0.287E+03 0.126E-01 -.833E-02 -.182E-01 -.462E-07 -.648E-06 -.494E-07

-.785E+01 -.119E+03 -.267E+03 0.804E+01 0.119E+03 0.267E+03 -.187E+00 0.172E-03 0.352E-01 -.117E-05 0.142E-05 -.127E-06

-.408E+00 0.206E+03 0.279E+03 0.409E+00 -.206E+03 -.279E+03 -.279E-02 0.713E-01 -

.466E-01 0.787E-06 0.754E-06 0.290E-05

-.604E-01 0.300E+02 0.294E+03 0.701E-01 -.299E+02 -.294E+03 -.945E-02 -.349E-01 0.103E-02 0.629E-07 0.566E-07 0.952E-06

-.206E+01 0.145E+03 -.282E+03 0.208E+01 -.145E+03 0.282E+03 -.189E-01 0.131E+00 0.258E-01 -.715E-06 -.963E-06 -.424E-07

-.256E+01 -.208E+02 -.285E+03 0.259E+01 0.208E+02 0.285E+03 -.291E-01 0.405E-01 0.320E-01 0.349E-06 0.225E-06 0.233E-06

-.548E+00 -.290E+02 0.291E+03 0.553E+00 0.290E+02 -.291E+03 -.282E-02 0.291E-01 -.253E-01 -.524E-06 0.740E-06 0.286E-06

0.604E-01 0.139E+03 0.289E+03 -.605E-01 -.139E+03 -.289E+03 -.337E-03 0.109E+00 -.210E-01 0.821E-06 0.119E-06 0.173E-05

-.289E+01 0.378E+02 -.286E+03 0.291E+01 -.377E+02 0.286E+03 -.143E-01 -.460E-02 0.213E-01 -.365E-06 -.258E-06 -.332E-07

-.513E+01 -.128E+03 -.271E+03 0.518E+01 0.128E+03 0.271E+03 -.462E-01 -.865E-01 0.382E-01 0.371E-06 -.469E-06 0.542E-06

0.405E+00 -.137E+03 0.280E+03 -.397E+00 0.137E+03 -.280E+03 -.967E-02 -.128E+00 -.159E-01 -.776E-06 -.593E-06 0.942E-06

0.194E+01 -.343E+03 0.233E+03 -.195E+01 0.344E+03 -.233E+03 0.910E-02 -.461E+00 -.550E-01 -.334E-06 -.977E-06 0.178E-05

-.252E+01 -.197E+03 -.259E+03 0.253E+01 0.197E+03 0.259E+03 -.931E-02 -.198E+00 0.371E-01 0.390E-06 -.947E-06 0.994E-06

0.691E+01 -.447E+03 -.198E+03 -.693E+01 0.448E+03 0.198E+03 0.947E-02 -.112E+01

0.891E-01 0.923E-06 -.326E-06 0.585E-06

-.451E+00 -.451E+03 0.204E+03 0.452E+00 0.452E+03 -.204E+03 -.206E-02 -.108E+01 -.113E+00 -.108E-05 -.209E-05 0.108E-06

0.172E+01 -.203E+03 0.269E+03 -.171E+01 0.203E+03 -.269E+03 -.480E-02 -.928E-01 -.322E-01 -.486E-06 -.819E-06 0.182E-05

-.210E+01 -.338E+03 -.222E+03 0.215E+01 0.338E+03 0.222E+03 -.441E-01 -.605E+00 0.541E-01 0.809E-06 -.726E-06 0.759E-06

0.218E+01 -.136E+03 0.282E+03 -.218E+01 0.136E+03 -.282E+03 -.634E-02 -.126E+00 -.965E-02 0.167E-06 -.996E-06 0.203E-05

0.671E+01 -.339E+03 0.238E+03 -.670E+01 0.340E+03 -.238E+03 -.126E-01 -.462E+00 -.463E-01 0.106E-05 -.451E-06 0.222E-05

0.678E+01 -.193E+03 -.258E+03 -.679E+01 0.193E+03 0.258E+03 0.108E-01 -.146E+00 0.634E-01 -.535E-07 -.609E-06 0.969E-06

0.313E+02 -.427E+03 -.198E+03 -.313E+02 0.428E+03 0.197E+03 0.717E-01 -.968E+00 0.135E+00 -.578E-06 0.423E-06 0.265E-06

0.544E+01 -.449E+03 0.209E+03 -.544E+01 0.450E+03 -.209E+03 0.654E-03 -.108E+01 -.801E-01 0.695E-06 -.139E-05 0.251E-05

0.368E+01 -.201E+03 0.272E+03 -.368E+01 0.201E+03 -.272E+03 -.714E-03 -.977E-01 -.308E-01 0.923E-06 -.603E-06 0.195E-05

0.124E+02 -.332E+03 -.223E+03 -.125E+02 0.332E+03 0.223E+03 0.120E+00 -.535E+00 0.317E-01 -.232E-06 -.182E-06 0.611E-06

0.218E+01 -.133E+03 0.283E+03 -.219E+01 0.133E+03 -.283E+03 0.540E-03 -.128E+00 -

.467E-02 0.108E-05 -.424E-06 0.100E-05

0.491E+01 -.332E+03 0.245E+03 -.487E+01 0.332E+03 -.245E+03 -.320E-01 -.476E+00 -.378E-01 0.134E-05 -.314E-06 -.681E-06

0.112E+02 -.182E+03 -.258E+03 -.113E+02 0.182E+03 0.258E+03 0.463E-01 -.993E-01 -.105E+00 0.503E-06 -.778E-07 0.167E-06

0.316E+02 -.399E+03 -.175E+03 -.319E+02 0.401E+03 0.174E+03 0.285E+00 -.140E+01 0.134E+01 0.118E-05 -.403E-05 0.104E-05

0.929E+01 -.443E+03 0.219E+03 -.929E+01 0.444E+03 -.219E+03 -.548E-02 -.109E+01 -.482E-01 0.161E-05 -.571E-06 0.112E-05

0.168E+01 -.196E+03 0.273E+03 -.169E+01 0.197E+03 -.273E+03 0.546E-02 -.109E+00 -.514E-01 0.141E-05 0.637E-07 -.182E-06

0.172E+02 -.310E+03 -.216E+03 -.175E+02 0.310E+03 0.216E+03 0.322E+00 -.220E+00 0.124E+00 0.660E-06 -.144E-05 0.549E-06

-.104E+01 -.132E+03 0.281E+03 0.103E+01 0.132E+03 -.281E+03 0.102E-01 -.127E+00 -.155E-03 0.962E-06 0.677E-06 -.894E-06

-.514E+01 -.332E+03 0.239E+03 0.513E+01 0.332E+03 -.239E+03 0.862E-02 -.494E+00 -.426E-01 0.897E-06 -.271E-06 -.347E-05

0.156E+01 -.170E+03 -.261E+03 -.168E+01 0.169E+03 0.261E+03 0.114E+00 0.361E+00 -.103E+00 -.257E-05 0.165E-06 -.451E-06

-.663E+01 -.303E+03 -.189E+03 0.619E+01 0.298E+03 0.185E+03 0.463E+00 0.503E+01 0.438E+01 -.153E-06 -.117E-05 0.812E-06

-.646E+00 -.436E+03 0.227E+03 0.644E+00 0.437E+03 -.227E+03 0.137E-02 -.120E+01 -

.484E-01 0.155E-05 -.568E-06 -.272E-05

-.303E+01 -.197E+03 0.268E+03 0.302E+01 0.197E+03 -.268E+03 0.145E-01 -.112E+00 -.432E-01 0.601E-06 0.926E-06 -.221E-05

0.320E+01 -.281E+03 -.215E+03 -.510E+01 0.280E+03 0.214E+03 0.190E+01 0.639E+00 0.822E+00 -.581E-05 -.319E-05 0.478E-06

-.274E+01 -.134E+03 0.277E+03 0.274E+01 0.134E+03 -.277E+03 0.246E-02 -.124E+00 -.188E-01 -.208E-06 0.127E-05 -.180E-05

-.599E+01 -.338E+03 0.230E+03 0.599E+01 0.339E+03 -.230E+03 0.114E-01 -.495E+00 -.466E-01 -.134E-05 -.485E-06 -.358E-05

-.648E+01 -.171E+03 -.257E+03 0.656E+01 0.170E+03 0.257E+03 -.736E-01 0.476E+00 0.814E-02 0.206E-05 -.111E-06 -.251E-06

-.441E+02 -.422E+03 -.184E+03 0.446E+02 0.423E+03 0.183E+03 -.556E+00 -.109E+01 0.639E+00 -.125E-05 -.346E-05 0.142E-05

-.867E+01 -.441E+03 0.211E+03 0.867E+01 0.443E+03 -.211E+03 0.143E-01 -.111E+01 -.763E-01 -.428E-06 -.815E-06 -.419E-05

-.292E+01 -.201E+03 0.265E+03 0.293E+01 0.201E+03 -.265E+03 -.912E-02 -.110E+00 -.207E-01 -.926E-06 0.775E-06 -.233E-05

-.144E+02 -.290E+03 -.209E+03 0.163E+02 0.289E+03 0.208E+03 -.197E+01 0.599E+00 0.785E+00 0.507E-05 -.283E-05 0.898E-06

-.138E+01 -.136E+03 0.277E+03 0.139E+01 0.136E+03 -.277E+03 -.101E-01 -.125E+00 -.242E-01 -.117E-05 0.611E-06 -.943E-06

-.277E+01 -.343E+03 0.230E+03 0.275E+01 0.343E+03 -.230E+03 0.235E-01 -.473E+00 -

.596E-01 -.151E-05 -.113E-05 -.124E-05

-.104E+02 -.189E+03 -.258E+03 0.104E+02 0.189E+03 0.258E+03 -.762E-01 -.139E+00 -.524E-01 -.472E-06 -.170E-06 0.370E-06

-.149E+02 -.446E+03 -.196E+03 0.150E+02 0.447E+03 0.196E+03 -.686E-01 -.112E+01 0.984E-01 -.189E-07 -.456E-06 0.961E-06

-.547E+01 -.448E+03 0.204E+03 0.547E+01 0.449E+03 -.203E+03 -.469E-02 -.108E+01 -.125E+00 -.221E-05 -.167E-05 -.295E-05

-.902E+00 -.203E+03 0.267E+03 0.910E+00 0.203E+03 -.267E+03 -.906E-02 -.102E+00 -.319E-01 -.150E-05 -.198E-06 -.386E-06

-.163E+02 -.329E+03 -.218E+03 0.166E+02 0.329E+03 0.218E+03 -.358E+00 -.481E+00 0.425E-01 -.603E-06 -.144E-05 0.113E-05

-.264E+01 -.250E+03 -.196E+03 0.156E+01 0.241E+03 0.190E+03 0.991E+00 0.787E+01 0.470E+01 0.538E-06 -.497E-05 0.172E-06

0.529E+02 -.518E+03 -.137E+03 -.540E+02 0.522E+03 0.140E+03 0.105E+01 -.395E+01 -.382E+01 -.210E-05 -.276E-05 0.127E-05

-.469E+02 -.588E+03 -.446E+03 0.530E+02 0.641E+03 0.480E+03 -.597E+01 -.518E+02 -.340E+02 0.283E-05 0.111E-04 0.119E-04

0.447E+01 0.287E+02 0.219E+02 -.291E-12 -.136E-11 0.131E-11 -.452E+01 -.286E+02 -.219E+02 0.152E-05 -.477E-04 0.865E-04

POSITION			TOTAL-FORCE (eV/Angst)		
1.24575	4.02870	5.43979	0.000043	0.001001	-0.000394
1.21024	4.07581	8.43726	-0.000979	0.002563	-0.001192
3.70862	4.02890	5.43965	0.000305	0.001873	-0.001078
3.67998	4.07733	8.43690	-0.004040	-0.000469	-0.002948
6.17157	4.02854	5.43942	-0.000013	-0.000156	-0.001738
6.14482	4.08292	8.43295	-0.002845	-0.003353	-0.003243
8.63513	4.02801	5.43869	0.000772	-0.000462	-0.001990
8.60339	4.08732	8.43089	-0.000142	-0.001224	-0.002282
11.09928	4.02784	5.43885	0.000873	0.001951	-0.002702
11.06021	4.08619	8.43099	-0.001744	0.000655	-0.000718
13.56311	4.02807	5.43972	0.000335	0.001602	-0.001607
13.52141	4.08047	8.43349	0.000411	-0.002304	0.000238
2.44241	15.48073	8.85224	-0.000613	-0.005188	0.002222
0.01714	15.44624	5.32469	0.000354	0.001554	-0.001169
4.86040	15.47728	8.86623	0.000880	0.000275	-0.000525
2.48016	15.44854	5.27562	0.000359	-0.001189	-0.000470
4.94382	15.44925	5.24869	0.001740	-0.002928	0.000257
12.31531	15.48242	9.00211	-0.004395	0.002061	0.005004
9.86772	15.44556	5.34176	0.000428	-0.001184	0.001055
14.76279	15.48245	8.89951	-0.006009	-0.000306	0.005357

12.33384	15.44510	5.36128	0.001352	-0.003220	-0.001231
7.40743	15.44616	5.26463	0.002417	0.001641	0.001400
6.44846	16.34427	7.40648	-0.001820	0.000574	0.004822
8.60064	16.47644	7.89249	0.005752	0.001144	0.006071
1.24544	5.11881	5.35500	0.000956	0.000269	-0.002504
2.44348	5.83889	8.62292	0.002417	-0.004460	0.001211
0.01380	5.79530	5.28573	0.002065	-0.002533	0.000469
1.21063	5.16420	8.54151	0.000256	-0.000503	-0.001847
2.44351	7.27931	8.74832	-0.000075	-0.001216	-0.000124
3.70866	5.11896	5.35390	-0.000431	-0.001523	0.000288
4.90800	5.84315	8.62123	-0.001089	0.003824	-0.000793
2.47701	5.79561	5.28397	0.001445	-0.000673	-0.002609
3.67679	5.16572	8.54000	-0.000125	0.001644	0.000002
4.90764	7.28398	8.74777	0.000735	-0.000608	0.001059
6.17184	5.11860	5.35433	0.001473	0.000505	0.000839
7.37096	5.84929	8.62094	-0.000643	0.007038	-0.002465
4.94029	5.79548	5.28340	0.000604	-0.002762	-0.001177
6.14080	5.17108	8.53715	-0.002512	0.002569	0.002524
7.37071	7.28983	8.75132	-0.001996	0.001627	0.000129
8.63543	5.11820	5.35521	0.001247	0.001479	-0.001128
9.83233	5.85166	8.62337	0.002775	0.000471	-0.001081
7.40374	5.79498	5.28512	0.003445	-0.002767	-0.001341

8.60194	5.17528	8.53759	-0.001845	-0.000378	-0.000147
9.83204	7.29110	8.75719	-0.001865	-0.002426	-0.002413
11.09930	5.11814	5.35578	-0.000873	-0.003214	-0.001423
12.29449	5.84673	8.62385	0.000074	0.005700	-0.002211
9.86750	5.79468	5.28678	-0.000754	-0.000801	0.001545
11.06261	5.17409	8.53894	0.002597	0.002772	-0.000328
12.29428	7.28729	8.75533	-0.004521	0.001225	-0.001526
13.56278	5.11829	5.35605	0.002662	0.000656	-0.002043
14.75895	5.83988	8.62434	-0.000208	-0.002693	-0.002232
12.33118	5.79480	5.28692	-0.004504	-0.001550	0.002589
13.52535	5.16844	8.54022	-0.003533	0.003851	-0.001363
14.75917	7.28012	8.75179	0.000897	0.002541	-0.000679
0.01434	7.23830	5.19017	0.000080	-0.000200	0.000067
1.24689	9.38061	5.13160	0.000537	-0.001848	-0.000013
1.21085	7.98059	8.79588	-0.000922	-0.000538	0.001524
2.44214	10.12243	8.87141	-0.000901	0.002787	-0.005027
0.01532	10.08686	5.14049	-0.002041	-0.000136	-0.002403
1.24606	7.94244	5.15775	0.002014	-0.002604	0.000827
1.21082	9.41592	8.85782	-0.000673	0.004570	0.000172
2.44072	11.55513	8.88414	-0.006177	-0.002286	0.001625
2.47747	7.23842	5.18585	0.002796	0.002893	0.001299
3.70997	9.38055	5.12566	-0.001074	-0.002997	0.000032

3.67534	7.98360	8.79349	-0.000561	0.000967	0.000929
4.90487	10.12925	8.87518	0.000387	-0.000624	-0.000065
2.47867	10.08713	5.12695	-0.002273	0.001510	0.000760
3.70939	7.94242	5.15441	0.000805	-0.004012	-0.001702
3.67589	9.41970	8.85445	-0.001589	0.002103	-0.000145
4.90263	11.56506	8.89086	0.000056	0.002014	0.000940
4.94085	7.23830	5.18552	-0.004694	0.002261	0.000820
6.17318	9.38002	5.13173	0.002052	0.002120	0.001818
6.13864	7.99044	8.79647	0.002385	-0.000464	-0.001602
7.36780	10.13760	8.89473	-0.001069	0.002937	0.000738
4.94196	10.08682	5.12700	0.004126	0.001474	-0.001158
6.17284	7.94199	5.15766	-0.000064	0.000548	0.003027
6.13939	9.42660	8.86164	0.000669	-0.000427	-0.002058
7.36410	11.57721	8.92935	0.001047	-0.002729	0.001747
7.40426	7.23794	5.19012	0.002144	0.001769	0.001062
8.63700	9.37970	5.14543	-0.000513	0.002960	0.000934
8.60086	7.99568	8.80617	0.001183	-0.000718	-0.001232
9.83068	10.14286	8.92842	-0.002294	0.001878	0.000059
7.40553	10.08627	5.14064	0.001175	-0.003586	0.003144
8.63637	7.94166	5.16555	0.002616	0.001785	-0.001413
8.60077	9.43254	8.88532	-0.006009	0.002577	-0.001321
9.82927	11.58244	9.00096	0.001087	0.004991	0.002086

9.86805	7.23787	5.19489	-0.000367	0.000106	-0.000236
11.10106	9.37979	5.15156	-0.003850	-0.001020	0.000645
11.06331	7.99411	8.80818	-0.000324	-0.001826	-0.000038
12.29815	10.12943	8.90340	-0.000250	-0.001262	0.001554
9.86930	10.08593	5.15631	-0.005461	-0.001471	0.001401
11.10021	7.94175	5.16862	-0.000620	-0.003077	0.001387
11.06206	9.43062	8.88839	0.004534	0.002035	0.002002
12.30255	11.56557	8.94694	0.001369	-0.001364	-0.002597
12.33169	7.23799	5.19447	-0.001026	0.000243	-0.001765
13.56437	9.38021	5.14435	0.000699	0.001665	-0.000591
13.52754	7.98555	8.80171	-0.000699	-0.002702	-0.003072
14.76233	10.12320	8.88285	-0.005325	0.000473	-0.001684
12.33257	10.08637	5.15511	0.002657	0.000524	-0.001546
13.56350	7.94214	5.16485	-0.000087	-0.000897	-0.000376
13.52731	9.42040	8.86925	-0.000071	0.003115	-0.000379
14.76430	11.55727	8.90646	-0.002821	-0.000143	0.001917
0.01611	11.52516	5.16621	-0.001083	-0.002534	0.000382
1.24770	13.67535	5.22209	0.001889	-0.002061	-0.002480
1.21217	12.26335	8.89409	0.001045	-0.000167	0.001134
2.43998	14.38728	8.86748	-0.002756	-0.000168	0.000740
0.01699	14.35408	5.27295	-0.000503	-0.000973	-0.001964
1.24794	12.22963	5.17275	0.001041	0.000868	-0.001360

1.21434	13.70818	8.88771	0.001835	0.003331	0.003608
2.47958	11.52580	5.14547	-0.001621	-0.000166	-0.001499
3.71218	13.67636	5.19535	0.004490	0.000872	0.001097
3.66932	12.26248	8.88184	-0.002462	0.000198	-0.000632
4.89370	14.38589	8.86075	0.002844	-0.002819	-0.002342
2.48000	14.35596	5.23149	0.001303	-0.001494	0.001670
3.71150	12.23022	5.15602	0.000906	-0.004508	0.001007
3.66212	13.70366	8.87117	-0.004911	0.005108	-0.000836
4.94290	11.52542	5.14351	-0.000060	-0.001729	-0.001611
6.17627	13.67505	5.20032	0.000854	0.000921	0.000076
6.13145	12.27911	8.90591	0.004552	0.006298	0.004556
7.36614	14.42967	8.88203	-0.005710	-0.003521	-0.001001
4.94347	14.35627	5.21375	0.000202	-0.002203	0.001170
6.17493	12.22917	5.16623	-0.001395	-0.001061	0.001538
6.11879	13.72336	8.87765	0.006058	0.004276	0.001624
7.40625	11.52413	5.16368	0.000920	-0.003293	0.000345
8.63876	13.67323	5.24377	0.001981	0.002410	-0.001341
8.58939	12.29067	9.00208	-0.003975	-0.002660	-0.005366
9.83855	14.39048	9.30305	0.020474	0.257825	0.204219
7.40672	14.35386	5.23530	-0.001100	-0.000842	-0.000698
8.63820	12.22778	5.19800	0.000321	-0.001185	0.001033
8.55571	13.73596	9.04598	0.019001	0.011946	0.021505

9.86985	11.52338	5.18893	0.001756	-0.001908	-0.000130
11.10099	13.67352	5.27669	0.003072	-0.000604	-0.001010
11.07378	12.27333	9.00891	0.000404	0.000555	-0.007050
12.30694	14.38896	9.00333	0.003262	-0.002306	0.001089
9.86934	14.35300	5.29564	0.002944	-0.000292	-0.000257
11.10161	12.22804	5.21650	-0.001144	-0.002669	0.001047
11.11464	13.70636	9.07877	-0.020657	0.020173	0.015780
12.33326	11.52411	5.18815	-0.000927	0.000321	0.000531
13.56430	13.67399	5.25995	0.001600	0.000256	0.000075
13.53626	12.26601	8.93587	-0.001453	0.003927	0.001864
14.76266	14.38906	8.90426	-0.002496	-0.000179	0.003825
12.33397	14.35288	5.30710	0.002720	-0.002241	-0.001794
13.56505	12.22870	5.20105	0.000064	0.000102	-0.001133
13.54921	13.70690	8.94399	-0.001717	-0.000711	0.001312
9.91126	15.53185	10.00972	-0.084476	-0.898780	-0.675561
7.28864	16.40884	8.69813	0.003063	-0.008712	-0.006429
10.02526	16.50365	10.64498	0.075087	0.614044	0.456807

---

total drift:	-0.044099	0.024206	-0.021585

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

---

free energy TOTEN = -1209.38425260 eV

energy without entropy= -1209.38425260 energy(sigma->0) = -1209.38425260

d Force = 0.5817810E-02[-0.236E-01, 0.353E-01] d Energy = 0.6060279E-02-0.242E-03

d Force = 0.6614734E+01[0.647E+01, 0.676E+01] d Ewald = 0.6615189E+01-0.455E-03

POTLOK: cpu time 0.1786: real time 0.1808

---

stress matrix after NEB project (eV)

-17.74740 -0.18399 0.08707

-0.18399 -15.02793 0.63651

0.08707 0.63651 -18.93295

FORCES: max atom, RMS 1.127530 0.112567

FORCE total and by dimension 1.364802 0.898780

Stress total and by dimension 30.002648 18.932955

Finite differences progress:

Degree of freedom: 3/ 6

Displacement: 1/ 2

Total: 5/ 12

LATTYP: Found a simple orthorhombic cell.

ALAT = 14.7806000000

B/A-ratio = 1.2466138046

C/A-ratio = 1.4433717170

Lattice vectors:

A1 = (-14.7806000000, 0.0000000000, 0.0000000000)

A2 = (0.0000000000, 0.0000000000, -18.4257000000)

A3 = (0.0000000000, -21.3339000000, 0.0000000000)

Analysis of symmetry for initial positions (statically):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The static configuration has the point symmetry C_1 .

Analysis of symmetry for dynamics (positions and initial velocities):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The dynamic configuration has the point symmetry C_1 .

Analysis of constrained symmetry for selective dynamics:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The constrained configuration has the point symmetry C_1 .

Analysis of structural, dynamic, and magnetic symmetry:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The magnetic configuration has the point symmetry C_1 .

Subroutine INISYM returns: Found 1 space group operations

(whereof 1 operations are pure point group operations),

and found 1 'primitive' translations

KPOINTS: KPT-Resolved Value to Generate K-Mesh: 0

Automatic generation of k-mesh.

Space group operators:

irot	det(A)	alpha	n_x	n_y	n_z	tau_x	tau_y	tau_z
1	1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Subroutine IBZKPT returns following result:

==========

Found 1 irreducible k-points:

Following reciprocal coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

Following cartesian coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

WAVPRE: cpu time 0.1214: real time 0.1308

FEWALD: cpu time 0.0028: real time 0.0028

ORTHCH: cpu time 0.9999: real time 1.0032

LOOP+: cpu time 189.6233: real time 190.6544

---------- Iteration 7(1) ----------

POTLOK: cpu time 0.1726: real time 0.1852

```
      SETDIJ:    cpu time       0.0101: real time       0.0101
      EDDIAG:    cpu time       1.9317: real time       1.9383
    RMM-DIIS:    cpu time       7.2476: real time       7.2728
      ORTHCH:    cpu time       0.3568: real time       0.3579
         DOS:    cpu time       0.0004: real time       0.0004
      CHARGE:    cpu time       0.5175: real time       0.5292
      MIXING:    cpu time       0.0046: real time       0.0046
      ----------------------------------------
        LOOP:    cpu time      10.2412: real time      10.2985

eigenvalue-minimisations    :    1948
total energy-change (2. order) :-0.2139138E-02    (-0.2038520E+00)
number of electron          518.9999725 magnetization             0.9999998
augmentation part            11.7339532 magnetization             0.0542403

Broyden mixing:
  rms(total) = 0.40495E-01        rms(broyden)= 0.40366E-01
  rms(prec ) = 0.41848E-01
  weight for this iteration         100.00

Free energy of the ion-electron system (eV)
  ----------------------------------------------------
```

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107340.52622411

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79944644

PAW double counting = 52181.73954105 -52244.66421629

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.00369845

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76851323 eV

energy without entropy = -1202.76851323 energy(sigma->0) = -1202.76851323

---------- Iteration 7(2) ----------

POTLOK: cpu time 0.1661: real time 0.1796

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9382: real time 1.9447

RMM-DIIS: cpu time 7.1090: real time 7.1447

ORTHCH: cpu time 0.3519: real time 0.3532

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5264: real time 0.5280

MIXING: cpu time 0.0048: real time 0.0048

LOOP: cpu time 10.1069: real time 10.1655

eigenvalue-minimisations : 1920

total energy-change (2. order) : 0.1368912E-02 (-0.1874428E-02)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7344455 magnetization 0.0542445

Broyden mixing:

rms(total) = 0.25760E-01 rms(broyden)= 0.25743E-01

rms(prec) = 0.26900E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9902

1.9902

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107339.78809066

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78746041

PAW double counting = 52176.74780927 -52239.66661101

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.73435046

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76714432 eV

energy without entropy = -1202.76714432 energy(sigma->0) = -1202.76714432

---------- Iteration 7(3) ----------

POTLOK: cpu time 0.1655: real time 0.1843

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9329: real time 1.9391

RMM-DIIS: cpu time 7.2696: real time 7.2984

ORTHCH: cpu time 0.3549: real time 0.3558

DOS: cpu time 0.0003: real time 0.0003

CHARGE: cpu time 0.5250: real time 0.5265

MIXING: cpu time 0.0056: real time 0.0055

LOOP: cpu time 10.2638: real time 10.3199

eigenvalue-minimisations : 1949

total energy-change (2. order) : 0.9021644E-03 (-0.2786433E-03)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7351164 magnetization 0.0542732

Broyden mixing:

rms(total) = 0.83391E-02 rms(broyden)= 0.83307E-02

rms(prec) = 0.90217E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5221

0.7604 2.2837

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107338.79029686

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78036774

PAW double counting = 52171.13401330 -52234.04781665

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.72914782

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76624216 eV

energy without entropy = -1202.76624216 energy(sigma->0) = -1202.76624216

---------- Iteration 7(4) ----------

POTLOK: cpu time 0.1708: real time 0.1738

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9304: real time 1.9372

RMM-DIIS: cpu time 7.3215: real time 7.3421

ORTHCH: cpu time 0.3527: real time 0.3535

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5257: real time 0.5274

MIXING: cpu time 0.0056: real time 0.0056

LOOP: cpu time 10.3173: real time 10.3502

eigenvalue-minimisations : 1949

total energy-change (2. order) : 0.1321276E-03 (-0.1846522E-04)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7347305 magnetization 0.0542739

Broyden mixing:

rms(total) = 0.38115E-02 rms(broyden)= 0.38103E-02

rms(prec) = 0.41544E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4649

2.3144 1.1925 0.8877

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107338.56373363

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78134183

PAW double counting = 52170.57072364 -52233.48439087

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.95668913

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76611003 eV

energy without entropy = -1202.76611003 energy(sigma->0) = -1202.76611003

---------- Iteration 7(5) ----------

POTLOK: cpu time 0.1728: real time 0.1872

SETDIJ: cpu time 0.0133: real time 0.0134

EDDIAG: cpu time 1.9337: real time 1.9403

RMM-DIIS: cpu time 7.2719: real time 7.3226

ORTHCH: cpu time 0.3549: real time 0.3559

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5252: real time 0.5268

MIXING: cpu time 0.0056: real time 0.0056

LOOP: cpu time 10.2777: real time 10.3523

eigenvalue-minimisations : 1951

total energy-change (2. order) :-0.2237332E-04 (-0.7551890E-05)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346652 magnetization 0.0542737

Broyden mixing:

rms(total) = 0.15731E-02 rms(broyden)= 0.15712E-02

rms(prec) = 0.18362E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4469

2.3670 1.7359 0.8424 0.8424

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107338.42916170

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78047359

PAW double counting = 52171.09310576 -52234.00673723

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.09045096

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76613240 eV

energy without entropy = -1202.76613240 energy(sigma->0) = -1202.76613240

---------- Iteration 7(6) ----------

POTLOK: cpu time 0.1649: real time 0.1827

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9293: real time 1.9355

RMM-DIIS: cpu time 7.1529: real time 7.1737

ORTHCH: cpu time 0.3525: real time 0.3535

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5257: real time 0.5273

MIXING: cpu time 0.0061: real time 0.0061

LOOP: cpu time 10.1418: real time 10.1893

eigenvalue-minimisations : 1915

total energy-change (2. order) :-0.4228455E-04 (-0.9407870E-06)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346301 magnetization 0.0542731

Broyden mixing:

rms(total) = 0.76035E-03 rms(broyden)= 0.76006E-03

rms(prec) = 0.10203E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4155

2.5187 2.0101 0.9546 0.9546 0.6397

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107338.27697556

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77984274

PAW double counting = 52171.59859384 -52234.51217744

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.24209639

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76617469 eV

energy without entropy = -1202.76617469 energy(sigma->0) = -1202.76617469

---------- Iteration 7(7) ----------

POTLOK: cpu time 0.1657: real time 0.1702

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9290: real time 1.9355

RMM-DIIS: cpu time 6.5726: real time 6.5913

ORTHCH: cpu time 0.3515: real time 0.3524

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5271: real time 0.5288

MIXING: cpu time 0.0057: real time 0.0057

LOOP: cpu time 9.5621: real time 9.5944

eigenvalue-minimisations : 1771

total energy-change (2. order) :-0.3451252E-04 (-0.2852795E-06)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346490 magnetization 0.0542736

Broyden mixing:

rms(total) = 0.39002E-03 rms(broyden)= 0.38989E-03

rms(prec) = 0.63962E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4257

2.6940 2.0786 1.3869 0.8957 0.8957 0.6034

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107338.16733192

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77919096

PAW double counting = 52171.83849560 -52234.75195544

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.35124654

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76620920 eV

energy without entropy = -1202.76620920 energy(sigma->0) = -1202.76620920

---------- Iteration 7(8) ----------

POTLOK: cpu time 0.1650: real time 0.1796

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9385: real time 1.9453

RMM-DIIS: cpu time 6.2617: real time 6.2805

ORTHCH: cpu time 0.3532: real time 0.3542

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5283: real time 0.5299

MIXING: cpu time 0.0061: real time 0.0061

LOOP: cpu time 9.2634: real time 9.3060

eigenvalue-minimisations : 1719

total energy-change (2. order) :-0.3890184E-04 (-0.2109867E-06)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346491 magnetization 0.0542744

Broyden mixing:

rms(total) = 0.23738E-03 rms(broyden)= 0.23729E-03

rms(prec) = 0.44477E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4343

2.7619 2.3142 1.5294 1.0050 1.0050 0.8188 0.6061

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107338.06040417

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77859283

PAW double counting = 52172.02624378 -52234.93960541

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.45771327

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76624810 eV

energy without entropy = -1202.76624810 energy(sigma->0) = -1202.76624810

---------- Iteration 7(9) ----------

POTLOK: cpu time 0.1672: real time 0.1815

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9317: real time 1.9378

RMM-DIIS: cpu time 6.2633: real time 6.2939

ORTHCH: cpu time 0.3522: real time 0.3532

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5264: real time 0.5280

MIXING: cpu time 0.0063: real time 0.0064

LOOP: cpu time 9.2578: real time 9.3115

eigenvalue-minimisations : 1709

total energy-change (2. order) :-0.4641464E-04 (-0.2610849E-06)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346243 magnetization 0.0542749

Broyden mixing:

rms(total) = 0.15526E-03 rms(broyden)= 0.15513E-03

rms(prec) = 0.29045E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5422

3.3743 2.5311 1.8210 1.3097 0.9818 0.9818 0.7248 0.6132

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107337.94682011

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77802398

PAW double counting = 52172.16659078 -52235.07990715

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.57082014

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76629452 eV

energy without entropy = -1202.76629452 energy(sigma->0) = -1202.76629452

---------- Iteration 7(10) ----------

POTLOK: cpu time 0.1660: real time 0.1800

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9295: real time 1.9362

RMM-DIIS: cpu time 6.2136: real time 6.2360

ORTHCH: cpu time 0.3516: real time 0.3528

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5276: real time 0.5294

MIXING: cpu time 0.0071: real time 0.0071

LOOP: cpu time 9.2058: real time 9.2519

eigenvalue-minimisations : 1699

total energy-change (2. order) :-0.4452311E-04 (-0.3351922E-06)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346244 magnetization 0.0542754

Broyden mixing:

rms(total) = 0.90092E-04 rms(broyden)= 0.90006E-04

rms(prec) = 0.15396E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6198

4.2719 2.5696 2.1286 1.2255 1.2255 0.9160 0.9160 0.7103 0.6149

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107337.82753027

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77732927

PAW double counting = 52172.21848733 -52235.13173157

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.68953193

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76633904 eV

energy without entropy = -1202.76633904 energy(sigma->0) = -1202.76633904

---------- Iteration 7(11) ----------

POTLOK: cpu time 0.1659: real time 0.1723

```
      SETDIJ:    cpu time       0.0101: real time       0.0101
      EDDIAG:    cpu time       1.9264: real time       1.9328
    RMM-DIIS:    cpu time       5.9173: real time       5.9479
      ORTHCH:    cpu time       0.3527: real time       0.3536
         DOS:    cpu time       0.0004: real time       0.0004
      CHARGE:    cpu time       0.5256: real time       0.5274
      MIXING:    cpu time       0.0072: real time       0.0072
      ----------------------------------------
        LOOP:    cpu time       8.9056: real time       8.9518

eigenvalue-minimisations    :    1612
total energy-change (2. order) :-0.1776376E-04    (-0.9800084E-07)
number of electron          518.9999725 magnetization             0.9999998
augmentation part             11.7346259 magnetization             0.0542755

Broyden mixing:
  rms(total) = 0.57527E-04        rms(broyden)= 0.57470E-04
  rms(prec ) = 0.95524E-04
  weight for this iteration         100.00

eigenvalues of (default mixing * dielectric matrix)
  average eigenvalue GAMMA=      1.6895
```

5.0538 2.6942 2.1806 1.5672 1.1223 1.1223 1.0259 0.8286 0.6180 0.6820

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107337.77554567

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77707251

PAW double counting = 52172.19284783 -52235.10608171

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.74128790

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76635680 eV

energy without entropy = -1202.76635680 energy(sigma->0) = -1202.76635680

---------- Iteration 7(12) ----------

POTLOK: cpu time 0.1672: real time 0.1933

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9284: real time 1.9345

RMM-DIIS: cpu time 5.6218: real time 5.6423

ORTHCH: cpu time 0.3521: real time 0.3530

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5264: real time 0.5279

MIXING: cpu time 0.0073: real time 0.0073

LOOP: cpu time 8.6137: real time 8.6689

eigenvalue-minimisations : 1516

total energy-change (2. order) :-0.1019438E-04 (-0.3578034E-07)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346212 magnetization 0.0542755

Broyden mixing:

rms(total) = 0.34322E-04 rms(broyden)= 0.34288E-04

rms(prec) = 0.59028E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7980

6.3117 2.7397 2.4119 2.0087 1.1878 1.1878 0.9519 0.9519 0.7504 0.6222

0.6535

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107337.75186794

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77702713

PAW double counting = 52172.16876679 -52235.08201964

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.76491148

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76636700 eV

energy without entropy = -1202.76636700 energy(sigma->0) = -1202.76636700

---------- Iteration 7(13) ----------

POTLOK: cpu time 0.1670: real time 0.1688

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9273: real time 1.9342

RMM-DIIS: cpu time 5.2973: real time 5.3205

ORTHCH: cpu time 0.3522: real time 0.3534

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5275: real time 0.5293

MIXING: cpu time 0.0082: real time 0.0083

LOOP: cpu time 8.2899: real time 8.3250

eigenvalue-minimisations : 1449

total energy-change (2. order) :-0.5859190E-05 (-0.1694890E-07)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346219 magnetization 0.0542755

Broyden mixing:

rms(total) = 0.20999E-04 rms(broyden)= 0.20990E-04

rms(prec) = 0.37591E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8293

6.7123 2.7597 2.7597 2.0356 1.4188 1.1594 1.1594 1.0012 0.9200 0.7548

0.6238 0.6473

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107337.73936204

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77700082

PAW double counting = 52172.16048669 -52235.07374233

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.77739414

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76637286 eV

energy without entropy = -1202.76637286 energy(sigma->0) = -1202.76637286

---------- Iteration 7(14) ----------

POTLOK: cpu time 0.1754: real time 0.1795

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9273: real time 1.9342

RMM-DIIS: cpu time 5.2029: real time 5.2223

ORTHCH: cpu time 0.3623: real time 0.3633

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5270: real time 0.5289

MIXING: cpu time 0.0084: real time 0.0084

LOOP: cpu time 8.2137: real time 8.2471

eigenvalue-minimisations : 1434

total energy-change (2. order) :-0.4589449E-05 (-0.1265121E-07)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346237 magnetization 0.0542755

Broyden mixing:

rms(total) = 0.15497E-04 rms(broyden)= 0.15483E-04

rms(prec) = 0.22560E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8645

7.0112 3.5498 2.6609 2.1848 1.8577 1.1551 1.1551 0.9808 0.9808 0.7137

0.7137 0.6231 0.6525

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107337.73290294

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77699284

PAW double counting = 52172.16744122 -52235.08069153

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.78385516

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76637745 eV

energy without entropy = -1202.76637745 energy(sigma->0) = -1202.76637745

---------- Iteration 7(15) ----------

POTLOK: cpu time 0.1674: real time 0.1684

SETDIJ: cpu time 0.0099: real time 0.0100

EDDIAG: cpu time 1.9261: real time 1.9321

RMM-DIIS: cpu time 4.8473: real time 4.8637

ORTHCH: cpu time 0.3517: real time 0.3526

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5263: real time 0.5280

MIXING: cpu time 0.0088: real time 0.0088

LOOP: cpu time 7.8380: real time 7.8639

eigenvalue-minimisations : 1313

total energy-change (2. order) :-0.1484572E-05 (-0.2964199E-08)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346228 magnetization 0.0542755

Broyden mixing:

rms(total) = 0.85364E-05 rms(broyden)= 0.85308E-05

rms(prec) = 0.13465E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9470

7.6403 4.3480 2.5578 2.5578 1.9458 1.2776 1.2776 1.0280 1.0280 0.8907

0.7801 0.6745 0.6262 0.6262

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107337.73110138

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77700111

PAW double counting = 52172.17367445 -52235.08692535

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.78566590

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76637893 eV

energy without entropy = -1202.76637893 energy(sigma->0) = -1202.76637893

---------- Iteration 7(16) ----------

POTLOK: cpu time 0.1666: real time 0.1854

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9359: real time 1.9421

RMM-DIIS: cpu time 4.8001: real time 4.8146

ORTHCH: cpu time 0.3522: real time 0.3531

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5265: real time 0.5283

MIXING: cpu time 0.0093: real time 0.0093

LOOP: cpu time 7.8012: real time 7.8433

eigenvalue-minimisations : 1304

total energy-change (2. order) :-0.1153370E-05 (-0.1350072E-08)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346220 magnetization 0.0542755

Broyden mixing:

rms(total) = 0.55531E-05 rms(broyden)= 0.55465E-05

rms(prec) = 0.86181E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9531

7.9416 4.7090 2.7096 2.4812 2.0021 1.3796 1.3796 1.0672 1.0672 0.9116

0.9116 0.8166 0.6708 0.6244 0.6244

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107337.73028244

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77700986

PAW double counting = 52172.17858345 -52235.09183535

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.78649374

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76638008 eV

energy without entropy = -1202.76638008 energy(sigma->0) = -1202.76638008

---------- Iteration 7(17) ----------

POTLOK: cpu time 0.1691: real time 0.1759

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9307: real time 1.9369

RMM-DIIS: cpu time 4.6918: real time 4.7108

ORTHCH: cpu time 0.3517: real time 0.3527

DOS: cpu time 0.0005: real time 0.0005

CHARGE: cpu time 0.5254: real time 0.5269

MIXING: cpu time 0.0097: real time 0.0097

LOOP: cpu time 7.6889: real time 7.7235

eigenvalue-minimisations : 1266

total energy-change (2. order) :-0.9856667E-06 (-0.5868444E-09)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346227 magnetization 0.0542756

Broyden mixing:

rms(total) = 0.29884E-05 rms(broyden)= 0.29844E-05

rms(prec) = 0.50045E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9713

8.1473 5.1233 2.8441 2.5214 2.1198 1.8887 1.2604 1.2604 1.0133 1.0133

0.8663 0.7849 0.7849 0.6639 0.6242 0.6242

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107337.72999445

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77701293

PAW double counting = 52172.17836433 -52235.09161614

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.78678588

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76638107 eV

energy without entropy = -1202.76638107 energy(sigma->0) = -1202.76638107

---------- Iteration 7(18) ----------

POTLOK: cpu time 0.1668: real time 0.1783

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9255: real time 1.9313

RMM-DIIS: cpu time 4.6122: real time 4.6368

ORTHCH: cpu time 0.3518: real time 0.3529

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5266: real time 0.5280

MIXING: cpu time 0.0098: real time 0.0098

LOOP: cpu time 7.6030: real time 7.6476

eigenvalue-minimisations : 1214

total energy-change (2. order) :-0.6188420E-06 (-0.3380043E-09)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346225 magnetization 0.0542756

Broyden mixing:

rms(total) = 0.18813E-05 rms(broyden)= 0.18800E-05

rms(prec) = 0.30684E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0391

8.4184 5.6363 3.4419 2.6531 2.3620 1.9704 1.3710 1.3710 1.0704 1.0704

0.9376 0.9376 0.8166 0.7055 0.6529 0.6251 0.6251

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107337.72988322

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77701935

PAW double counting = 52172.17724323 -52235.09049604

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.78690314

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76638169 eV

energy without entropy = -1202.76638169 energy(sigma->0) = -1202.76638169

---------- Iteration 7(19) ----------

POTLOK: cpu time 0.1667: real time 0.1731

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9262: real time 1.9326

RMM-DIIS: cpu time 4.3504: real time 4.3824

ORTHCH: cpu time 0.3526: real time 0.3537

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5268: real time 0.5285

MIXING: cpu time 0.0106: real time 0.0106

LOOP: cpu time 7.3438: real time 7.3913

eigenvalue-minimisations : 1066

total energy-change (2. order) :-0.1389053E-06 (-0.1303970E-09)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346223 magnetization 0.0542756

Broyden mixing:

rms(total) = 0.12728E-05 rms(broyden)= 0.12717E-05

rms(prec) = 0.18956E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0369

8.5887 5.8850 3.7893 2.6078 2.4506 1.9594 1.7031 1.2431 1.2431 1.0096

1.0096 0.8770 0.8550 0.8550 0.6901 0.6462 0.6259 0.6259

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107337.72977979

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77702392

PAW double counting = 52172.17638940 -52235.08964272

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.78701077

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76638183 eV

energy without entropy = -1202.76638183 energy(sigma->0) = -1202.76638183

---------- Iteration 7(20) ----------

POTLOK: cpu time 0.1658: real time 0.1820

SETDIJ: cpu time 0.0099: real time 0.0100

EDDIAG: cpu time 1.9263: real time 1.9328

RMM-DIIS: cpu time 4.0824: real time 4.0952

ORTHCH: cpu time 0.3539: real time 0.3550

DOS: cpu time 0.0004: real time 0.0004

LOOP: cpu time 6.5387: real time 6.5753

eigenvalue-minimisations : 923

total energy-change (2. order) :-0.2884190E-07 (-0.6986411E-10)

number of electron 518.9999725 magnetization 0.9999998

augmentation part 11.7346223 magnetization 0.0542756

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91332.05595134

-Hartree energ DENC = -107337.72971084

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77702350

PAW double counting = 52172.17618307 -52235.08943589

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.78707983

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76638186 eV

energy without entropy = -1202.76638186 energy(sigma->0) = -1202.76638186

---

average (electrostatic) potential at core

the test charge radii are 0.5201 0.6991 1.0621 0.7215

(the norm of the test charge is 1.0000)

1 -40.7553	2 -40.7533	3 -40.7546	4 -40.7534	5 -40.7553
6 -40.7575	7 -40.7549	8 -40.7628	9 -40.7545	10 -40.7622
11 -40.7560	12 -40.7580	13 -40.6541	14 -40.6990	15 -40.7739
16 -40.7012	17 -40.6948	18 -40.8630	19 -40.6824	20 -40.6706
21 -40.6916	22 -40.6642	23 -40.0836	24 -40.1314	25 -57.4616
26 -57.6729	27 -57.6596	28 -57.4716	29 -57.6669	30 -57.4616
31 -57.6727	32 -57.6592	33 -57.4696	34 -57.6718	35 -57.4624
36 -57.6746	37 -57.6592	38 -57.4718	39 -57.6776	40 -57.4614
41 -57.6786	42 -57.6594	43 -57.4767	44 -57.6922	45 -57.4614
46 -57.6775	47 -57.6602	48 -57.4769	49 -57.6833	50 -57.4626
51 -57.6742	52 -57.6599	53 -57.4746	54 -57.6696	55 -57.6396
56 -57.6657	57 -57.6904	58 -57.6871	59 -57.6694	60 -57.6721
61 -57.6938	62 -57.6786	63 -57.6398	64 -57.6652	65 -57.6925
66 -57.6985	67 -57.6677	68 -57.6719	69 -57.6976	70 -57.7052
71 -57.6393	72 -57.6666	73 -57.7001	74 -57.7257	75 -57.6685
76 -57.6725	77 -57.7099	78 -57.7562	79 -57.6395	80 -57.6692
81 -57.7139	82 -57.7561	83 -57.6718	84 -57.6740	85 -57.7414
86 -57.8465	87 -57.6419	88 -57.6699	89 -57.7158	90 -57.7210
91 -57.6766	92 -57.6743	93 -57.7459	94 -57.7644	95 -57.6403
96 -57.6680	97 -57.6995	98 -57.6944	99 -57.6738	100 -57.6730
101 -57.7117	102 -57.6899	103 -57.6633	104 -57.6341	105 -57.6495
106 -57.2950	107 -57.3913	108 -57.6343	109 -57.6020	110 -57.6622

111 -57.6340	112 -57.6461	113 -57.3145	114 -57.3971	115 -57.6335
116 -57.6040	117 -57.6615	118 -57.6257	119 -57.7024	120 -57.6904
121 -57.3906	122 -57.6323	123 -57.7144	124 -57.6624	125 -57.6286
126 -57.8393	127 -58.3323	128 -57.3639	129 -57.6376	130 -58.1528
131 -57.6705	132 -57.6379	133 -57.8067	134 -57.4229	135 -57.3754
136 -57.6416	137 -58.0870	138 -57.6668	139 -57.6336	140 -57.6754
141 -57.3043	142 -57.3814	143 -57.6369	144 -57.6523	145 -60.8075
146 -57.3154	147 -81.1856			

E-fermi : -2.3810 XC(G=0): -2.7340 alpha+bet : -2.2521

spin component 1

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-26.8137	1.00000
2	-21.5728	1.00000
3	-21.4749	1.00000
4	-21.1056	1.00000

5	-21.0724	1.00000
6	-21.0191	1.00000
7	-20.9820	1.00000
8	-20.9801	1.00000
9	-20.8946	1.00000
10	-20.5645	1.00000
11	-20.5072	1.00000
12	-20.4152	1.00000
13	-20.4014	1.00000
14	-20.1334	1.00000
15	-19.9796	1.00000
16	-19.7117	1.00000
17	-19.6317	1.00000
18	-19.6034	1.00000
19	-19.5877	1.00000
20	-19.5319	1.00000
21	-19.5302	1.00000
22	-19.5022	1.00000
23	-19.4845	1.00000
24	-19.1195	1.00000
25	-19.0795	1.00000
26	-18.9827	1.00000

27	-18.9682	1.00000
28	-18.9067	1.00000
29	-18.7372	1.00000
30	-18.5128	1.00000
31	-18.3632	1.00000
32	-18.2789	1.00000
33	-18.2556	1.00000
34	-18.1877	1.00000
35	-18.1856	1.00000
36	-18.0833	1.00000
37	-18.0794	1.00000
38	-17.5723	1.00000
39	-17.3172	1.00000
40	-17.2918	1.00000
41	-17.2864	1.00000
42	-17.2136	1.00000
43	-17.2068	1.00000
44	-17.1826	1.00000
45	-17.0274	1.00000
46	-16.9540	1.00000
47	-16.9362	1.00000
48	-16.8966	1.00000

49	-16.8947	1.00000
50	-16.8534	1.00000
51	-16.8451	1.00000
52	-16.8254	1.00000
53	-16.8226	1.00000
54	-16.7326	1.00000
55	-16.7295	1.00000
56	-16.1887	1.00000
57	-15.7331	1.00000
58	-15.6956	1.00000
59	-15.6646	1.00000
60	-15.6413	1.00000
61	-15.6194	1.00000
62	-15.5571	1.00000
63	-15.5531	1.00000
64	-15.1837	1.00000
65	-14.8142	1.00000
66	-14.6133	1.00000
67	-14.5812	1.00000
68	-14.5381	1.00000
69	-14.5017	1.00000
70	-14.4724	1.00000

71	-14.4467	1.00000
72	-14.3377	1.00000
73	-14.3092	1.00000
74	-14.2830	1.00000
75	-14.2757	1.00000
76	-14.1856	1.00000
77	-14.1818	1.00000
78	-13.8938	1.00000
79	-13.7650	1.00000
80	-13.5978	1.00000
81	-13.5519	1.00000
82	-13.5328	1.00000
83	-13.5020	1.00000
84	-13.4505	1.00000
85	-13.3673	1.00000
86	-13.3488	1.00000
87	-13.1937	1.00000
88	-12.7901	1.00000
89	-12.7632	1.00000
90	-12.7310	1.00000
91	-12.6993	1.00000
92	-12.6899	1.00000

93	-12.6277	1.00000
94	-12.4643	1.00000
95	-12.4494	1.00000
96	-12.3856	1.00000
97	-12.3282	1.00000
98	-12.2162	1.00000
99	-12.2065	1.00000
100	-12.1689	1.00000
101	-11.9463	1.00000
102	-11.6886	1.00000
103	-11.6289	1.00000
104	-11.6143	1.00000
105	-11.5706	1.00000
106	-11.0955	1.00000
107	-11.0528	1.00000
108	-10.9010	1.00000
109	-10.8905	1.00000
110	-10.8338	1.00000
111	-10.7140	1.00000
112	-10.6807	1.00000
113	-10.6645	1.00000
114	-10.6500	1.00000

115	-10.5925	1.00000
116	-10.5840	1.00000
117	-10.5755	1.00000
118	-10.5716	1.00000
119	-10.5293	1.00000
120	-10.5285	1.00000
121	-10.5137	1.00000
122	-10.5059	1.00000
123	-10.3823	1.00000
124	-10.2946	1.00000
125	-10.2592	1.00000
126	-10.1906	1.00000
127	-10.1895	1.00000
128	-10.0382	1.00000
129	-9.9923	1.00000
130	-9.8898	1.00000
131	-9.8630	1.00000
132	-9.7950	1.00000
133	-9.7891	1.00000
134	-9.7470	1.00000
135	-9.6797	1.00000
136	-9.4481	1.00000

137	-9.4268	1.00000
138	-9.3977	1.00000
139	-9.3908	1.00000
140	-9.3811	1.00000
141	-9.3719	1.00000
142	-9.3134	1.00000
143	-9.3061	1.00000
144	-9.2939	1.00000
145	-9.2843	1.00000
146	-9.2707	1.00000
147	-9.0929	1.00000
148	-9.0065	1.00000
149	-8.9793	1.00000
150	-8.9602	1.00000
151	-8.9482	1.00000
152	-8.7956	1.00000
153	-8.7486	1.00000
154	-8.7378	1.00000
155	-8.7210	1.00000
156	-8.7118	1.00000
157	-8.6904	1.00000
158	-8.6803	1.00000

159	-8.6718	1.00000
160	-8.6564	1.00000
161	-8.5972	1.00000
162	-8.5859	1.00000
163	-8.5789	1.00000
164	-8.5705	1.00000
165	-8.4915	1.00000
166	-8.4606	1.00000
167	-8.4390	1.00000
168	-8.3484	1.00000
169	-8.3005	1.00000
170	-8.2770	1.00000
171	-8.2670	1.00000
172	-8.2362	1.00000
173	-8.2351	1.00000
174	-8.1544	1.00000
175	-8.1480	1.00000
176	-8.0798	1.00000
177	-8.0472	1.00000
178	-8.0292	1.00000
179	-8.0246	1.00000
180	-7.9761	1.00000

181	-7.9677	1.00000
182	-7.9273	1.00000
183	-7.9036	1.00000
184	-7.8879	1.00000
185	-7.8755	1.00000
186	-7.8034	1.00000
187	-7.8002	1.00000
188	-7.7501	1.00000
189	-7.7135	1.00000
190	-7.6697	1.00000
191	-7.6031	1.00000
192	-7.5881	1.00000
193	-7.5790	1.00000
194	-7.5509	1.00000
195	-7.4835	1.00000
196	-7.4830	1.00000
197	-7.4321	1.00000
198	-7.3281	1.00000
199	-7.2523	1.00000
200	-7.1558	1.00000
201	-7.0693	1.00000
202	-7.0447	1.00000

203	-7.0314	1.00000
204	-7.0167	1.00000
205	-6.9997	1.00000
206	-6.9929	1.00000
207	-6.9785	1.00000
208	-6.8694	1.00000
209	-6.8235	1.00000
210	-6.8044	1.00000
211	-6.7962	1.00000
212	-6.7349	1.00000
213	-6.6894	1.00000
214	-6.4746	1.00000
215	-6.4287	1.00000
216	-6.3995	1.00000
217	-6.3941	1.00000
218	-6.3774	1.00000
219	-6.3759	1.00000
220	-6.3206	1.00000
221	-6.3110	1.00000
222	-6.2410	1.00000
223	-6.2326	1.00000
224	-6.2322	1.00000

225	-6.0810	1.00000
226	-6.0416	1.00000
227	-5.7962	1.00000
228	-5.7561	1.00000
229	-5.6978	1.00000
230	-5.6441	1.00000
231	-5.6404	1.00000
232	-5.5626	1.00000
233	-5.5333	1.00000
234	-5.4714	1.00000
235	-5.4430	1.00000
236	-5.1680	1.00000
237	-5.0621	1.00000
238	-5.0543	1.00000
239	-5.0216	1.00000
240	-4.9929	1.00000
241	-4.9142	1.00000
242	-4.8568	1.00000
243	-4.8263	1.00000
244	-4.7935	1.00000
245	-4.6833	1.00000
246	-4.5759	1.00000

247	-4.5746	1.00000
248	-4.5099	1.00000
249	-4.4488	1.00000
250	-4.3873	1.00000
251	-4.2957	1.00000
252	-4.2700	1.00000
253	-4.2159	1.00000
254	-3.5680	1.00000
255	-3.3578	1.00000
256	-3.2062	1.00000
257	-2.9420	1.00000
258	-2.8515	1.00000
259	-2.8271	1.00000
260	-2.6112	1.00000
261	-1.9113	0.00000
262	-1.7716	0.00000
263	-1.7224	0.00000
264	-1.3492	0.00000
265	-1.3214	0.00000
266	-1.2003	0.00000
267	-0.7487	0.00000
268	-0.5876	0.00000

269	-0.5069	0.00000
270	-0.3111	0.00000
271	-0.3091	0.00000
272	-0.2933	0.00000
273	-0.1861	0.00000
274	-0.0610	0.00000
275	-0.0540	0.00000
276	-0.0130	0.00000
277	0.0320	0.00000
278	0.0799	0.00000
279	0.1699	0.00000
280	0.2175	0.00000
281	0.2448	0.00000
282	0.4189	0.00000
283	0.4438	0.00000
284	0.4787	0.00000
285	0.5968	0.00000
286	0.6689	0.00000
287	0.8181	0.00000
288	0.8727	0.00000
289	1.0468	0.00000
290	1.0867	0.00000

291	1.1168	0.00000
292	1.1603	0.00000
293	1.2226	0.00000
294	1.2431	0.00000
295	1.2856	0.00000
296	1.3135	0.00000
297	1.3451	0.00000
298	1.4095	0.00000
299	1.4641	0.00000
300	1.4837	0.00000
301	1.5508	0.00000
302	1.5855	0.00000
303	1.6227	0.00000
304	1.6766	0.00000
305	1.7493	0.00000
306	1.7615	0.00000
307	1.8722	0.00000
308	1.8917	0.00000
309	1.9037	0.00000
310	1.9115	0.00000
311	2.1270	0.00000
312	2.1889	0.00000

313	2.2068	0.00000
314	2.2336	0.00000
315	2.2745	0.00000
316	2.2915	0.00000
317	2.3311	0.00000
318	2.3516	0.00000
319	2.3703	0.00000
320	2.3960	0.00000
321	2.4172	0.00000
322	2.4292	0.00000
323	2.4395	0.00000
324	2.4532	0.00000
325	2.4617	0.00000
326	2.5260	0.00000
327	2.5402	0.00000
328	2.7017	0.00000
329	2.7286	0.00000
330	2.7517	0.00000
331	2.7552	0.00000
332	2.7648	0.00000
333	2.8118	0.00000
334	2.8316	0.00000

335	2.8638	0.00000
336	2.8910	0.00000
337	2.9233	0.00000
338	2.9456	0.00000
339	2.9779	0.00000
340	3.0046	0.00000
341	3.0334	0.00000
342	3.0431	0.00000
343	3.0658	0.00000
344	3.0838	0.00000
345	3.1508	0.00000
346	3.1624	0.00000
347	3.1799	0.00000
348	3.1921	0.00000
349	3.3019	0.00000
350	3.3240	0.00000
351	3.3532	0.00000
352	3.3680	0.00000
353	3.3900	0.00000
354	3.4347	0.00000
355	3.4770	0.00000
356	3.4825	0.00000

357	3.4857	0.00000
358	3.4961	0.00000
359	3.6348	0.00000
360	3.6730	0.00000
361	3.6881	0.00000
362	3.7343	0.00000
363	3.7494	0.00000
364	3.7574	0.00000
365	3.7722	0.00000
366	3.7929	0.00000
367	3.8106	0.00000
368	3.8320	0.00000
369	3.8369	0.00000
370	3.8527	0.00000
371	3.8756	0.00000
372	3.8826	0.00000
373	3.9102	0.00000
374	3.9227	0.00000
375	3.9333	0.00000
376	3.9575	0.00000
377	3.9718	0.00000
378	3.9849	0.00000

379	4.0165	0.00000
380	4.0696	0.00000
381	4.1649	0.00000
382	4.2465	0.00000
383	4.2583	0.00000
384	4.2586	0.00000
385	4.2857	0.00000
386	4.3140	0.00000
387	4.3277	0.00000
388	4.3416	0.00000
389	4.3701	0.00000
390	4.3800	0.00000
391	4.4174	0.00000
392	4.4451	0.00000
393	4.4693	0.00000
394	4.4804	0.00000
395	4.4864	0.00000
396	4.4962	0.00000
397	4.5179	0.00000
398	4.5500	0.00000
399	4.5899	0.00000
400	4.6079	0.00000

401	4.6267	0.00000
402	4.6423	0.00000
403	4.6567	0.00000
404	4.6791	0.00000
405	4.7035	0.00000
406	4.7314	0.00000
407	4.7469	0.00000
408	4.7676	0.00000
409	4.7828	0.00000
410	4.7839	0.00000
411	4.7973	0.00000
412	4.8292	0.00000
413	4.8632	0.00000
414	4.8716	0.00000
415	4.8981	0.00000
416	4.9317	0.00000
417	4.9835	0.00000
418	5.0041	0.00000
419	5.0104	0.00000
420	5.0346	0.00000
421	5.0385	0.00000
422	5.0642	0.00000

423	5.0814	0.00000
424	5.1151	0.00000
425	5.1174	0.00000
426	5.1367	0.00000
427	5.1406	0.00000
428	5.1519	0.00000
429	5.1747	0.00000
430	5.1846	0.00000
431	5.1879	0.00000
432	5.2165	0.00000
433	5.2345	0.00000
434	5.2414	0.00000
435	5.2558	0.00000
436	5.2880	0.00000
437	5.2945	0.00000
438	5.3087	0.00000
439	5.3322	0.00000
440	5.3483	0.00000
441	5.3661	0.00000
442	5.3731	0.00000
443	5.3907	0.00000
444	5.4213	0.00000

445	5.4528	0.00000
446	5.4636	0.00000
447	5.4813	0.00000
448	5.4945	0.00000
449	5.5170	0.00000
450	5.5489	0.00000
451	5.5673	0.00000
452	5.5742	0.00000
453	5.5956	0.00000
454	5.6130	0.00000
455	5.6576	0.00000
456	5.6807	0.00000
457	5.7090	0.00000
458	5.7227	0.00000
459	5.7438	0.00000
460	5.7576	0.00000
461	5.7810	0.00000
462	5.7881	0.00000
463	5.7941	0.00000
464	5.7996	0.00000
465	5.8071	0.00000
466	5.8230	0.00000

467	5.8418	0.00000
468	5.8542	0.00000
469	5.8720	0.00000
470	5.8793	0.00000
471	5.8849	0.00000
472	5.9072	0.00000
473	5.9137	0.00000
474	5.9397	0.00000
475	5.9526	0.00000
476	5.9716	0.00000
477	5.9790	0.00000
478	6.0032	0.00000
479	6.0111	0.00000
480	6.0738	0.00000

spin component 2

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-26.8069	1.00000
2	-21.5716	1.00000
3	-21.4733	1.00000

4	-21.1037	1.00000
5	-21.0715	1.00000
6	-21.0164	1.00000
7	-20.9806	1.00000
8	-20.9782	1.00000
9	-20.8840	1.00000
10	-20.5616	1.00000
11	-20.5039	1.00000
12	-20.4041	1.00000
13	-20.3917	1.00000
14	-20.1293	1.00000
15	-19.9563	1.00000
16	-19.7090	1.00000
17	-19.6304	1.00000
18	-19.6013	1.00000
19	-19.5814	1.00000
20	-19.5306	1.00000
21	-19.5284	1.00000
22	-19.4795	1.00000
23	-19.4649	1.00000
24	-19.1171	1.00000
25	-19.0771	1.00000

26	-18.9728	1.00000
27	-18.9586	1.00000
28	-18.9019	1.00000
29	-18.7075	1.00000
30	-18.5098	1.00000
31	-18.3562	1.00000
32	-18.2508	1.00000
33	-18.2304	1.00000
34	-18.1824	1.00000
35	-18.1802	1.00000
36	-18.0631	1.00000
37	-18.0597	1.00000
38	-17.5689	1.00000
39	-17.3012	1.00000
40	-17.2912	1.00000
41	-17.2769	1.00000
42	-17.2113	1.00000
43	-17.2099	1.00000
44	-17.1797	1.00000
45	-17.0235	1.00000
46	-16.9452	1.00000
47	-16.9260	1.00000

48	-16.8740	1.00000
49	-16.8729	1.00000
50	-16.8326	1.00000
51	-16.8266	1.00000
52	-16.8216	1.00000
53	-16.8189	1.00000
54	-16.7345	1.00000
55	-16.7283	1.00000
56	-16.1860	1.00000
57	-15.7323	1.00000
58	-15.6619	1.00000
59	-15.6478	1.00000
60	-15.6242	1.00000
61	-15.5699	1.00000
62	-15.5311	1.00000
63	-15.5283	1.00000
64	-15.1800	1.00000
65	-14.8120	1.00000
66	-14.6112	1.00000
67	-14.5637	1.00000
68	-14.5037	1.00000
69	-14.5019	1.00000

70	-14.4683	1.00000
71	-14.4422	1.00000
72	-14.3343	1.00000
73	-14.3016	1.00000
74	-14.2713	1.00000
75	-14.2672	1.00000
76	-14.1675	1.00000
77	-14.1642	1.00000
78	-13.8929	1.00000
79	-13.7626	1.00000
80	-13.5953	1.00000
81	-13.5414	1.00000
82	-13.5217	1.00000
83	-13.4984	1.00000
84	-13.4488	1.00000
85	-13.3469	1.00000
86	-13.3441	1.00000
87	-13.1921	1.00000
88	-12.7840	1.00000
89	-12.7537	1.00000
90	-12.7223	1.00000
91	-12.6807	1.00000

92	-12.6740	1.00000
93	-12.6255	1.00000
94	-12.4518	1.00000
95	-12.4346	1.00000
96	-12.3820	1.00000
97	-12.3273	1.00000
98	-12.2116	1.00000
99	-12.2013	1.00000
100	-12.1673	1.00000
101	-11.9436	1.00000
102	-11.6858	1.00000
103	-11.6109	1.00000
104	-11.5951	1.00000
105	-11.5650	1.00000
106	-11.0937	1.00000
107	-11.0496	1.00000
108	-10.8917	1.00000
109	-10.8800	1.00000
110	-10.8309	1.00000
111	-10.7080	1.00000
112	-10.6795	1.00000
113	-10.6617	1.00000

114	-10.6450	1.00000
115	-10.5846	1.00000
116	-10.5773	1.00000
117	-10.5725	1.00000
118	-10.5686	1.00000
119	-10.5187	1.00000
120	-10.5178	1.00000
121	-10.5046	1.00000
122	-10.4999	1.00000
123	-10.3815	1.00000
124	-10.2938	1.00000
125	-10.2584	1.00000
126	-10.1872	1.00000
127	-10.1861	1.00000
128	-10.0331	1.00000
129	-9.9823	1.00000
130	-9.8871	1.00000
131	-9.8596	1.00000
132	-9.7863	1.00000
133	-9.7800	1.00000
134	-9.7451	1.00000
135	-9.6765	1.00000

136	-9.4462	1.00000
137	-9.4234	1.00000
138	-9.3870	1.00000
139	-9.3818	1.00000
140	-9.3729	1.00000
141	-9.3624	1.00000
142	-9.3110	1.00000
143	-9.3038	1.00000
144	-9.2932	1.00000
145	-9.2816	1.00000
146	-9.2497	1.00000
147	-9.0917	1.00000
148	-9.0029	1.00000
149	-8.9691	1.00000
150	-8.9460	1.00000
151	-8.9403	1.00000
152	-8.7931	1.00000
153	-8.7407	1.00000
154	-8.7354	1.00000
155	-8.7154	1.00000
156	-8.7083	1.00000
157	-8.6731	1.00000

158	-8.6669	1.00000
159	-8.6591	1.00000
160	-8.6557	1.00000
161	-8.5798	1.00000
162	-8.5738	1.00000
163	-8.5689	1.00000
164	-8.5522	1.00000
165	-8.4911	1.00000
166	-8.4600	1.00000
167	-8.4374	1.00000
168	-8.3458	1.00000
169	-8.2976	1.00000
170	-8.2752	1.00000
171	-8.2363	1.00000
172	-8.2325	1.00000
173	-8.2304	1.00000
174	-8.1443	1.00000
175	-8.1367	1.00000
176	-8.0765	1.00000
177	-8.0451	1.00000
178	-8.0166	1.00000
179	-8.0096	1.00000

180	-7.9716	1.00000
181	-7.9626	1.00000
182	-7.9233	1.00000
183	-7.8941	1.00000
184	-7.8740	1.00000
185	-7.8666	1.00000
186	-7.7947	1.00000
187	-7.7909	1.00000
188	-7.7406	1.00000
189	-7.6821	1.00000
190	-7.6394	1.00000
191	-7.6009	1.00000
192	-7.5802	1.00000
193	-7.5580	1.00000
194	-7.5434	1.00000
195	-7.4755	1.00000
196	-7.4753	1.00000
197	-7.4310	1.00000
198	-7.3272	1.00000
199	-7.2390	1.00000
200	-7.1526	1.00000
201	-7.0592	1.00000

202	-7.0393	1.00000
203	-7.0184	1.00000
204	-6.9885	1.00000
205	-6.9807	1.00000
206	-6.9756	1.00000
207	-6.9441	1.00000
208	-6.8658	1.00000
209	-6.8193	1.00000
210	-6.7983	1.00000
211	-6.7911	1.00000
212	-6.7281	1.00000
213	-6.6801	1.00000
214	-6.4714	1.00000
215	-6.3986	1.00000
216	-6.3862	1.00000
217	-6.3813	1.00000
218	-6.3666	1.00000
219	-6.3418	1.00000
220	-6.3077	1.00000
221	-6.2790	1.00000
222	-6.2326	1.00000
223	-6.2310	1.00000

224	-6.2266	1.00000
225	-6.0503	1.00000
226	-6.0130	1.00000
227	-5.7597	1.00000
228	-5.7153	1.00000
229	-5.6962	1.00000
230	-5.6386	1.00000
231	-5.6262	1.00000
232	-5.5475	1.00000
233	-5.5265	1.00000
234	-5.4450	1.00000
235	-5.4155	1.00000
236	-5.1458	1.00000
237	-5.0633	1.00000
238	-5.0301	1.00000
239	-5.0259	1.00000
240	-4.9635	1.00000
241	-4.8813	1.00000
242	-4.8576	1.00000
243	-4.8066	1.00000
244	-4.7816	1.00000
245	-4.6531	1.00000

246	-4.5821	1.00000
247	-4.5790	1.00000
248	-4.4799	1.00000
249	-4.4245	1.00000
250	-4.3984	1.00000
251	-4.2995	1.00000
252	-4.2312	1.00000
253	-4.1785	1.00000
254	-3.5419	1.00000
255	-3.3124	1.00000
256	-3.1469	1.00000
257	-2.9469	1.00000
258	-2.8024	1.00000
259	-2.7438	1.00000
260	-2.0644	0.00000
261	-1.9173	0.00000
262	-1.7263	0.00000
263	-1.6826	0.00000
264	-1.3083	0.00000
265	-1.2864	0.00000
266	-1.1641	0.00000
267	-0.7274	0.00000

268	-0.5870	0.00000
269	-0.5144	0.00000
270	-0.2840	0.00000
271	-0.2810	0.00000
272	-0.2632	0.00000
273	-0.1595	0.00000
274	-0.0621	0.00000
275	-0.0516	0.00000
276	0.0108	0.00000
277	0.0372	0.00000
278	0.0748	0.00000
279	0.2051	0.00000
280	0.2526	0.00000
281	0.2765	0.00000
282	0.4310	0.00000
283	0.4496	0.00000
284	0.4801	0.00000
285	0.6013	0.00000
286	0.6892	0.00000
287	0.8210	0.00000
288	0.8795	0.00000
289	1.0567	0.00000

290	1.1037	0.00000
291	1.1395	0.00000
292	1.1743	0.00000
293	1.2314	0.00000
294	1.2493	0.00000
295	1.3068	0.00000
296	1.3188	0.00000
297	1.3587	0.00000
298	1.4287	0.00000
299	1.4774	0.00000
300	1.5007	0.00000
301	1.5759	0.00000
302	1.6017	0.00000
303	1.6505	0.00000
304	1.6854	0.00000
305	1.7570	0.00000
306	1.7715	0.00000
307	1.8773	0.00000
308	1.8971	0.00000
309	1.9067	0.00000
310	1.9185	0.00000
311	2.1427	0.00000

312	2.1994	0.00000
313	2.2186	0.00000
314	2.2529	0.00000
315	2.2885	0.00000
316	2.2960	0.00000
317	2.3365	0.00000
318	2.3595	0.00000
319	2.3811	0.00000
320	2.4059	0.00000
321	2.4265	0.00000
322	2.4343	0.00000
323	2.4497	0.00000
324	2.4586	0.00000
325	2.4666	0.00000
326	2.5286	0.00000
327	2.5459	0.00000
328	2.7068	0.00000
329	2.7349	0.00000
330	2.7518	0.00000
331	2.7581	0.00000
332	2.7737	0.00000
333	2.8261	0.00000

334	2.8445	0.00000
335	2.8765	0.00000
336	2.9024	0.00000
337	2.9320	0.00000
338	2.9551	0.00000
339	2.9827	0.00000
340	3.0062	0.00000
341	3.0373	0.00000
342	3.0500	0.00000
343	3.0715	0.00000
344	3.0913	0.00000
345	3.1533	0.00000
346	3.1706	0.00000
347	3.1887	0.00000
348	3.2006	0.00000
349	3.3075	0.00000
350	3.3287	0.00000
351	3.3615	0.00000
352	3.3716	0.00000
353	3.3933	0.00000
354	3.4402	0.00000
355	3.4824	0.00000

356	3.4905	0.00000
357	3.4930	0.00000
358	3.5023	0.00000
359	3.6398	0.00000
360	3.6769	0.00000
361	3.7005	0.00000
362	3.7396	0.00000
363	3.7535	0.00000
364	3.7593	0.00000
365	3.7771	0.00000
366	3.7976	0.00000
367	3.8134	0.00000
368	3.8396	0.00000
369	3.8471	0.00000
370	3.8663	0.00000
371	3.8793	0.00000
372	3.8916	0.00000
373	3.9217	0.00000
374	3.9344	0.00000
375	3.9473	0.00000
376	3.9597	0.00000
377	3.9826	0.00000

378	3.9872	0.00000
379	4.0223	0.00000
380	4.0790	0.00000
381	4.1713	0.00000
382	4.2602	0.00000
383	4.2616	0.00000
384	4.2697	0.00000
385	4.2933	0.00000
386	4.3222	0.00000
387	4.3345	0.00000
388	4.3508	0.00000
389	4.3799	0.00000
390	4.3847	0.00000
391	4.4232	0.00000
392	4.4491	0.00000
393	4.4747	0.00000
394	4.4831	0.00000
395	4.4925	0.00000
396	4.4994	0.00000
397	4.5215	0.00000
398	4.5545	0.00000
399	4.5930	0.00000

400	4.6106	0.00000
401	4.6284	0.00000
402	4.6459	0.00000
403	4.6598	0.00000
404	4.6850	0.00000
405	4.7083	0.00000
406	4.7372	0.00000
407	4.7518	0.00000
408	4.7710	0.00000
409	4.7862	0.00000
410	4.7894	0.00000
411	4.8029	0.00000
412	4.8339	0.00000
413	4.8689	0.00000
414	4.8843	0.00000
415	4.9033	0.00000
416	4.9423	0.00000
417	4.9934	0.00000
418	5.0095	0.00000
419	5.0127	0.00000
420	5.0377	0.00000
421	5.0438	0.00000

422	5.0685	0.00000
423	5.0857	0.00000
424	5.1185	0.00000
425	5.1216	0.00000
426	5.1407	0.00000
427	5.1441	0.00000
428	5.1687	0.00000
429	5.1793	0.00000
430	5.1881	0.00000
431	5.1927	0.00000
432	5.2214	0.00000
433	5.2369	0.00000
434	5.2448	0.00000
435	5.2614	0.00000
436	5.2968	0.00000
437	5.3018	0.00000
438	5.3117	0.00000
439	5.3365	0.00000
440	5.3523	0.00000
441	5.3699	0.00000
442	5.3806	0.00000
443	5.3937	0.00000

444	5.4297	0.00000
445	5.4591	0.00000
446	5.4703	0.00000
447	5.4867	0.00000
448	5.4991	0.00000
449	5.5237	0.00000
450	5.5673	0.00000
451	5.5729	0.00000
452	5.5934	0.00000
453	5.6081	0.00000
454	5.6227	0.00000
455	5.6699	0.00000
456	5.6915	0.00000
457	5.7179	0.00000
458	5.7272	0.00000
459	5.7482	0.00000
460	5.7626	0.00000
461	5.7888	0.00000
462	5.7910	0.00000
463	5.7972	0.00000
464	5.8034	0.00000
465	5.8198	0.00000

466	5.8253	0.00000
467	5.8542	0.00000
468	5.8611	0.00000
469	5.8799	0.00000
470	5.8855	0.00000
471	5.8896	0.00000
472	5.9057	0.00000
473	5.9216	0.00000
474	5.9484	0.00000
475	5.9557	0.00000
476	5.9725	0.00000
477	5.9780	0.00000
478	5.9977	0.00000
479	6.0175	0.00000
480	6.0528	0.00000

---

soft charge-density along one line, spin component 1

0 1 2 3 4 5 6 7

8 9

total charge-density along one line

soft charge-density along one line, spin component 2

0 1 2 3 4 5 6 7

8 9

total charge-density along one line

pseudopotential strength for first ion, spin component: 1

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

pseudopotential strength for first ion, spin component: 2

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

total augmentation occupancy for first ion, spin component: 1

3.579 -0.646 0.444 -0.034 -0.000

-0.646 0.130 -0.082 0.006 0.000

0.444 -0.082 0.056 -0.003 -0.000

-0.034 0.006 -0.003 0.011 0.000

-0.000 0.000 -0.000 0.000 0.007

total augmentation occupancy for first ion, spin component: 2

-0.000 0.000 -0.000 0.000 0.000

0.000 -0.000 0.000 -0.000 -0.000

-0.000 0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

---------- aborting loop because EDIFF is reached ----------

total charge

# of ion	s	p	d	tot

1	0.646	0.043	0.000	0.690
2	0.646	0.043	0.000	0.690
3	0.646	0.043	0.000	0.690
4	0.646	0.043	0.000	0.690
5	0.646	0.043	0.000	0.690
6	0.646	0.043	0.000	0.690
7	0.646	0.043	0.000	0.690
8	0.646	0.043	0.000	0.690
9	0.646	0.043	0.000	0.690
10	0.646	0.043	0.000	0.690
11	0.646	0.043	0.000	0.690
12	0.646	0.043	0.000	0.690
13	0.646	0.043	0.000	0.689
14	0.646	0.043	0.000	0.689
15	0.648	0.045	0.000	0.693
16	0.646	0.043	0.000	0.689
17	0.646	0.043	0.000	0.689
18	0.646	0.043	0.000	0.689
19	0.646	0.043	0.000	0.689
20	0.646	0.043	0.000	0.689
21	0.646	0.043	0.000	0.689
22	0.646	0.044	0.000	0.690

23	0.542	0.015	0.000	0.557
24	0.541	0.015	0.000	0.556
25	0.870	1.763	0.000	2.633
26	0.867	1.785	0.000	2.653
27	0.867	1.786	0.000	2.653
28	0.870	1.762	0.000	2.632
29	0.865	1.783	0.000	2.648
30	0.870	1.763	0.000	2.633
31	0.867	1.786	0.000	2.653
32	0.867	1.786	0.000	2.653
33	0.870	1.762	0.000	2.632
34	0.865	1.783	0.000	2.648
35	0.870	1.763	0.000	2.633
36	0.868	1.787	0.000	2.654
37	0.867	1.786	0.000	2.653
38	0.870	1.763	0.000	2.633
39	0.865	1.784	0.000	2.649
40	0.870	1.763	0.000	2.633
41	0.868	1.787	0.000	2.655
42	0.867	1.786	0.000	2.653
43	0.871	1.764	0.000	2.634
44	0.865	1.783	0.000	2.648

45	0.870	1.763	0.000	2.633
46	0.867	1.786	0.000	2.653
47	0.867	1.786	0.000	2.653
48	0.871	1.763	0.000	2.634
49	0.865	1.783	0.000	2.648
50	0.870	1.763	0.000	2.633
51	0.867	1.786	0.000	2.653
52	0.867	1.786	0.000	2.653
53	0.870	1.762	0.000	2.632
54	0.865	1.784	0.000	2.648
55	0.865	1.784	0.000	2.649
56	0.865	1.786	0.000	2.651
57	0.866	1.787	0.000	2.653
58	0.866	1.790	0.000	2.656
59	0.865	1.786	0.000	2.651
60	0.866	1.786	0.000	2.651
61	0.866	1.788	0.000	2.654
62	0.867	1.791	0.000	2.658
63	0.865	1.784	0.000	2.649
64	0.865	1.786	0.000	2.651
65	0.866	1.787	0.000	2.652
66	0.865	1.788	0.000	2.653

67	0.865	1.786	0.000	2.651
68	0.866	1.785	0.000	2.651
69	0.865	1.787	0.000	2.652
70	0.866	1.787	0.000	2.653
71	0.865	1.784	0.000	2.649
72	0.865	1.786	0.000	2.651
73	0.866	1.786	0.000	2.652
74	0.864	1.785	0.000	2.649
75	0.865	1.786	0.000	2.651
76	0.866	1.786	0.000	2.651
77	0.865	1.786	0.000	2.651
78	0.865	1.784	0.000	2.649
79	0.865	1.784	0.000	2.649
80	0.865	1.786	0.000	2.651
81	0.865	1.785	0.000	2.650
82	0.863	1.782	0.000	2.645
83	0.865	1.786	0.000	2.651
84	0.866	1.786	0.000	2.651
85	0.865	1.784	0.000	2.648
86	0.862	1.774	0.000	2.636
87	0.865	1.784	0.000	2.649
88	0.865	1.787	0.000	2.652

89	0.865	1.785	0.000	2.650
90	0.865	1.788	0.000	2.653
91	0.865	1.786	0.000	2.651
92	0.866	1.786	0.000	2.651
93	0.864	1.783	0.000	2.647
94	0.866	1.785	0.000	2.651
95	0.865	1.784	0.000	2.649
96	0.865	1.786	0.000	2.651
97	0.866	1.787	0.000	2.653
98	0.866	1.789	0.000	2.655
99	0.865	1.786	0.000	2.651
100	0.866	1.786	0.000	2.651
101	0.865	1.787	0.000	2.652
102	0.867	1.790	0.000	2.657
103	0.865	1.786	0.000	2.651
104	0.867	1.785	0.000	2.653
105	0.866	1.786	0.000	2.652
106	0.870	1.778	0.000	2.648
107	0.869	1.765	0.000	2.635
108	0.865	1.783	0.000	2.648
109	0.869	1.789	0.000	2.658
110	0.865	1.786	0.000	2.651

111	0.867	1.785	0.000	2.653
112	0.867	1.789	0.000	2.655
113	0.871	1.782	0.000	2.653
114	0.869	1.765	0.000	2.634
115	0.865	1.783	0.000	2.648
116	0.870	1.791	0.000	2.661
117	0.865	1.786	0.000	2.651
118	0.867	1.786	0.000	2.653
119	0.865	1.782	0.000	2.647
120	0.857	1.707	0.000	2.564
121	0.869	1.765	0.000	2.634
122	0.865	1.783	0.000	2.648
123	0.866	1.778	0.000	2.644
124	0.866	1.786	0.000	2.652
125	0.868	1.785	0.000	2.653
126	0.862	1.776	0.000	2.638
127	0.851	1.837	0.000	2.688
128	0.870	1.767	0.000	2.637
129	0.865	1.783	0.000	2.648
130	0.860	1.757	0.000	2.617
131	0.866	1.786	0.000	2.652
132	0.867	1.784	0.000	2.652

133	0.864	1.787	0.000	2.651
134	0.869	1.789	0.000	2.659
135	0.869	1.767	0.000	2.636
136	0.865	1.783	0.000	2.648
137	0.866	1.772	0.000	2.638
138	0.866	1.786	0.000	2.652
139	0.867	1.785	0.000	2.652
140	0.866	1.788	0.000	2.654
141	0.870	1.779	0.000	2.649
142	0.869	1.766	0.000	2.635
143	0.865	1.783	0.000	2.648
144	0.869	1.790	0.000	2.659
145	0.940	1.713	0.000	2.653
146	1.240	1.545	0.075	2.860
147	1.632	3.515	0.000	5.147
---	---	---	---	---
tot	123.061	221.537	0.075	344.673

magnetization (x)

# of ion	s	p	d	tot
1	0.000	-0.000	0.000	0.000
2	-0.000	0.000	0.000	-0.000
3	0.000	-0.000	0.000	0.000
4	-0.000	0.000	0.000	-0.000
5	0.000	-0.000	0.000	0.000
6	-0.000	0.000	0.000	-0.000
7	0.000	-0.000	0.000	0.000
8	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	0.000
10	-0.000	0.000	0.000	-0.000
11	0.000	-0.000	0.000	0.000
12	-0.000	0.000	0.000	-0.000
13	0.000	-0.000	0.000	0.000
14	-0.004	0.002	0.000	-0.002
15	0.000	-0.000	0.000	0.000
16	-0.004	0.002	0.000	-0.002
17	-0.004	0.002	0.000	-0.002
18	0.000	-0.000	0.000	0.000
19	-0.003	0.001	0.000	-0.002
20	0.000	-0.000	0.000	0.000

21	-0.003	0.002	0.000	-0.002
22	-0.003	0.002	0.000	-0.002
23	-0.000	0.000	0.000	-0.000
24	-0.000	0.000	0.000	-0.000
25	-0.000	-0.007	0.000	-0.008
26	-0.000	-0.002	0.000	-0.002
27	0.000	0.003	0.000	0.003
28	0.000	0.005	0.000	0.005
29	0.000	0.003	0.000	0.003
30	-0.000	-0.007	0.000	-0.008
31	-0.000	-0.002	0.000	-0.002
32	0.000	0.003	0.000	0.003
33	0.000	0.005	0.000	0.005
34	0.000	0.002	0.000	0.002
35	-0.000	-0.007	0.000	-0.008
36	-0.000	-0.002	0.000	-0.002
37	0.000	0.003	0.000	0.003
38	0.000	0.006	0.000	0.007
39	0.000	0.002	0.000	0.002
40	-0.000	-0.007	0.000	-0.008
41	-0.000	-0.002	0.000	-0.002
42	0.000	0.002	0.000	0.003

43	0.000	0.005	0.000	0.006
44	0.000	0.004	0.000	0.004
45	-0.000	-0.007	0.000	-0.008
46	-0.000	-0.002	0.000	-0.002
47	0.000	0.003	0.000	0.003
48	0.000	0.005	0.000	0.006
49	0.000	0.001	0.000	0.002
50	-0.000	-0.007	0.000	-0.008
51	-0.000	-0.002	0.000	-0.002
52	0.000	0.002	0.000	0.003
53	0.000	0.006	0.000	0.007
54	0.000	0.002	0.000	0.002
55	-0.000	-0.005	0.000	-0.006
56	-0.000	-0.007	0.000	-0.007
57	-0.000	-0.001	0.000	-0.001
58	-0.000	-0.001	0.000	-0.001
59	0.000	0.006	0.000	0.007
60	0.000	0.003	0.000	0.003
61	0.000	0.001	0.000	0.001
62	0.000	0.003	0.000	0.003
63	-0.000	-0.005	0.000	-0.006
64	-0.000	-0.007	0.000	-0.007

65	-0.000	-0.001	0.000	-0.001
66	-0.000	-0.001	0.000	-0.001
67	0.000	0.006	0.000	0.006
68	0.000	0.003	0.000	0.003
69	0.000	0.001	0.000	0.001
70	0.000	0.002	0.000	0.002
71	-0.000	-0.005	0.000	-0.006
72	-0.000	-0.007	0.000	-0.007
73	-0.000	-0.001	0.000	-0.001
74	-0.000	-0.002	0.000	-0.002
75	0.000	0.006	0.000	0.007
76	0.000	0.003	0.000	0.004
77	0.000	0.003	0.000	0.003
78	0.000	0.001	0.000	0.001
79	-0.000	-0.005	0.000	-0.006
80	-0.000	-0.007	0.000	-0.007
81	-0.000	-0.001	0.000	-0.002
82	-0.000	-0.002	0.000	-0.002
83	0.001	0.007	0.000	0.008
84	0.000	0.003	0.000	0.003
85	0.000	0.002	0.000	0.002
86	0.000	0.005	0.000	0.006

87	-0.000	-0.005	0.000	-0.005
88	-0.000	-0.007	0.000	-0.007
89	-0.000	-0.001	0.000	-0.002
90	-0.000	-0.002	0.000	-0.002
91	0.001	0.008	0.000	0.008
92	0.000	0.003	0.000	0.003
93	0.000	0.002	0.000	0.003
94	0.000	0.001	0.000	0.001
95	-0.000	-0.005	0.000	-0.006
96	-0.000	-0.007	0.000	-0.007
97	-0.000	-0.001	0.000	-0.001
98	-0.000	-0.001	0.000	-0.001
99	0.001	0.007	0.000	0.007
100	0.000	0.003	0.000	0.004
101	0.000	0.003	0.000	0.003
102	0.000	0.002	0.000	0.002
103	-0.001	-0.010	0.000	-0.011
104	-0.003	-0.028	0.000	-0.031
105	-0.000	-0.001	0.000	-0.002
106	-0.000	-0.004	0.000	-0.005
107	0.007	0.116	0.000	0.122
108	0.001	0.010	0.000	0.011

109	0.000	0.001	0.000	0.001
110	-0.001	-0.010	0.000	-0.011
111	-0.003	-0.028	0.000	-0.031
112	-0.000	-0.001	0.000	-0.002
113	-0.000	-0.003	0.000	-0.004
114	0.007	0.120	0.000	0.127
115	0.001	0.010	0.000	0.011
116	0.000	0.001	0.000	0.002
117	-0.001	-0.010	0.000	-0.011
118	-0.003	-0.026	0.000	-0.029
119	-0.000	-0.002	0.000	-0.002
120	-0.000	-0.002	0.000	-0.002
121	0.007	0.115	0.000	0.122
122	0.001	0.010	0.000	0.010
123	0.000	0.003	0.000	0.003
124	-0.001	-0.010	0.000	-0.011
125	-0.003	-0.024	0.000	-0.027
126	-0.000	-0.002	0.000	-0.002
127	-0.000	0.001	0.000	0.001
128	0.006	0.105	0.000	0.111
129	0.001	0.009	0.000	0.010
130	0.000	0.004	0.000	0.004

131	-0.001	-0.009	0.000	-0.010
132	-0.003	-0.024	0.000	-0.027
133	-0.000	-0.002	0.000	-0.002
134	-0.000	-0.002	0.000	-0.002
135	0.006	0.097	0.000	0.102
136	0.001	0.009	0.000	0.010
137	0.000	0.004	0.000	0.005
138	-0.001	-0.010	0.000	-0.011
139	-0.003	-0.026	0.000	-0.029
140	-0.000	-0.002	0.000	-0.002
141	-0.000	-0.003	0.000	-0.004
142	0.006	0.105	0.000	0.111
143	0.001	0.010	0.000	0.010
144	0.000	0.002	0.000	0.003
145	0.000	0.005	0.000	0.006
146	-0.000	0.000	-0.000	0.000
147	0.000	0.004	0.000	0.004
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tot	0.001	0.513	-0.000	0.514

CHARGE: cpu time 0.5235: real time 0.5252

FORLOC: cpu time 0.0200: real time 0.0201

FORNL : cpu time 2.0384: real time 2.0448

STRESS: cpu time 6.0970: real time 6.1160

FORCOR: cpu time 0.1398: real time 0.1402

FORHAR: cpu time 0.0333: real time 0.0333

MIXING: cpu time 0.0111: real time 0.0112

OFIELD: cpu time 0.0001: real time 0.0001

DFTD3 V3.0 Rev 1

Edisp (eV) -6.61770

E6 (eV) : -3.9313

E8 (eV) : -2.6864

% E8 : 40.59

FORVDW: cpu time 1.7972: real time 1.8472

FORCE on cell =-STRESS in cart. coord. units (eV):

Direction	XX	YY	ZZ	XY	YZ	ZX
Alpha Z	233.50077	233.50077	233.50077			
Ewald	107584.52914	23479.74489	-39732.34816	9.13457	3452.92080	128.52653

Hartree	106100.37983	25036.38731	-23799.03742	-6.90535	2946.17447	93.24988
E(xc)	-1914.21384	-1916.57416	-1979.87604	0.12990	1.82079	0.13116
Local	**********	-53965.01629	57025.20455	1.05127	-6357.24027	-218.37047
n-local	-472.61689	-482.35104	-439.55293	-0.66624	-0.65189	-0.31204
augment	-38.30400	-38.57162	-34.33035	0.01319	-0.98585	-0.00019
Kinetic	7634.96845	7638.89241	8713.84728	-3.06602	-41.67713	-3.21174
Fock	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
vdW	-2.64076	-1.49092	-6.59328	0.00117	-0.07441	0.01175
Total	-17.73860	-15.47866	-19.18559	-0.30749	0.28651	0.02489
in kB	-4.89152	-4.26833	-5.29053	-0.08479	0.07901	0.00686

external pressure = -4.82 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

energy-cutoff : 400.00

volume of cell : 5810.14

direct lattice vectors			reciprocal lattice vectors		
14.780600000	0.000000000	0.000000000	0.067656252	0.000000000	0.000000000
0.000000000	21.333900000	0.000000000	0.000000000	0.046873755	0.000000000
0.000000000	0.000000000	18.425700000	0.000000000	0.000000000	0.054272022

length of vectors

14.780600000 21.333900000 18.425700000 0.067656252 0.046873755 0.054272022

FORCES acting on ions

electron-ion (+dipol) ewald-force non-local-force convergence-correction

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0.453E-02 0.154E+03 0.361E+02 -.303E-02 -.160E+03 -.357E+02 -.180E-02 0.566E+01 -.438E+00 -.161E-06 -.456E-06 -.498E-06

-.186E-01 0.155E+03 -.340E+02 0.162E-01 -.160E+03 0.335E+02 0.116E-02 0.565E+01 0.541E+00 0.299E-06 0.204E-06 0.191E-06

0.184E+00 0.154E+03 0.360E+02 -.184E+00 -.160E+03 -.356E+02 0.713E-05 0.565E+01 -.443E+00 0.169E-06 -.492E-06 -.334E-06

0.112E+00 0.155E+03 -.341E+02 -.988E-01 -.160E+03 0.336E+02 -.175E-01 0.565E+01 0.535E+00 0.785E-07 0.631E-07 0.385E-06

0.172E+00 0.154E+03 0.362E+02 -.173E+00 -.160E+03 -.357E+02 0.116E-02 0.566E+01 -.440E+00 0.324E-06 -.617E-06 -.495E-06

0.126E+00 0.154E+03 -.340E+02 -.108E+00 -.160E+03 0.334E+02 -.211E-01 0.565E+01 0.541E+00 -.234E-06 -.105E-06 -.109E-06

-.192E-01 0.154E+03 0.363E+02 0.180E-01 -.160E+03 -.359E+02 0.159E-02 0.566E+01 -

.431E+00 0.195E-06 -.713E-06 -.822E-06

-.128E-01 0.154E+03 -.338E+02 0.197E-01 -.160E+03 0.332E+02 -.721E-02 0.565E+01 0.555E+00 -.277E-06 -.159E-06 -.817E-06

-.182E+00 0.154E+03 0.363E+02 0.182E+00 -.160E+03 -.359E+02 0.256E-03 0.566E+01 -.429E+00 -.166E-06 -.692E-06 -.969E-06

-.128E+00 0.155E+03 -.337E+02 0.115E+00 -.160E+03 0.331E+02 0.109E-01 0.565E+01 0.561E+00 -.556E-07 -.143E-07 -.102E-05

-.174E+00 0.154E+03 0.362E+02 0.176E+00 -.160E+03 -.358E+02 -.176E-02 0.566E+01 -.432E+00 -.361E-06 -.550E-06 -.801E-06

-.115E+00 0.155E+03 -.338E+02 0.959E-01 -.160E+03 0.332E+02 0.192E-01 0.565E+01 0.555E+00 0.190E-06 0.172E-06 -.514E-06

0.228E+01 -.150E+03 -.387E+02 -.227E+01 0.156E+03 0.386E+02 -.103E-01 -.566E+01 0.766E-01 -.344E-06 0.928E-06 -.685E-07

-.419E+00 -.151E+03 0.388E+02 0.420E+00 0.157E+03 -.386E+02 -.128E-02 -.567E+01 -.269E+00 0.218E-06 0.689E-06 0.951E-07

0.136E+02 -.146E+03 -.413E+02 -.138E+02 0.151E+03 0.413E+02 0.257E+00 -.567E+01 -.348E-01 0.703E-07 0.550E-06 -.917E-08

0.162E+01 -.151E+03 0.402E+02 -.162E+01 0.156E+03 -.400E+02 -.101E-02 -.567E+01 -.229E+00 -.238E-06 0.477E-06 -.572E-06

0.353E+01 -.149E+03 0.443E+02 -.352E+01 0.155E+03 -.441E+02 -.204E-02 -.567E+01 -.180E+00 -.440E-06 0.345E-06 -.267E-06

-.149E+02 -.146E+03 -.330E+02 0.150E+02 0.151E+03 0.330E+02 -.958E-01 -.566E+01

0.469E-01 -.996E-06 0.517E-06 -.430E-07

-.297E+01 -.149E+03 0.432E+02 0.296E+01 0.155E+03 -.430E+02 0.115E-01 -.567E+01 -.241E+00 0.196E-06 0.494E-06 0.124E-05

-.380E+01 -.150E+03 -.385E+02 0.380E+01 0.156E+03 0.385E+02 -.609E-02 -.566E+01 0.238E-01 -.132E-06 0.884E-06 -.319E-06

-.208E+01 -.151E+03 0.395E+02 0.208E+01 0.156E+03 -.392E+02 0.149E-02 -.566E+01 -.282E+00 0.476E-06 0.668E-06 0.927E-06

0.820E-02 -.148E+03 0.486E+02 -.675E-03 0.154E+03 -.484E+02 -.548E-02 -.570E+01 -.158E+00 -.267E-06 0.404E-06 0.767E-06

0.196E+02 -.103E+03 0.222E+02 -.212E+02 0.103E+03 -.246E+02 0.153E+01 0.138E+00 0.238E+01 0.497E-06 0.628E-06 -.301E-06

-.191E+02 -.103E+03 0.154E+02 0.215E+02 0.103E+03 -.169E+02 -.241E+01 -.120E+00 0.152E+01 0.656E-06 0.495E-06 0.608E-06

0.710E-01 0.461E+03 0.202E+03 -.743E-01 -.462E+03 -.201E+03 0.384E-02 0.102E+01 -.219E+00 -.643E-06 -.313E-06 -.123E-05

0.212E+00 0.353E+03 -.234E+03 -.212E+00 -.353E+03 0.234E+03 0.260E-02 0.443E+00 -.371E-01 0.456E-06 0.731E-07 0.230E-05

-.254E-01 0.351E+03 0.240E+03 0.240E-01 -.351E+03 -.241E+03 0.316E-02 0.408E+00 0.565E-01 -.984E-06 -.786E-08 -.161E-05

-.173E+00 0.462E+03 -.195E+03 0.180E+00 -.463E+03 0.195E+03 -.662E-02 0.105E+01 0.233E+00 0.105E-05 0.133E-05 0.157E-05

-.623E-01 0.210E+03 -.272E+03 0.663E-01 -.210E+03 0.272E+03 -.446E-02 0.942E-01

0.560E-01 0.278E-06 -.110E-05 0.168E-05

0.562E+00 0.461E+03 0.202E+03 -.565E+00 -.462E+03 -.201E+03 0.201E-02 0.102E+01 -.214E+00 0.529E-06 -.421E-06 -.639E-06

0.106E+01 0.352E+03 -.234E+03 -.107E+01 -.353E+03 0.234E+03 0.160E-01 0.449E+00 -.425E-01 -.500E-06 -.579E-07 0.151E-05

0.413E+00 0.351E+03 0.240E+03 -.415E+00 -.351E+03 -.240E+03 0.303E-02 0.408E+00 0.493E-01 -.815E-07 0.126E-06 -.495E-06

0.578E+00 0.462E+03 -.195E+03 -.584E+00 -.463E+03 0.195E+03 0.480E-02 0.105E+01 0.235E+00 0.217E-07 0.646E-06 0.221E-05

0.690E+00 0.210E+03 -.272E+03 -.695E+00 -.210E+03 0.272E+03 0.609E-02 0.919E-01 0.617E-01 -.397E-06 -.848E-06 0.113E-05

0.426E+00 0.461E+03 0.202E+03 -.429E+00 -.462E+03 -.202E+03 0.383E-02 0.102E+01 -.213E+00 0.111E-05 -.879E-06 -.157E-05

0.939E+00 0.352E+03 -.233E+03 -.955E+00 -.352E+03 0.233E+03 0.151E-01 0.442E+00 -.377E-01 -.116E-05 0.579E-06 -.787E-06

0.479E+00 0.351E+03 0.241E+03 -.481E+00 -.351E+03 -.241E+03 0.249E-02 0.406E+00 0.513E-01 0.834E-06 -.147E-06 -.714E-06

0.705E+00 0.462E+03 -.194E+03 -.716E+00 -.463E+03 0.194E+03 0.784E-02 0.106E+01 0.242E+00 -.112E-05 0.733E-06 0.235E-06

0.725E+00 0.210E+03 -.271E+03 -.734E+00 -.210E+03 0.271E+03 0.655E-02 0.918E-01 0.592E-01 -.671E-06 0.130E-06 -.222E-06

-.181E+00 0.461E+03 0.202E+03 0.178E+00 -.462E+03 -.202E+03 0.448E-02 0.102E+01 -

.218E+00 0.731E-06 -.130E-05 -.308E-05

-.294E+00 0.352E+03 -.233E+03 0.298E+00 -.352E+03 0.233E+03 -.212E-02 0.441E+00 -.300E-01 -.323E-06 0.158E-05 -.231E-05

0.409E-01 0.351E+03 0.241E+03 -.399E-01 -.351E+03 -.241E+03 0.222E-02 0.410E+00 0.559E-01 0.965E-06 -.566E-06 -.208E-05

0.504E-01 0.462E+03 -.194E+03 -.565E-01 -.463E+03 0.194E+03 0.394E-02 0.106E+01 0.232E+00 -.809E-06 0.148E-05 -.231E-05

-.477E-01 0.210E+03 -.271E+03 0.457E-01 -.210E+03 0.271E+03 -.272E-03 0.940E-01 0.323E-01 -.354E-07 0.800E-06 -.107E-05

-.552E+00 0.461E+03 0.202E+03 0.550E+00 -.462E+03 -.202E+03 0.768E-03 0.102E+01 -.220E+00 -.493E-06 -.124E-05 -.361E-05

-.119E+01 0.352E+03 -.233E+03 0.120E+01 -.353E+03 0.233E+03 -.162E-01 0.448E+00 -.331E-01 0.606E-06 0.140E-05 -.174E-05

-.352E+00 0.351E+03 0.241E+03 0.349E+00 -.351E+03 -.241E+03 0.206E-02 0.414E+00 0.625E-01 0.140E-06 -.768E-06 -.317E-05

-.412E+00 0.462E+03 -.194E+03 0.426E+00 -.463E+03 0.194E+03 -.115E-01 0.106E+01 0.230E+00 0.219E-07 0.217E-05 -.299E-05

-.561E+00 0.210E+03 -.271E+03 0.566E+00 -.210E+03 0.271E+03 -.943E-02 0.922E-01 0.525E-01 0.261E-06 0.661E-06 -.679E-06

-.475E+00 0.461E+03 0.202E+03 0.475E+00 -.462E+03 -.202E+03 0.308E-02 0.102E+01 -.220E+00 -.125E-05 -.710E-06 -.265E-05

-.806E+00 0.353E+03 -.234E+03 0.820E+00 -.353E+03 0.234E+03 -.149E-01 0.448E+00 -

.393E-01 0.873E-06 0.683E-06 0.579E-06

-.374E+00 0.351E+03 0.241E+03 0.369E+00 -.351E+03 -.241E+03 0.975E-03 0.411E+00 0.627E-01 -.872E-06 -.472E-06 -.292E-05

-.595E+00 0.462E+03 -.194E+03 0.608E+00 -.463E+03 0.194E+03 -.170E-01 0.105E+01 0.234E+00 0.907E-06 0.205E-05 -.110E-05

-.588E+00 0.210E+03 -.272E+03 0.599E+00 -.210E+03 0.272E+03 -.102E-01 0.999E-01 0.567E-01 0.566E-06 -.334E-06 0.698E-06

-.960E-02 0.206E+03 0.279E+03 0.130E-01 -.206E+03 -.279E+03 -.361E-02 0.689E-01 -.410E-01 -.722E-06 0.308E-06 -.124E-05

0.667E+00 0.303E+02 0.296E+03 -.662E+00 -.302E+02 -.296E+03 -.469E-02 -.408E-01 0.770E-02 -.937E-07 0.502E-06 -.129E-05

-.846E+00 0.144E+03 -.282E+03 0.848E+00 -.144E+03 0.282E+03 -.317E-02 0.137E+00 0.286E-01 0.346E-06 -.106E-05 0.102E-05

0.534E+00 -.215E+02 -.285E+03 -.534E+00 0.214E+02 0.285E+03 -.779E-03 0.392E-01 0.185E-01 0.334E-07 -.125E-05 -.240E-06

0.496E+00 -.294E+02 0.293E+03 -.493E+00 0.294E+02 -.293E+03 -.555E-02 0.256E-01 -.301E-01 0.259E-06 0.102E-06 -.106E-05

0.524E+00 0.139E+03 0.289E+03 -.524E+00 -.139E+03 -.289E+03 0.179E-02 0.104E+00 -.247E-01 -.428E-06 0.680E-06 -.913E-06

-.127E+01 0.364E+02 -.287E+03 0.127E+01 -.364E+02 0.287E+03 -.405E-04 -.696E-02 0.137E-01 -.219E-06 -.112E-05 0.152E-06

0.167E+01 -.130E+03 -.271E+03 -.169E+01 0.130E+03 0.271E+03 0.107E-01 -.876E-01

0.371E-01 -.133E-06 -.790E-06 -.658E-06

0.397E+00 0.207E+03 0.280E+03 -.395E+00 -.207E+03 -.280E+03 0.706E-03 0.698E-01 -.369E-01 -.173E-06 0.664E-06 -.496E-06

0.921E+00 0.312E+02 0.296E+03 -.924E+00 -.311E+02 -.296E+03 0.225E-02 -.408E-01 0.124E-01 -.112E-06 0.606E-06 -.109E-05

0.133E+01 0.144E+03 -.282E+03 -.133E+01 -.144E+03 0.282E+03 0.504E-02 0.127E+00 0.279E-01 0.511E-07 -.133E-05 0.115E-05

0.342E+01 -.199E+02 -.285E+03 -.343E+01 0.199E+02 0.285E+03 0.136E-01 0.420E-01 0.134E-01 0.464E-06 -.105E-05 0.189E-07

0.139E+01 -.287E+02 0.294E+03 -.139E+01 0.287E+02 -.294E+03 -.349E-02 0.254E-01 -.305E-01 -.626E-07 0.680E-06 -.164E-05

0.678E+00 0.139E+03 0.290E+03 -.679E+00 -.139E+03 -.290E+03 0.612E-03 0.103E+00 -.294E-01 0.165E-06 0.751E-06 -.536E-06

0.160E+01 0.367E+02 -.287E+03 -.159E+01 -.367E+02 0.287E+03 -.128E-01 -.199E-01 0.127E-01 0.358E-06 -.129E-05 0.144E-06

0.612E+01 -.125E+03 -.271E+03 -.614E+01 0.125E+03 0.271E+03 0.222E-01 -.888E-01 0.146E-01 0.399E-06 -.101E-05 -.155E-06

0.368E+00 0.207E+03 0.280E+03 -.373E+00 -.207E+03 -.280E+03 0.104E-03 0.687E-01 -.364E-01 0.580E-06 0.301E-06 -.553E-06

-.353E-01 0.319E+02 0.296E+03 0.266E-01 -.319E+02 -.296E+03 0.106E-01 -.360E-01 0.141E-01 -.327E-07 -.294E-06 -.401E-06

0.210E+01 0.144E+03 -.281E+03 -.211E+01 -.144E+03 0.281E+03 0.121E-01 0.121E+00

0.238E-01 -.355E-06 -.447E-06 0.420E-06

0.303E+01 -.172E+02 -.283E+03 -.306E+01 0.171E+02 0.283E+03 0.249E-01 0.890E-01 0.599E-01 0.628E-06 -.112E-06 0.488E-06

0.106E+01 -.272E+02 0.294E+03 -.106E+01 0.272E+02 -.294E+03 0.289E-02 0.245E-01 -.374E-01 -.406E-06 0.170E-06 -.857E-06

0.977E-01 0.140E+03 0.290E+03 -.992E-01 -.140E+03 -.290E+03 0.130E-02 0.107E+00 -.230E-01 0.553E-06 0.153E-07 -.740E-06

0.277E+01 0.387E+02 -.286E+03 -.277E+01 -.387E+02 0.286E+03 0.157E-02 -.994E-02 0.288E-01 -.875E-07 -.795E-06 0.283E-06

0.596E+01 -.115E+03 -.267E+03 -.612E+01 0.115E+03 0.267E+03 0.156E+00 0.446E-02 0.129E+00 0.441E-06 -.136E-05 0.477E-06

-.242E+00 0.207E+03 0.280E+03 0.239E+00 -.207E+03 -.280E+03 0.439E-02 0.719E-01 -.385E-01 0.696E-06 -.402E-06 -.134E-05

-.114E+01 0.314E+02 0.294E+03 0.113E+01 -.314E+02 -.294E+03 0.921E-02 -.309E-01 0.565E-02 0.102E-06 -.117E-05 0.762E-07

0.595E+00 0.144E+03 -.281E+03 -.612E+00 -.144E+03 0.281E+03 0.178E-01 0.127E+00 0.438E-01 0.316E-07 0.522E-06 -.359E-06

-.939E+00 -.159E+02 -.286E+03 0.931E+00 0.158E+02 0.286E+03 0.587E-02 0.929E-01 0.798E-01 0.316E-06 0.201E-06 0.656E-06

-.640E+00 -.265E+02 0.293E+03 0.636E+00 0.265E+02 -.293E+03 0.494E-02 0.236E-01 -.268E-01 -.254E-06 -.901E-06 0.340E-06

-.534E+00 0.139E+03 0.289E+03 0.529E+00 -.139E+03 -.289E+03 0.656E-02 0.114E+00 -

.212E-01 0.431E-06 -.717E-06 -.120E-05

0.779E+00 0.408E+02 -.287E+03 -.791E+00 -.408E+02 0.287E+03 0.514E-02 0.296E-02 -.191E-01 0.354E-06 0.124E-06 0.372E-06

-.459E+00 -.113E+03 -.276E+03 0.425E+00 0.113E+03 0.277E+03 0.348E-01 0.629E-01 -.268E+00 0.437E-06 0.631E-06 0.713E-06

-.572E+00 0.206E+03 0.279E+03 0.570E+00 -.206E+03 -.279E+03 0.115E-02 0.724E-01 -.454E-01 0.223E-06 -.772E-06 -.205E-05

-.785E+00 0.304E+02 0.294E+03 0.788E+00 -.304E+02 -.294E+03 -.756E-02 -.306E-01 -.118E-02 0.129E-06 -.127E-05 -.886E-07

-.123E+01 0.144E+03 -.281E+03 0.125E+01 -.145E+03 0.281E+03 -.158E-01 0.123E+00 0.504E-01 -.154E-06 0.875E-06 -.546E-06

-.366E+01 -.174E+02 -.283E+03 0.369E+01 0.173E+02 0.283E+03 -.313E-01 0.118E+00 0.578E-01 -.902E-06 0.193E-06 0.391E-06

-.130E+01 -.277E+02 0.291E+03 0.129E+01 0.277E+02 -.291E+03 -.131E-02 0.343E-01 -.217E-01 0.135E-06 -.143E-05 0.864E-06

-.348E+00 0.139E+03 0.289E+03 0.347E+00 -.139E+03 -.289E+03 0.661E-05 0.112E+00 -.145E-01 -.114E-06 -.785E-06 -.151E-05

-.830E+00 0.400E+02 -.287E+03 0.822E+00 -.400E+02 0.287E+03 0.125E-01 -.664E-02 -.183E-01 -.233E-06 0.340E-06 0.249E-06

-.786E+01 -.119E+03 -.267E+03 0.806E+01 0.119E+03 0.267E+03 -.193E+00 0.627E-02 0.339E-01 -.689E-06 -.109E-05 0.318E-06

-.410E+00 0.206E+03 0.279E+03 0.411E+00 -.206E+03 -.279E+03 -.280E-02 0.718E-01 -

.463E-01 -.621E-06 -.413E-06 -.199E-05

-.658E-01 0.300E+02 0.294E+03 0.756E-01 -.299E+02 -.294E+03 -.950E-02 -.345E-01 0.141E-02 0.176E-08 -.439E-06 -.756E-06

-.206E+01 0.145E+03 -.282E+03 0.208E+01 -.145E+03 0.282E+03 -.190E-01 0.133E+00 0.255E-01 0.830E-07 0.284E-07 0.142E-06

-.257E+01 -.208E+02 -.285E+03 0.259E+01 0.208E+02 0.285E+03 -.291E-01 0.414E-01 0.316E-01 -.519E-06 -.846E-06 0.450E-08

-.556E+00 -.290E+02 0.291E+03 0.561E+00 0.290E+02 -.291E+03 -.287E-02 0.294E-01 -.248E-01 0.321E-06 -.984E-06 0.200E-06

0.577E-01 0.139E+03 0.289E+03 -.578E-01 -.139E+03 -.289E+03 -.343E-03 0.109E+00 -.207E-01 -.595E-06 -.493E-07 -.137E-05

-.290E+01 0.378E+02 -.286E+03 0.291E+01 -.378E+02 0.286E+03 -.151E-01 -.277E-02 0.206E-01 -.197E-06 -.408E-06 0.233E-06

-.514E+01 -.128E+03 -.271E+03 0.519E+01 0.128E+03 0.271E+03 -.466E-01 -.858E-01 0.375E-01 -.475E-06 -.668E-06 -.207E-06

0.394E+00 -.137E+03 0.280E+03 -.386E+00 0.137E+03 -.280E+03 -.972E-02 -.127E+00 -.154E-01 0.767E-06 -.117E-06 -.905E-06

0.193E+01 -.343E+03 0.233E+03 -.194E+01 0.344E+03 -.233E+03 0.913E-02 -.460E+00 -.543E-01 0.478E-06 0.111E-05 -.183E-05

-.253E+01 -.197E+03 -.259E+03 0.254E+01 0.197E+03 0.259E+03 -.963E-02 -.197E+00 0.367E-01 -.668E-06 -.563E-06 -.580E-06

0.691E+01 -.447E+03 -.198E+03 -.693E+01 0.448E+03 0.198E+03 0.985E-02 -.112E+01

0.872E-01 -.926E-06 0.121E-05 -.326E-06

-.476E+00 -.451E+03 0.204E+03 0.477E+00 0.452E+03 -.204E+03 -.207E-02 -.108E+01 -.112E+00 0.107E-05 0.216E-05 -.974E-07

0.171E+01 -.203E+03 0.269E+03 -.170E+01 0.203E+03 -.269E+03 -.481E-02 -.925E-01 -.317E-01 0.458E-06 0.206E-06 -.188E-05

-.211E+01 -.338E+03 -.222E+03 0.216E+01 0.338E+03 0.222E+03 -.444E-01 -.603E+00 0.535E-01 -.995E-06 -.178E-07 -.454E-06

0.218E+01 -.136E+03 0.282E+03 -.218E+01 0.136E+03 -.282E+03 -.638E-02 -.126E+00 -.917E-02 -.993E-07 0.254E-06 -.220E-05

0.672E+01 -.339E+03 0.238E+03 -.671E+01 0.340E+03 -.238E+03 -.128E-01 -.461E+00 -.456E-01 -.987E-06 0.630E-06 -.231E-05

0.679E+01 -.193E+03 -.259E+03 -.680E+01 0.193E+03 0.258E+03 0.114E-01 -.145E+00 0.633E-01 0.494E-06 -.107E-05 -.542E-06

0.313E+02 -.427E+03 -.198E+03 -.313E+02 0.428E+03 0.197E+03 0.734E-01 -.972E+00 0.136E+00 0.499E-06 0.360E-06 -.136E-06

0.544E+01 -.449E+03 0.209E+03 -.544E+01 0.450E+03 -.209E+03 0.549E-03 -.108E+01 -.795E-01 -.542E-06 0.169E-05 -.253E-05

0.369E+01 -.201E+03 0.272E+03 -.369E+01 0.201E+03 -.272E+03 -.758E-03 -.975E-01 -.303E-01 -.688E-06 0.471E-07 -.206E-05

0.124E+02 -.332E+03 -.223E+03 -.125E+02 0.332E+03 0.223E+03 0.121E+00 -.534E+00 0.312E-01 0.383E-06 -.679E-06 -.275E-06

0.219E+01 -.133E+03 0.283E+03 -.220E+01 0.133E+03 -.283E+03 0.543E-03 -.128E+00 -

.417E-02 -.865E-06 -.193E-06 -.103E-05

0.494E+01 -.332E+03 0.245E+03 -.491E+01 0.332E+03 -.245E+03 -.319E-01 -.476E+00 -.372E-01 -.142E-05 0.383E-07 0.660E-06

0.112E+02 -.182E+03 -.258E+03 -.113E+02 0.182E+03 0.258E+03 0.481E-01 -.984E-01 -.104E+00 0.688E-06 -.156E-05 0.101E-06

0.319E+02 -.399E+03 -.175E+03 -.322E+02 0.401E+03 0.174E+03 0.307E+00 -.143E+01 0.131E+01 0.332E-05 0.338E-05 0.587E-06

0.931E+01 -.443E+03 0.219E+03 -.931E+01 0.444E+03 -.219E+03 -.576E-02 -.110E+01 -.483E-01 -.160E-05 0.751E-06 -.114E-05

0.170E+01 -.196E+03 0.273E+03 -.171E+01 0.197E+03 -.273E+03 0.553E-02 -.109E+00 -.508E-01 -.126E-05 -.628E-06 0.282E-06

0.172E+02 -.310E+03 -.216E+03 -.175E+02 0.310E+03 0.216E+03 0.328E+00 -.218E+00 0.122E+00 0.797E-06 0.435E-07 -.134E-06

-.103E+01 -.132E+03 0.281E+03 0.102E+01 0.132E+03 -.281E+03 0.104E-01 -.127E+00 0.458E-03 -.793E-06 -.115E-05 0.125E-05

-.511E+01 -.331E+03 0.239E+03 0.510E+01 0.332E+03 -.239E+03 0.904E-02 -.494E+00 -.412E-01 -.320E-06 -.528E-07 0.395E-05

0.160E+01 -.170E+03 -.261E+03 -.172E+01 0.169E+03 0.261E+03 0.121E+00 0.383E+00 -.836E-01 0.266E-05 -.264E-06 0.516E-06

-.644E+01 -.299E+03 -.189E+03 0.594E+01 0.294E+03 0.185E+03 0.481E+00 0.503E+01 0.370E+01 0.969E-06 0.937E-05 0.382E-05

-.600E+00 -.436E+03 0.227E+03 0.597E+00 0.437E+03 -.227E+03 0.191E-02 -.120E+01 -

.477E-01 -.125E-05 0.410E-06 0.284E-05

-.302E+01 -.197E+03 0.268E+03 0.300E+01 0.197E+03 -.268E+03 0.147E-01 -.111E+00 -.424E-01 -.345E-06 -.128E-05 0.279E-05

0.345E+01 -.280E+03 -.215E+03 -.540E+01 0.280E+03 0.214E+03 0.193E+01 0.646E+00 0.820E+00 0.621E-05 0.429E-05 0.102E-05

-.274E+01 -.134E+03 0.277E+03 0.274E+01 0.134E+03 -.277E+03 0.249E-02 -.123E+00 -.181E-01 0.139E-06 -.145E-05 0.251E-05

-.602E+01 -.338E+03 0.230E+03 0.602E+01 0.339E+03 -.230E+03 0.111E-01 -.494E+00 -.453E-01 0.829E-06 0.360E-06 0.423E-05

-.652E+01 -.171E+03 -.257E+03 0.660E+01 0.170E+03 0.257E+03 -.813E-01 0.495E+00 0.278E-01 -.217E-05 0.248E-06 0.368E-06

-.443E+02 -.422E+03 -.184E+03 0.449E+02 0.423E+03 0.183E+03 -.570E+00 -.111E+01 0.615E+00 -.312E-05 0.402E-05 -.284E-06

-.867E+01 -.441E+03 0.211E+03 0.866E+01 0.442E+03 -.211E+03 0.144E-01 -.111E+01 -.742E-01 0.487E-06 0.638E-06 0.488E-05

-.294E+01 -.201E+03 0.265E+03 0.294E+01 0.201E+03 -.265E+03 -.921E-02 -.110E+00 -.200E-01 0.603E-06 -.110E-05 0.297E-05

-.146E+02 -.290E+03 -.209E+03 0.166E+02 0.289E+03 0.209E+03 -.199E+01 0.610E+00 0.782E+00 -.525E-05 0.453E-05 0.607E-06

-.139E+01 -.136E+03 0.277E+03 0.140E+01 0.136E+03 -.277E+03 -.103E-01 -.125E+00 -.236E-01 0.820E-06 -.102E-05 0.140E-05

-.281E+01 -.343E+03 0.230E+03 0.278E+01 0.343E+03 -.230E+03 0.234E-01 -.473E+00 -

.588E-01 0.128E-05 0.101E-05 0.142E-05

-.104E+02 -.189E+03 -.258E+03 0.105E+02 0.189E+03 0.258E+03 -.780E-01 -.139E+00 -.527E-01 -.978E-06 -.115E-05 -.156E-06

-.150E+02 -.446E+03 -.196E+03 0.150E+02 0.447E+03 0.196E+03 -.700E-01 -.113E+01 0.101E+00 -.564E-06 0.178E-05 -.791E-06

-.552E+01 -.448E+03 0.204E+03 0.552E+01 0.449E+03 -.204E+03 -.501E-02 -.109E+01 -.124E+00 0.167E-05 0.163E-05 0.348E-05

-.922E+00 -.203E+03 0.267E+03 0.930E+00 0.203E+03 -.267E+03 -.914E-02 -.102E+00 -.314E-01 0.116E-05 -.356E-06 0.595E-06

-.163E+02 -.329E+03 -.218E+03 0.167E+02 0.329E+03 0.218E+03 -.362E+00 -.480E+00 0.433E-01 -.123E-05 0.114E-05 -.860E-06

-.405E+01 -.263E+03 -.192E+03 0.316E+01 0.256E+03 0.188E+03 0.968E+00 0.773E+01 0.509E+01 0.584E-08 0.310E-05 0.343E-06

0.532E+02 -.518E+03 -.137E+03 -.543E+02 0.522E+03 0.141E+03 0.106E+01 -.396E+01 -.382E+01 0.483E-05 0.256E-05 0.369E-06

-.462E+02 -.582E+03 -.447E+03 0.519E+02 0.632E+03 0.481E+03 -.576E+01 -.501E+02 -.346E+02 -.300E-05 -.172E-04 -.132E-04

0.425E+01 0.269E+02 0.228E+02 -.320E-12 -.591E-11 0.114E-11 -.430E+01 -.269E+02 -.228E+02 0.123E-05 0.957E-05 -.361E-04

POSITION			TOTAL-FORCE (eV/Angst)		
1.24575	4.02870	5.43979	0.000042	0.001049	-0.000445
1.21024	4.07581	8.43726	-0.000989	0.002667	-0.001108
3.70862	4.02890	5.43965	0.000312	0.001920	-0.001132
3.67998	4.07733	8.43690	-0.004028	-0.000363	-0.002868
6.17157	4.02854	5.43942	-0.000000	-0.000107	-0.001789
6.14482	4.08292	8.43295	-0.002822	-0.003245	-0.003154
8.63513	4.02801	5.43869	0.000784	-0.000409	-0.002036
8.60339	4.08732	8.43089	-0.000124	-0.001121	-0.002157
11.09928	4.02784	5.43885	0.000875	0.002006	-0.002744
11.06021	4.08619	8.43099	-0.001745	0.000761	-0.000585
13.56311	4.02807	5.43972	0.000331	0.001653	-0.001654
13.52141	4.08047	8.43349	0.000396	-0.002198	0.000337
2.44241	15.48073	8.85224	-0.000629	-0.005348	0.002409
0.01714	15.44624	5.32469	0.000339	0.001522	-0.001244
4.86040	15.47728	8.86623	0.001315	0.000160	-0.000193
2.48016	15.44854	5.27562	0.000369	-0.001214	-0.000572
4.94382	15.44925	5.24869	0.001823	-0.003067	0.000337
12.31531	15.48242	9.00211	-0.004208	0.001119	0.003381
9.86772	15.44556	5.34176	0.000428	-0.001034	0.000747
14.76279	15.48245	8.89951	-0.006252	-0.000631	0.005661

12.33384	15.44510	5.36128	0.001370	-0.003208	-0.001349
7.40743	15.44616	5.26463	0.002328	0.001451	0.001363
6.44846	16.34427	7.40648	-0.003594	-0.002958	-0.000796
8.60064	16.47644	7.89249	0.004495	0.003036	0.004190
1.24544	5.11881	5.35500	0.000938	0.000057	-0.002429
2.44348	5.83889	8.62292	0.002425	-0.004399	0.001207
0.01380	5.79530	5.28573	0.002090	-0.002379	0.000453
1.21063	5.16420	8.54151	0.000256	-0.000523	-0.001960
2.44351	7.27931	8.74832	-0.000081	-0.001292	-0.000146
3.70866	5.11896	5.35390	-0.000417	-0.001728	0.000360
4.90800	5.84315	8.62123	-0.001073	0.003840	-0.000739
2.47701	5.79561	5.28397	0.001455	-0.000525	-0.002626
3.67679	5.16572	8.54000	-0.000117	0.001638	-0.000104
4.90764	7.28398	8.74777	0.000665	-0.000608	0.000986
6.17184	5.11860	5.35433	0.001483	0.000279	0.000933
7.37096	5.84929	8.62094	-0.000598	0.007143	-0.002459
4.94029	5.79548	5.28340	0.000601	-0.002616	-0.001193
6.14080	5.17108	8.53715	-0.002521	0.002506	0.002383
7.37071	7.28983	8.75132	-0.001971	0.001588	0.000124
8.63543	5.11820	5.35521	0.001234	0.001226	-0.001031
9.83233	5.85166	8.62337	0.002803	0.000848	-0.001129
7.40374	5.79498	5.28512	0.003469	-0.002610	-0.001355

8.60194	5.17528	8.53759	-0.001933	-0.000474	-0.000297
9.83204	7.29110	8.75719	-0.001802	-0.002785	-0.002475
11.09930	5.11814	5.35578	-0.000863	-0.003472	-0.001325
12.29449	5.84673	8.62385	-0.000020	0.005800	-0.002208
9.86750	5.79468	5.28678	-0.000741	-0.000633	0.001536
11.06261	5.17409	8.53894	0.002722	0.002601	-0.000483
12.29428	7.28729	8.75533	-0.004545	0.001153	-0.001533
13.56278	5.11829	5.35605	0.002652	0.000418	-0.001944
14.75895	5.83988	8.62434	-0.000248	-0.002622	-0.002182
12.33118	5.79480	5.28692	-0.004504	-0.001387	0.002576
13.52535	5.16844	8.54022	-0.003478	0.003743	-0.001514
14.75917	7.28012	8.75179	0.000992	0.002541	-0.000738
0.01434	7.23830	5.19017	0.000093	-0.000213	0.000069
1.24689	9.38061	5.13160	0.000550	-0.001870	-0.000008
1.21085	7.98059	8.79588	-0.000944	-0.000421	0.001545
2.44214	10.12243	8.87141	-0.000902	0.003790	-0.005015
0.01532	10.08686	5.14049	-0.002038	-0.000134	-0.002412
1.24606	7.94244	5.15775	0.002005	-0.002598	0.000814
1.21082	9.41592	8.85782	-0.000852	0.004210	0.000179
2.44072	11.55513	8.88414	-0.006100	-0.003293	0.001630
2.47747	7.23842	5.18585	0.002796	0.002864	0.001306
3.70997	9.38055	5.12566	-0.001092	-0.003019	0.000039

3.67534	7.98360	8.79349	-0.000564	0.001132	0.000951
4.90487	10.12925	8.87518	0.000116	0.000102	0.000108
2.47867	10.08713	5.12695	-0.002262	0.001496	0.000752
3.70939	7.94242	5.15441	0.000837	-0.004008	-0.001714
3.67589	9.41970	8.85445	-0.001328	0.001763	-0.000165
4.90263	11.56506	8.89086	-0.000897	0.000900	0.000860
4.94085	7.23830	5.18552	-0.004715	0.002244	0.000822
6.17318	9.38002	5.13173	0.002004	0.002068	0.001829
6.13864	7.99044	8.79647	0.002532	-0.000160	-0.001754
7.36780	10.13760	8.89473	-0.000213	0.003379	0.000401
4.94196	10.08682	5.12700	0.004143	0.001484	-0.001170
6.17284	7.94199	5.15766	-0.000040	0.000566	0.003019
6.13939	9.42660	8.86164	0.000868	-0.000400	-0.002326
7.36410	11.57721	8.92935	-0.002356	-0.001661	0.005213
7.40426	7.23794	5.19012	0.002143	0.001760	0.001066
8.63700	9.37970	5.14543	-0.000570	0.002931	0.000948
8.60086	7.99568	8.80617	0.001019	-0.000358	-0.000927
9.83068	10.14286	8.92842	-0.002209	0.003185	-0.001468
7.40553	10.08627	5.14064	0.001235	-0.003565	0.003129
8.63637	7.94166	5.16555	0.002609	0.001788	-0.001421
8.60077	9.43254	8.88532	-0.006121	0.002174	-0.001235
9.82927	11.58244	9.00096	0.001103	0.001549	-0.000078

9.86805	7.23787	5.19489	-0.000369	0.000095	-0.000212
11.10106	9.37979	5.15156	-0.003811	-0.001043	0.000658
11.06331	7.99411	8.80818	-0.000207	-0.001424	0.000253
12.29815	10.12943	8.90340	-0.001399	-0.000916	0.001186
9.86930	10.08593	5.15631	-0.005441	-0.001447	0.001399
11.10021	7.94175	5.16862	-0.000583	-0.003076	0.001376
11.06206	9.43062	8.88839	0.004702	0.001606	0.002104
12.30255	11.56557	8.94694	0.005255	-0.000360	0.000937
12.33169	7.23799	5.19447	-0.001035	0.000245	-0.001760
13.56437	9.38021	5.14435	0.000754	0.001626	-0.000579
13.52754	7.98555	8.80171	-0.000824	-0.002427	-0.003173
14.76233	10.12320	8.88285	-0.005090	0.001335	-0.001566
12.33257	10.08637	5.15511	0.002625	0.000546	-0.001552
13.56350	7.94214	5.16485	-0.000083	-0.000886	-0.000386
13.52731	9.42040	8.86925	-0.000248	0.003163	-0.000707
14.76430	11.55727	8.90646	-0.001606	-0.001277	0.001577
0.01611	11.52516	5.16621	-0.001072	-0.002592	0.000382
1.24770	13.67535	5.22209	0.001787	-0.002593	-0.002504
1.21217	12.26335	8.89409	0.000168	-0.000503	0.001209
2.43998	14.38728	8.86748	-0.002605	0.001981	0.000866
0.01699	14.35408	5.27295	-0.000380	-0.000339	-0.001993
1.24794	12.22963	5.17275	0.001066	0.000835	-0.001384

1.21434	13.70818	8.88771	0.002263	0.001354	0.003913
2.47958	11.52580	5.14547	-0.001609	-0.000230	-0.001483
3.71218	13.67636	5.19535	0.004778	0.000286	0.001019
3.66932	12.26248	8.88184	-0.001731	-0.000194	-0.000636
4.89370	14.38589	8.86075	0.005115	-0.000097	-0.002575
2.48000	14.35596	5.23149	0.001263	-0.000843	0.001690
3.71150	12.23022	5.15602	0.000897	-0.004557	0.000991
3.66212	13.70366	8.87117	-0.005489	0.003219	-0.000485
4.94290	11.52542	5.14351	-0.000079	-0.001823	-0.001611
6.17627	13.67505	5.20032	0.000855	0.000270	0.000026
6.13145	12.27911	8.90591	0.005983	0.006745	0.004668
7.36614	14.42967	8.88203	0.005256	0.002866	0.001472
4.94347	14.35627	5.21375	0.000009	-0.001573	0.000949
6.17493	12.22917	5.16623	-0.001446	-0.001033	0.001552
6.11879	13.72336	8.87765	0.004547	-0.001919	-0.001448
7.40625	11.52413	5.16368	0.000904	-0.003410	0.000343
8.63876	13.67323	5.24377	0.001722	0.001783	-0.001332
8.58939	12.29067	9.00208	0.002885	0.003884	0.003505
9.83855	14.39048	9.30305	-0.012399	-0.277034	-0.204616
7.40672	14.35386	5.23530	-0.001177	0.000142	-0.000822
8.63820	12.22778	5.19800	0.000297	-0.001296	0.001065
8.55571	13.73596	9.04598	-0.016493	-0.022572	-0.012501

9.86985	11.52338	5.18893	0.001747	-0.002042	-0.000109
11.10099	13.67352	5.27669	0.003296	-0.001125	-0.000979
11.07378	12.27333	9.00891	-0.007305	0.007162	0.001371
12.30694	14.38896	9.00333	-0.005488	0.000172	0.001699
9.86934	14.35300	5.29564	0.002910	0.000345	0.000155
11.10161	12.22804	5.21650	-0.001082	-0.002781	0.001049
11.11464	13.70636	9.07877	0.023956	-0.020418	-0.015110
12.33326	11.52411	5.18815	-0.000925	0.000244	0.000520
13.56430	13.67399	5.25995	0.001528	-0.000302	0.000068
13.53626	12.26601	8.93587	-0.003164	0.004520	0.002335
14.76266	14.38906	8.90426	-0.004927	0.002691	0.003417
12.33397	14.35288	5.30710	0.002823	-0.001532	-0.001747
13.56505	12.22870	5.20105	0.000141	0.000086	-0.001160
13.54921	13.70690	8.94399	0.000378	-0.006527	0.000746
9.91126	15.53185	9.97972	0.085178	0.886225	0.686340
7.28864	16.40884	8.69813	-0.003087	0.000137	0.000960
10.02526	16.50365	10.64498	-0.064465	-0.580825	-0.449644

---

total drift:	-0.044807	0.025133	-0.021448

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

---

free energy TOTEN = -1209.38408620 eV

energy without entropy= -1209.38408620 energy(sigma->0) = -1209.38408620

d Force =-0.1616872E-03[-0.206E-01, 0.203E-01] d Energy =-0.1663951E-03 0.471E-05

d Force =-0.5670744E+01[-0.563E+01,-0.571E+01] d Ewald =-0.5670359E+01-0.386E-03

POTLOK: cpu time 0.1747: real time 0.1753

---

stress matrix after NEB project (eV)

-17.73860 -0.30749 0.02489

-0.30749 -15.47866 0.28651

0.02489 0.28651 -19.18559

FORCES: max atom, RMS 1.124150 0.110884

FORCE total and by dimension 1.344398 0.886225

Stress total and by dimension 30.375779 19.185585

Finite differences progress:

Degree of freedom: 3/ 6

Displacement: 2/ 2

Total: 6/ 12

LATTYP: Found a simple orthorhombic cell.

ALAT = 14.7806000000

B/A-ratio = 1.2466138046

C/A-ratio = 1.4433717170

Lattice vectors:

A1 = (-14.7806000000, 0.0000000000, 0.0000000000)

A2 = (0.0000000000, 0.0000000000, -18.4257000000)

A3 = (0.0000000000, -21.3339000000, 0.0000000000)

Analysis of symmetry for initial positions (statically):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The static configuration has the point symmetry C_1 .

Analysis of symmetry for dynamics (positions and initial velocities):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The dynamic configuration has the point symmetry C_1 .

Analysis of constrained symmetry for selective dynamics:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The constrained configuration has the point symmetry C_1 .

Analysis of structural, dynamic, and magnetic symmetry:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The magnetic configuration has the point symmetry C_1 .

Subroutine INISYM returns: Found 1 space group operations

(whereof 1 operations are pure point group operations),

and found 1 'primitive' translations

KPOINTS: KPT-Resolved Value to Generate K-Mesh: 0

Automatic generation of k-mesh.

Space group operators:

irot	det(A)	alpha	n_x	n_y	n_z	tau_x	tau_y	tau_z
1	1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Subroutine IBZKPT returns following result:

==========

Found 1 irreducible k-points:

Following reciprocal coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

Following cartesian coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

WAVPRE: cpu time 0.1238: real time 0.1412

FEWALD: cpu time 0.0027: real time 0.0027

ORTHCH: cpu time 1.0094: real time 1.0124

LOOP+: cpu time 189.5011: real time 190.5091

---------- Iteration 8(1) ----------

POTLOK: cpu time 0.1708: real time 0.1837

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9347: real time 1.9416

RMM-DIIS: cpu time 7.2591: real time 7.2979

ORTHCH: cpu time 0.3520: real time 0.3535

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5250: real time 0.5266

MIXING: cpu time 0.0045: real time 0.0046

LOOP: cpu time 10.2566: real time 10.3182

eigenvalue-minimisations : 1948

total energy-change (2. order) :-0.8666827E-02 (-0.1705332E+00)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7351772 magnetization 0.0542874

Broyden mixing:

rms(total) = 0.25305E-01 rms(broyden)= 0.25060E-01

rms(prec) = 0.26183E-01

weight for this iteration 100.00

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107333.84643981

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77783157

PAW double counting = 52172.17608102 -52235.08933354

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.04555585

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77504865 eV

energy without entropy = -1202.77504865 energy(sigma->0) = -1202.77504865

---------- Iteration 8(2) ----------

POTLOK: cpu time 0.1693: real time 0.1764

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9241: real time 1.9306

RMM-DIIS: cpu time 7.1355: real time 7.1713

ORTHCH: cpu time 0.3552: real time 0.3563

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5207: real time 0.5225

MIXING: cpu time 0.0048: real time 0.0048

LOOP: cpu time 10.1202: real time 10.1724

eigenvalue-minimisations : 1920

total energy-change (2. order) : 0.3763119E-02 (-0.1155641E-02)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7371129 magnetization 0.0542824

Broyden mixing:

rms(total) = 0.16508E-01 rms(broyden)= 0.16490E-01

rms(prec) = 0.17113E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3913

1.3913

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.18242975

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.77523350

PAW double counting = 52172.83012727 -52235.74238613

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.70419838

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77128553 eV

energy without entropy = -1202.77128553 energy(sigma->0) = -1202.77128553

---------- Iteration 8(3) ----------

POTLOK: cpu time 0.1650: real time 0.1932

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9229: real time 1.9292

RMM-DIIS: cpu time 7.2932: real time 7.3243

ORTHCH: cpu time 0.3521: real time 0.3532

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5220: real time 0.5237

MIXING: cpu time 0.0051: real time 0.0050

LOOP: cpu time 10.2709: real time 10.3394

eigenvalue-minimisations : 1953

total energy-change (2. order) : 0.1935985E-03 (-0.8671447E-04)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7359441 magnetization 0.0542805

Broyden mixing:

rms(total) = 0.77920E-02 rms(broyden)= 0.77861E-02

rms(prec) = 0.81280E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4432

0.7044 2.1821

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.44901308

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78437426

PAW double counting = 52173.98997359 -52236.90588047

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.44291419

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77109194 eV

energy without entropy = -1202.77109194 energy(sigma->0) = -1202.77109194

---------- Iteration 8(4) ----------

POTLOK: cpu time 0.1664: real time 0.1808

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9251: real time 1.9310

RMM-DIIS: cpu time 7.2803: real time 7.3206

ORTHCH: cpu time 0.3541: real time 0.3551

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5225: real time 0.5242

MIXING: cpu time 0.0052: real time 0.0052

LOOP: cpu time 10.2641: real time 10.3275

eigenvalue-minimisations : 1942

total energy-change (2. order) : 0.6034963E-05 (-0.1496626E-04)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7363183 magnetization 0.0542766

Broyden mixing:

rms(total) = 0.24291E-02 rms(broyden)= 0.24277E-02

rms(prec) = 0.26141E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3527

2.1983 1.0607 0.7990

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.63107490

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78389677

PAW double counting = 52174.54836216 -52237.46494781

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.25969009

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77108590 eV

energy without entropy = -1202.77108590 energy(sigma->0) = -1202.77108590

---------- Iteration 8(5) ----------

POTLOK: cpu time 0.1663: real time 0.1672

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9304: real time 1.9367

RMM-DIIS: cpu time 7.0852: real time 7.1160

ORTHCH: cpu time 0.3531: real time 0.3540

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5222: real time 0.5239

MIXING: cpu time 0.0055: real time 0.0055

LOOP: cpu time 10.0734: real time 10.1138

eigenvalue-minimisations : 1917

total energy-change (2. order) : 0.5937443E-05 (-0.1235139E-05)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7364924 magnetization 0.0542758

Broyden mixing:

rms(total) = 0.11161E-02 rms(broyden)= 0.11149E-02

rms(prec) = 0.12062E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4603

2.2627 1.9160 0.8312 0.8312

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.69686883

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78340286

PAW double counting = 52174.50475961 -52237.42137682

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.19336474

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77107996 eV

energy without entropy = -1202.77107996 energy(sigma->0) = -1202.77107996

---------- Iteration 8(6) ----------

POTLOK: cpu time 0.1656: real time 0.1874

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9245: real time 1.9312

RMM-DIIS: cpu time 6.9353: real time 6.9584

ORTHCH: cpu time 0.3517: real time 0.3529

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5210: real time 0.5226

MIXING: cpu time 0.0058: real time 0.0059

LOOP: cpu time 9.9142: real time 9.9688

eigenvalue-minimisations : 1867

total energy-change (2. order) :-0.4614099E-05 (-0.5461309E-06)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7365157 magnetization 0.0542763

Broyden mixing:

rms(total) = 0.43886E-03 rms(broyden)= 0.43818E-03

rms(prec) = 0.52734E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3598

2.4239 1.9405 0.8682 0.8682 0.6982

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.78180394

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78374752

PAW double counting = 52174.37799265 -52237.29489332

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.10849545

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77108458 eV

energy without entropy = -1202.77108458 energy(sigma->0) = -1202.77108458

---------- Iteration 8(7) ----------

POTLOK: cpu time 0.1658: real time 0.1794

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9364: real time 1.9428

RMM-DIIS: cpu time 5.9864: real time 6.0210

ORTHCH: cpu time 0.3512: real time 0.3524

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5219: real time 0.5235

MIXING: cpu time 0.0063: real time 0.0063

LOOP: cpu time 8.9785: real time 9.0359

eigenvalue-minimisations : 1623

total energy-change (2. order) :-0.4034904E-05 (-0.6103102E-07)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7364982 magnetization 0.0542757

Broyden mixing:

rms(total) = 0.21633E-03 rms(broyden)= 0.21627E-03

rms(prec) = 0.31068E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3697

2.5677 1.6954 1.5826 0.8785 0.8785 0.6158

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.81740817

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78404116

PAW double counting = 52174.33640527 -52237.25340167

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.07309317

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77108861 eV

energy without entropy = -1202.77108861 energy(sigma->0) = -1202.77108861

---------- Iteration 8(8) ----------

POTLOK: cpu time 0.1677: real time 0.1693

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9208: real time 1.9276

RMM-DIIS: cpu time 5.9946: real time 6.0301

ORTHCH: cpu time 0.3518: real time 0.3529

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5217: real time 0.5235

MIXING: cpu time 0.0065: real time 0.0065

LOOP: cpu time 8.9737: real time 9.0206

eigenvalue-minimisations : 1653

total energy-change (2. order) :-0.6054557E-05 (-0.6476519E-07)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7364875 magnetization 0.0542754

Broyden mixing:

rms(total) = 0.12765E-03 rms(broyden)= 0.12757E-03

rms(prec) = 0.21555E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3458

2.6200 2.0974 1.1577 1.1577 0.8988 0.8799 0.6094

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.85896059

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78431170

PAW double counting = 52174.28678995 -52237.20384993

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.03175377

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77109467 eV

energy without entropy = -1202.77109467 energy(sigma->0) = -1202.77109467

---------- Iteration 8(9) ----------

POTLOK: cpu time 0.1680: real time 0.1827

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9243: real time 1.9309

RMM-DIIS: cpu time 5.2808: real time 5.3055

ORTHCH: cpu time 0.3519: real time 0.3531

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5216: real time 0.5234

MIXING: cpu time 0.0069: real time 0.0068

LOOP: cpu time 8.2640: real time 8.3130

eigenvalue-minimisations : 1447

total energy-change (2. order) :-0.5858972E-05 (-0.1389906E-07)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7364957 magnetization 0.0542754

Broyden mixing:

rms(total) = 0.74072E-04 rms(broyden)= 0.74012E-04

rms(prec) = 0.14578E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4258

2.7002 2.5165 1.5157 1.5157 0.8947 0.8947 0.7557 0.6130

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.89329601

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78443403

PAW double counting = 52174.24668424 -52237.16375704

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.99753372

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77110053 eV

energy without entropy = -1202.77110053 energy(sigma->0) = -1202.77110053

---------- Iteration 8(10) ----------

POTLOK: cpu time 0.1669: real time 0.1850

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9205: real time 1.9269

RMM-DIIS: cpu time 5.5274: real time 5.5628

ORTHCH: cpu time 0.3534: real time 0.3544

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5218: real time 0.5235

MIXING: cpu time 0.0071: real time 0.0073

LOOP: cpu time 8.5077: real time 8.5704

eigenvalue-minimisations : 1514

total energy-change (2. order) :-0.9110845E-05 (-0.2879863E-07)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7365030 magnetization 0.0542751

Broyden mixing:

rms(total) = 0.64571E-04 rms(broyden)= 0.64492E-04

rms(prec) = 0.95178E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5018

3.6519 2.5625 1.9194 1.1347 1.1347 0.9832 0.7986 0.7162 0.6150

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.94414752

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78465590

PAW double counting = 52174.20702139 -52237.12411219

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.94689518

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77110964 eV

energy without entropy = -1202.77110964 energy(sigma->0) = -1202.77110964

---------- Iteration 8(11) ----------

POTLOK: cpu time 0.1622: real time 0.1939

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9202: real time 1.9264

RMM-DIIS: cpu time 5.2492: real time 5.2711

ORTHCH: cpu time 0.3544: real time 0.3555

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5217: real time 0.5235

MIXING: cpu time 0.0076: real time 0.0076

LOOP: cpu time 8.2258: real time 8.2885

eigenvalue-minimisations : 1439

total energy-change (2. order) :-0.4980837E-05 (-0.1438706E-07)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7365003 magnetization 0.0542750

Broyden mixing:

rms(total) = 0.32486E-04 rms(broyden)= 0.32463E-04

rms(prec) = 0.53014E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5527

4.2357 2.5387 1.9872 1.3381 1.3381 0.9891 0.9891 0.8100 0.6833 0.6176

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.97094552

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78479925

PAW double counting = 52174.19717616 -52237.11428249

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.92022999

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77111462 eV

energy without entropy = -1202.77111462 energy(sigma->0) = -1202.77111462

---------- Iteration 8(12) ----------

POTLOK: cpu time 0.1693: real time 0.1719

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9204: real time 1.9270

RMM-DIIS: cpu time 5.0260: real time 5.0484

ORTHCH: cpu time 0.3518: real time 0.3530

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5219: real time 0.5234

MIXING: cpu time 0.0078: real time 0.0078

LOOP: cpu time 8.0075: real time 8.0420

eigenvalue-minimisations : 1385

total energy-change (2. order) :-0.4510330E-05 (-0.6240977E-08)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7364992 magnetization 0.0542750

Broyden mixing:

rms(total) = 0.25908E-04 rms(broyden)= 0.25899E-04

rms(prec) = 0.37909E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7110

5.7014 2.6406 2.4090 1.8627 1.1257 1.1257 0.9701 0.8492 0.8492 0.6671

0.6200

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.98525759

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78485014

PAW double counting = 52174.20257913 -52237.11968784

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.90597093

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77111913 eV

energy without entropy = -1202.77111913 energy(sigma->0) = -1202.77111913

---------- Iteration 8(13) ----------

POTLOK: cpu time 0.1664: real time 0.1685

SETDIJ: cpu time 0.0099: real time 0.0099

EDDIAG: cpu time 1.9242: real time 1.9309

RMM-DIIS: cpu time 4.8412: real time 4.8557

ORTHCH: cpu time 0.3530: real time 0.3540

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5219: real time 0.5236

MIXING: cpu time 0.0080: real time 0.0080

LOOP: cpu time 7.8251: real time 7.8510

eigenvalue-minimisations : 1328

total energy-change (2. order) :-0.3746609E-05 (-0.4127137E-08)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7365016 magnetization 0.0542750

Broyden mixing:

rms(total) = 0.10946E-04 rms(broyden)= 0.10925E-04

rms(prec) = 0.18382E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7062

6.2524 2.7305 2.4638 1.8425 1.1459 1.1459 1.0078 1.0078 0.7977 0.7977

0.6209 0.6611

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.99576467

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78486582

PAW double counting = 52174.20794104 -52237.12504533

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.89548770

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77112288 eV

energy without entropy = -1202.77112288 energy(sigma->0) = -1202.77112288

---------- Iteration 8(14) ----------

POTLOK: cpu time 0.1674: real time 0.1850

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9228: real time 1.9290

RMM-DIIS: cpu time 4.6582: real time 4.6851

ORTHCH: cpu time 0.3523: real time 0.3534

DOS: cpu time 0.0004: real time 0.0003

CHARGE: cpu time 0.5213: real time 0.5230

MIXING: cpu time 0.0084: real time 0.0085

LOOP: cpu time 7.6409: real time 7.6944

eigenvalue-minimisations : 1248

total energy-change (2. order) :-0.1628337E-05 (-0.1187039E-08)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7365021 magnetization 0.0542750

Broyden mixing:

rms(total) = 0.77999E-05 rms(broyden)= 0.77958E-05

rms(prec) = 0.12749E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8027

6.9163 2.9779 2.6034 2.1046 1.8933 1.1380 1.1380 0.9828 0.8594 0.8594

0.6969 0.6239 0.6416

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.99783520

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78486574

PAW double counting = 52174.20761190 -52237.12471694

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.89341797

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77112450 eV

energy without entropy = -1202.77112450 energy(sigma->0) = -1202.77112450

---------- Iteration 8(15) ----------

POTLOK: cpu time 0.1672: real time 0.1860

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9242: real time 1.9306

RMM-DIIS: cpu time 4.6990: real time 4.7145

ORTHCH: cpu time 0.3531: real time 0.3543

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5222: real time 0.5240

MIXING: cpu time 0.0089: real time 0.0089

LOOP: cpu time 7.6850: real time 7.7289

eigenvalue-minimisations : 1250

total energy-change (2. order) :-0.1102169E-05 (-0.9883729E-09)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7365019 magnetization 0.0542750

Broyden mixing:

rms(total) = 0.53381E-05 rms(broyden)= 0.53365E-05

rms(prec) = 0.76826E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8573

7.4376 3.8432 2.6237 2.3246 1.8086 1.1291 1.1291 1.0310 1.0310 0.8514

0.8514 0.6846 0.6285 0.6285

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.99925099

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78486259

PAW double counting = 52174.20656734 -52237.12367372

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.89199880

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77112561 eV

energy without entropy = -1202.77112561 energy(sigma->0) = -1202.77112561

---------- Iteration 8(16) ----------

POTLOK: cpu time 0.1679: real time 0.1711

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9231: real time 1.9295

RMM-DIIS: cpu time 4.3071: real time 4.3203

ORTHCH: cpu time 0.3541: real time 0.3549

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5212: real time 0.5229

MIXING: cpu time 0.0094: real time 0.0095

LOOP: cpu time 7.2932: real time 7.3187

eigenvalue-minimisations : 1069

total energy-change (2. order) :-0.3068344E-06 (-0.3625598E-09)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7365017 magnetization 0.0542750

Broyden mixing:

rms(total) = 0.28531E-05 rms(broyden)= 0.28509E-05

rms(prec) = 0.44350E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8557

7.6506 4.2327 2.6012 2.3485 1.7819 1.3643 1.1862 1.1862 1.0333 0.8636

0.8636 0.7882 0.6799 0.6272 0.6272

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.99963121

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78485831

PAW double counting = 52174.20608348 -52237.12318980

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.89161465

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77112591 eV

energy without entropy = -1202.77112591 energy(sigma->0) = -1202.77112591

---------- Iteration 8(17) ----------

POTLOK: cpu time 0.1661: real time 0.1669

SETDIJ: cpu time 0.0099: real time 0.0100

EDDIAG: cpu time 1.9237: real time 1.9294

RMM-DIIS: cpu time 4.1750: real time 4.1898

ORTHCH: cpu time 0.3552: real time 0.3563

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5208: real time 0.5225

MIXING: cpu time 0.0094: real time 0.0094

LOOP: cpu time 7.1606: real time 7.1846

eigenvalue-minimisations : 996

total energy-change (2. order) :-0.1465960E-06 (-0.1535287E-09)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7365017 magnetization 0.0542750

Broyden mixing:

rms(total) = 0.19033E-05 rms(broyden)= 0.19016E-05

rms(prec) = 0.29257E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9198

7.9137 4.8137 2.6295 2.6295 2.1778 1.7832 1.1519 1.1519 1.0595 1.0595

0.8596 0.8596 0.7100 0.6642 0.6241 0.6288

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.99968499

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78485404

PAW double counting = 52174.20554231 -52237.12264815

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.89155724

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77112606 eV

energy without entropy = -1202.77112606 energy(sigma->0) = -1202.77112606

---------- Iteration 8(18) ----------

POTLOK: cpu time 0.1679: real time 0.1804

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9205: real time 1.9276

RMM-DIIS: cpu time 4.1260: real time 4.1545

ORTHCH: cpu time 0.3544: real time 0.3554

DOS: cpu time 0.0003: real time 0.0003

LOOP: cpu time 6.5791: real time 6.6283

eigenvalue-minimisations : 963

total energy-change (2. order) :-0.7541530E-07 (-0.9362644E-10)

number of electron 518.9999732 magnetization 0.9999998

augmentation part 11.7365017 magnetization 0.0542750

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91328.42168117

-Hartree energ DENC = -107334.99968340

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78485036

PAW double counting = 52174.20512007 -52237.12222572

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.89155540

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77112613 eV

energy without entropy = -1202.77112613 energy(sigma->0) = -1202.77112613

---

average (electrostatic) potential at core

the test charge radii are 0.5201 0.6991 1.0621 0.7215

(the norm of the test charge is 1.0000)

1 -40.7532	2 -40.7511	3 -40.7525	4 -40.7511	5 -40.7532
6 -40.7554	7 -40.7528	8 -40.7606	9 -40.7524	10 -40.7600
11 -40.7539	12 -40.7559	13 -40.6507	14 -40.6965	15 -40.7709
16 -40.6988	17 -40.6927	18 -40.8587	19 -40.6797	20 -40.6673
21 -40.6890	22 -40.6623	23 -40.0888	24 -40.1297	25 -57.4593
26 -57.6704	27 -57.6573	28 -57.4692	29 -57.6640	30 -57.4593
31 -57.6702	32 -57.6569	33 -57.4671	34 -57.6689	35 -57.4601
36 -57.6721	37 -57.6569	38 -57.4694	39 -57.6747	40 -57.4591
41 -57.6761	42 -57.6571	43 -57.4743	44 -57.6893	45 -57.4591
46 -57.6750	47 -57.6579	48 -57.4744	49 -57.6804	50 -57.4603
51 -57.6717	52 -57.6576	53 -57.4721	54 -57.6667	55 -57.6372
56 -57.6632	57 -57.6875	58 -57.6839	59 -57.6669	60 -57.6697
61 -57.6907	62 -57.6754	63 -57.6374	64 -57.6627	65 -57.6896
66 -57.6953	67 -57.6652	68 -57.6695	69 -57.6944	70 -57.7018
71 -57.6369	72 -57.6641	73 -57.6972	74 -57.7222	75 -57.6661
76 -57.6701	77 -57.7066	78 -57.7516	79 -57.6371	80 -57.6667

81 -57.7110	82 -57.7527	83 -57.6693	84 -57.6716	85 -57.7381
86 -57.8421	87 -57.6395	88 -57.6674	89 -57.7129	90 -57.7178
91 -57.6740	92 -57.6719	93 -57.7426	94 -57.7606	95 -57.6379
96 -57.6655	97 -57.6966	98 -57.6913	99 -57.6713	100 -57.6706
101 -57.7085	102 -57.6865	103 -57.6608	104 -57.6315	105 -57.6462
106 -57.2908	107 -57.3886	108 -57.6317	109 -57.5982	110 -57.6597
111 -57.6314	112 -57.6428	113 -57.3100	114 -57.3943	115 -57.6310
116 -57.6002	117 -57.6589	118 -57.6232	119 -57.6987	120 -57.6841
121 -57.3880	122 -57.6298	123 -57.7101	124 -57.6599	125 -57.6259
126 -57.8333	127 -58.3306	128 -57.3614	129 -57.6350	130 -58.1428
131 -57.6678	132 -57.6351	133 -57.8023	134 -57.4168	135 -57.3725
136 -57.6389	137 -58.0802	138 -57.6642	139 -57.6309	140 -57.6719
141 -57.3000	142 -57.3787	143 -57.6343	144 -57.6482	145 -60.8417
146 -57.3165	147 -81.2580			

E-fermi : -2.3169 XC(G=0): -2.7344 alpha+bet : -2.2521

spin component 1

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-26.9562	1.00000
2	-21.5691	1.00000
3	-21.4721	1.00000
4	-21.1003	1.00000
5	-21.0692	1.00000
6	-21.0153	1.00000
7	-20.9793	1.00000
8	-20.9773	1.00000
9	-20.8917	1.00000
10	-20.5584	1.00000
11	-20.5039	1.00000
12	-20.4122	1.00000
13	-20.3987	1.00000
14	-20.1270	1.00000
15	-19.9764	1.00000
16	-19.7039	1.00000
17	-19.6281	1.00000
18	-19.6002	1.00000
19	-19.5846	1.00000
20	-19.5293	1.00000

21	-19.5275	1.00000
22	-19.4993	1.00000
23	-19.4817	1.00000
24	-19.1125	1.00000
25	-19.0760	1.00000
26	-18.9791	1.00000
27	-18.9655	1.00000
28	-18.9012	1.00000
29	-18.7342	1.00000
30	-18.5053	1.00000
31	-18.3598	1.00000
32	-18.2760	1.00000
33	-18.2528	1.00000
34	-18.1842	1.00000
35	-18.1821	1.00000
36	-18.0805	1.00000
37	-18.0767	1.00000
38	-17.5622	1.00000
39	-17.3140	1.00000
40	-17.2883	1.00000
41	-17.2833	1.00000
42	-17.2106	1.00000

43	-17.2042	1.00000
44	-17.1774	1.00000
45	-17.0234	1.00000
46	-16.9509	1.00000
47	-16.9333	1.00000
48	-16.8938	1.00000
49	-16.8920	1.00000
50	-16.8507	1.00000
51	-16.8424	1.00000
52	-16.8218	1.00000
53	-16.8195	1.00000
54	-16.7300	1.00000
55	-16.7269	1.00000
56	-16.1780	1.00000
57	-15.7302	1.00000
58	-15.6928	1.00000
59	-15.6611	1.00000
60	-15.6378	1.00000
61	-15.6168	1.00000
62	-15.5544	1.00000
63	-15.5505	1.00000
64	-15.1761	1.00000

65	-14.8107	1.00000
66	-14.6091	1.00000
67	-14.5787	1.00000
68	-14.5355	1.00000
69	-14.4990	1.00000
70	-14.4693	1.00000
71	-14.4431	1.00000
72	-14.3346	1.00000
73	-14.3063	1.00000
74	-14.2804	1.00000
75	-14.2727	1.00000
76	-14.1831	1.00000
77	-14.1793	1.00000
78	-13.8912	1.00000
79	-13.7606	1.00000
80	-13.5943	1.00000
81	-13.5491	1.00000
82	-13.5301	1.00000
83	-13.4985	1.00000
84	-13.4465	1.00000
85	-13.3648	1.00000
86	-13.3462	1.00000

87	-13.1895	1.00000
88	-12.7871	1.00000
89	-12.7601	1.00000
90	-12.7279	1.00000
91	-12.6967	1.00000
92	-12.6869	1.00000
93	-12.6247	1.00000
94	-12.4618	1.00000
95	-12.4470	1.00000
96	-12.3825	1.00000
97	-12.3246	1.00000
98	-12.2137	1.00000
99	-12.2040	1.00000
100	-12.1657	1.00000
101	-11.9488	1.00000
102	-11.6851	1.00000
103	-11.6283	1.00000
104	-11.6117	1.00000
105	-11.5781	1.00000
106	-11.1006	1.00000
107	-11.0708	1.00000
108	-10.8992	1.00000

109	-10.8882	1.00000
110	-10.8324	1.00000
111	-10.7113	1.00000
112	-10.6798	1.00000
113	-10.6623	1.00000
114	-10.6472	1.00000
115	-10.5900	1.00000
116	-10.5816	1.00000
117	-10.5723	1.00000
118	-10.5685	1.00000
119	-10.5268	1.00000
120	-10.5260	1.00000
121	-10.5112	1.00000
122	-10.5034	1.00000
123	-10.3792	1.00000
124	-10.2937	1.00000
125	-10.2568	1.00000
126	-10.1882	1.00000
127	-10.1871	1.00000
128	-10.0636	1.00000
129	-10.0251	1.00000
130	-9.8911	1.00000

131	-9.8652	1.00000
132	-9.7943	1.00000
133	-9.7867	1.00000
134	-9.7549	1.00000
135	-9.6900	1.00000
136	-9.4495	1.00000
137	-9.4257	1.00000
138	-9.3956	1.00000
139	-9.3885	1.00000
140	-9.3802	1.00000
141	-9.3697	1.00000
142	-9.3108	1.00000
143	-9.3039	1.00000
144	-9.2981	1.00000
145	-9.2849	1.00000
146	-9.2704	1.00000
147	-9.0920	1.00000
148	-9.0044	1.00000
149	-8.9848	1.00000
150	-8.9577	1.00000
151	-8.9552	1.00000
152	-8.7934	1.00000

153	-8.7462	1.00000
154	-8.7350	1.00000
155	-8.7185	1.00000
156	-8.7092	1.00000
157	-8.6877	1.00000
158	-8.6784	1.00000
159	-8.6690	1.00000
160	-8.6542	1.00000
161	-8.5949	1.00000
162	-8.5835	1.00000
163	-8.5766	1.00000
164	-8.5682	1.00000
165	-8.4883	1.00000
166	-8.4573	1.00000
167	-8.4365	1.00000
168	-8.3459	1.00000
169	-8.2978	1.00000
170	-8.2749	1.00000
171	-8.2641	1.00000
172	-8.2337	1.00000
173	-8.2327	1.00000
174	-8.1521	1.00000

175	-8.1456	1.00000
176	-8.0779	1.00000
177	-8.0446	1.00000
178	-8.0266	1.00000
179	-8.0219	1.00000
180	-7.9734	1.00000
181	-7.9649	1.00000
182	-7.9249	1.00000
183	-7.9010	1.00000
184	-7.8855	1.00000
185	-7.8728	1.00000
186	-7.8012	1.00000
187	-7.7978	1.00000
188	-7.7481	1.00000
189	-7.7109	1.00000
190	-7.6665	1.00000
191	-7.6002	1.00000
192	-7.5852	1.00000
193	-7.5761	1.00000
194	-7.5477	1.00000
195	-7.4810	1.00000
196	-7.4805	1.00000

197	-7.4293	1.00000
198	-7.3249	1.00000
199	-7.2498	1.00000
200	-7.1590	1.00000
201	-7.0668	1.00000
202	-7.0422	1.00000
203	-7.0285	1.00000
204	-7.0138	1.00000
205	-6.9970	1.00000
206	-6.9901	1.00000
207	-6.9758	1.00000
208	-6.8667	1.00000
209	-6.8211	1.00000
210	-6.8020	1.00000
211	-6.7936	1.00000
212	-6.7324	1.00000
213	-6.6878	1.00000
214	-6.4713	1.00000
215	-6.4254	1.00000
216	-6.3963	1.00000
217	-6.3915	1.00000
218	-6.3744	1.00000

219	-6.3728	1.00000
220	-6.3176	1.00000
221	-6.3076	1.00000
222	-6.2372	1.00000
223	-6.2301	1.00000
224	-6.2296	1.00000
225	-6.0781	1.00000
226	-6.0379	1.00000
227	-5.7931	1.00000
228	-5.7525	1.00000
229	-5.6943	1.00000
230	-5.6416	1.00000
231	-5.6378	1.00000
232	-5.5593	1.00000
233	-5.5308	1.00000
234	-5.4682	1.00000
235	-5.4396	1.00000
236	-5.1665	1.00000
237	-5.0591	1.00000
238	-5.0510	1.00000
239	-5.0186	1.00000
240	-4.9894	1.00000

241	-4.9112	1.00000
242	-4.8540	1.00000
243	-4.8228	1.00000
244	-4.7902	1.00000
245	-4.6820	1.00000
246	-4.5730	1.00000
247	-4.5717	1.00000
248	-4.5060	1.00000
249	-4.4461	1.00000
250	-4.3842	1.00000
251	-4.2932	1.00000
252	-4.2661	1.00000
253	-4.2131	1.00000
254	-3.5595	1.00000
255	-3.3549	1.00000
256	-3.2015	1.00000
257	-2.9396	1.00000
258	-2.8487	1.00000
259	-2.8241	1.00000
260	-2.6075	1.00000
261	-1.9089	0.00000
262	-1.7685	0.00000

263	-1.7194	0.00000
264	-1.3466	0.00000
265	-1.3125	0.00000
266	-1.1949	0.00000
267	-0.7456	0.00000
268	-0.5850	0.00000
269	-0.5028	0.00000
270	-0.3083	0.00000
271	-0.3062	0.00000
272	-0.2905	0.00000
273	-0.1837	0.00000
274	-0.0584	0.00000
275	-0.0506	0.00000
276	-0.0108	0.00000
277	0.0346	0.00000
278	0.0838	0.00000
279	0.1726	0.00000
280	0.2202	0.00000
281	0.2476	0.00000
282	0.4195	0.00000
283	0.4471	0.00000
284	0.4814	0.00000

285	0.5972	0.00000
286	0.6737	0.00000
287	0.8185	0.00000
288	0.8729	0.00000
289	1.0477	0.00000
290	1.0889	0.00000
291	1.1206	0.00000
292	1.1621	0.00000
293	1.2230	0.00000
294	1.2443	0.00000
295	1.2875	0.00000
296	1.3141	0.00000
297	1.3465	0.00000
298	1.4115	0.00000
299	1.4664	0.00000
300	1.4822	0.00000
301	1.5533	0.00000
302	1.5867	0.00000
303	1.6237	0.00000
304	1.6777	0.00000
305	1.7506	0.00000
306	1.7629	0.00000

307	1.8732	0.00000
308	1.8937	0.00000
309	1.9045	0.00000
310	1.9133	0.00000
311	2.1228	0.00000
312	2.1872	0.00000
313	2.2082	0.00000
314	2.2346	0.00000
315	2.2752	0.00000
316	2.2918	0.00000
317	2.3313	0.00000
318	2.3532	0.00000
319	2.3719	0.00000
320	2.3980	0.00000
321	2.4197	0.00000
322	2.4299	0.00000
323	2.4396	0.00000
324	2.4530	0.00000
325	2.4614	0.00000
326	2.5231	0.00000
327	2.5380	0.00000
328	2.7009	0.00000

329	2.7282	0.00000
330	2.7529	0.00000
331	2.7562	0.00000
332	2.7648	0.00000
333	2.8143	0.00000
334	2.8334	0.00000
335	2.8593	0.00000
336	2.8909	0.00000
337	2.9238	0.00000
338	2.9463	0.00000
339	2.9786	0.00000
340	3.0052	0.00000
341	3.0342	0.00000
342	3.0436	0.00000
343	3.0659	0.00000
344	3.0847	0.00000
345	3.1503	0.00000
346	3.1617	0.00000
347	3.1795	0.00000
348	3.1914	0.00000
349	3.3008	0.00000
350	3.3226	0.00000

351	3.3523	0.00000
352	3.3672	0.00000
353	3.3889	0.00000
354	3.4317	0.00000
355	3.4764	0.00000
356	3.4841	0.00000
357	3.4860	0.00000
358	3.4981	0.00000
359	3.6336	0.00000
360	3.6726	0.00000
361	3.6879	0.00000
362	3.7322	0.00000
363	3.7508	0.00000
364	3.7586	0.00000
365	3.7723	0.00000
366	3.7937	0.00000
367	3.8117	0.00000
368	3.8334	0.00000
369	3.8379	0.00000
370	3.8516	0.00000
371	3.8762	0.00000
372	3.8836	0.00000

373	3.9099	0.00000
374	3.9235	0.00000
375	3.9336	0.00000
376	3.9573	0.00000
377	3.9722	0.00000
378	3.9838	0.00000
379	4.0160	0.00000
380	4.0681	0.00000
381	4.1645	0.00000
382	4.2460	0.00000
383	4.2574	0.00000
384	4.2582	0.00000
385	4.2853	0.00000
386	4.3130	0.00000
387	4.3271	0.00000
388	4.3410	0.00000
389	4.3708	0.00000
390	4.3808	0.00000
391	4.4173	0.00000
392	4.4447	0.00000
393	4.4690	0.00000
394	4.4800	0.00000

395	4.4857	0.00000
396	4.4961	0.00000
397	4.5169	0.00000
398	4.5505	0.00000
399	4.5898	0.00000
400	4.6077	0.00000
401	4.6270	0.00000
402	4.6421	0.00000
403	4.6565	0.00000
404	4.6793	0.00000
405	4.7038	0.00000
406	4.7312	0.00000
407	4.7463	0.00000
408	4.7669	0.00000
409	4.7829	0.00000
410	4.7836	0.00000
411	4.7971	0.00000
412	4.8280	0.00000
413	4.8630	0.00000
414	4.8718	0.00000
415	4.8976	0.00000
416	4.9310	0.00000

417	4.9839	0.00000
418	5.0043	0.00000
419	5.0106	0.00000
420	5.0350	0.00000
421	5.0389	0.00000
422	5.0639	0.00000
423	5.0815	0.00000
424	5.1141	0.00000
425	5.1175	0.00000
426	5.1369	0.00000
427	5.1405	0.00000
428	5.1534	0.00000
429	5.1747	0.00000
430	5.1848	0.00000
431	5.1877	0.00000
432	5.2148	0.00000
433	5.2351	0.00000
434	5.2401	0.00000
435	5.2554	0.00000
436	5.2891	0.00000
437	5.2953	0.00000
438	5.3087	0.00000

439	5.3315	0.00000
440	5.3489	0.00000
441	5.3667	0.00000
442	5.3736	0.00000
443	5.3921	0.00000
444	5.4203	0.00000
445	5.4533	0.00000
446	5.4628	0.00000
447	5.4815	0.00000
448	5.4947	0.00000
449	5.5187	0.00000
450	5.5494	0.00000
451	5.5666	0.00000
452	5.5748	0.00000
453	5.5954	0.00000
454	5.6149	0.00000
455	5.6577	0.00000
456	5.6813	0.00000
457	5.7090	0.00000
458	5.7222	0.00000
459	5.7436	0.00000
460	5.7572	0.00000

461	5.7813	0.00000
462	5.7891	0.00000
463	5.7948	0.00000
464	5.8005	0.00000
465	5.8069	0.00000
466	5.8231	0.00000
467	5.8426	0.00000
468	5.8540	0.00000
469	5.8728	0.00000
470	5.8804	0.00000
471	5.8856	0.00000
472	5.9087	0.00000
473	5.9134	0.00000
474	5.9396	0.00000
475	5.9505	0.00000
476	5.9696	0.00000
477	5.9761	0.00000
478	6.0009	0.00000
479	6.0102	0.00000
480	6.0669	0.00000

spin component 2

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-26.9495	1.00000
2	-21.5679	1.00000
3	-21.4706	1.00000
4	-21.0984	1.00000
5	-21.0683	1.00000
6	-21.0126	1.00000
7	-20.9779	1.00000
8	-20.9755	1.00000
9	-20.8811	1.00000
10	-20.5554	1.00000
11	-20.5005	1.00000
12	-20.4012	1.00000
13	-20.3890	1.00000
14	-20.1228	1.00000
15	-19.9533	1.00000
16	-19.7011	1.00000
17	-19.6269	1.00000
18	-19.5981	1.00000
19	-19.5782	1.00000

20	-19.5280	1.00000
21	-19.5257	1.00000
22	-19.4766	1.00000
23	-19.4623	1.00000
24	-19.1101	1.00000
25	-19.0736	1.00000
26	-18.9692	1.00000
27	-18.9560	1.00000
28	-18.8964	1.00000
29	-18.7045	1.00000
30	-18.5022	1.00000
31	-18.3527	1.00000
32	-18.2478	1.00000
33	-18.2276	1.00000
34	-18.1790	1.00000
35	-18.1767	1.00000
36	-18.0604	1.00000
37	-18.0571	1.00000
38	-17.5588	1.00000
39	-17.2977	1.00000
40	-17.2877	1.00000
41	-17.2740	1.00000

42	-17.2083	1.00000
43	-17.2072	1.00000
44	-17.1744	1.00000
45	-17.0195	1.00000
46	-16.9421	1.00000
47	-16.9229	1.00000
48	-16.8712	1.00000
49	-16.8702	1.00000
50	-16.8299	1.00000
51	-16.8235	1.00000
52	-16.8185	1.00000
53	-16.8160	1.00000
54	-16.7318	1.00000
55	-16.7257	1.00000
56	-16.1754	1.00000
57	-15.7294	1.00000
58	-15.6584	1.00000
59	-15.6441	1.00000
60	-15.6215	1.00000
61	-15.5673	1.00000
62	-15.5285	1.00000
63	-15.5257	1.00000

64	-15.1724	1.00000
65	-14.8085	1.00000
66	-14.6069	1.00000
67	-14.5612	1.00000
68	-14.5010	1.00000
69	-14.4992	1.00000
70	-14.4653	1.00000
71	-14.4387	1.00000
72	-14.3312	1.00000
73	-14.2986	1.00000
74	-14.2686	1.00000
75	-14.2645	1.00000
76	-14.1651	1.00000
77	-14.1617	1.00000
78	-13.8903	1.00000
79	-13.7582	1.00000
80	-13.5916	1.00000
81	-13.5385	1.00000
82	-13.5190	1.00000
83	-13.4949	1.00000
84	-13.4448	1.00000
85	-13.3443	1.00000

86	-13.3416	1.00000
87	-13.1880	1.00000
88	-12.7807	1.00000
89	-12.7506	1.00000
90	-12.7190	1.00000
91	-12.6782	1.00000
92	-12.6712	1.00000
93	-12.6225	1.00000
94	-12.4492	1.00000
95	-12.4321	1.00000
96	-12.3790	1.00000
97	-12.3237	1.00000
98	-12.2091	1.00000
99	-12.1988	1.00000
100	-12.1642	1.00000
101	-11.9460	1.00000
102	-11.6822	1.00000
103	-11.6117	1.00000
104	-11.5925	1.00000
105	-11.5710	1.00000
106	-11.0984	1.00000
107	-11.0681	1.00000

108	-10.8901	1.00000
109	-10.8777	1.00000
110	-10.8295	1.00000
111	-10.7053	1.00000
112	-10.6786	1.00000
113	-10.6593	1.00000
114	-10.6423	1.00000
115	-10.5821	1.00000
116	-10.5746	1.00000
117	-10.5695	1.00000
118	-10.5656	1.00000
119	-10.5162	1.00000
120	-10.5153	1.00000
121	-10.5021	1.00000
122	-10.4974	1.00000
123	-10.3784	1.00000
124	-10.2928	1.00000
125	-10.2559	1.00000
126	-10.1848	1.00000
127	-10.1836	1.00000
128	-10.0541	1.00000
129	-10.0175	1.00000

130	-9.8883	1.00000
131	-9.8628	1.00000
132	-9.7861	1.00000
133	-9.7777	1.00000
134	-9.7524	1.00000
135	-9.6875	1.00000
136	-9.4478	1.00000
137	-9.4223	1.00000
138	-9.3846	1.00000
139	-9.3797	1.00000
140	-9.3725	1.00000
141	-9.3601	1.00000
142	-9.3084	1.00000
143	-9.3011	1.00000
144	-9.2974	1.00000
145	-9.2836	1.00000
146	-9.2482	1.00000
147	-9.0908	1.00000
148	-9.0009	1.00000
149	-8.9787	1.00000
150	-8.9439	1.00000
151	-8.9428	1.00000

152	-8.7909	1.00000
153	-8.7382	1.00000
154	-8.7326	1.00000
155	-8.7129	1.00000
156	-8.7059	1.00000
157	-8.6706	1.00000
158	-8.6643	1.00000
159	-8.6567	1.00000
160	-8.6535	1.00000
161	-8.5776	1.00000
162	-8.5715	1.00000
163	-8.5667	1.00000
164	-8.5497	1.00000
165	-8.4879	1.00000
166	-8.4567	1.00000
167	-8.4349	1.00000
168	-8.3432	1.00000
169	-8.2947	1.00000
170	-8.2733	1.00000
171	-8.2336	1.00000
172	-8.2300	1.00000
173	-8.2279	1.00000

174	-8.1419	1.00000
175	-8.1344	1.00000
176	-8.0746	1.00000
177	-8.0425	1.00000
178	-8.0138	1.00000
179	-8.0073	1.00000
180	-7.9688	1.00000
181	-7.9599	1.00000
182	-7.9208	1.00000
183	-7.8914	1.00000
184	-7.8717	1.00000
185	-7.8640	1.00000
186	-7.7924	1.00000
187	-7.7885	1.00000
188	-7.7387	1.00000
189	-7.6794	1.00000
190	-7.6365	1.00000
191	-7.5980	1.00000
192	-7.5774	1.00000
193	-7.5551	1.00000
194	-7.5401	1.00000
195	-7.4730	1.00000

196	-7.4729	1.00000
197	-7.4282	1.00000
198	-7.3240	1.00000
199	-7.2365	1.00000
200	-7.1559	1.00000
201	-7.0561	1.00000
202	-7.0367	1.00000
203	-7.0162	1.00000
204	-6.9857	1.00000
205	-6.9779	1.00000
206	-6.9728	1.00000
207	-6.9414	1.00000
208	-6.8630	1.00000
209	-6.8168	1.00000
210	-6.7959	1.00000
211	-6.7884	1.00000
212	-6.7257	1.00000
213	-6.6784	1.00000
214	-6.4681	1.00000
215	-6.3955	1.00000
216	-6.3832	1.00000
217	-6.3788	1.00000

218	-6.3635	1.00000
219	-6.3389	1.00000
220	-6.3038	1.00000
221	-6.2761	1.00000
222	-6.2299	1.00000
223	-6.2285	1.00000
224	-6.2229	1.00000
225	-6.0474	1.00000
226	-6.0094	1.00000
227	-5.7568	1.00000
228	-5.7118	1.00000
229	-5.6926	1.00000
230	-5.6361	1.00000
231	-5.6234	1.00000
232	-5.5444	1.00000
233	-5.5237	1.00000
234	-5.4418	1.00000
235	-5.4122	1.00000
236	-5.1445	1.00000
237	-5.0605	1.00000
238	-5.0266	1.00000
239	-5.0229	1.00000

240	-4.9599	1.00000
241	-4.8784	1.00000
242	-4.8548	1.00000
243	-4.8032	1.00000
244	-4.7782	1.00000
245	-4.6516	1.00000
246	-4.5792	1.00000
247	-4.5761	1.00000
248	-4.4761	1.00000
249	-4.4218	1.00000
250	-4.3954	1.00000
251	-4.2970	1.00000
252	-4.2273	1.00000
253	-4.1757	1.00000
254	-3.5332	1.00000
255	-3.3095	1.00000
256	-3.1421	1.00000
257	-2.9446	1.00000
258	-2.7996	1.00000
259	-2.7406	1.00000
260	-2.0613	0.00000
261	-1.9149	0.00000

262	-1.7233	0.00000
263	-1.6795	0.00000
264	-1.3007	0.00000
265	-1.2815	0.00000
266	-1.1598	0.00000
267	-0.7242	0.00000
268	-0.5844	0.00000
269	-0.5103	0.00000
270	-0.2812	0.00000
271	-0.2781	0.00000
272	-0.2604	0.00000
273	-0.1570	0.00000
274	-0.0586	0.00000
275	-0.0487	0.00000
276	0.0127	0.00000
277	0.0396	0.00000
278	0.0787	0.00000
279	0.2077	0.00000
280	0.2553	0.00000
281	0.2792	0.00000
282	0.4331	0.00000
283	0.4515	0.00000

284	0.4827	0.00000
285	0.6019	0.00000
286	0.6941	0.00000
287	0.8213	0.00000
288	0.8796	0.00000
289	1.0574	0.00000
290	1.1070	0.00000
291	1.1417	0.00000
292	1.1766	0.00000
293	1.2319	0.00000
294	1.2502	0.00000
295	1.3088	0.00000
296	1.3195	0.00000
297	1.3601	0.00000
298	1.4306	0.00000
299	1.4786	0.00000
300	1.4999	0.00000
301	1.5777	0.00000
302	1.6028	0.00000
303	1.6523	0.00000
304	1.6864	0.00000
305	1.7581	0.00000

306	1.7730	0.00000
307	1.8771	0.00000
308	1.8994	0.00000
309	1.9076	0.00000
310	1.9210	0.00000
311	2.1390	0.00000
312	2.1984	0.00000
313	2.2198	0.00000
314	2.2532	0.00000
315	2.2892	0.00000
316	2.2964	0.00000
317	2.3366	0.00000
318	2.3609	0.00000
319	2.3827	0.00000
320	2.4080	0.00000
321	2.4283	0.00000
322	2.4352	0.00000
323	2.4503	0.00000
324	2.4579	0.00000
325	2.4670	0.00000
326	2.5257	0.00000
327	2.5437	0.00000

328	2.7060	0.00000
329	2.7344	0.00000
330	2.7530	0.00000
331	2.7589	0.00000
332	2.7734	0.00000
333	2.8289	0.00000
334	2.8465	0.00000
335	2.8721	0.00000
336	2.9022	0.00000
337	2.9325	0.00000
338	2.9557	0.00000
339	2.9835	0.00000
340	3.0068	0.00000
341	3.0382	0.00000
342	3.0504	0.00000
343	3.0717	0.00000
344	3.0921	0.00000
345	3.1528	0.00000
346	3.1704	0.00000
347	3.1882	0.00000
348	3.1995	0.00000
349	3.3065	0.00000

350	3.3273	0.00000
351	3.3607	0.00000
352	3.3707	0.00000
353	3.3922	0.00000
354	3.4372	0.00000
355	3.4818	0.00000
356	3.4916	0.00000
357	3.4938	0.00000
358	3.5045	0.00000
359	3.6385	0.00000
360	3.6764	0.00000
361	3.7003	0.00000
362	3.7380	0.00000
363	3.7547	0.00000
364	3.7604	0.00000
365	3.7772	0.00000
366	3.7985	0.00000
367	3.8145	0.00000
368	3.8407	0.00000
369	3.8472	0.00000
370	3.8659	0.00000
371	3.8800	0.00000

372	3.8929	0.00000
373	3.9209	0.00000
374	3.9353	0.00000
375	3.9481	0.00000
376	3.9591	0.00000
377	3.9825	0.00000
378	3.9864	0.00000
379	4.0219	0.00000
380	4.0774	0.00000
381	4.1709	0.00000
382	4.2586	0.00000
383	4.2622	0.00000
384	4.2690	0.00000
385	4.2928	0.00000
386	4.3211	0.00000
387	4.3338	0.00000
388	4.3502	0.00000
389	4.3807	0.00000
390	4.3856	0.00000
391	4.4231	0.00000
392	4.4487	0.00000
393	4.4740	0.00000

394	4.4827	0.00000
395	4.4923	0.00000
396	4.4991	0.00000
397	4.5203	0.00000
398	4.5550	0.00000
399	4.5929	0.00000
400	4.6104	0.00000
401	4.6288	0.00000
402	4.6456	0.00000
403	4.6595	0.00000
404	4.6852	0.00000
405	4.7086	0.00000
406	4.7369	0.00000
407	4.7514	0.00000
408	4.7703	0.00000
409	4.7868	0.00000
410	4.7889	0.00000
411	4.8028	0.00000
412	4.8328	0.00000
413	4.8682	0.00000
414	4.8848	0.00000
415	4.9027	0.00000

416	4.9417	0.00000
417	4.9937	0.00000
418	5.0096	0.00000
419	5.0130	0.00000
420	5.0383	0.00000
421	5.0441	0.00000
422	5.0682	0.00000
423	5.0858	0.00000
424	5.1175	0.00000
425	5.1216	0.00000
426	5.1409	0.00000
427	5.1439	0.00000
428	5.1698	0.00000
429	5.1794	0.00000
430	5.1884	0.00000
431	5.1926	0.00000
432	5.2197	0.00000
433	5.2375	0.00000
434	5.2434	0.00000
435	5.2611	0.00000
436	5.2978	0.00000
437	5.3025	0.00000

438	5.3118	0.00000
439	5.3358	0.00000
440	5.3528	0.00000
441	5.3706	0.00000
442	5.3812	0.00000
443	5.3949	0.00000
444	5.4289	0.00000
445	5.4594	0.00000
446	5.4692	0.00000
447	5.4871	0.00000
448	5.4990	0.00000
449	5.5256	0.00000
450	5.5676	0.00000
451	5.5726	0.00000
452	5.5943	0.00000
453	5.6074	0.00000
454	5.6246	0.00000
455	5.6700	0.00000
456	5.6921	0.00000
457	5.7181	0.00000
458	5.7268	0.00000
459	5.7479	0.00000

460	5.7622	0.00000
461	5.7892	0.00000
462	5.7921	0.00000
463	5.7977	0.00000
464	5.8038	0.00000
465	5.8200	0.00000
466	5.8253	0.00000
467	5.8549	0.00000
468	5.8607	0.00000
469	5.8816	0.00000
470	5.8864	0.00000
471	5.8908	0.00000
472	5.9074	0.00000
473	5.9209	0.00000
474	5.9472	0.00000
475	5.9537	0.00000
476	5.9702	0.00000
477	5.9772	0.00000
478	5.9950	0.00000
479	6.0159	0.00000
480	6.0491	0.00000

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soft charge-density along one line, spin component 1

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

soft charge-density along one line, spin component 2

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

pseudopotential strength for first ion, spin component: 1

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

pseudopotential strength for first ion, spin component: 2

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

total augmentation occupancy for first ion, spin component: 1

3.579 -0.646 0.444 -0.034 -0.000

-0.646 0.130 -0.082 0.006 0.000

0.444 -0.082 0.056 -0.003 -0.000

-0.034 0.006 -0.003 0.011 0.000

-0.000 0.000 -0.000 0.000 0.007

total augmentation occupancy for first ion, spin component: 2

-0.000 0.000 -0.000 0.000 0.000

0.000 -0.000 0.000 -0.000 -0.000

-0.000 0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

---------- aborting loop because EDIFF is reached ----------

total charge

# of ion	s	p	d	tot
1	0.646	0.043	0.000	0.690
2	0.646	0.043	0.000	0.690
3	0.646	0.043	0.000	0.690
4	0.646	0.043	0.000	0.690
5	0.646	0.043	0.000	0.690
6	0.646	0.043	0.000	0.690
7	0.646	0.043	0.000	0.690
8	0.646	0.043	0.000	0.690
9	0.646	0.043	0.000	0.690
10	0.646	0.043	0.000	0.690
11	0.646	0.043	0.000	0.690
12	0.646	0.043	0.000	0.690
13	0.646	0.043	0.000	0.689
14	0.646	0.043	0.000	0.689
15	0.648	0.045	0.000	0.693
16	0.646	0.043	0.000	0.689

17	0.646	0.043	0.000	0.689
18	0.646	0.043	0.000	0.689
19	0.646	0.043	0.000	0.689
20	0.646	0.043	0.000	0.689
21	0.646	0.043	0.000	0.689
22	0.646	0.044	0.000	0.690
23	0.541	0.015	0.000	0.557
24	0.541	0.015	0.000	0.556
25	0.870	1.763	0.000	2.633
26	0.867	1.785	0.000	2.653
27	0.867	1.786	0.000	2.653
28	0.870	1.762	0.000	2.632
29	0.865	1.783	0.000	2.648
30	0.870	1.763	0.000	2.633
31	0.867	1.786	0.000	2.653
32	0.867	1.786	0.000	2.653
33	0.870	1.762	0.000	2.632
34	0.865	1.783	0.000	2.648
35	0.870	1.763	0.000	2.633
36	0.868	1.787	0.000	2.654
37	0.867	1.786	0.000	2.653
38	0.870	1.763	0.000	2.633

39	0.865	1.784	0.000	2.649
40	0.870	1.763	0.000	2.633
41	0.868	1.787	0.000	2.655
42	0.867	1.786	0.000	2.653
43	0.871	1.764	0.000	2.634
44	0.865	1.783	0.000	2.648
45	0.870	1.763	0.000	2.633
46	0.867	1.786	0.000	2.653
47	0.867	1.786	0.000	2.653
48	0.871	1.763	0.000	2.634
49	0.865	1.783	0.000	2.648
50	0.870	1.763	0.000	2.633
51	0.867	1.786	0.000	2.653
52	0.867	1.786	0.000	2.653
53	0.870	1.762	0.000	2.632
54	0.865	1.784	0.000	2.648
55	0.865	1.784	0.000	2.649
56	0.865	1.786	0.000	2.651
57	0.866	1.787	0.000	2.653
58	0.866	1.790	0.000	2.656
59	0.865	1.786	0.000	2.651
60	0.866	1.786	0.000	2.651

61	0.866	1.788	0.000	2.654
62	0.867	1.791	0.000	2.658
63	0.865	1.784	0.000	2.649
64	0.865	1.786	0.000	2.651
65	0.866	1.787	0.000	2.652
66	0.865	1.788	0.000	2.653
67	0.865	1.786	0.000	2.651
68	0.866	1.785	0.000	2.651
69	0.865	1.787	0.000	2.652
70	0.866	1.787	0.000	2.653
71	0.865	1.784	0.000	2.649
72	0.865	1.786	0.000	2.651
73	0.866	1.786	0.000	2.652
74	0.864	1.785	0.000	2.649
75	0.865	1.786	0.000	2.651
76	0.866	1.786	0.000	2.651
77	0.865	1.786	0.000	2.651
78	0.865	1.784	0.000	2.649
79	0.865	1.784	0.000	2.649
80	0.865	1.786	0.000	2.651
81	0.865	1.785	0.000	2.650
82	0.863	1.782	0.000	2.645

83	0.865	1.786	0.000	2.651
84	0.866	1.786	0.000	2.651
85	0.865	1.784	0.000	2.648
86	0.862	1.774	0.000	2.636
87	0.865	1.784	0.000	2.649
88	0.865	1.787	0.000	2.652
89	0.865	1.785	0.000	2.650
90	0.865	1.788	0.000	2.653
91	0.865	1.786	0.000	2.651
92	0.866	1.786	0.000	2.651
93	0.864	1.783	0.000	2.647
94	0.866	1.785	0.000	2.651
95	0.865	1.784	0.000	2.649
96	0.865	1.786	0.000	2.651
97	0.866	1.787	0.000	2.653
98	0.866	1.789	0.000	2.655
99	0.865	1.786	0.000	2.651
100	0.866	1.786	0.000	2.651
101	0.865	1.787	0.000	2.652
102	0.867	1.790	0.000	2.657
103	0.865	1.786	0.000	2.651
104	0.867	1.785	0.000	2.653

105	0.866	1.786	0.000	2.652
106	0.870	1.778	0.000	2.648
107	0.869	1.765	0.000	2.635
108	0.865	1.783	0.000	2.648
109	0.869	1.789	0.000	2.658
110	0.865	1.786	0.000	2.651
111	0.867	1.785	0.000	2.653
112	0.867	1.789	0.000	2.655
113	0.871	1.782	0.000	2.653
114	0.869	1.765	0.000	2.634
115	0.865	1.783	0.000	2.648
116	0.870	1.791	0.000	2.661
117	0.865	1.786	0.000	2.651
118	0.867	1.786	0.000	2.653
119	0.865	1.782	0.000	2.647
120	0.857	1.707	0.000	2.564
121	0.869	1.765	0.000	2.634
122	0.865	1.783	0.000	2.648
123	0.866	1.778	0.000	2.644
124	0.866	1.786	0.000	2.652
125	0.867	1.785	0.000	2.653
126	0.862	1.776	0.000	2.638

127	0.849	1.830	0.000	2.679
128	0.870	1.767	0.000	2.637
129	0.865	1.783	0.000	2.648
130	0.860	1.757	0.000	2.617
131	0.866	1.786	0.000	2.652
132	0.867	1.784	0.000	2.652
133	0.864	1.787	0.000	2.651
134	0.869	1.789	0.000	2.659
135	0.869	1.767	0.000	2.636
136	0.865	1.783	0.000	2.648
137	0.866	1.772	0.000	2.638
138	0.866	1.786	0.000	2.652
139	0.867	1.785	0.000	2.652
140	0.866	1.788	0.000	2.654
141	0.870	1.779	0.000	2.649
142	0.869	1.766	0.000	2.635
143	0.865	1.783	0.000	2.648
144	0.869	1.790	0.000	2.659
145	0.941	1.716	0.000	2.657
146	1.240	1.546	0.074	2.860
147	1.633	3.524	0.000	5.157

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tot 123.061 221.544 0.074 344.679

magnetization (x)

# of ion	s	p	d	tot
1	0.000	-0.000	0.000	0.000
2	-0.000	0.000	0.000	-0.000
3	0.000	-0.000	0.000	0.000
4	-0.000	0.000	0.000	-0.000
5	0.000	-0.000	0.000	0.000
6	-0.000	0.000	0.000	-0.000
7	0.000	-0.000	0.000	0.000
8	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	0.000
10	-0.000	0.000	0.000	-0.000
11	0.000	-0.000	0.000	0.000
12	-0.000	0.000	0.000	-0.000
13	0.000	-0.000	0.000	0.000
14	-0.004	0.002	0.000	-0.002

15	0.000	-0.000	0.000	0.000
16	-0.004	0.002	0.000	-0.002
17	-0.004	0.002	0.000	-0.002
18	0.000	-0.000	0.000	0.000
19	-0.003	0.001	0.000	-0.002
20	0.000	-0.000	0.000	0.000
21	-0.003	0.002	0.000	-0.002
22	-0.003	0.002	0.000	-0.002
23	-0.000	0.000	0.000	-0.000
24	-0.000	0.000	0.000	-0.000
25	-0.000	-0.007	0.000	-0.008
26	-0.000	-0.002	0.000	-0.002
27	0.000	0.003	0.000	0.003
28	0.000	0.005	0.000	0.005
29	0.000	0.003	0.000	0.003
30	-0.000	-0.007	0.000	-0.008
31	-0.000	-0.002	0.000	-0.002
32	0.000	0.003	0.000	0.003
33	0.000	0.005	0.000	0.005
34	0.000	0.002	0.000	0.002
35	-0.000	-0.007	0.000	-0.008
36	-0.000	-0.002	0.000	-0.002

37	0.000	0.003	0.000	0.003
38	0.000	0.006	0.000	0.007
39	0.000	0.002	0.000	0.002
40	-0.000	-0.007	0.000	-0.008
41	-0.000	-0.002	0.000	-0.002
42	0.000	0.002	0.000	0.003
43	0.000	0.005	0.000	0.006
44	0.000	0.004	0.000	0.004
45	-0.000	-0.007	0.000	-0.008
46	-0.000	-0.002	0.000	-0.002
47	0.000	0.003	0.000	0.003
48	0.000	0.005	0.000	0.006
49	0.000	0.001	0.000	0.002
50	-0.000	-0.007	0.000	-0.008
51	-0.000	-0.002	0.000	-0.002
52	0.000	0.002	0.000	0.003
53	0.000	0.006	0.000	0.007
54	0.000	0.002	0.000	0.002
55	-0.000	-0.005	0.000	-0.006
56	-0.000	-0.007	0.000	-0.007
57	-0.000	-0.001	0.000	-0.001
58	-0.000	-0.001	0.000	-0.001

59	0.000	0.006	0.000	0.007
60	0.000	0.003	0.000	0.003
61	0.000	0.001	0.000	0.001
62	0.000	0.003	0.000	0.003
63	-0.000	-0.005	0.000	-0.006
64	-0.000	-0.007	0.000	-0.007
65	-0.000	-0.001	0.000	-0.001
66	-0.000	-0.001	0.000	-0.001
67	0.000	0.006	0.000	0.006
68	0.000	0.003	0.000	0.003
69	0.000	0.001	0.000	0.001
70	0.000	0.002	0.000	0.002
71	-0.000	-0.005	0.000	-0.006
72	-0.000	-0.007	0.000	-0.007
73	-0.000	-0.001	0.000	-0.001
74	-0.000	-0.002	0.000	-0.002
75	0.000	0.006	0.000	0.007
76	0.000	0.003	0.000	0.004
77	0.000	0.003	0.000	0.003
78	0.000	0.001	0.000	0.001
79	-0.000	-0.005	0.000	-0.006
80	-0.000	-0.007	0.000	-0.007

81	-0.000	-0.001	0.000	-0.002
82	-0.000	-0.002	0.000	-0.002
83	0.001	0.007	0.000	0.008
84	0.000	0.003	0.000	0.003
85	0.000	0.002	0.000	0.002
86	0.000	0.005	0.000	0.006
87	-0.000	-0.005	0.000	-0.005
88	-0.000	-0.007	0.000	-0.007
89	-0.000	-0.001	0.000	-0.002
90	-0.000	-0.002	0.000	-0.002
91	0.001	0.008	0.000	0.008
92	0.000	0.003	0.000	0.003
93	0.000	0.002	0.000	0.003
94	0.000	0.001	0.000	0.001
95	-0.000	-0.005	0.000	-0.006
96	-0.000	-0.007	0.000	-0.007
97	-0.000	-0.001	0.000	-0.001
98	-0.000	-0.001	0.000	-0.001
99	0.001	0.007	0.000	0.007
100	0.000	0.003	0.000	0.004
101	0.000	0.003	0.000	0.003
102	0.000	0.002	0.000	0.002

103	-0.001	-0.010	0.000	-0.011
104	-0.003	-0.028	0.000	-0.031
105	-0.000	-0.001	0.000	-0.002
106	-0.000	-0.004	0.000	-0.005
107	0.007	0.116	0.000	0.122
108	0.001	0.010	0.000	0.011
109	0.000	0.001	0.000	0.001
110	-0.001	-0.010	0.000	-0.011
111	-0.003	-0.028	0.000	-0.031
112	-0.000	-0.001	0.000	-0.002
113	-0.000	-0.003	0.000	-0.004
114	0.007	0.120	0.000	0.127
115	0.001	0.010	0.000	0.011
116	0.000	0.001	0.000	0.002
117	-0.001	-0.010	0.000	-0.011
118	-0.003	-0.026	0.000	-0.029
119	-0.000	-0.002	0.000	-0.002
120	-0.000	-0.002	0.000	-0.002
121	0.007	0.115	0.000	0.122
122	0.001	0.010	0.000	0.010
123	0.000	0.003	0.000	0.003
124	-0.001	-0.010	0.000	-0.011

125	-0.003	-0.024	0.000	-0.027
126	-0.000	-0.002	0.000	-0.002
127	-0.000	0.001	0.000	0.001
128	0.006	0.105	0.000	0.111
129	0.001	0.009	0.000	0.010
130	0.000	0.004	0.000	0.004
131	-0.001	-0.009	0.000	-0.010
132	-0.003	-0.024	0.000	-0.027
133	-0.000	-0.002	0.000	-0.002
134	-0.000	-0.002	0.000	-0.002
135	0.006	0.097	0.000	0.102
136	0.001	0.009	0.000	0.010
137	0.000	0.004	0.000	0.005
138	-0.001	-0.010	0.000	-0.011
139	-0.003	-0.026	0.000	-0.029
140	-0.000	-0.002	0.000	-0.002
141	-0.000	-0.003	0.000	-0.004
142	0.006	0.105	0.000	0.111
143	0.001	0.010	0.000	0.010
144	0.000	0.002	0.000	0.003
145	0.000	0.005	0.000	0.006
146	-0.000	0.000	-0.000	0.000

147 0.000 0.004 0.000 0.004

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tot 0.001 0.513 -0.000 0.514

CHARGE: cpu time 0.5202: real time 0.5217

FORLOC: cpu time 0.0199: real time 0.0200

FORNL : cpu time 2.0656: real time 2.0734

STRESS: cpu time 6.2093: real time 6.2301

FORCOR: cpu time 0.1408: real time 0.1412

FORHAR: cpu time 0.0332: real time 0.0333

MIXING: cpu time 0.0102: real time 0.0102

OFIELD: cpu time 0.0001: real time 0.0001

DFTD3 V3.0 Rev 1

Edisp (eV) -6.61780

E6 (eV) : -3.9313

E8 (eV) : -2.6865

% E8 : 40.60

FORVDW: cpu time 1.5387: real time 1.5800

FORCE on cell =-STRESS in cart. coord. units (eV):

Direction	XX	YY	ZZ	XY	YZ	ZX
Alpha Z	233.50077	233.50077	233.50077			
Ewald	107580.56416	23476.25992	-39728.53249	12.81117	3454.40125	130.01950
Hartree	106097.84647	25032.29041	-23795.13714	-5.61600	2947.16446	93.56749
E(xc)	-1914.22256	-1916.57845	-1979.88707	0.14252	1.82064	0.13697
Local	**********	-53957.14430	57017.43389	-3.50925	-6359.69187	-219.96202
n-local	-472.65215	-482.43338	-439.52334	-0.74008	-0.68555	-0.35685
augment	-38.29444	-38.58728	-34.30652	-0.00145	-0.97752	-0.00638
Kinetic	7635.00902	7638.78787	8713.93626	-3.33509	-41.57385	-3.36746
Fock	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
vdW	-2.64308	-1.49218	-6.59370	0.00143	-0.07450	0.01086
Total	-17.75778	-15.39663	-19.10934	-0.24675	0.38306	0.04210
in kB	-4.89681	-4.24571	-5.26951	-0.06804	0.10563	0.01161

external pressure = -4.80 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

energy-cutoff : 400.00

volume of cell : 5810.14

direct lattice vectors reciprocal lattice vectors

14.780600000 0.000000000 0.000000000 0.067656252 0.000000000 0.000000000

0.000000000 21.333900000 0.000000000 0.000000000 0.046873755 0.000000000

0.000000000 0.000000000 18.425700000 0.000000000 0.000000000 0.054272022

length of vectors

14.780600000 21.333900000 18.425700000 0.067656252 0.046873755 0.054272022

FORCES acting on ions

electron-ion (+dipol) ewald-force non-local-force convergence-correction

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0.409E-02 0.154E+03 0.361E+02 -.260E-02 -.160E+03 -.357E+02 -.180E-02 0.566E+01 -.438E+00 0.115E-06 0.473E-06 -.130E-06

-.193E-01 0.155E+03 -.340E+02 0.169E-01 -.160E+03 0.335E+02 0.116E-02 0.565E+01 0.541E+00 -.344E-06 0.355E-06 -.598E-06

0.184E+00 0.154E+03 0.360E+02 -.184E+00 -.160E+03 -.356E+02 0.945E-05 0.565E+01 -.443E+00 -.875E-07 0.439E-06 -.690E-07

0.111E+00 0.155E+03 -.341E+02 -.980E-01 -.160E+03 0.336E+02 -.175E-01 0.565E+01

0.535E+00 0.495E-06 0.297E-06 -.563E-06

0.171E+00 0.154E+03 0.362E+02 -.173E+00 -.160E+03 -.357E+02 0.116E-02 0.566E+01 -.440E+00 -.247E-06 0.281E-06 0.613E-06

0.126E+00 0.154E+03 -.340E+02 -.108E+00 -.160E+03 0.334E+02 -.211E-01 0.565E+01 0.541E+00 0.708E-06 -.328E-06 0.235E-06

-.187E-01 0.154E+03 0.363E+02 0.176E-01 -.160E+03 -.359E+02 0.159E-02 0.566E+01 -.431E+00 -.151E-06 0.141E-06 0.123E-05

-.120E-01 0.154E+03 -.338E+02 0.189E-01 -.160E+03 0.332E+02 -.721E-02 0.565E+01 0.555E+00 0.268E-06 -.849E-06 0.925E-06

-.181E+00 0.154E+03 0.363E+02 0.181E+00 -.160E+03 -.359E+02 0.254E-03 0.566E+01 -.429E+00 0.128E-06 0.205E-06 0.117E-05

-.127E+00 0.155E+03 -.337E+02 0.114E+00 -.160E+03 0.331E+02 0.109E-01 0.565E+01 0.561E+00 -.390E-06 -.789E-06 0.885E-06

-.174E+00 0.154E+03 0.362E+02 0.176E+00 -.160E+03 -.358E+02 -.177E-02 0.566E+01 -.432E+00 0.243E-06 0.328E-06 0.509E-06

-.115E+00 0.155E+03 -.338E+02 0.958E-01 -.160E+03 0.332E+02 0.192E-01 0.565E+01 0.555E+00 -.741E-06 -.253E-06 0.140E-06

0.227E+01 -.150E+03 -.386E+02 -.226E+01 0.156E+03 0.386E+02 -.103E-01 -.566E+01 0.767E-01 0.139E-06 -.643E-06 -.223E-06

-.419E+00 -.151E+03 0.388E+02 0.420E+00 0.157E+03 -.386E+02 -.128E-02 -.567E+01 -.269E+00 0.160E-06 -.229E-06 0.123E-06

0.136E+02 -.146E+03 -.413E+02 -.138E+02 0.151E+03 0.413E+02 0.257E+00 -.567E+01 -

.348E-01 0.186E-06 -.678E-06 -.602E-06

0.162E+01 -.151E+03 0.402E+02 -.162E+01 0.156E+03 -.400E+02 -.993E-03 -.567E+01 -.229E+00 0.754E-07 -.247E-06 0.654E-06

0.352E+01 -.149E+03 0.443E+02 -.352E+01 0.155E+03 -.441E+02 -.197E-02 -.567E+01 -.180E+00 0.278E-06 -.471E-06 0.374E-06

-.149E+02 -.146E+03 -.329E+02 0.150E+02 0.151E+03 0.329E+02 -.952E-01 -.566E+01 0.482E-01 -.287E-06 -.756E-06 0.455E-06

-.297E+01 -.149E+03 0.432E+02 0.296E+01 0.155E+03 -.430E+02 0.114E-01 -.567E+01 -.241E+00 -.407E-06 -.581E-06 -.997E-06

-.381E+01 -.150E+03 -.385E+02 0.381E+01 0.156E+03 0.385E+02 -.611E-02 -.566E+01 0.239E-01 0.579E-06 -.658E-06 -.236E-06

-.207E+01 -.151E+03 0.395E+02 0.207E+01 0.156E+03 -.392E+02 0.151E-02 -.566E+01 -.282E+00 0.165E-06 -.516E-06 -.780E-06

0.277E-02 -.148E+03 0.486E+02 0.490E-02 0.154E+03 -.484E+02 -.556E-02 -.569E+01 -.158E+00 -.224E-06 -.708E-06 -.258E-06

0.196E+02 -.103E+03 0.222E+02 -.212E+02 0.103E+03 -.246E+02 0.153E+01 0.139E+00 0.238E+01 0.137E-06 -.111E-05 0.521E-06

-.191E+02 -.103E+03 0.153E+02 0.216E+02 0.103E+03 -.168E+02 -.241E+01 -.119E+00 0.152E+01 -.936E-06 -.779E-06 0.154E-05

0.696E-01 0.461E+03 0.202E+03 -.729E-01 -.462E+03 -.201E+03 0.384E-02 0.102E+01 -.219E+00 0.609E-06 0.963E-06 -.114E-05

0.209E+00 0.353E+03 -.234E+03 -.209E+00 -.353E+03 0.234E+03 0.259E-02 0.443E+00 -

.370E-01 0.107E-06 0.215E-06 -.308E-05

-.257E-01 0.351E+03 0.240E+03 0.244E-01 -.351E+03 -.241E+03 0.315E-02 0.408E+00

0.564E-01 0.117E-05 -.297E-07 -.640E-06

-.176E+00 0.462E+03 -.195E+03 0.182E+00 -.463E+03 0.195E+03 -.663E-02 0.105E+01

0.233E+00 -.765E-06 0.617E-06 -.274E-05

-.657E-01 0.210E+03 -.272E+03 0.698E-01 -.210E+03 0.272E+03 -.446E-02 0.937E-01

0.560E-01 0.115E-06 0.937E-06 -.216E-05

0.560E+00 0.461E+03 0.202E+03 -.563E+00 -.462E+03 -.201E+03 0.202E-02 0.102E+01 -

.214E+00 -.659E-06 0.836E-06 -.878E-06

0.105E+01 0.352E+03 -.234E+03 -.107E+01 -.353E+03 0.234E+03 0.160E-01 0.448E+00 -

.425E-01 0.114E-05 -.976E-06 -.163E-05

0.411E+00 0.351E+03 0.240E+03 -.413E+00 -.351E+03 -.240E+03 0.304E-02 0.408E+00

0.491E-01 -.280E-07 -.616E-07 -.143E-05

0.576E+00 0.462E+03 -.195E+03 -.581E+00 -.463E+03 0.195E+03 0.480E-02 0.105E+01

0.235E+00 0.122E-05 0.311E-06 -.262E-05

0.687E+00 0.210E+03 -.272E+03 -.693E+00 -.210E+03 0.272E+03 0.599E-02 0.913E-01

0.616E-01 0.232E-06 0.159E-06 -.121E-05

0.426E+00 0.461E+03 0.202E+03 -.428E+00 -.462E+03 -.202E+03 0.385E-02 0.102E+01 -

.214E+00 -.130E-05 0.411E-06 0.139E-05

0.940E+00 0.352E+03 -.233E+03 -.956E+00 -.352E+03 0.233E+03 0.151E-01 0.441E+00 -

.377E-01 0.743E-06 -.287E-05 0.754E-06

0.477E+00 0.351E+03 0.241E+03 -.479E+00 -.351E+03 -.241E+03 0.250E-02 0.406E+00

0.512E-01 -.120E-05 -.157E-06 -.172E-06

0.704E+00 0.462E+03 -.194E+03 -.715E+00 -.463E+03 0.194E+03 0.786E-02 0.106E+01 0.242E+00 0.163E-05 -.218E-05 0.640E-07

0.726E+00 0.210E+03 -.271E+03 -.735E+00 -.210E+03 0.271E+03 0.652E-02 0.911E-01 0.592E-01 0.478E-07 -.108E-05 0.227E-06

-.180E+00 0.461E+03 0.202E+03 0.176E+00 -.462E+03 -.202E+03 0.448E-02 0.102E+01 -.218E+00 -.695E-06 0.399E-06 0.339E-05

-.291E+00 0.352E+03 -.233E+03 0.295E+00 -.352E+03 0.233E+03 -.216E-02 0.440E+00 -.299E-01 -.109E-06 -.400E-05 0.180E-05

0.412E-01 0.351E+03 0.241E+03 -.402E-01 -.351E+03 -.241E+03 0.223E-02 0.409E+00 0.558E-01 -.125E-05 -.113E-06 0.197E-05

0.528E-01 0.462E+03 -.194E+03 -.589E-01 -.463E+03 0.194E+03 0.393E-02 0.106E+01 0.232E+00 0.627E-06 -.441E-05 0.231E-05

-.438E-01 0.210E+03 -.271E+03 0.420E-01 -.210E+03 0.271E+03 -.258E-03 0.933E-01 0.324E-01 -.129E-06 -.187E-05 0.904E-06

-.550E+00 0.461E+03 0.202E+03 0.548E+00 -.462E+03 -.202E+03 0.759E-03 0.102E+01 -.220E+00 0.734E-06 0.495E-06 0.316E-05

-.119E+01 0.352E+03 -.233E+03 0.120E+01 -.353E+03 0.233E+03 -.162E-01 0.447E+00 -.330E-01 -.107E-05 -.275E-05 0.548E-06

-.351E+00 0.351E+03 0.241E+03 0.347E+00 -.351E+03 -.241E+03 0.206E-02 0.413E+00 0.624E-01 0.134E-06 -.971E-08 0.272E-05

-.409E+00 0.462E+03 -.194E+03 0.423E+00 -.463E+03 0.194E+03 -.115E-01 0.106E+01

0.230E+00 -.963E-06 -.420E-05 0.215E-05

-.559E+00 0.210E+03 -.271E+03 0.563E+00 -.210E+03 0.271E+03 -.937E-02 0.915E-01 0.525E-01 -.313E-06 -.119E-05 0.101E-06

-.475E+00 0.461E+03 0.202E+03 0.474E+00 -.462E+03 -.202E+03 0.307E-02 0.102E+01 -.220E+00 0.131E-05 0.707E-06 0.929E-06

-.807E+00 0.353E+03 -.234E+03 0.821E+00 -.353E+03 0.234E+03 -.149E-01 0.447E+00 -.393E-01 -.823E-06 -.714E-06 -.193E-05

-.373E+00 0.351E+03 0.241E+03 0.367E+00 -.351E+03 -.241E+03 0.959E-03 0.411E+00 0.626E-01 0.117E-05 -.509E-07 0.152E-05

-.594E+00 0.462E+03 -.194E+03 0.607E+00 -.463E+03 0.194E+03 -.170E-01 0.105E+01 0.234E+00 -.178E-05 -.191E-05 -.285E-06

-.589E+00 0.210E+03 -.272E+03 0.600E+00 -.210E+03 0.272E+03 -.102E-01 0.993E-01 0.567E-01 0.264E-07 0.196E-06 -.150E-05

-.980E-02 0.206E+03 0.279E+03 0.131E-01 -.206E+03 -.279E+03 -.360E-02 0.687E-01 -.412E-01 0.111E-05 -.146E-05 -.710E-06

0.665E+00 0.303E+02 0.296E+03 -.660E+00 -.302E+02 -.296E+03 -.467E-02 -.409E-01 0.754E-02 0.294E-06 -.122E-05 0.253E-06

-.850E+00 0.144E+03 -.282E+03 0.851E+00 -.144E+03 0.282E+03 -.314E-02 0.137E+00 0.286E-01 0.794E-07 0.668E-06 -.149E-05

0.524E+00 -.215E+02 -.285E+03 -.525E+00 0.214E+02 0.285E+03 -.791E-03 0.388E-01 0.186E-01 0.211E-06 0.147E-05 0.802E-07

0.497E+00 -.294E+02 0.293E+03 -.494E+00 0.294E+02 -.293E+03 -.552E-02 0.255E-01 -

.303E-01 0.422E-06 -.549E-06 0.381E-06

0.522E+00 0.139E+03 0.289E+03 -.522E+00 -.139E+03 -.289E+03 0.179E-02 0.104E+00 -.248E-01 0.516E-06 -.156E-05 -.733E-06

-.127E+01 0.364E+02 -.287E+03 0.127E+01 -.364E+02 0.287E+03 -.234E-04 -.746E-02 0.137E-01 0.379E-06 0.112E-05 -.402E-06

0.165E+01 -.130E+03 -.271E+03 -.167E+01 0.130E+03 0.271E+03 0.107E-01 -.878E-01 0.371E-01 0.337E-06 0.168E-05 0.677E-06

0.395E+00 0.207E+03 0.280E+03 -.393E+00 -.207E+03 -.280E+03 0.714E-03 0.696E-01 -.370E-01 -.646E-07 -.169E-05 -.110E-05

0.916E+00 0.312E+02 0.296E+03 -.920E+00 -.311E+02 -.296E+03 0.226E-02 -.409E-01 0.122E-01 -.363E-06 -.110E-05 0.292E-06

0.132E+01 0.144E+03 -.282E+03 -.133E+01 -.144E+03 0.282E+03 0.501E-02 0.126E+00 0.279E-01 0.172E-06 0.801E-06 -.133E-05

0.341E+01 -.199E+02 -.285E+03 -.342E+01 0.199E+02 0.285E+03 0.134E-01 0.415E-01 0.136E-01 -.783E-06 0.103E-05 0.194E-06

0.139E+01 -.287E+02 0.294E+03 -.138E+01 0.287E+02 -.294E+03 -.347E-02 0.253E-01 -.307E-01 0.897E-08 -.671E-06 0.832E-06

0.676E+00 0.139E+03 0.290E+03 -.676E+00 -.139E+03 -.290E+03 0.623E-03 0.103E+00 -.295E-01 -.650E-06 -.155E-05 -.548E-06

0.159E+01 0.367E+02 -.287E+03 -.158E+01 -.366E+02 0.287E+03 -.128E-01 -.204E-01 0.128E-01 -.415E-07 0.110E-05 -.224E-06

0.610E+01 -.125E+03 -.271E+03 -.612E+01 0.125E+03 0.271E+03 0.218E-01 -.893E-01

0.146E-01 -.750E-06 0.175E-05 -.174E-07

0.366E+00 0.207E+03 0.280E+03 -.371E+00 -.207E+03 -.280E+03 0.110E-03 0.685E-01 -.365E-01 -.118E-05 -.144E-05 -.294E-06

-.384E-01 0.319E+02 0.296E+03 0.298E-01 -.318E+02 -.296E+03 0.106E-01 -.361E-01 0.139E-01 -.542E-06 -.201E-06 0.533E-07

0.210E+01 0.144E+03 -.281E+03 -.211E+01 -.144E+03 0.281E+03 0.120E-01 0.120E+00 0.240E-01 0.404E-07 -.275E-06 -.225E-06

0.303E+01 -.172E+02 -.283E+03 -.306E+01 0.171E+02 0.283E+03 0.242E-01 0.865E-01 0.609E-01 -.775E-06 0.485E-06 0.624E-07

0.105E+01 -.272E+02 0.294E+03 -.105E+01 0.272E+02 -.294E+03 0.289E-02 0.244E-01 -.376E-01 -.223E-06 -.552E-07 0.384E-06

0.961E-01 0.140E+03 0.290E+03 -.977E-01 -.140E+03 -.290E+03 0.131E-02 0.107E+00 -.232E-01 -.110E-05 -.840E-06 0.167E-06

0.277E+01 0.387E+02 -.286E+03 -.277E+01 -.387E+02 0.286E+03 0.936E-03 -.110E-01 0.291E-01 -.759E-06 0.323E-06 0.253E-06

0.596E+01 -.115E+03 -.267E+03 -.611E+01 0.115E+03 0.267E+03 0.152E+00 0.211E-03 0.131E+00 -.923E-06 0.428E-05 -.890E-06

-.241E+00 0.207E+03 0.280E+03 0.239E+00 -.207E+03 -.280E+03 0.438E-02 0.717E-01 -.387E-01 -.108E-05 -.891E-06 0.954E-06

-.114E+01 0.314E+02 0.294E+03 0.113E+01 -.314E+02 -.294E+03 0.917E-02 -.311E-01 0.546E-02 -.603E-06 0.470E-06 -.289E-06

0.598E+00 0.144E+03 -.281E+03 -.616E+00 -.144E+03 0.281E+03 0.178E-01 0.126E+00

0.437E-01 -.538E-06 -.916E-06 0.653E-06

-.926E+00 -.159E+02 -.286E+03 0.918E+00 0.158E+02 0.285E+03 0.595E-02 0.909E-01

0.802E-01 -.370E-06 -.148E-05 0.701E-07

-.642E+00 -.265E+02 0.293E+03 0.638E+00 0.265E+02 -.293E+03 0.490E-02 0.235E-01 -

.270E-01 -.382E-06 0.847E-06 -.451E-06

-.532E+00 0.139E+03 0.289E+03 0.528E+00 -.139E+03 -.289E+03 0.654E-02 0.114E+00 -

.213E-01 -.608E-06 -.377E-06 0.729E-06

0.785E+00 0.408E+02 -.287E+03 -.797E+00 -.408E+02 0.287E+03 0.523E-02 0.206E-02 -

.191E-01 -.773E-06 -.732E-06 0.410E-06

-.429E+00 -.113E+03 -.276E+03 0.394E+00 0.113E+03 0.276E+03 0.362E-01 0.603E-01 -

.268E+00 -.427E-06 0.141E-05 -.105E-05

-.569E+00 0.206E+03 0.279E+03 0.568E+00 -.206E+03 -.279E+03 0.114E-02 0.721E-01 -

.455E-01 0.170E-07 -.782E-06 0.128E-05

-.780E+00 0.304E+02 0.294E+03 0.783E+00 -.304E+02 -.294E+03 -.756E-02 -.308E-01 -

.136E-02 0.401E-06 0.158E-06 -.436E-06

-.123E+01 0.144E+03 -.281E+03 0.124E+01 -.145E+03 0.281E+03 -.158E-01 0.122E+00

0.504E-01 0.193E-06 -.107E-05 0.637E-06

-.365E+01 -.174E+02 -.283E+03 0.368E+01 0.173E+02 0.283E+03 -.310E-01 0.117E+00

0.585E-01 0.597E-06 0.445E-06 0.153E-06

-.129E+01 -.277E+02 0.291E+03 0.129E+01 0.277E+02 -.291E+03 -.133E-02 0.341E-01 -

.219E-01 -.300E-06 0.929E-06 -.104E-05

-.345E+00 0.139E+03 0.289E+03 0.344E+00 -.139E+03 -.289E+03 0.814E-05 0.112E+00 -

.146E-01 0.583E-06 -.545E-06 0.493E-06

-.821E+00 0.400E+02 -.287E+03 0.813E+00 -.400E+02 0.287E+03 0.127E-01 -.738E-02 -.183E-01 0.301E-06 -.908E-06 0.466E-06

-.785E+01 -.119E+03 -.267E+03 0.804E+01 0.119E+03 0.267E+03 -.191E+00 0.501E-02 0.342E-01 0.582E-06 0.439E-05 -.411E-06

-.408E+00 0.206E+03 0.279E+03 0.409E+00 -.206E+03 -.279E+03 -.280E-02 0.716E-01 -.464E-01 0.119E-05 -.112E-05 0.540E-06

-.630E-01 0.300E+02 0.294E+03 0.728E-01 -.299E+02 -.294E+03 -.948E-02 -.347E-01 0.124E-02 0.804E-06 -.513E-06 -.107E-06

-.206E+01 0.145E+03 -.282E+03 0.208E+01 -.145E+03 0.282E+03 -.190E-01 0.132E+00 0.257E-01 0.547E-07 -.409E-06 -.491E-06

-.257E+01 -.208E+02 -.285E+03 0.260E+01 0.208E+02 0.285E+03 -.291E-01 0.409E-01 0.317E-01 0.105E-05 0.102E-05 0.398E-07

-.549E+00 -.290E+02 0.291E+03 0.554E+00 0.290E+02 -.291E+03 -.286E-02 0.293E-01 -.250E-01 0.487E-06 0.373E-06 -.509E-06

0.591E-01 0.139E+03 0.289E+03 -.593E-01 -.139E+03 -.289E+03 -.335E-03 0.109E+00 -.208E-01 0.126E-05 -.107E-05 -.216E-06

-.290E+01 0.378E+02 -.286E+03 0.291E+01 -.378E+02 0.286E+03 -.149E-01 -.338E-02 0.210E-01 0.950E-06 0.244E-06 0.282E-07

-.515E+01 -.128E+03 -.271E+03 0.519E+01 0.128E+03 0.271E+03 -.463E-01 -.862E-01 0.379E-01 0.114E-05 0.112E-05 0.161E-06

0.396E+00 -.137E+03 0.280E+03 -.388E+00 0.137E+03 -.280E+03 -.968E-02 -.127E+00 -

.156E-01 0.109E-06 0.336E-06 0.786E-06

0.192E+01 -.343E+03 0.233E+03 -.193E+01 0.344E+03 -.233E+03 0.916E-02 -.460E+00 -.546E-01 0.263E-06 0.635E-06 0.201E-05

-.255E+01 -.197E+03 -.259E+03 0.256E+01 0.197E+03 0.259E+03 -.944E-02 -.197E+00 0.369E-01 0.120E-05 0.153E-05 0.553E-06

0.688E+01 -.447E+03 -.198E+03 -.689E+01 0.448E+03 0.198E+03 0.984E-02 -.112E+01 0.880E-01 0.660E-06 -.158E-05 -.231E-06

-.473E+00 -.451E+03 0.204E+03 0.474E+00 0.452E+03 -.204E+03 -.202E-02 -.108E+01 -.112E+00 0.216E-06 0.141E-06 0.723E-06

0.170E+01 -.203E+03 0.269E+03 -.170E+01 0.203E+03 -.269E+03 -.479E-02 -.926E-01 -.319E-01 0.251E-06 0.740E-06 0.168E-05

-.214E+01 -.338E+03 -.222E+03 0.219E+01 0.338E+03 0.222E+03 -.441E-01 -.604E+00 0.537E-01 0.168E-05 -.156E-06 0.882E-07

0.218E+01 -.136E+03 0.282E+03 -.217E+01 0.136E+03 -.282E+03 -.634E-02 -.126E+00 -.938E-02 0.278E-06 0.343E-06 0.166E-05

0.671E+01 -.339E+03 0.238E+03 -.669E+01 0.340E+03 -.238E+03 -.127E-01 -.461E+00 -.459E-01 0.875E-06 0.857E-06 0.203E-05

0.676E+01 -.193E+03 -.259E+03 -.678E+01 0.193E+03 0.258E+03 0.111E-01 -.145E+00 0.633E-01 -.509E-06 0.204E-05 0.371E-06

0.312E+02 -.427E+03 -.198E+03 -.313E+02 0.428E+03 0.197E+03 0.726E-01 -.969E+00 0.135E+00 0.652E-06 -.164E-05 -.174E-05

0.543E+01 -.449E+03 0.209E+03 -.543E+01 0.450E+03 -.209E+03 0.673E-03 -.108E+01 -

.797E-01 0.558E-06 0.311E-06 0.263E-05

0.368E+01 -.201E+03 0.272E+03 -.367E+01 0.201E+03 -.272E+03 -.710E-03 -.975E-01 -.305E-01 0.402E-06 0.113E-05 0.166E-05

0.124E+02 -.332E+03 -.223E+03 -.125E+02 0.332E+03 0.223E+03 0.121E+00 -.534E+00 0.314E-01 -.115E-06 0.199E-06 -.362E-06

0.219E+01 -.133E+03 0.283E+03 -.219E+01 0.133E+03 -.283E+03 0.560E-03 -.128E+00 -.440E-02 0.248E-06 0.104E-05 0.734E-06

0.492E+01 -.332E+03 0.245E+03 -.489E+01 0.332E+03 -.245E+03 -.319E-01 -.476E+00 -.374E-01 0.101E-05 0.160E-05 -.206E-06

0.112E+02 -.182E+03 -.258E+03 -.113E+02 0.183E+03 0.258E+03 0.468E-01 -.985E-01 -.104E+00 0.804E-06 0.460E-05 -.924E-06

0.317E+02 -.399E+03 -.175E+03 -.320E+02 0.401E+03 0.174E+03 0.295E+00 -.142E+01 0.132E+01 0.311E-05 -.287E-05 0.174E-05

0.929E+01 -.443E+03 0.219E+03 -.929E+01 0.444E+03 -.219E+03 -.553E-02 -.109E+01 -.482E-01 0.106E-05 0.529E-06 0.115E-05

0.169E+01 -.196E+03 0.273E+03 -.169E+01 0.197E+03 -.273E+03 0.551E-02 -.108E+00 -.511E-01 0.499E-06 0.197E-05 -.196E-06

0.172E+02 -.310E+03 -.216E+03 -.175E+02 0.310E+03 0.216E+03 0.325E+00 -.219E+00 0.123E+00 0.211E-05 -.191E-06 -.109E-05

-.103E+01 -.132E+03 0.281E+03 0.102E+01 0.132E+03 -.281E+03 0.103E-01 -.127E+00 0.160E-03 -.166E-06 0.173E-05 -.108E-05

-.511E+01 -.332E+03 0.239E+03 0.510E+01 0.332E+03 -.239E+03 0.874E-02 -.494E+00 -

.418E-01 -.153E-05 0.100E-05 -.322E-05

0.160E+01 -.170E+03 -.261E+03 -.173E+01 0.169E+03 0.261E+03 0.116E+00 0.369E+00 -.938E-01 -.549E-05 0.755E-05 -.119E-05

-.623E+01 -.301E+03 -.189E+03 0.575E+01 0.296E+03 0.185E+03 0.441E+00 0.503E+01 0.404E+01 -.553E-05 -.267E-05 0.133E-05

-.619E+00 -.436E+03 0.227E+03 0.616E+00 0.437E+03 -.227E+03 0.155E-02 -.120E+01 -.477E-01 -.579E-06 0.276E-06 -.159E-05

-.302E+01 -.197E+03 0.268E+03 0.300E+01 0.197E+03 -.268E+03 0.146E-01 -.111E+00 -.428E-01 -.676E-06 0.201E-05 -.249E-05

0.339E+01 -.281E+03 -.215E+03 -.530E+01 0.280E+03 0.214E+03 0.191E+01 0.635E+00 0.816E+00 -.160E-04 -.381E-05 -.139E-05

-.273E+01 -.134E+03 0.277E+03 0.273E+01 0.134E+03 -.277E+03 0.244E-02 -.123E+00 -.185E-01 -.492E-06 0.162E-05 -.233E-05

-.599E+01 -.338E+03 0.230E+03 0.599E+01 0.339E+03 -.230E+03 0.112E-01 -.494E+00 -.459E-01 -.355E-06 -.667E-07 -.351E-05

-.646E+01 -.171E+03 -.257E+03 0.654E+01 0.170E+03 0.257E+03 -.794E-01 0.490E+00 0.185E-01 0.532E-05 0.878E-05 -.924E-06

-.442E+02 -.422E+03 -.184E+03 0.448E+02 0.423E+03 0.183E+03 -.564E+00 -.110E+01 0.620E+00 -.302E-05 -.836E-05 0.624E-06

-.865E+01 -.441E+03 0.211E+03 0.864E+01 0.443E+03 -.211E+03 0.143E-01 -.111E+01 -.751E-01 -.132E-05 -.988E-06 -.422E-05

-.292E+01 -.201E+03 0.265E+03 0.293E+01 0.201E+03 -.265E+03 -.919E-02 -.110E+00 -

.203E-01 -.212E-06 0.153E-05 -.242E-05

-.144E+02 -.290E+03 -.209E+03 0.164E+02 0.289E+03 0.208E+03 -.198E+01 0.614E+00 0.784E+00 0.162E-04 -.100E-04 -.275E-05

-.138E+01 -.136E+03 0.277E+03 0.139E+01 0.136E+03 -.277E+03 -.102E-01 -.125E+00 -.239E-01 0.497E-07 0.105E-05 -.103E-05

-.279E+01 -.343E+03 0.230E+03 0.277E+01 0.343E+03 -.230E+03 0.235E-01 -.473E+00 -.592E-01 -.114E-06 0.378E-06 -.725E-06

-.104E+02 -.189E+03 -.258E+03 0.105E+02 0.189E+03 0.258E+03 -.772E-01 -.140E+00 -.523E-01 -.109E-05 0.328E-05 -.387E-06

-.150E+02 -.446E+03 -.196E+03 0.151E+02 0.447E+03 0.196E+03 -.688E-01 -.113E+01 0.991E-01 0.139E-05 -.261E-05 -.788E-06

-.548E+01 -.448E+03 0.204E+03 0.549E+01 0.449E+03 -.204E+03 -.487E-02 -.109E+01 -.125E+00 0.181E-06 -.108E-05 -.273E-05

-.913E+00 -.203E+03 0.267E+03 0.921E+00 0.203E+03 -.267E+03 -.910E-02 -.102E+00 -.316E-01 -.192E-06 0.995E-06 -.252E-06

-.163E+02 -.329E+03 -.218E+03 0.167E+02 0.329E+03 0.218E+03 -.360E+00 -.481E+00 0.423E-01 -.221E-05 -.217E-05 -.676E-06

-.291E+00 -.257E+03 -.194E+03 -.719E+00 0.249E+03 0.190E+03 0.109E+01 0.779E+01 0.488E+01 -.703E-05 0.238E-04 0.199E-04

0.529E+02 -.518E+03 -.137E+03 -.540E+02 0.522E+03 0.141E+03 0.106E+01 -.396E+01 -.382E+01 0.358E-05 -.462E-05 0.286E-05

-.487E+02 -.585E+03 -.446E+03 0.554E+02 0.636E+03 0.480E+03 -.669E+01 -.508E+02 -

.342E+02 -.110E-04 -.215E-04 -.627E-05

0.513E+01 0.276E+02 0.223E+02 -.298E-12 0.114E-12 0.307E-11 -.517E+01 -.276E+02 -.223E+02 -.152E-04 -.191E-04 0.249E-05

POSITION			TOTAL-FORCE (eV/Angst)		
1.24575	4.02870	5.43979	0.000053	0.001036	-0.000413
1.21024	4.07581	8.43726	-0.000974	0.002627	-0.001136
3.70862	4.02890	5.43965	0.000320	0.001907	-0.001098
3.67998	4.07733	8.43690	-0.004024	-0.000405	-0.002889
6.17157	4.02854	5.43942	0.000007	-0.000122	-0.001757
6.14482	4.08292	8.43295	-0.002821	-0.003288	-0.003184
8.63513	4.02801	5.43869	0.000793	-0.000426	-0.002008
8.60339	4.08732	8.43089	-0.000118	-0.001161	-0.002205
11.09928	4.02784	5.43885	0.000888	0.001990	-0.002715
11.06021	4.08619	8.43099	-0.001730	0.000723	-0.000630
13.56311	4.02807	5.43972	0.000345	0.001639	-0.001623
13.52141	4.08047	8.43349	0.000415	-0.002239	0.000308
2.44241	15.48073	8.85224	-0.000634	-0.005296	0.002334
0.01714	15.44624	5.32469	0.000352	0.001538	-0.001197

4.86040	15.47728	8.86623	0.001051	0.000257	-0.000307
2.48016	15.44854	5.27562	0.000368	-0.001193	-0.000518
4.94382	15.44925	5.24869	0.001772	-0.002965	0.000273
12.31531	15.48242	9.00211	-0.003760	0.000025	0.005725
9.86772	15.44556	5.34176	0.000461	-0.001090	0.000891
14.76279	15.48245	8.89951	-0.006208	-0.000554	0.005512
12.33384	15.44510	5.36128	0.001374	-0.003217	-0.001270
7.40743	15.44616	5.26463	0.002398	0.001618	0.001310
6.44846	16.34427	7.40648	-0.003117	-0.000537	0.001993
8.60064	16.47644	7.89249	0.005002	0.002163	0.004785
1.24544	5.11881	5.35500	0.000952	0.000161	-0.002448
2.44348	5.83889	8.62292	0.002451	-0.004416	0.001221
0.01380	5.79530	5.28573	0.002092	-0.002445	0.000470
1.21063	5.16420	8.54151	0.000264	-0.000515	-0.001905
2.44351	7.27931	8.74832	-0.000060	-0.001249	-0.000128
3.70866	5.11896	5.35390	-0.000417	-0.001621	0.000338
4.90800	5.84315	8.62123	-0.001087	0.003836	-0.000761
2.47701	5.79561	5.28397	0.001467	-0.000590	-0.002608
3.67679	5.16572	8.54000	-0.000117	0.001644	-0.000046
4.90764	7.28398	8.74777	0.000716	-0.000631	0.001023
6.17184	5.11860	5.35433	0.001490	0.000401	0.000897
7.37096	5.84929	8.62094	-0.000637	0.007120	-0.002441

4.94029	5.79548	5.28340	0.000620	-0.002681	-0.001175
6.14080	5.17108	8.53715	-0.002476	0.002541	0.002460
7.37071	7.28983	8.75132	-0.002016	0.001619	0.000141
8.63543	5.11820	5.35521	0.001253	0.001351	-0.001061
9.83233	5.85166	8.62337	0.002859	0.000699	-0.001090
7.40374	5.79498	5.28512	0.003471	-0.002684	-0.001340
8.60194	5.17528	8.53759	-0.001889	-0.000421	-0.000228
9.83204	7.29110	8.75719	-0.001714	-0.002632	-0.002437
11.09930	5.11814	5.35578	-0.000858	-0.003348	-0.001362
12.29449	5.84673	8.62385	0.000008	0.005782	-0.002205
9.86750	5.79468	5.28678	-0.000730	-0.000706	0.001548
11.06261	5.17409	8.53894	0.002672	0.002639	-0.000406
12.29428	7.28729	8.75533	-0.004551	0.001154	-0.001526
13.56278	5.11829	5.35605	0.002668	0.000529	-0.001976
14.75895	5.83988	8.62434	-0.000239	-0.002625	-0.002183
12.33118	5.79480	5.28692	-0.004491	-0.001450	0.002591
13.52535	5.16844	8.54022	-0.003476	0.003779	-0.001443
14.75917	7.28012	8.75179	0.000963	0.002577	-0.000694
0.01434	7.23830	5.19017	0.000093	-0.000201	0.000078
1.24689	9.38061	5.13160	0.000553	-0.001854	0.000001
1.21085	7.98059	8.79588	-0.000933	-0.000467	0.001528
2.44214	10.12243	8.87141	-0.000852	0.003334	-0.005003

0.01532	10.08686	5.14049	-0.002027	-0.000129	-0.002399
1.24606	7.94244	5.15775	0.002025	-0.002590	0.000829
1.21082	9.41592	8.85782	-0.000783	0.004347	0.000183
2.44072	11.55513	8.88414	-0.006026	-0.002822	0.001620
2.47747	7.23842	5.18585	0.002809	0.002883	0.001313
3.70997	9.38055	5.12566	-0.001077	-0.003001	0.000045
3.67534	7.98360	8.79349	-0.000577	0.001078	0.000960
4.90487	10.12925	8.87518	0.000276	-0.000198	0.000009
2.47867	10.08713	5.12695	-0.002250	0.001507	0.000764
3.70939	7.94242	5.15441	0.000838	-0.004007	-0.001699
3.67589	9.41970	8.85445	-0.001486	0.001935	-0.000154
4.90263	11.56506	8.89086	-0.000226	0.001429	0.000926
4.94085	7.23830	5.18552	-0.004699	0.002257	0.000832
6.17318	9.38002	5.13173	0.002028	0.002105	0.001832
6.13864	7.99044	8.79647	0.002477	-0.000285	-0.001685
7.36780	10.13760	8.89473	-0.001106	0.003365	0.000774
4.94196	10.08682	5.12700	0.004158	0.001480	-0.001154
6.17284	7.94199	5.15766	-0.000035	0.000562	0.003030
6.13939	9.42660	8.86164	0.000875	-0.000523	-0.002160
7.36410	11.57721	8.92935	-0.000475	-0.002956	0.003519
7.40426	7.23794	5.19012	0.002148	0.001772	0.001076
8.63700	9.37970	5.14543	-0.000537	0.002949	0.000955

8.60086	7.99568	8.80617	0.001079	-0.000420	-0.001086
9.83068	10.14286	8.92842	-0.002009	0.002627	-0.000681
7.40553	10.08627	5.14064	0.001228	-0.003558	0.003147
8.63637	7.94166	5.16555	0.002633	0.001801	-0.001409
8.60077	9.43254	8.88532	-0.006017	0.002272	-0.001292
9.82927	11.58244	9.00096	0.001429	0.003031	0.000981
9.86805	7.23787	5.19489	-0.000352	0.000107	-0.000213
11.10106	9.37979	5.15156	-0.003824	-0.001024	0.000658
11.06331	7.99411	8.80818	-0.000262	-0.001628	0.000133
12.29815	10.12943	8.90340	-0.001435	-0.001186	0.001216
9.86930	10.08593	5.15631	-0.005430	-0.001443	0.001407
11.10021	7.94175	5.16862	-0.000585	-0.003070	0.001389
11.06206	9.43062	8.88839	0.004678	0.001810	0.002095
12.30255	11.56557	8.94694	0.004129	0.000128	-0.000783
12.33169	7.23799	5.19447	-0.001026	0.000249	-0.001751
13.56437	9.38021	5.14435	0.000744	0.001650	-0.000575
13.52754	7.98555	8.80171	-0.000786	-0.002555	-0.003097
14.76233	10.12320	8.88285	-0.005178	0.000929	-0.001574
12.33257	10.08637	5.15511	0.002653	0.000554	-0.001541
13.56350	7.94214	5.16485	-0.000069	-0.000882	-0.000372
13.52731	9.42040	8.86925	-0.000050	0.003282	-0.000579
14.76430	11.55727	8.90646	-0.002223	-0.000842	0.001886

0.01611	11.52516	5.16621	-0.001070	-0.002567	0.000390
1.24770	13.67535	5.22209	0.001817	-0.002373	-0.002486
1.21217	12.26335	8.89409	0.000475	-0.000277	0.001167
2.43998	14.38728	8.86748	-0.002592	0.001042	0.000803
0.01699	14.35408	5.27295	-0.000405	-0.000577	-0.001961
1.24794	12.22963	5.17275	0.001071	0.000858	-0.001363
1.21434	13.70818	8.88771	0.002039	0.002139	0.003812
2.47958	11.52580	5.14547	-0.001603	-0.000190	-0.001479
3.71218	13.67636	5.19535	0.004631	0.000577	0.001061
3.66932	12.26248	8.88184	-0.002255	0.000062	-0.000592
4.89370	14.38589	8.86075	0.004040	-0.001010	-0.002745
2.48000	14.35596	5.23149	0.001304	-0.001117	0.001694
3.71150	12.23022	5.15602	0.000926	-0.004545	0.001006
3.66212	13.70366	8.87117	-0.005473	0.004091	-0.000619
4.94290	11.52542	5.14351	-0.000074	-0.001755	-0.001602
6.17627	13.67505	5.20032	0.000855	0.000587	0.000065
6.13145	12.27911	8.90591	0.005517	0.006096	0.004660
7.36614	14.42967	8.88203	0.000015	-0.002186	0.000454
4.94347	14.35627	5.21375	0.000105	-0.001923	0.001079
6.17493	12.22917	5.16623	-0.001406	-0.001043	0.001534
6.11879	13.72336	8.87765	0.006121	0.001689	0.000029
7.40625	11.52413	5.16368	0.000915	-0.003347	0.000351

8.63876	13.67323	5.24377	0.001914	0.002069	-0.001306
8.58939	12.29067	9.00208	-0.003074	0.001840	-0.001914
9.83855	14.39048	9.30305	-0.038707	0.002935	0.005987
7.40672	14.35386	5.23530	-0.001160	-0.000358	-0.000662
8.63820	12.22778	5.19800	0.000324	-0.001221	0.001037
8.55571	13.73596	9.04598	0.004576	-0.011247	0.001852
9.86985	11.52338	5.18893	0.001764	-0.001975	-0.000114
11.10099	13.67352	5.27669	0.003216	-0.000911	-0.001001
11.07378	12.27333	9.00891	-0.007104	0.003038	-0.001834
12.30694	14.38896	9.00333	-0.001397	-0.000397	0.000408
9.86934	14.35300	5.29564	0.002942	0.000081	0.000006
11.10161	12.22804	5.21650	-0.001095	-0.002708	0.001060
11.11464	13.70636	9.07877	0.010335	0.006002	0.001213
12.33326	11.52411	5.18815	-0.000917	0.000275	0.000534
13.56430	13.67399	5.25995	0.001544	-0.000086	0.000071
13.53626	12.26601	8.93587	-0.002220	0.004210	0.002242
14.76266	14.38906	8.90426	-0.003794	0.001709	0.003576
12.33397	14.35288	5.30710	0.002800	-0.001789	-0.001761
13.56505	12.22870	5.20105	0.000126	0.000108	-0.001136
13.54921	13.70690	8.94399	-0.001206	-0.004623	-0.000181
9.91126	15.53185	9.99472	0.085272	0.117122	0.079603
7.28864	16.40884	8.69813	0.004494	-0.005520	0.000451

10.04026 16.50365 10.64498 -0.049510 -0.117431 -0.078773

---

total drift: -0.046322 0.023736 -0.022868

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

---

free energy TOTEN = -1209.38892592 eV

energy without entropy= -1209.38892592 energy(sigma->0) = -1209.38892592

d Force = 0.4889757E-02[0.451E-03, 0.933E-02] d Energy = 0.4839720E-02 0.500E-04

d Force = 0.3634532E+01[0.367E+01, 0.360E+01] d Ewald = 0.3634270E+01 0.262E-03

POTLOK: cpu time 0.4253: real time 0.4261

---

stress matrix after NEB project (eV)

-17.75778 -0.24675 0.04210

-0.24675 -15.39663 0.38306

0.04210 0.38306 -19.10934

FORCES: max atom, RMS 0.165305 0.018401

FORCE total and by dimension 0.223097 0.117431

Stress total and by dimension 30.298197 19.109341

Finite differences progress:

Degree of freedom: 4/ 6

Displacement: 1/ 2

Total: 7/ 12

LATTYP: Found a simple orthorhombic cell.

ALAT = 14.7806000000

B/A-ratio = 1.2466138046

C/A-ratio = 1.4433717170

Lattice vectors:

A1 = (-14.7806000000, 0.0000000000, 0.0000000000)

A2 = (0.0000000000, 0.0000000000, -18.4257000000)

A3 = (0.0000000000, -21.3339000000, 0.0000000000)

Analysis of symmetry for initial positions (statically):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The static configuration has the point symmetry C_1 .

Analysis of symmetry for dynamics (positions and initial velocities):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The dynamic configuration has the point symmetry C_1 .

Analysis of constrained symmetry for selective dynamics:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The constrained configuration has the point symmetry C_1 .

Analysis of structural, dynamic, and magnetic symmetry:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The magnetic configuration has the point symmetry C_1 .

Subroutine INISYM returns: Found 1 space group operations

(whereof 1 operations are pure point group operations),

and found 1 'primitive' translations

KPOINTS: KPT-Resolved Value to Generate K-Mesh: 0

Automatic generation of k-mesh.

Space group operators:

irot det(A) alpha n_x n_y n_z tau_x tau_y tau_z

1 1.000000 0.000000 1.000000 0.000000 0.000000 0.000000 0.000000 0.000000

Subroutine IBZKPT returns following result:

==========

Found 1 irreducible k-points:

Following reciprocal coordinates:

Coordinates Weight

0.000000 0.000000 0.000000 1.000000

Following cartesian coordinates:

Coordinates Weight

0.000000 0.000000 0.000000 1.000000

WAVPRE: cpu time 0.1187: real time 0.1400

FEWALD: cpu time 0.0025: real time 0.0025

ORTHCH: cpu time 0.9987: real time 1.0021

LOOP+: cpu time 168.1882: real time 169.1781

---------- Iteration 9(1) ----------

POTLOK: cpu time 0.1688: real time 0.1795

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9312: real time 1.9369

RMM-DIIS: cpu time 7.1124: real time 7.1325

ORTHCH: cpu time 0.3527: real time 0.3536

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5262: real time 0.5277

MIXING: cpu time 0.0043: real time 0.0043

LOOP: cpu time 10.1060: real time 10.1448

eigenvalue-minimisations : 1926

total energy-change (2. order) :-0.1734973E-01 (-0.4931775E+00)

number of electron 518.9999717 magnetization 0.9999998

augmentation part 11.7335032 magnetization 0.0542805

Broyden mixing:

rms(total) = 0.37533E-01 rms(broyden)= 0.36933E-01

rms(prec) = 0.38397E-01

weight for this iteration 100.00

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.25642576

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79702159

PAW double counting = 52174.20513944 -52237.12224524

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.23745418

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.78847579 eV

energy without entropy = -1202.78847579 energy(sigma->0) = -1202.78847579

---------- Iteration 9(2) ----------

POTLOK: cpu time 0.1661: real time 0.1741

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9264: real time 1.9326

RMM-DIIS: cpu time 7.2788: real time 7.3071

ORTHCH: cpu time 0.3545: real time 0.3553

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5272: real time 0.5288

MIXING: cpu time 0.0048: real time 0.0048

LOOP: cpu time 10.2683: real time 10.3133

eigenvalue-minimisations : 1940

total energy-change (2. order) : 0.1619721E-01 (-0.3190486E-02)

number of electron 518.9999717 magnetization 0.9999998

augmentation part 11.7409495 magnetization 0.0542641

Broyden mixing:

rms(total) = 0.29615E-01 rms(broyden)= 0.29553E-01

rms(prec) = 0.31329E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 0.6684

0.6684

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.38119694

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.78206895

PAW double counting = 52175.80804047 -52238.71915954

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.08751988

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77227858 eV

energy without entropy = -1202.77227858 energy(sigma->0) = -1202.77227858

---------- Iteration 9(3) ----------

POTLOK: cpu time 0.1650: real time 0.1852

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9251: real time 1.9317

RMM-DIIS: cpu time 7.1128: real time 7.1490

ORTHCH: cpu time 0.3525: real time 0.3537

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5279: real time 0.5295

MIXING: cpu time 0.0050: real time 0.0050

LOOP: cpu time 10.0987: real time 10.1647

eigenvalue-minimisations : 1924

total energy-change (2. order) : 0.1335664E-02 (-0.1007045E-03)

number of electron 518.9999717 magnetization 0.9999998

augmentation part 11.7386796 magnetization 0.0542695

Broyden mixing:

rms(total) = 0.15109E-01 rms(broyden)= 0.15105E-01

rms(prec) = 0.15740E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3823

0.6750 2.0897

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.49145479

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79858338

PAW double counting = 52176.78977678 -52239.70615217

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.98718448

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77094292 eV

energy without entropy = -1202.77094292 energy(sigma->0) = -1202.77094292

---------- Iteration 9(4) ----------

POTLOK: cpu time 0.1646: real time 0.1826

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9351: real time 1.9416

RMM-DIIS: cpu time 7.1426: real time 7.1717

ORTHCH: cpu time 0.3529: real time 0.3539

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5276: real time 0.5294

MIXING: cpu time 0.0055: real time 0.0055

LOOP: cpu time 10.1388: real time 10.1951

eigenvalue-minimisations : 1926

total energy-change (2. order) :-0.3047246E-03 (-0.2111535E-03)

number of electron 518.9999717 magnetization 0.9999998

augmentation part 11.7362388 magnetization 0.0542774

Broyden mixing:

rms(total) = 0.92556E-02 rms(broyden)= 0.92409E-02

rms(prec) = 0.99766E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.2368

2.0591 0.8256 0.8256

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.68228853

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81393589

PAW double counting = 52178.93235672 -52241.85471189

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.80602819

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77124764 eV

energy without entropy = -1202.77124764 energy(sigma->0) = -1202.77124764

-- Iteration 9(5) --

POTLOK: cpu time 0.1646: real time 0.1673

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9261: real time 1.9324

RMM-DIIS: cpu time 6.9454: real time 6.9851

ORTHCH: cpu time 0.3531: real time 0.3541

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5276: real time 0.5293

MIXING: cpu time 0.0055: real time 0.0056

LOOP: cpu time 9.9326: real time 9.9842

eigenvalue-minimisations : 1904

total energy-change (2. order) : 0.1718227E-03 (-0.2217663E-04)

number of electron 518.9999717 magnetization 0.9999998

augmentation part 11.7374550 magnetization 0.0542733

Broyden mixing:

rms(total) = 0.18791E-02 rms(broyden)= 0.18717E-02

rms(prec) = 0.19947E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3455

2.0607 1.5529 0.8843 0.8843

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.65137255

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80667957

PAW double counting = 52178.89831957 -52241.81846607

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.83172471

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77107582 eV

energy without entropy = -1202.77107582 energy(sigma->0) = -1202.77107582

---------- Iteration 9(6) ----------

POTLOK: cpu time 0.1657: real time 0.1945

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9279: real time 1.9340

RMM-DIIS: cpu time 6.8415: real time 6.8734

ORTHCH: cpu time 0.3521: real time 0.3531

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5267: real time 0.5284

MIXING: cpu time 0.0058: real time 0.0059

LOOP: cpu time 9.8304: real time 9.9000

eigenvalue-minimisations : 1837

total energy-change (2. order) :-0.9360323E-05 (-0.2543957E-05)

number of electron 518.9999717 magnetization 0.9999998

augmentation part 11.7377575 magnetization 0.0542728

Broyden mixing:

rms(total) = 0.62766E-03 rms(broyden)= 0.62176E-03

rms(prec) = 0.67327E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3586

2.3728 1.7539 0.9211 0.9211 0.8240

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.66924929

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80544126

PAW double counting = 52179.05129183 -52241.97127589

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.81278145

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77108518 eV

energy without entropy = -1202.77108518 energy(sigma->0) = -1202.77108518

---------- Iteration 9(7) ----------

POTLOK: cpu time 0.1651: real time 0.1775

```
      SETDIJ:    cpu time       0.0101: real time       0.0101
      EDDIAG:    cpu time       1.9271: real time       1.9341
    RMM-DIIS:    cpu time       6.1134: real time       6.1323
      ORTHCH:    cpu time       0.3533: real time       0.3545
         DOS:    cpu time       0.0004: real time       0.0004
      CHARGE:    cpu time       0.5271: real time       0.5291
      MIXING:    cpu time       0.0059: real time       0.0059
      ----------------------------------------
        LOOP:    cpu time       9.1023: real time       9.1438

eigenvalue-minimisations    :    1663
total energy-change (2. order) :-0.4139642E-05    (-0.1532753E-06)
number of electron          518.9999717 magnetization             0.9999998
augmentation part             11.7376924 magnetization             0.0542725

Broyden mixing:
  rms(total) = 0.15188E-03        rms(broyden)= 0.15162E-03
  rms(prec ) = 0.20266E-03
  weight for this iteration          100.00

eigenvalues of (default mixing * dielectric matrix)
  average eigenvalue GAMMA=       1.3100
```

2.4904 1.6754 1.2257 0.8878 0.8878 0.6931

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.69077239

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80604697

PAW double counting = 52179.15307302 -52242.07332631

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.79159898

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77108932 eV

energy without entropy = -1202.77108932 energy(sigma->0) = -1202.77108932

---------- Iteration 9(8) ----------

POTLOK: cpu time 0.1664: real time 0.1717

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9290: real time 1.9351

RMM-DIIS: cpu time 5.2633: real time 5.2889

ORTHCH: cpu time 0.3519: real time 0.3529

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5266: real time 0.5282

MIXING: cpu time 0.0064: real time 0.0064

LOOP: cpu time 8.2541: real time 8.2937

eigenvalue-minimisations : 1442

total energy-change (2. order) :-0.2708715E-05 (-0.1569063E-07)

number of electron 518.9999717 magnetization 0.9999998

augmentation part 11.7376818 magnetization 0.0542725

Broyden mixing:

rms(total) = 0.11809E-03 rms(broyden)= 0.11804E-03

rms(prec) = 0.16395E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3616

2.5497 1.8725 1.6586 0.9329 0.9329 0.9223 0.6620

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.70036625

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80614204

PAW double counting = 52179.16946208 -52242.08974770

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.78207056

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77109203 eV

energy without entropy = -1202.77109203 energy(sigma->0) = -1202.77109203

---------- Iteration 9(9) ----------

POTLOK: cpu time 0.1624: real time 0.1638

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9264: real time 1.9324

RMM-DIIS: cpu time 5.3372: real time 5.3537

ORTHCH: cpu time 0.3541: real time 0.3551

DOS: cpu time 0.0007: real time 0.0007

CHARGE: cpu time 0.5270: real time 0.5288

MIXING: cpu time 0.0069: real time 0.0069

LOOP: cpu time 8.3248: real time 8.3515

eigenvalue-minimisations : 1456

total energy-change (2. order) :-0.5067712E-05 (-0.1921821E-07)

number of electron 518.9999717 magnetization 0.9999998

augmentation part 11.7377078 magnetization 0.0542725

Broyden mixing:

rms(total) = 0.82181E-04 rms(broyden)= 0.82023E-04

rms(prec) = 0.10997E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3779

2.7052 2.3668 1.6660 1.0773 0.9039 0.9039 0.7545 0.6454

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.71694638

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80608981

PAW double counting = 52179.17393062 -52242.09418614

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.76547337

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77109710 eV

energy without entropy = -1202.77109710 energy(sigma->0) = -1202.77109710

---------- Iteration 9(10) ----------

POTLOK: cpu time 0.1646: real time 0.1832

SETDIJ: cpu time 0.0100: real time 0.0101

```
      EDDIAG:  cpu time        1.9265: real time        1.9325
  RMM-DIIS:  cpu time        5.0499: real time        5.0721
     ORTHCH:  cpu time        0.3534: real time        0.3543
        DOS:  cpu time        0.0004: real time        0.0004
     CHARGE:  cpu time        0.5270: real time        0.5285
     MIXING:  cpu time        0.0074: real time        0.0074
     ----------------------------------------
       LOOP:  cpu time        8.0393: real time        8.0886

eigenvalue-minimisations  :  1372
total energy-change (2. order) :-0.3401743E-05  (-0.7747360E-08)
number of electron       518.9999717 magnetization             0.9999998
augmentation part         11.7377020 magnetization             0.0542724

Broyden mixing:
 rms(total) = 0.42582E-04        rms(broyden)= 0.42574E-04
 rms(prec ) = 0.65016E-04
 weight for this iteration        100.00

eigenvalues of (default mixing * dielectric matrix)
 average eigenvalue GAMMA=      1.4414
 3.1707   2.5124   1.6843   1.4549   0.9402   0.9402   0.9363   0.7068   0.6269
```

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.72846849

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80619806

PAW double counting = 52179.17114116 -52242.09141362

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.75404598

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77110050 eV

energy without entropy = -1202.77110050 energy(sigma->0) = -1202.77110050

---------- Iteration 9(11) ----------

POTLOK: cpu time 0.1638: real time 0.1758

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9270: real time 1.9333

RMM-DIIS: cpu time 5.1263: real time 5.1445

ORTHCH: cpu time 0.3529: real time 0.3538

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5268: real time 0.5282

MIXING: cpu time 0.0077: real time 0.0077

LOOP: cpu time 8.1148: real time 8.1537

eigenvalue-minimisations : 1411

total energy-change (2. order) :-0.3861001E-05 (-0.1241886E-07)

number of electron 518.9999717 magnetization 0.9999998

augmentation part 11.7376912 magnetization 0.0542723

Broyden mixing:

rms(total) = 0.45803E-04 rms(broyden)= 0.45756E-04

rms(prec) = 0.55507E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5395

4.0852 2.5470 2.0206 1.7704 0.9263 0.9263 0.9956 0.8253 0.6804 0.6181

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.74224850

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80633808

PAW double counting = 52179.16367385 -52242.08396786

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.74038829

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77110436 eV

energy without entropy = -1202.77110436 energy(sigma->0) = -1202.77110436

---------- Iteration 9(12) ----------

POTLOK: cpu time 0.1636: real time 0.1646

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9340: real time 1.9401

RMM-DIIS: cpu time 4.6911: real time 4.7304

ORTHCH: cpu time 0.3519: real time 0.3530

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5251: real time 0.5271

MIXING: cpu time 0.0076: real time 0.0076

LOOP: cpu time 7.6836: real time 7.7331

eigenvalue-minimisations : 1256

total energy-change (2. order) :-0.2120614E-05 (-0.3380649E-08)

number of electron 518.9999717 magnetization 0.9999998

augmentation part 11.7376960 magnetization 0.0542723

Broyden mixing:

rms(total) = 0.15520E-04 rms(broyden)= 0.15500E-04

rms(prec) = 0.22561E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6183

5.1089 2.5823 2.3305 1.7567 0.9484 0.9484 1.0031 1.0031 0.8278 0.6744

0.6175

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.74899295

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80634651

PAW double counting = 52179.15742871 -52242.07771417

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.73366294

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77110648 eV

energy without entropy = -1202.77110648 energy(sigma->0) = -1202.77110648

--- Iteration 9(13) ---

POTLOK: cpu time 0.1649: real time 0.1714

SETDIJ: cpu time 0.0103: real time 0.0103

```
      EDDIAG:  cpu time        1.9249: real time        1.9312
 RMM-DIIS:  cpu time        4.6482: real time        4.6631
      ORTHCH:  cpu time        0.3517: real time        0.3527
         DOS:  cpu time        0.0004: real time        0.0004
      CHARGE:  cpu time        0.5273: real time        0.5288
      MIXING:  cpu time        0.0077: real time        0.0077
      ----------------------------------------
        LOOP:  cpu time        7.6354: real time        7.6656

eigenvalue-minimisations  :  1230
total energy-change (2. order) :-0.1290311E-05  (-0.1693089E-08)
number of electron       518.9999717 magnetization             0.9999998
augmentation part         11.7376988 magnetization             0.0542723

Broyden mixing:
 rms(total) = 0.93735E-05        rms(broyden)= 0.93489E-05
 rms(prec ) = 0.13964E-04
 weight for this iteration         100.00

eigenvalues of (default mixing * dielectric matrix)
 average eigenvalue GAMMA=      1.6561
 5.8660   2.6321   2.3608   1.6136   1.6136   0.9455   0.9455   0.9923   0.8828   0.7392
```

0.6630 0.6183

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.75223280

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80634614

PAW double counting = 52179.15536535 -52242.07564561

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.73042921

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77110777 eV

energy without entropy = -1202.77110777 energy(sigma->0) = -1202.77110777

---------- Iteration 9(14) ----------

POTLOK: cpu time 0.1661: real time 0.1856

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9252: real time 1.9312

RMM-DIIS: cpu time 4.4064: real time 4.4204

ORTHCH: cpu time 0.3541: real time 0.3550

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5275: real time 0.5293

MIXING: cpu time 0.0083: real time 0.0083

LOOP: cpu time 7.3981: real time 7.4402

eigenvalue-minimisations : 1106

total energy-change (2. order) :-0.7251365E-06 (-0.5900080E-09)

number of electron 518.9999717 magnetization 0.9999998

augmentation part 11.7376982 magnetization 0.0542723

Broyden mixing:

rms(total) = 0.54163E-05 rms(broyden)= 0.54149E-05

rms(prec) = 0.90962E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7214

6.5229 2.6972 2.3239 2.1003 1.8620 1.0690 1.0690 0.9399 0.9399 0.8776

0.7114 0.6175 0.6482

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.75341963

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80635141

PAW double counting = 52179.15567500 -52242.07595609

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.72924756

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77110849 eV

energy without entropy = -1202.77110849 energy(sigma->0) = -1202.77110849

---------- Iteration 9(15) ----------

POTLOK: cpu time 0.1723: real time 0.1818

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9281: real time 1.9339

RMM-DIIS: cpu time 4.6068: real time 4.6194

ORTHCH: cpu time 0.3536: real time 0.3546

DOS: cpu time 0.0004: real time 0.0003

CHARGE: cpu time 0.5271: real time 0.5286

MIXING: cpu time 0.0087: real time 0.0087

LOOP: cpu time 7.6070: real time 7.6376

eigenvalue-minimisations : 1203

total energy-change (2. order) :-0.7044800E-06 (-0.7706298E-09)

number of electron 518.9999717 magnetization 0.9999998

augmentation part 11.7376977 magnetization 0.0542723

Broyden mixing:

rms(total) = 0.39530E-05 rms(broyden)= 0.39501E-05

rms(prec) = 0.57370E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7899

7.2710 3.3063 2.5428 2.1602 1.7329 1.1884 1.1884 0.9497 0.9497 0.9692

0.8454 0.6962 0.6184 0.6396

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.75428956

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80635021

PAW double counting = 52179.15639172 -52242.07667326

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.72837668

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77110920 eV

energy without entropy = -1202.77110920 energy(sigma->0) = -1202.77110920

---------- Iteration 9(16) ----------

POTLOK: cpu time 0.1705: real time 0.1715

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9310: real time 1.9376

RMM-DIIS: cpu time 4.2390: real time 4.2590

ORTHCH: cpu time 0.3557: real time 0.3566

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5275: real time 0.5292

MIXING: cpu time 0.0090: real time 0.0090

LOOP: cpu time 7.2429: real time 7.2733

eigenvalue-minimisations : 1044

total energy-change (2. order) :-0.2212691E-06 (-0.3020570E-09)

number of electron 518.9999717 magnetization 0.9999998

augmentation part 11.7376984 magnetization 0.0542723

Broyden mixing:

rms(total) = 0.32558E-05 rms(broyden)= 0.32522E-05

rms(prec) = 0.41645E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8413

7.7676 3.8844 2.5573 2.1913 1.8173 1.8173 1.0527 1.0527 0.9430 0.9430

0.8708 0.7782 0.6880 0.6202 0.6363

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.75450542

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80634214

PAW double counting = 52179.15634018 -52242.07662039

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.72815430

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77110942 eV

energy without entropy = -1202.77110942 energy(sigma->0) = -1202.77110942

---------- Iteration 9(17) ----------

POTLOK: cpu time 0.1660: real time 0.1719

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9285: real time 1.9347

RMM-DIIS: cpu time 4.1667: real time 4.1886

ORTHCH: cpu time 0.3571: real time 0.3583

DOS: cpu time 0.0003: real time 0.0003

LOOP: cpu time 6.6286: real time 6.6639

eigenvalue-minimisations : 963

total energy-change (2. order) :-0.8141069E-07 (-0.1034053E-09)

number of electron 518.9999717 magnetization 0.9999998

augmentation part 11.7376984 magnetization 0.0542723

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91329.99480157

-Hartree energ DENC = -107336.75447821

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80634141

PAW double counting = 52179.15622873 -52242.07650972

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.72818007

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77110950 eV

energy without entropy = -1202.77110950 energy(sigma->0) = -1202.77110950

---

average (electrostatic) potential at core

the test charge radii are 0.5201 0.6991 1.0621 0.7215

(the norm of the test charge is 1.0000)

1 -40.7525	2 -40.7504	3 -40.7518	4 -40.7505	5 -40.7525
6 -40.7547	7 -40.7522	8 -40.7599	9 -40.7518	10 -40.7595
11 -40.7532	12 -40.7553	13 -40.6496	14 -40.6957	15 -40.7691
16 -40.6978	17 -40.6914	18 -40.8625	19 -40.6788	20 -40.6669
21 -40.6883	22 -40.6609	23 -40.0814	24 -40.1261	25 -57.4586
26 -57.6697	27 -57.6566	28 -57.4684	29 -57.6632	30 -57.4585
31 -57.6695	32 -57.6562	33 -57.4664	34 -57.6680	35 -57.4593
36 -57.6713	37 -57.6562	38 -57.4686	39 -57.6740	40 -57.4584
41 -57.6754	42 -57.6564	43 -57.4735	44 -57.6885	45 -57.4584
46 -57.6743	47 -57.6572	48 -57.4738	49 -57.6796	50 -57.4596
51 -57.6710	52 -57.6569	53 -57.4714	54 -57.6660	55 -57.6364
56 -57.6624	57 -57.6867	58 -57.6830	59 -57.6661	60 -57.6689
61 -57.6897	62 -57.6744	63 -57.6366	64 -57.6618	65 -57.6888
66 -57.6944	67 -57.6643	68 -57.6687	69 -57.6935	70 -57.7007
71 -57.6361	72 -57.6632	73 -57.6965	74 -57.7216	75 -57.6652
76 -57.6693	77 -57.7058	78 -57.7514	79 -57.6363	80 -57.6658
81 -57.7102	82 -57.7519	83 -57.6685	84 -57.6708	85 -57.7372
86 -57.8413	87 -57.6387	88 -57.6665	89 -57.7121	90 -57.7167

91 -57.6732	92 -57.6711	93 -57.7420	94 -57.7591	95 -57.6371
96 -57.6647	97 -57.6958	98 -57.6903	99 -57.6705	100 -57.6698
101 -57.7075	102 -57.6856	103 -57.6599	104 -57.6305	105 -57.6452
106 -57.2894	107 -57.3876	108 -57.6308	109 -57.5971	110 -57.6588
111 -57.6304	112 -57.6418	113 -57.3083	114 -57.3933	115 -57.6300
116 -57.5989	117 -57.6580	118 -57.6221	119 -57.6979	120 -57.6825
121 -57.3869	122 -57.6288	123 -57.7089	124 -57.6590	125 -57.6249
126 -57.8338	127 -58.3274	128 -57.3602	129 -57.6341	130 -58.1448
131 -57.6669	132 -57.6342	133 -57.7995	134 -57.4164	135 -57.3715
136 -57.6381	137 -58.0765	138 -57.6634	139 -57.6299	140 -57.6709
141 -57.2987	142 -57.3777	143 -57.6334	144 -57.6475	145 -60.8509
146 -57.3124	147 -81.2833			

E-fermi : -2.3342 XC(G=0): -2.7343 alpha+bet : -2.2521

spin component 1

k-point 1 : 0.0000 0.0000 0.0000

band No. band energies occupation

1	-27.0132	1.00000
2	-21.5682	1.00000
3	-21.4713	1.00000
4	-21.0994	1.00000
5	-21.0684	1.00000
6	-21.0145	1.00000
7	-20.9785	1.00000
8	-20.9765	1.00000
9	-20.8908	1.00000
10	-20.5575	1.00000
11	-20.5031	1.00000
12	-20.4114	1.00000
13	-20.3978	1.00000
14	-20.1262	1.00000
15	-19.9756	1.00000
16	-19.7031	1.00000
17	-19.6273	1.00000
18	-19.5994	1.00000
19	-19.5837	1.00000
20	-19.5284	1.00000
21	-19.5266	1.00000
22	-19.4984	1.00000

23	-19.4809	1.00000
24	-19.1118	1.00000
25	-19.0751	1.00000
26	-18.9783	1.00000
27	-18.9646	1.00000
28	-18.9004	1.00000
29	-18.7333	1.00000
30	-18.5045	1.00000
31	-18.3589	1.00000
32	-18.2751	1.00000
33	-18.2519	1.00000
34	-18.1833	1.00000
35	-18.1812	1.00000
36	-18.0796	1.00000
37	-18.0758	1.00000
38	-17.5616	1.00000
39	-17.3131	1.00000
40	-17.2874	1.00000
41	-17.2825	1.00000
42	-17.2098	1.00000
43	-17.2033	1.00000
44	-17.1766	1.00000

45	-17.0226	1.00000
46	-16.9501	1.00000
47	-16.9324	1.00000
48	-16.8930	1.00000
49	-16.8911	1.00000
50	-16.8499	1.00000
51	-16.8415	1.00000
52	-16.8209	1.00000
53	-16.8187	1.00000
54	-16.7292	1.00000
55	-16.7260	1.00000
56	-16.1773	1.00000
57	-15.7294	1.00000
58	-15.6918	1.00000
59	-15.6601	1.00000
60	-15.6368	1.00000
61	-15.6160	1.00000
62	-15.5535	1.00000
63	-15.5496	1.00000
64	-15.1747	1.00000
65	-14.8095	1.00000
66	-14.6083	1.00000

67	-14.5779	1.00000
68	-14.5347	1.00000
69	-14.4981	1.00000
70	-14.4683	1.00000
71	-14.4422	1.00000
72	-14.3337	1.00000
73	-14.3054	1.00000
74	-14.2795	1.00000
75	-14.2719	1.00000
76	-14.1823	1.00000
77	-14.1784	1.00000
78	-13.8898	1.00000
79	-13.7597	1.00000
80	-13.5933	1.00000
81	-13.5482	1.00000
82	-13.5292	1.00000
83	-13.4975	1.00000
84	-13.4457	1.00000
85	-13.3639	1.00000
86	-13.3453	1.00000
87	-13.1888	1.00000
88	-12.7862	1.00000

89	-12.7593	1.00000
90	-12.7272	1.00000
91	-12.6959	1.00000
92	-12.6861	1.00000
93	-12.6237	1.00000
94	-12.4609	1.00000
95	-12.4461	1.00000
96	-12.3818	1.00000
97	-12.3238	1.00000
98	-12.2128	1.00000
99	-12.2032	1.00000
100	-12.1649	1.00000
101	-11.9489	1.00000
102	-11.6848	1.00000
103	-11.6281	1.00000
104	-11.6109	1.00000
105	-11.5803	1.00000
106	-11.1072	1.00000
107	-11.0758	1.00000
108	-10.8987	1.00000
109	-10.8875	1.00000
110	-10.8322	1.00000

111	-10.7106	1.00000
112	-10.6804	1.00000
113	-10.6623	1.00000
114	-10.6464	1.00000
115	-10.5892	1.00000
116	-10.5808	1.00000
117	-10.5715	1.00000
118	-10.5677	1.00000
119	-10.5260	1.00000
120	-10.5252	1.00000
121	-10.5104	1.00000
122	-10.5026	1.00000
123	-10.3784	1.00000
124	-10.2946	1.00000
125	-10.2566	1.00000
126	-10.1875	1.00000
127	-10.1863	1.00000
128	-10.0816	1.00000
129	-10.0395	1.00000
130	-9.8918	1.00000
131	-9.8657	1.00000
132	-9.7945	1.00000

133	-9.7859	1.00000
134	-9.7585	1.00000
135	-9.6933	1.00000
136	-9.4500	1.00000
137	-9.4254	1.00000
138	-9.3949	1.00000
139	-9.3878	1.00000
140	-9.3798	1.00000
141	-9.3691	1.00000
142	-9.3103	1.00000
143	-9.3039	1.00000
144	-9.3001	1.00000
145	-9.2852	1.00000
146	-9.2702	1.00000
147	-9.0919	1.00000
148	-9.0041	1.00000
149	-8.9873	1.00000
150	-8.9569	1.00000
151	-8.9563	1.00000
152	-8.7929	1.00000
153	-8.7454	1.00000
154	-8.7342	1.00000

155	-8.7177	1.00000
156	-8.7085	1.00000
157	-8.6869	1.00000
158	-8.6779	1.00000
159	-8.6682	1.00000
160	-8.6535	1.00000
161	-8.5943	1.00000
162	-8.5825	1.00000
163	-8.5759	1.00000
164	-8.5675	1.00000
165	-8.4875	1.00000
166	-8.4570	1.00000
167	-8.4356	1.00000
168	-8.3451	1.00000
169	-8.2971	1.00000
170	-8.2745	1.00000
171	-8.2634	1.00000
172	-8.2329	1.00000
173	-8.2318	1.00000
174	-8.1512	1.00000
175	-8.1448	1.00000
176	-8.0773	1.00000

177	-8.0440	1.00000
178	-8.0258	1.00000
179	-8.0213	1.00000
180	-7.9727	1.00000
181	-7.9641	1.00000
182	-7.9240	1.00000
183	-7.9002	1.00000
184	-7.8847	1.00000
185	-7.8719	1.00000
186	-7.8003	1.00000
187	-7.7969	1.00000
188	-7.7471	1.00000
189	-7.7102	1.00000
190	-7.6658	1.00000
191	-7.5994	1.00000
192	-7.5844	1.00000
193	-7.5754	1.00000
194	-7.5468	1.00000
195	-7.4802	1.00000
196	-7.4796	1.00000
197	-7.4279	1.00000
198	-7.3239	1.00000

199	-7.2489	1.00000
200	-7.1551	1.00000
201	-7.0659	1.00000
202	-7.0416	1.00000
203	-7.0277	1.00000
204	-7.0130	1.00000
205	-6.9961	1.00000
206	-6.9892	1.00000
207	-6.9749	1.00000
208	-6.8661	1.00000
209	-6.8202	1.00000
210	-6.8011	1.00000
211	-6.7926	1.00000
212	-6.7316	1.00000
213	-6.6859	1.00000
214	-6.4705	1.00000
215	-6.4246	1.00000
216	-6.3956	1.00000
217	-6.3907	1.00000
218	-6.3736	1.00000
219	-6.3720	1.00000
220	-6.3167	1.00000

221	-6.3068	1.00000
222	-6.2364	1.00000
223	-6.2292	1.00000
224	-6.2288	1.00000
225	-6.0771	1.00000
226	-6.0372	1.00000
227	-5.7921	1.00000
228	-5.7518	1.00000
229	-5.6934	1.00000
230	-5.6407	1.00000
231	-5.6366	1.00000
232	-5.5585	1.00000
233	-5.5299	1.00000
234	-5.4673	1.00000
235	-5.4388	1.00000
236	-5.1647	1.00000
237	-5.0582	1.00000
238	-5.0500	1.00000
239	-5.0178	1.00000
240	-4.9885	1.00000
241	-4.9098	1.00000
242	-4.8531	1.00000

243	-4.8220	1.00000
244	-4.7893	1.00000
245	-4.6802	1.00000
246	-4.5722	1.00000
247	-4.5708	1.00000
248	-4.5051	1.00000
249	-4.4451	1.00000
250	-4.3833	1.00000
251	-4.2924	1.00000
252	-4.2653	1.00000
253	-4.2123	1.00000
254	-3.5582	1.00000
255	-3.3541	1.00000
256	-3.2002	1.00000
257	-2.9389	1.00000
258	-2.8479	1.00000
259	-2.8232	1.00000
260	-2.6062	1.00000
261	-1.9082	0.00000
262	-1.7672	0.00000
263	-1.7184	0.00000
264	-1.3435	0.00000

265	-1.2981	0.00000
266	-1.1864	0.00000
267	-0.7436	0.00000
268	-0.5842	0.00000
269	-0.5012	0.00000
270	-0.3074	0.00000
271	-0.3053	0.00000
272	-0.2896	0.00000
273	-0.1825	0.00000
274	-0.0573	0.00000
275	-0.0488	0.00000
276	-0.0098	0.00000
277	0.0354	0.00000
278	0.0850	0.00000
279	0.1734	0.00000
280	0.2208	0.00000
281	0.2485	0.00000
282	0.4210	0.00000
283	0.4485	0.00000
284	0.4821	0.00000
285	0.5983	0.00000
286	0.6757	0.00000

287	0.8190	0.00000
288	0.8735	0.00000
289	1.0465	0.00000
290	1.0846	0.00000
291	1.1210	0.00000
292	1.1629	0.00000
293	1.2234	0.00000
294	1.2445	0.00000
295	1.2875	0.00000
296	1.3142	0.00000
297	1.3463	0.00000
298	1.4117	0.00000
299	1.4658	0.00000
300	1.4836	0.00000
301	1.5531	0.00000
302	1.5869	0.00000
303	1.6252	0.00000
304	1.6777	0.00000
305	1.7508	0.00000
306	1.7634	0.00000
307	1.8735	0.00000
308	1.8950	0.00000

309	1.9051	0.00000
310	1.9135	0.00000
311	2.1235	0.00000
312	2.1868	0.00000
313	2.2085	0.00000
314	2.2355	0.00000
315	2.2758	0.00000
316	2.2918	0.00000
317	2.3315	0.00000
318	2.3537	0.00000
319	2.3723	0.00000
320	2.3977	0.00000
321	2.4204	0.00000
322	2.4300	0.00000
323	2.4402	0.00000
324	2.4535	0.00000
325	2.4616	0.00000
326	2.5239	0.00000
327	2.5373	0.00000
328	2.7010	0.00000
329	2.7286	0.00000
330	2.7533	0.00000

331	2.7565	0.00000
332	2.7644	0.00000
333	2.8147	0.00000
334	2.8342	0.00000
335	2.8589	0.00000
336	2.8912	0.00000
337	2.9243	0.00000
338	2.9464	0.00000
339	2.9785	0.00000
340	3.0051	0.00000
341	3.0341	0.00000
342	3.0443	0.00000
343	3.0660	0.00000
344	3.0849	0.00000
345	3.1498	0.00000
346	3.1630	0.00000
347	3.1797	0.00000
348	3.1920	0.00000
349	3.3005	0.00000
350	3.3226	0.00000
351	3.3520	0.00000
352	3.3673	0.00000

353	3.3895	0.00000
354	3.4326	0.00000
355	3.4763	0.00000
356	3.4851	0.00000
357	3.4857	0.00000
358	3.4986	0.00000
359	3.6342	0.00000
360	3.6730	0.00000
361	3.6859	0.00000
362	3.7322	0.00000
363	3.7515	0.00000
364	3.7589	0.00000
365	3.7721	0.00000
366	3.7936	0.00000
367	3.8121	0.00000
368	3.8341	0.00000
369	3.8382	0.00000
370	3.8519	0.00000
371	3.8767	0.00000
372	3.8838	0.00000
373	3.9101	0.00000
374	3.9241	0.00000

375	3.9340	0.00000
376	3.9576	0.00000
377	3.9726	0.00000
378	3.9838	0.00000
379	4.0163	0.00000
380	4.0697	0.00000
381	4.1646	0.00000
382	4.2466	0.00000
383	4.2576	0.00000
384	4.2582	0.00000
385	4.2851	0.00000
386	4.3130	0.00000
387	4.3277	0.00000
388	4.3410	0.00000
389	4.3712	0.00000
390	4.3810	0.00000
391	4.4174	0.00000
392	4.4444	0.00000
393	4.4686	0.00000
394	4.4803	0.00000
395	4.4865	0.00000
396	4.4963	0.00000

397	4.5173	0.00000
398	4.5504	0.00000
399	4.5907	0.00000
400	4.6078	0.00000
401	4.6273	0.00000
402	4.6429	0.00000
403	4.6568	0.00000
404	4.6796	0.00000
405	4.7040	0.00000
406	4.7317	0.00000
407	4.7465	0.00000
408	4.7670	0.00000
409	4.7832	0.00000
410	4.7835	0.00000
411	4.7972	0.00000
412	4.8284	0.00000
413	4.8632	0.00000
414	4.8722	0.00000
415	4.8977	0.00000
416	4.9312	0.00000
417	4.9835	0.00000
418	5.0045	0.00000

419	5.0105	0.00000
420	5.0350	0.00000
421	5.0392	0.00000
422	5.0651	0.00000
423	5.0818	0.00000
424	5.1143	0.00000
425	5.1173	0.00000
426	5.1365	0.00000
427	5.1409	0.00000
428	5.1539	0.00000
429	5.1753	0.00000
430	5.1850	0.00000
431	5.1878	0.00000
432	5.2154	0.00000
433	5.2353	0.00000
434	5.2408	0.00000
435	5.2558	0.00000
436	5.2895	0.00000
437	5.2956	0.00000
438	5.3088	0.00000
439	5.3317	0.00000
440	5.3493	0.00000

441	5.3670	0.00000
442	5.3736	0.00000
443	5.3928	0.00000
444	5.4210	0.00000
445	5.4533	0.00000
446	5.4640	0.00000
447	5.4816	0.00000
448	5.4943	0.00000
449	5.5187	0.00000
450	5.5499	0.00000
451	5.5691	0.00000
452	5.5752	0.00000
453	5.5954	0.00000
454	5.6155	0.00000
455	5.6577	0.00000
456	5.6813	0.00000
457	5.7094	0.00000
458	5.7230	0.00000
459	5.7436	0.00000
460	5.7575	0.00000
461	5.7815	0.00000
462	5.7895	0.00000

463	5.7951	0.00000
464	5.8009	0.00000
465	5.8073	0.00000
466	5.8232	0.00000
467	5.8426	0.00000
468	5.8538	0.00000
469	5.8732	0.00000
470	5.8814	0.00000
471	5.8859	0.00000
472	5.9092	0.00000
473	5.9144	0.00000
474	5.9412	0.00000
475	5.9507	0.00000
476	5.9695	0.00000
477	5.9746	0.00000
478	5.9986	0.00000
479	6.0082	0.00000
480	6.0630	0.00000

spin component 2

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-27.0065	1.00000
2	-21.5671	1.00000
3	-21.4697	1.00000
4	-21.0975	1.00000
5	-21.0675	1.00000
6	-21.0118	1.00000
7	-20.9770	1.00000
8	-20.9746	1.00000
9	-20.8803	1.00000
10	-20.5546	1.00000
11	-20.4997	1.00000
12	-20.4003	1.00000
13	-20.3882	1.00000
14	-20.1221	1.00000
15	-19.9525	1.00000
16	-19.7004	1.00000
17	-19.6260	1.00000
18	-19.5973	1.00000
19	-19.5773	1.00000
20	-19.5271	1.00000
21	-19.5249	1.00000

22	-19.4758	1.00000
23	-19.4614	1.00000
24	-19.1094	1.00000
25	-19.0727	1.00000
26	-18.9684	1.00000
27	-18.9551	1.00000
28	-18.8957	1.00000
29	-18.7037	1.00000
30	-18.5015	1.00000
31	-18.3519	1.00000
32	-18.2470	1.00000
33	-18.2268	1.00000
34	-18.1781	1.00000
35	-18.1758	1.00000
36	-18.0595	1.00000
37	-18.0562	1.00000
38	-17.5582	1.00000
39	-17.2969	1.00000
40	-17.2868	1.00000
41	-17.2732	1.00000
42	-17.2074	1.00000
43	-17.2064	1.00000

44	-17.1737	1.00000
45	-17.0186	1.00000
46	-16.9412	1.00000
47	-16.9220	1.00000
48	-16.8704	1.00000
49	-16.8693	1.00000
50	-16.8290	1.00000
51	-16.8226	1.00000
52	-16.8176	1.00000
53	-16.8152	1.00000
54	-16.7309	1.00000
55	-16.7249	1.00000
56	-16.1747	1.00000
57	-15.7287	1.00000
58	-15.6574	1.00000
59	-15.6432	1.00000
60	-15.6208	1.00000
61	-15.5663	1.00000
62	-15.5276	1.00000
63	-15.5249	1.00000
64	-15.1710	1.00000
65	-14.8073	1.00000

66	-14.6061	1.00000
67	-14.5603	1.00000
68	-14.5001	1.00000
69	-14.4983	1.00000
70	-14.4643	1.00000
71	-14.4378	1.00000
72	-14.3303	1.00000
73	-14.2977	1.00000
74	-14.2678	1.00000
75	-14.2636	1.00000
76	-14.1642	1.00000
77	-14.1608	1.00000
78	-13.8889	1.00000
79	-13.7573	1.00000
80	-13.5907	1.00000
81	-13.5376	1.00000
82	-13.5181	1.00000
83	-13.4940	1.00000
84	-13.4440	1.00000
85	-13.3434	1.00000
86	-13.3408	1.00000
87	-13.1872	1.00000

88	-12.7799	1.00000
89	-12.7498	1.00000
90	-12.7183	1.00000
91	-12.6773	1.00000
92	-12.6704	1.00000
93	-12.6215	1.00000
94	-12.4484	1.00000
95	-12.4312	1.00000
96	-12.3782	1.00000
97	-12.3230	1.00000
98	-12.2082	1.00000
99	-12.1980	1.00000
100	-12.1633	1.00000
101	-11.9461	1.00000
102	-11.6819	1.00000
103	-11.6122	1.00000
104	-11.5917	1.00000
105	-11.5726	1.00000
106	-11.1048	1.00000
107	-11.0733	1.00000
108	-10.8895	1.00000
109	-10.8770	1.00000

110	-10.8292	1.00000
111	-10.7046	1.00000
112	-10.6793	1.00000
113	-10.6593	1.00000
114	-10.6415	1.00000
115	-10.5812	1.00000
116	-10.5738	1.00000
117	-10.5687	1.00000
118	-10.5647	1.00000
119	-10.5154	1.00000
120	-10.5145	1.00000
121	-10.5012	1.00000
122	-10.4966	1.00000
123	-10.3775	1.00000
124	-10.2936	1.00000
125	-10.2557	1.00000
126	-10.1840	1.00000
127	-10.1828	1.00000
128	-10.0694	1.00000
129	-10.0342	1.00000
130	-9.8890	1.00000
131	-9.8635	1.00000

132	-9.7867	1.00000
133	-9.7769	1.00000
134	-9.7556	1.00000
135	-9.6910	1.00000
136	-9.4483	1.00000
137	-9.4219	1.00000
138	-9.3837	1.00000
139	-9.3790	1.00000
140	-9.3724	1.00000
141	-9.3593	1.00000
142	-9.3079	1.00000
143	-9.3008	1.00000
144	-9.2993	1.00000
145	-9.2845	1.00000
146	-9.2478	1.00000
147	-9.0907	1.00000
148	-9.0006	1.00000
149	-8.9822	1.00000
150	-8.9437	1.00000
151	-8.9424	1.00000
152	-8.7904	1.00000
153	-8.7374	1.00000

154	-8.7318	1.00000
155	-8.7122	1.00000
156	-8.7053	1.00000
157	-8.6698	1.00000
158	-8.6635	1.00000
159	-8.6560	1.00000
160	-8.6528	1.00000
161	-8.5770	1.00000
162	-8.5708	1.00000
163	-8.5659	1.00000
164	-8.5487	1.00000
165	-8.4871	1.00000
166	-8.4564	1.00000
167	-8.4340	1.00000
168	-8.3423	1.00000
169	-8.2939	1.00000
170	-8.2729	1.00000
171	-8.2329	1.00000
172	-8.2291	1.00000
173	-8.2271	1.00000
174	-8.1411	1.00000
175	-8.1335	1.00000

176	-8.0741	1.00000
177	-8.0419	1.00000
178	-8.0129	1.00000
179	-8.0069	1.00000
180	-7.9682	1.00000
181	-7.9591	1.00000
182	-7.9199	1.00000
183	-7.8906	1.00000
184	-7.8709	1.00000
185	-7.8631	1.00000
186	-7.7915	1.00000
187	-7.7876	1.00000
188	-7.7376	1.00000
189	-7.6786	1.00000
190	-7.6358	1.00000
191	-7.5971	1.00000
192	-7.5765	1.00000
193	-7.5543	1.00000
194	-7.5395	1.00000
195	-7.4721	1.00000
196	-7.4720	1.00000
197	-7.4269	1.00000

198	-7.3230	1.00000
199	-7.2356	1.00000
200	-7.1520	1.00000
201	-7.0551	1.00000
202	-7.0360	1.00000
203	-7.0154	1.00000
204	-6.9850	1.00000
205	-6.9771	1.00000
206	-6.9719	1.00000
207	-6.9406	1.00000
208	-6.8624	1.00000
209	-6.8159	1.00000
210	-6.7950	1.00000
211	-6.7875	1.00000
212	-6.7248	1.00000
213	-6.6765	1.00000
214	-6.4672	1.00000
215	-6.3946	1.00000
216	-6.3825	1.00000
217	-6.3779	1.00000
218	-6.3626	1.00000
219	-6.3381	1.00000

220	-6.3030	1.00000
221	-6.2753	1.00000
222	-6.2291	1.00000
223	-6.2277	1.00000
224	-6.2221	1.00000
225	-6.0465	1.00000
226	-6.0086	1.00000
227	-5.7558	1.00000
228	-5.7111	1.00000
229	-5.6918	1.00000
230	-5.6353	1.00000
231	-5.6223	1.00000
232	-5.5436	1.00000
233	-5.5229	1.00000
234	-5.4408	1.00000
235	-5.4114	1.00000
236	-5.1425	1.00000
237	-5.0597	1.00000
238	-5.0257	1.00000
239	-5.0219	1.00000
240	-4.9590	1.00000
241	-4.8770	1.00000

242	-4.8539	1.00000
243	-4.8023	1.00000
244	-4.7773	1.00000
245	-4.6499	1.00000
246	-4.5783	1.00000
247	-4.5752	1.00000
248	-4.4752	1.00000
249	-4.4208	1.00000
250	-4.3944	1.00000
251	-4.2962	1.00000
252	-4.2264	1.00000
253	-4.1749	1.00000
254	-3.5318	1.00000
255	-3.3087	1.00000
256	-3.1408	1.00000
257	-2.9439	1.00000
258	-2.7988	1.00000
259	-2.7396	1.00000
260	-2.0600	0.00000
261	-1.9142	0.00000
262	-1.7220	0.00000
263	-1.6784	0.00000

264	-1.2865	0.00000
265	-1.2750	0.00000
266	-1.1545	0.00000
267	-0.7223	0.00000
268	-0.5835	0.00000
269	-0.5087	0.00000
270	-0.2803	0.00000
271	-0.2773	0.00000
272	-0.2594	0.00000
273	-0.1558	0.00000
274	-0.0569	0.00000
275	-0.0477	0.00000
276	0.0140	0.00000
277	0.0405	0.00000
278	0.0799	0.00000
279	0.2085	0.00000
280	0.2559	0.00000
281	0.2801	0.00000
282	0.4350	0.00000
283	0.4524	0.00000
284	0.4832	0.00000
285	0.6030	0.00000

286	0.6960	0.00000
287	0.8219	0.00000
288	0.8804	0.00000
289	1.0543	0.00000
290	1.1038	0.00000
291	1.1427	0.00000
292	1.1775	0.00000
293	1.2321	0.00000
294	1.2506	0.00000
295	1.3086	0.00000
296	1.3199	0.00000
297	1.3600	0.00000
298	1.4306	0.00000
299	1.4785	0.00000
300	1.5012	0.00000
301	1.5773	0.00000
302	1.6032	0.00000
303	1.6537	0.00000
304	1.6864	0.00000
305	1.7582	0.00000
306	1.7736	0.00000
307	1.8774	0.00000

308	1.9004	0.00000
309	1.9083	0.00000
310	1.9214	0.00000
311	2.1398	0.00000
312	2.1979	0.00000
313	2.2202	0.00000
314	2.2541	0.00000
315	2.2895	0.00000
316	2.2964	0.00000
317	2.3368	0.00000
318	2.3614	0.00000
319	2.3831	0.00000
320	2.4079	0.00000
321	2.4286	0.00000
322	2.4353	0.00000
323	2.4512	0.00000
324	2.4585	0.00000
325	2.4673	0.00000
326	2.5265	0.00000
327	2.5431	0.00000
328	2.7061	0.00000
329	2.7347	0.00000

330	2.7535	0.00000
331	2.7594	0.00000
332	2.7729	0.00000
333	2.8291	0.00000
334	2.8473	0.00000
335	2.8718	0.00000
336	2.9025	0.00000
337	2.9329	0.00000
338	2.9559	0.00000
339	2.9833	0.00000
340	3.0067	0.00000
341	3.0380	0.00000
342	3.0512	0.00000
343	3.0717	0.00000
344	3.0924	0.00000
345	3.1523	0.00000
346	3.1716	0.00000
347	3.1885	0.00000
348	3.2001	0.00000
349	3.3062	0.00000
350	3.3274	0.00000
351	3.3603	0.00000

352	3.3708	0.00000
353	3.3927	0.00000
354	3.4381	0.00000
355	3.4816	0.00000
356	3.4916	0.00000
357	3.4944	0.00000
358	3.5051	0.00000
359	3.6392	0.00000
360	3.6769	0.00000
361	3.6982	0.00000
362	3.7380	0.00000
363	3.7552	0.00000
364	3.7608	0.00000
365	3.7770	0.00000
366	3.7984	0.00000
367	3.8149	0.00000
368	3.8413	0.00000
369	3.8475	0.00000
370	3.8661	0.00000
371	3.8805	0.00000
372	3.8932	0.00000
373	3.9209	0.00000

374	3.9359	0.00000
375	3.9487	0.00000
376	3.9594	0.00000
377	3.9828	0.00000
378	3.9865	0.00000
379	4.0222	0.00000
380	4.0791	0.00000
381	4.1710	0.00000
382	4.2595	0.00000
383	4.2621	0.00000
384	4.2688	0.00000
385	4.2928	0.00000
386	4.3211	0.00000
387	4.3343	0.00000
388	4.3502	0.00000
389	4.3811	0.00000
390	4.3858	0.00000
391	4.4232	0.00000
392	4.4485	0.00000
393	4.4737	0.00000
394	4.4834	0.00000
395	4.4929	0.00000

396	4.4991	0.00000
397	4.5207	0.00000
398	4.5549	0.00000
399	4.5938	0.00000
400	4.6105	0.00000
401	4.6290	0.00000
402	4.6464	0.00000
403	4.6598	0.00000
404	4.6855	0.00000
405	4.7088	0.00000
406	4.7375	0.00000
407	4.7515	0.00000
408	4.7704	0.00000
409	4.7867	0.00000
410	4.7890	0.00000
411	4.8029	0.00000
412	4.8332	0.00000
413	4.8684	0.00000
414	4.8852	0.00000
415	4.9029	0.00000
416	4.9418	0.00000
417	4.9932	0.00000

418	5.0099	0.00000
419	5.0128	0.00000
420	5.0383	0.00000
421	5.0444	0.00000
422	5.0694	0.00000
423	5.0860	0.00000
424	5.1177	0.00000
425	5.1214	0.00000
426	5.1406	0.00000
427	5.1442	0.00000
428	5.1704	0.00000
429	5.1799	0.00000
430	5.1887	0.00000
431	5.1927	0.00000
432	5.2204	0.00000
433	5.2378	0.00000
434	5.2440	0.00000
435	5.2615	0.00000
436	5.2980	0.00000
437	5.3029	0.00000
438	5.3119	0.00000
439	5.3361	0.00000

440	5.3532	0.00000
441	5.3708	0.00000
442	5.3812	0.00000
443	5.3955	0.00000
444	5.4292	0.00000
445	5.4595	0.00000
446	5.4706	0.00000
447	5.4871	0.00000
448	5.4988	0.00000
449	5.5257	0.00000
450	5.5680	0.00000
451	5.5747	0.00000
452	5.5947	0.00000
453	5.6076	0.00000
454	5.6252	0.00000
455	5.6700	0.00000
456	5.6920	0.00000
457	5.7188	0.00000
458	5.7274	0.00000
459	5.7479	0.00000
460	5.7626	0.00000
461	5.7896	0.00000

462	5.7926	0.00000
463	5.7981	0.00000
464	5.8041	0.00000
465	5.8203	0.00000
466	5.8254	0.00000
467	5.8545	0.00000
468	5.8610	0.00000
469	5.8825	0.00000
470	5.8867	0.00000
471	5.8912	0.00000
472	5.9082	0.00000
473	5.9214	0.00000
474	5.9494	0.00000
475	5.9540	0.00000
476	5.9704	0.00000
477	5.9767	0.00000
478	5.9926	0.00000
479	6.0137	0.00000
480	6.0463	0.00000

---

soft charge-density along one line, spin component 1

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

soft charge-density along one line, spin component 2

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

pseudopotential strength for first ion, spin component: 1

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

pseudopotential strength for first ion, spin component: 2

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

total augmentation occupancy for first ion, spin component: 1

3.579 -0.646 0.444 -0.034 -0.000

-0.646 0.130 -0.082 0.006 0.000

0.444 -0.082 0.056 -0.003 -0.000

-0.034 0.006 -0.003 0.011 0.000

-0.000 0.000 -0.000 0.000 0.007

total augmentation occupancy for first ion, spin component: 2

-0.000 0.000 -0.000 0.000 0.000

0.000 -0.000 0.000 -0.000 -0.000

-0.000 0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

---------- aborting loop because EDIFF is reached ----------

total charge

# of ion	s	p	d	tot
1	0.646	0.043	0.000	0.690
2	0.646	0.043	0.000	0.690
3	0.646	0.043	0.000	0.690
4	0.646	0.043	0.000	0.690
5	0.646	0.043	0.000	0.690
6	0.646	0.043	0.000	0.690
7	0.646	0.043	0.000	0.690
8	0.646	0.043	0.000	0.690
9	0.646	0.043	0.000	0.690
10	0.646	0.043	0.000	0.690
11	0.646	0.043	0.000	0.690
12	0.646	0.043	0.000	0.690
13	0.646	0.043	0.000	0.689
14	0.646	0.043	0.000	0.689
15	0.648	0.045	0.000	0.693
16	0.646	0.043	0.000	0.689
17	0.646	0.043	0.000	0.689
18	0.646	0.043	0.000	0.689

19	0.646	0.043	0.000	0.689
20	0.646	0.043	0.000	0.689
21	0.646	0.043	0.000	0.689
22	0.646	0.044	0.000	0.690
23	0.542	0.015	0.000	0.557
24	0.541	0.015	0.000	0.556
25	0.870	1.763	0.000	2.633
26	0.867	1.785	0.000	2.653
27	0.867	1.786	0.000	2.653
28	0.870	1.762	0.000	2.632
29	0.865	1.783	0.000	2.648
30	0.870	1.763	0.000	2.633
31	0.867	1.786	0.000	2.653
32	0.867	1.786	0.000	2.653
33	0.870	1.762	0.000	2.632
34	0.865	1.783	0.000	2.648
35	0.870	1.763	0.000	2.633
36	0.868	1.787	0.000	2.654
37	0.867	1.786	0.000	2.653
38	0.870	1.763	0.000	2.633
39	0.865	1.784	0.000	2.649
40	0.870	1.763	0.000	2.633

41	0.868	1.787	0.000	2.655
42	0.867	1.786	0.000	2.653
43	0.871	1.764	0.000	2.634
44	0.865	1.783	0.000	2.648
45	0.870	1.763	0.000	2.633
46	0.867	1.786	0.000	2.653
47	0.867	1.786	0.000	2.653
48	0.871	1.763	0.000	2.634
49	0.865	1.783	0.000	2.648
50	0.870	1.763	0.000	2.633
51	0.867	1.786	0.000	2.653
52	0.867	1.786	0.000	2.653
53	0.870	1.762	0.000	2.632
54	0.865	1.784	0.000	2.648
55	0.865	1.784	0.000	2.649
56	0.865	1.786	0.000	2.651
57	0.866	1.787	0.000	2.653
58	0.866	1.790	0.000	2.656
59	0.865	1.786	0.000	2.651
60	0.866	1.786	0.000	2.651
61	0.866	1.788	0.000	2.654
62	0.867	1.791	0.000	2.658

63	0.865	1.784	0.000	2.649
64	0.865	1.786	0.000	2.651
65	0.866	1.787	0.000	2.652
66	0.865	1.788	0.000	2.653
67	0.865	1.786	0.000	2.651
68	0.866	1.785	0.000	2.651
69	0.865	1.787	0.000	2.652
70	0.866	1.787	0.000	2.653
71	0.865	1.784	0.000	2.649
72	0.865	1.786	0.000	2.651
73	0.866	1.786	0.000	2.652
74	0.864	1.785	0.000	2.649
75	0.865	1.786	0.000	2.651
76	0.866	1.786	0.000	2.651
77	0.865	1.786	0.000	2.651
78	0.865	1.784	0.000	2.649
79	0.865	1.784	0.000	2.649
80	0.865	1.786	0.000	2.651
81	0.865	1.785	0.000	2.650
82	0.863	1.782	0.000	2.645
83	0.865	1.786	0.000	2.651
84	0.866	1.786	0.000	2.651

85	0.865	1.784	0.000	2.648
86	0.862	1.774	0.000	2.636
87	0.865	1.784	0.000	2.649
88	0.865	1.787	0.000	2.652
89	0.865	1.785	0.000	2.650
90	0.865	1.788	0.000	2.653
91	0.865	1.786	0.000	2.651
92	0.866	1.786	0.000	2.651
93	0.864	1.783	0.000	2.647
94	0.866	1.785	0.000	2.651
95	0.865	1.784	0.000	2.649
96	0.865	1.786	0.000	2.651
97	0.866	1.787	0.000	2.653
98	0.866	1.789	0.000	2.655
99	0.865	1.786	0.000	2.651
100	0.866	1.786	0.000	2.651
101	0.865	1.787	0.000	2.652
102	0.867	1.790	0.000	2.657
103	0.865	1.786	0.000	2.651
104	0.867	1.785	0.000	2.653
105	0.866	1.786	0.000	2.652
106	0.870	1.778	0.000	2.648

107	0.869	1.765	0.000	2.635
108	0.865	1.783	0.000	2.648
109	0.869	1.789	0.000	2.658
110	0.865	1.786	0.000	2.651
111	0.867	1.785	0.000	2.653
112	0.867	1.789	0.000	2.655
113	0.871	1.782	0.000	2.653
114	0.869	1.765	0.000	2.634
115	0.865	1.783	0.000	2.648
116	0.870	1.791	0.000	2.661
117	0.865	1.786	0.000	2.651
118	0.867	1.786	0.000	2.653
119	0.865	1.782	0.000	2.647
120	0.857	1.707	0.000	2.564
121	0.869	1.765	0.000	2.634
122	0.865	1.783	0.000	2.648
123	0.866	1.778	0.000	2.644
124	0.866	1.786	0.000	2.652
125	0.867	1.785	0.000	2.653
126	0.862	1.776	0.000	2.638
127	0.849	1.831	0.000	2.680
128	0.870	1.767	0.000	2.637

129	0.865	1.783	0.000	2.648
130	0.860	1.757	0.000	2.617
131	0.866	1.786	0.000	2.652
132	0.867	1.784	0.000	2.652
133	0.864	1.787	0.000	2.651
134	0.869	1.790	0.000	2.659
135	0.869	1.767	0.000	2.636
136	0.865	1.783	0.000	2.648
137	0.866	1.772	0.000	2.638
138	0.866	1.786	0.000	2.652
139	0.867	1.785	0.000	2.652
140	0.866	1.788	0.000	2.654
141	0.870	1.779	0.000	2.649
142	0.869	1.766	0.000	2.635
143	0.865	1.783	0.000	2.648
144	0.869	1.790	0.000	2.659
145	0.943	1.720	0.000	2.663
146	1.240	1.546	0.074	2.860
147	1.634	3.528	0.000	5.162
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tot	123.063	221.552	0.074	344.690

magnetization (x)

# of ion	s	p	d	tot
1	0.000	-0.000	0.000	0.000
2	-0.000	0.000	0.000	-0.000
3	0.000	-0.000	0.000	0.000
4	-0.000	0.000	0.000	-0.000
5	0.000	-0.000	0.000	0.000
6	-0.000	0.000	0.000	-0.000
7	0.000	-0.000	0.000	0.000
8	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	0.000
10	-0.000	0.000	0.000	-0.000
11	0.000	-0.000	0.000	0.000
12	-0.000	0.000	0.000	-0.000
13	0.000	-0.000	0.000	0.000
14	-0.004	0.002	0.000	-0.002
15	0.000	-0.000	0.000	0.000
16	-0.004	0.002	0.000	-0.002

17	-0.004	0.002	0.000	-0.002
18	0.000	-0.000	0.000	0.000
19	-0.003	0.001	0.000	-0.002
20	0.000	-0.000	0.000	0.000
21	-0.003	0.002	0.000	-0.002
22	-0.003	0.002	0.000	-0.002
23	-0.000	0.000	0.000	-0.000
24	-0.000	0.000	0.000	-0.000
25	-0.000	-0.007	0.000	-0.008
26	-0.000	-0.002	0.000	-0.002
27	0.000	0.003	0.000	0.003
28	0.000	0.005	0.000	0.005
29	0.000	0.003	0.000	0.003
30	-0.000	-0.007	0.000	-0.008
31	-0.000	-0.002	0.000	-0.002
32	0.000	0.003	0.000	0.003
33	0.000	0.005	0.000	0.005
34	0.000	0.002	0.000	0.002
35	-0.000	-0.007	0.000	-0.008
36	-0.000	-0.002	0.000	-0.002
37	0.000	0.003	0.000	0.003
38	0.000	0.006	0.000	0.007

39	0.000	0.002	0.000	0.002
40	-0.000	-0.007	0.000	-0.008
41	-0.000	-0.002	0.000	-0.002
42	0.000	0.002	0.000	0.003
43	0.000	0.005	0.000	0.006
44	0.000	0.004	0.000	0.004
45	-0.000	-0.007	0.000	-0.008
46	-0.000	-0.002	0.000	-0.002
47	0.000	0.003	0.000	0.003
48	0.000	0.005	0.000	0.006
49	0.000	0.001	0.000	0.001
50	-0.000	-0.007	0.000	-0.008
51	-0.000	-0.002	0.000	-0.002
52	0.000	0.002	0.000	0.003
53	0.000	0.006	0.000	0.007
54	0.000	0.002	0.000	0.002
55	-0.000	-0.005	0.000	-0.006
56	-0.000	-0.007	0.000	-0.007
57	-0.000	-0.001	0.000	-0.001
58	-0.000	-0.001	0.000	-0.001
59	0.000	0.006	0.000	0.007
60	0.000	0.003	0.000	0.003

61	0.000	0.001	0.000	0.001
62	0.000	0.003	0.000	0.003
63	-0.000	-0.005	0.000	-0.006
64	-0.000	-0.007	0.000	-0.007
65	-0.000	-0.001	0.000	-0.001
66	-0.000	-0.001	0.000	-0.001
67	0.000	0.006	0.000	0.006
68	0.000	0.003	0.000	0.003
69	0.000	0.001	0.000	0.001
70	0.000	0.002	0.000	0.002
71	-0.000	-0.005	0.000	-0.006
72	-0.000	-0.007	0.000	-0.007
73	-0.000	-0.001	0.000	-0.001
74	-0.000	-0.002	0.000	-0.002
75	0.000	0.006	0.000	0.007
76	0.000	0.003	0.000	0.004
77	0.000	0.003	0.000	0.003
78	0.000	0.001	0.000	0.001
79	-0.000	-0.005	0.000	-0.006
80	-0.000	-0.007	0.000	-0.007
81	-0.000	-0.001	0.000	-0.002
82	-0.000	-0.002	0.000	-0.002

83	0.001	0.007	0.000	0.008
84	0.000	0.003	0.000	0.003
85	0.000	0.002	0.000	0.002
86	0.000	0.005	0.000	0.006
87	-0.000	-0.005	0.000	-0.005
88	-0.000	-0.007	0.000	-0.007
89	-0.000	-0.001	0.000	-0.002
90	-0.000	-0.002	0.000	-0.002
91	0.001	0.008	0.000	0.008
92	0.000	0.003	0.000	0.003
93	0.000	0.002	0.000	0.003
94	0.000	0.001	0.000	0.001
95	-0.000	-0.005	0.000	-0.006
96	-0.000	-0.007	0.000	-0.007
97	-0.000	-0.001	0.000	-0.001
98	-0.000	-0.001	0.000	-0.001
99	0.001	0.007	0.000	0.007
100	0.000	0.003	0.000	0.004
101	0.000	0.003	0.000	0.003
102	0.000	0.002	0.000	0.002
103	-0.001	-0.010	0.000	-0.011
104	-0.003	-0.028	0.000	-0.031

105	-0.000	-0.001	0.000	-0.002
106	-0.000	-0.004	0.000	-0.005
107	0.007	0.116	0.000	0.122
108	0.001	0.010	0.000	0.011
109	0.000	0.001	0.000	0.001
110	-0.001	-0.010	0.000	-0.011
111	-0.003	-0.028	0.000	-0.031
112	-0.000	-0.001	0.000	-0.002
113	-0.000	-0.003	0.000	-0.004
114	0.007	0.120	0.000	0.127
115	0.001	0.010	0.000	0.011
116	0.000	0.001	0.000	0.002
117	-0.001	-0.010	0.000	-0.011
118	-0.003	-0.026	0.000	-0.029
119	-0.000	-0.002	0.000	-0.002
120	-0.000	-0.002	0.000	-0.002
121	0.007	0.115	0.000	0.122
122	0.001	0.010	0.000	0.010
123	0.000	0.003	0.000	0.003
124	-0.001	-0.010	0.000	-0.011
125	-0.003	-0.024	0.000	-0.027
126	-0.000	-0.002	0.000	-0.002

127	-0.000	0.001	0.000	0.001
128	0.006	0.105	0.000	0.111
129	0.001	0.009	0.000	0.010
130	0.000	0.004	0.000	0.004
131	-0.001	-0.009	0.000	-0.010
132	-0.003	-0.024	0.000	-0.027
133	-0.000	-0.002	0.000	-0.002
134	-0.000	-0.002	0.000	-0.002
135	0.006	0.097	0.000	0.102
136	0.001	0.009	0.000	0.010
137	0.000	0.004	0.000	0.005
138	-0.001	-0.010	0.000	-0.011
139	-0.003	-0.026	0.000	-0.029
140	-0.000	-0.002	0.000	-0.002
141	-0.000	-0.003	0.000	-0.004
142	0.006	0.105	0.000	0.111
143	0.001	0.010	0.000	0.010
144	0.000	0.002	0.000	0.003
145	0.000	0.005	0.000	0.006
146	-0.000	0.000	-0.000	0.000
147	0.000	0.004	0.000	0.004

---

tot 0.001 0.513 -0.000 0.514

CHARGE: cpu time 0.5247: real time 0.5264

FORLOC: cpu time 0.0199: real time 0.0199

FORNL : cpu time 2.0412: real time 2.0486

STRESS: cpu time 6.1199: real time 6.1414

FORCOR: cpu time 0.1415: real time 0.1446

FORHAR: cpu time 0.0329: real time 0.0330

MIXING: cpu time 0.0099: real time 0.0100

OFIELD: cpu time 0.0001: real time 0.0001

DFTD3 V3.0 Rev 1

Edisp (eV) -6.61778

E6 (eV) : -3.9313

E8 (eV) : -2.6865

% E8 : 40.60

FORVDW: cpu time 1.8307: real time 1.8578

FORCE on cell =-STRESS in cart. coord. units (eV):

Direction	XX	YY	ZZ	XY	YZ	ZX
Alpha Z	233.50077	233.50077	233.50077			
Ewald	107578.82113	23477.72195	-39726.67839	6.61667	3455.37498	126.96661
Hartree	106097.66684	25032.87846	-23793.79132	-7.84487	2947.15814	92.80971
E(xc)	-1914.25008	-1916.59708	-1979.90705	0.12110	1.82367	0.12318
Local	**********	-53958.90031	57014.32649	4.28808	-6360.43687	-216.56288
n-local	-472.65521	-482.49881	-439.56650	-0.62040	-0.71886	-0.27918
augment	-38.28098	-38.59421	-34.30844	0.02120	-0.98379	0.00707
Kinetic	7635.27983	7638.80264	8714.01536	-2.83799	-41.61945	-3.01282
Fock	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
vdW	-2.64087	-1.49209	-6.59252	0.00135	-0.07442	0.01253
Total	-17.73381	-15.17868	-19.00161	-0.25487	0.52340	0.06422
in kB	-4.89020	-4.18560	-5.23980	-0.07028	0.14433	0.01771

external pressure = -4.77 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

energy-cutoff : 400.00

volume of cell : 5810.14

direct lattice vectors reciprocal lattice vectors

14.780600000 0.000000000 0.000000000 0.067656252 0.000000000 0.000000000

0.000000000 21.333900000 0.000000000 0.000000000 0.046873755 0.000000000

0.000000000 0.000000000 18.425700000 0.000000000 0.000000000 0.054272022

length of vectors

14.780600000 21.333900000 18.425700000 0.067656252 0.046873755 0.054272022

FORCES acting on ions

electron-ion (+dipol) ewald-force non-local-force convergence-correction

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0.512E-02 0.154E+03 0.361E+02 -.361E-02 -.160E+03 -.357E+02 -.180E-02 0.566E+01 -.438E+00 -.417E-06 0.163E-07 0.707E-06

-.178E-01 0.155E+03 -.340E+02 0.154E-01 -.160E+03 0.335E+02 0.115E-02 0.565E+01 0.541E+00 -.183E-05 -.438E-06 0.124E-06

0.185E+00 0.154E+03 0.360E+02 -.185E+00 -.160E+03 -.356E+02 0.708E-05 0.565E+01 -.443E+00 -.290E-06 0.858E-06 -.545E-06

0.113E+00 0.155E+03 -.341E+02 -.996E-01 -.160E+03 0.336E+02 -.175E-01 0.565E+01 0.535E+00 -.128E-05 0.159E-05 -.807E-06

0.171E+00 0.154E+03 0.362E+02 -.173E+00 -.160E+03 -.357E+02 0.116E-02 0.566E+01 -

.440E+00 0.146E-06 0.102E-05 -.740E-06

0.126E+00 0.154E+03 -.340E+02 -.108E+00 -.160E+03 0.334E+02 -.211E-01 0.565E+01 0.541E+00 0.692E-06 0.200E-05 -.960E-06

-.198E-01 0.154E+03 0.363E+02 0.186E-01 -.160E+03 -.359E+02 0.159E-02 0.566E+01 -.431E+00 0.346E-06 0.386E-06 0.279E-06

-.137E-01 0.154E+03 -.338E+02 0.205E-01 -.160E+03 0.332E+02 -.720E-02 0.565E+01 0.555E+00 0.169E-05 0.635E-06 -.241E-06

-.182E+00 0.154E+03 0.363E+02 0.183E+00 -.160E+03 -.359E+02 0.257E-03 0.566E+01 -.429E+00 0.258E-06 -.323E-06 0.144E-05

-.129E+00 0.155E+03 -.337E+02 0.116E+00 -.160E+03 0.331E+02 0.109E-01 0.565E+01 0.561E+00 0.113E-05 -.116E-05 0.589E-06

-.174E+00 0.154E+03 0.362E+02 0.176E+00 -.160E+03 -.358E+02 -.177E-02 0.566E+01 -.432E+00 -.420E-07 -.541E-06 0.166E-05

-.115E+00 0.155E+03 -.338E+02 0.959E-01 -.160E+03 0.332E+02 0.192E-01 0.565E+01 0.555E+00 -.413E-06 -.180E-05 0.801E-06

0.229E+01 -.150E+03 -.387E+02 -.228E+01 0.156E+03 0.386E+02 -.104E-01 -.566E+01 0.767E-01 0.758E-06 -.367E-06 -.633E-06

-.413E+00 -.151E+03 0.388E+02 0.414E+00 0.157E+03 -.386E+02 -.129E-02 -.567E+01 -.269E+00 0.810E-06 -.613E-06 -.321E-07

0.136E+02 -.146E+03 -.413E+02 -.139E+02 0.151E+03 0.413E+02 0.257E+00 -.567E+01 -.348E-01 -.596E-06 -.626E-06 -.843E-06

0.163E+01 -.151E+03 0.402E+02 -.163E+01 0.156E+03 -.400E+02 -.101E-02 -.567E+01 -

.229E+00 0.457E-06 -.180E-06 0.645E-06

0.353E+01 -.149E+03 0.443E+02 -.352E+01 0.155E+03 -.441E+02 -.202E-02 -.567E+01 -.180E+00 -.663E-07 -.118E-06 0.492E-06

-.148E+02 -.146E+03 -.330E+02 0.149E+02 0.151E+03 0.330E+02 -.963E-01 -.566E+01 0.492E-01 -.771E-06 -.223E-05 -.611E-06

-.298E+01 -.149E+03 0.432E+02 0.297E+01 0.155E+03 -.430E+02 0.115E-01 -.567E+01 -.241E+00 -.669E-06 -.797E-06 -.513E-06

-.378E+01 -.150E+03 -.385E+02 0.378E+01 0.156E+03 0.385E+02 -.629E-02 -.566E+01 0.240E-01 0.141E-05 -.149E-05 -.999E-06

-.208E+01 -.151E+03 0.395E+02 0.208E+01 0.156E+03 -.392E+02 0.151E-02 -.566E+01 -.282E+00 -.260E-07 -.114E-05 -.518E-06

0.443E-03 -.148E+03 0.486E+02 0.715E-02 0.154E+03 -.484E+02 -.551E-02 -.570E+01 -.158E+00 -.474E-06 -.339E-06 -.464E-07

0.196E+02 -.103E+03 0.222E+02 -.212E+02 0.103E+03 -.246E+02 0.154E+01 0.138E+00 0.238E+01 -.921E-06 -.847E-06 -.897E-06

-.192E+02 -.103E+03 0.154E+02 0.216E+02 0.103E+03 -.169E+02 -.241E+01 -.119E+00 0.152E+01 -.633E-06 -.160E-05 -.126E-05

0.729E-01 0.461E+03 0.202E+03 -.762E-01 -.462E+03 -.201E+03 0.382E-02 0.102E+01 -.219E+00 -.174E-06 0.757E-06 0.163E-05

0.214E+00 0.353E+03 -.234E+03 -.215E+00 -.353E+03 0.234E+03 0.260E-02 0.443E+00 -.370E-01 -.258E-05 -.177E-06 -.201E-05

-.240E-01 0.351E+03 0.240E+03 0.226E-01 -.351E+03 -.241E+03 0.314E-02 0.408E+00

0.564E-01 0.296E-06 0.564E-06 0.252E-05

-.171E+00 0.462E+03 -.195E+03 0.177E+00 -.463E+03 0.195E+03 -.665E-02 0.105E+01 0.233E+00 -.410E-05 -.236E-05 -.628E-06

-.587E-01 0.210E+03 -.272E+03 0.628E-01 -.210E+03 0.272E+03 -.451E-02 0.935E-01 0.560E-01 -.115E-05 0.794E-06 -.160E-05

0.564E+00 0.461E+03 0.202E+03 -.566E+00 -.462E+03 -.201E+03 0.201E-02 0.102E+01 -.214E+00 -.183E-06 0.274E-05 -.202E-05

0.106E+01 0.352E+03 -.234E+03 -.108E+01 -.353E+03 0.234E+03 0.160E-01 0.448E+00 -.424E-01 -.401E-06 0.297E-05 -.287E-05

0.415E+00 0.351E+03 0.240E+03 -.417E+00 -.351E+03 -.240E+03 0.301E-02 0.408E+00 0.491E-01 0.306E-06 0.172E-05 -.617E-06

0.581E+00 0.462E+03 -.195E+03 -.586E+00 -.463E+03 0.195E+03 0.479E-02 0.105E+01 0.235E+00 -.286E-05 0.355E-05 -.299E-05

0.691E+00 0.210E+03 -.272E+03 -.697E+00 -.210E+03 0.272E+03 0.608E-02 0.912E-01 0.616E-01 -.839E-08 0.184E-05 -.176E-05

0.426E+00 0.461E+03 0.202E+03 -.429E+00 -.462E+03 -.202E+03 0.385E-02 0.102E+01 -.214E+00 0.248E-07 0.305E-05 -.254E-05

0.938E+00 0.352E+03 -.233E+03 -.954E+00 -.352E+03 0.233E+03 0.151E-01 0.441E+00 -.377E-01 0.225E-05 0.162E-05 -.204E-05

0.479E+00 0.351E+03 0.241E+03 -.481E+00 -.351E+03 -.241E+03 0.249E-02 0.406E+00 0.512E-01 0.663E-07 0.241E-05 -.259E-05

0.705E+00 0.462E+03 -.194E+03 -.716E+00 -.463E+03 0.194E+03 0.786E-02 0.106E+01

0.242E+00 0.175E-05 0.475E-05 -.319E-05

0.723E+00 0.210E+03 -.271E+03 -.732E+00 -.210E+03 0.271E+03 0.656E-02 0.910E-01 0.593E-01 0.998E-06 0.118E-05 -.126E-05

-.183E+00 0.461E+03 0.202E+03 0.180E+00 -.462E+03 -.202E+03 0.450E-02 0.102E+01 -.218E+00 0.817E-07 0.158E-05 0.540E-06

-.297E+00 0.352E+03 -.233E+03 0.301E+00 -.352E+03 0.233E+03 -.198E-02 0.440E+00 -.299E-01 0.198E-05 -.251E-05 -.519E-06

0.395E-01 0.351E+03 0.241E+03 -.385E-01 -.351E+03 -.241E+03 0.224E-02 0.409E+00 0.557E-01 -.363E-06 0.202E-05 -.131E-05

0.476E-01 0.462E+03 -.194E+03 -.538E-01 -.463E+03 0.194E+03 0.401E-02 0.106E+01 0.232E+00 0.380E-05 0.317E-06 -.127E-05

-.517E-01 0.210E+03 -.271E+03 0.496E-01 -.210E+03 0.271E+03 -.234E-03 0.933E-01 0.324E-01 0.592E-06 -.470E-06 -.701E-06

-.553E+00 0.461E+03 0.202E+03 0.551E+00 -.462E+03 -.202E+03 0.775E-03 0.102E+01 -.220E+00 0.125E-06 -.167E-06 0.401E-05

-.119E+01 0.352E+03 -.233E+03 0.120E+01 -.353E+03 0.233E+03 -.163E-01 0.447E+00 -.330E-01 0.437E-06 -.442E-05 0.383E-06

-.354E+00 0.351E+03 0.241E+03 0.351E+00 -.351E+03 -.241E+03 0.207E-02 0.413E+00 0.623E-01 -.444E-06 0.957E-06 0.174E-05

-.414E+00 0.462E+03 -.194E+03 0.428E+00 -.463E+03 0.194E+03 -.115E-01 0.106E+01 0.230E+00 0.236E-05 -.514E-05 0.805E-06

-.563E+00 0.210E+03 -.271E+03 0.567E+00 -.210E+03 0.271E+03 -.946E-02 0.914E-01

0.525E-01 0.298E-06 -.155E-05 -.661E-06

-.475E+00 0.461E+03 0.202E+03 0.474E+00 -.462E+03 -.202E+03 0.306E-02 0.102E+01 -.220E+00 0.143E-06 -.710E-06 0.450E-05

-.804E+00 0.353E+03 -.234E+03 0.818E+00 -.353E+03 0.234E+03 -.150E-01 0.447E+00 -.393E-01 -.177E-05 -.369E-05 -.300E-06

-.375E+00 0.351E+03 0.241E+03 0.369E+00 -.351E+03 -.241E+03 0.962E-03 0.411E+00 0.626E-01 0.119E-06 0.306E-06 0.368E-05

-.594E+00 0.462E+03 -.194E+03 0.608E+00 -.463E+03 0.194E+03 -.170E-01 0.105E+01 0.234E+00 -.927E-06 -.657E-05 0.129E-05

-.586E+00 0.210E+03 -.272E+03 0.597E+00 -.210E+03 0.272E+03 -.102E-01 0.991E-01 0.566E-01 -.771E-06 -.110E-05 -.996E-06

-.780E-02 0.206E+03 0.279E+03 0.112E-01 -.206E+03 -.279E+03 -.361E-02 0.686E-01 -.412E-01 0.629E-06 0.336E-06 0.146E-05

0.671E+00 0.303E+02 0.296E+03 -.666E+00 -.302E+02 -.296E+03 -.469E-02 -.410E-01 0.750E-02 0.630E-06 -.182E-07 0.736E-06

-.842E+00 0.144E+03 -.282E+03 0.844E+00 -.144E+03 0.282E+03 -.321E-02 0.137E+00 0.287E-01 -.844E-06 0.580E-06 -.119E-05

0.543E+00 -.215E+02 -.285E+03 -.544E+00 0.214E+02 0.285E+03 -.781E-03 0.387E-01 0.186E-01 -.396E-06 0.644E-06 -.103E-05

0.502E+00 -.294E+02 0.293E+03 -.499E+00 0.294E+02 -.293E+03 -.554E-02 0.254E-01 -.304E-01 0.296E-06 0.280E-06 0.104E-05

0.526E+00 0.139E+03 0.289E+03 -.527E+00 -.139E+03 -.289E+03 0.178E-02 0.103E+00 -

.248E-01 0.799E-06 0.146E-06 0.450E-06

-.126E+01 0.364E+02 -.287E+03 0.126E+01 -.364E+02 0.287E+03 -.671E-04 -.763E-02 0.139E-01 -.342E-06 0.774E-06 -.807E-06

0.168E+01 -.130E+03 -.271E+03 -.170E+01 0.130E+03 0.271E+03 0.106E-01 -.879E-01 0.372E-01 0.310E-06 0.165E-05 -.119E-05

0.399E+00 0.207E+03 0.280E+03 -.397E+00 -.207E+03 -.280E+03 0.701E-03 0.695E-01 -.371E-01 0.747E-06 0.359E-06 -.607E-06

0.923E+00 0.312E+02 0.296E+03 -.926E+00 -.311E+02 -.296E+03 0.224E-02 -.410E-01 0.122E-01 0.586E-06 -.331E-06 -.234E-06

0.133E+01 0.144E+03 -.282E+03 -.134E+01 -.144E+03 0.282E+03 0.498E-02 0.126E+00 0.279E-01 -.213E-06 0.137E-05 -.145E-05

0.342E+01 -.199E+02 -.285E+03 -.344E+01 0.199E+02 0.285E+03 0.136E-01 0.412E-01 0.137E-01 0.381E-07 0.146E-05 -.149E-05

0.139E+01 -.287E+02 0.294E+03 -.139E+01 0.287E+02 -.294E+03 -.350E-02 0.252E-01 -.307E-01 0.467E-06 -.194E-07 0.647E-06

0.680E+00 0.139E+03 0.290E+03 -.680E+00 -.139E+03 -.290E+03 0.611E-03 0.103E+00 -.295E-01 0.561E-06 0.768E-08 -.118E-05

0.161E+01 0.367E+02 -.287E+03 -.159E+01 -.367E+02 0.287E+03 -.128E-01 -.206E-01 0.128E-01 -.211E-06 0.119E-05 -.125E-05

0.613E+01 -.125E+03 -.271E+03 -.615E+01 0.125E+03 0.271E+03 0.220E-01 -.894E-01 0.148E-01 -.144E-06 0.148E-05 -.194E-05

0.368E+00 0.207E+03 0.280E+03 -.373E+00 -.207E+03 -.280E+03 0.102E-03 0.684E-01 -

.365E-01 0.953E-07 0.531E-06 -.196E-05

-.375E-01 0.319E+02 0.296E+03 0.288E-01 -.318E+02 -.296E+03 0.106E-01 -.362E-01 0.139E-01 -.216E-06 -.245E-06 -.588E-06

0.210E+01 0.144E+03 -.281E+03 -.211E+01 -.144E+03 0.281E+03 0.122E-01 0.120E+00 0.241E-01 0.561E-06 0.109E-05 -.131E-05

0.303E+01 -.171E+02 -.283E+03 -.305E+01 0.171E+02 0.283E+03 0.246E-01 0.878E-01 0.606E-01 0.423E-06 0.209E-05 -.126E-05

0.106E+01 -.272E+02 0.294E+03 -.106E+01 0.272E+02 -.294E+03 0.287E-02 0.243E-01 -.376E-01 0.164E-06 -.797E-07 0.337E-08

0.966E-01 0.140E+03 0.290E+03 -.982E-01 -.140E+03 -.290E+03 0.129E-02 0.107E+00 -.232E-01 -.283E-06 0.659E-07 -.151E-05

0.277E+01 0.387E+02 -.286E+03 -.277E+01 -.387E+02 0.286E+03 0.140E-02 -.107E-01 0.294E-01 0.236E-06 0.145E-05 -.123E-05

0.595E+01 -.115E+03 -.267E+03 -.611E+01 0.115E+03 0.267E+03 0.155E+00 0.282E-02 0.129E+00 -.384E-06 0.166E-05 -.207E-05

-.243E+00 0.207E+03 0.280E+03 0.241E+00 -.207E+03 -.280E+03 0.439E-02 0.716E-01 -.387E-01 -.645E-06 0.583E-06 -.118E-05

-.115E+01 0.314E+02 0.294E+03 0.114E+01 -.314E+02 -.294E+03 0.920E-02 -.311E-01 0.542E-02 -.719E-06 0.864E-07 0.589E-08

0.591E+00 0.144E+03 -.281E+03 -.608E+00 -.144E+03 0.281E+03 0.178E-01 0.126E+00 0.438E-01 0.303E-06 0.907E-06 -.823E-06

-.954E+00 -.159E+02 -.286E+03 0.945E+00 0.158E+02 0.285E+03 0.603E-02 0.907E-01

0.802E-01 -.374E-06 -.238E-06 -.125E-05

-.646E+00 -.265E+02 0.293E+03 0.642E+00 0.265E+02 -.293E+03 0.491E-02 0.234E-01 -.271E-01 -.374E-06 0.151E-06 0.730E-08

-.537E+00 0.139E+03 0.289E+03 0.532E+00 -.139E+03 -.289E+03 0.656E-02 0.114E+00 -.214E-01 -.918E-06 0.234E-06 -.246E-06

0.771E+00 0.408E+02 -.287E+03 -.783E+00 -.408E+02 0.287E+03 0.506E-02 0.215E-02 -.190E-01 0.129E-06 0.616E-06 -.902E-06

-.490E+00 -.113E+03 -.276E+03 0.457E+00 0.113E+03 0.276E+03 0.334E-01 0.601E-01 -.268E+00 -.209E-05 0.494E-07 -.220E-05

-.574E+00 0.206E+03 0.279E+03 0.572E+00 -.206E+03 -.279E+03 0.117E-02 0.720E-01 -.455E-01 -.827E-06 0.470E-06 0.832E-06

-.787E+00 0.304E+02 0.294E+03 0.790E+00 -.304E+02 -.294E+03 -.753E-02 -.309E-01 -.139E-02 -.360E-06 0.400E-06 0.854E-06

-.123E+01 0.144E+03 -.281E+03 0.125E+01 -.145E+03 0.281E+03 -.157E-01 0.122E+00 0.504E-01 0.650E-06 -.130E-06 -.712E-06

-.366E+01 -.174E+02 -.283E+03 0.369E+01 0.173E+02 0.283E+03 -.307E-01 0.116E+00 0.590E-01 -.947E-08 0.964E-06 -.108E-05

-.130E+01 -.277E+02 0.291E+03 0.130E+01 0.277E+02 -.291E+03 -.130E-02 0.340E-01 -.219E-01 -.536E-06 0.353E-06 0.410E-06

-.350E+00 0.139E+03 0.289E+03 0.349E+00 -.139E+03 -.289E+03 0.250E-04 0.112E+00 -.146E-01 -.481E-06 0.451E-06 0.136E-05

-.837E+00 0.400E+02 -.287E+03 0.829E+00 -.400E+02 0.287E+03 0.124E-01 -.758E-02 -

.182E-01 -.392E-06 -.629E-07 -.908E-06

-.787E+01 -.119E+03 -.267E+03 0.806E+01 0.119E+03 0.267E+03 -.188E+00 0.148E-02 0.349E-01 0.179E-05 -.101E-05 -.252E-05

-.410E+00 0.206E+03 0.279E+03 0.411E+00 -.206E+03 -.279E+03 -.280E-02 0.715E-01 -.464E-01 -.138E-07 0.380E-06 0.222E-05

-.631E-01 0.300E+02 0.294E+03 0.729E-01 -.299E+02 -.294E+03 -.948E-02 -.347E-01 0.120E-02 0.128E-06 0.351E-06 0.123E-05

-.206E+01 0.145E+03 -.282E+03 0.208E+01 -.145E+03 0.282E+03 -.189E-01 0.132E+00 0.256E-01 -.373E-06 -.863E-06 -.894E-06

-.256E+01 -.209E+02 -.285E+03 0.258E+01 0.208E+02 0.285E+03 -.291E-01 0.410E-01 0.319E-01 0.289E-06 0.315E-06 -.630E-06

-.555E+00 -.290E+02 0.291E+03 0.559E+00 0.290E+02 -.291E+03 -.284E-02 0.292E-01 -.251E-01 -.348E-07 0.413E-06 0.974E-06

0.589E-01 0.139E+03 0.289E+03 -.591E-01 -.139E+03 -.289E+03 -.347E-03 0.109E+00 -.208E-01 0.341E-06 0.430E-06 0.171E-05

-.290E+01 0.377E+02 -.286E+03 0.291E+01 -.377E+02 0.286E+03 -.146E-01 -.399E-02 0.209E-01 0.631E-06 0.215E-06 -.743E-06

-.512E+01 -.128E+03 -.271E+03 0.517E+01 0.128E+03 0.271E+03 -.464E-01 -.862E-01 0.377E-01 0.554E-06 -.117E-06 -.115E-05

0.404E+00 -.137E+03 0.280E+03 -.396E+00 0.137E+03 -.280E+03 -.971E-02 -.127E+00 -.156E-01 0.370E-06 0.182E-06 0.107E-05

0.195E+01 -.343E+03 0.233E+03 -.195E+01 0.344E+03 -.233E+03 0.906E-02 -.461E+00 -

.547E-01 0.137E-05 0.217E-06 0.174E-05

-.251E+01 -.197E+03 -.259E+03 0.252E+01 0.197E+03 0.259E+03 -.950E-02 -.198E+00 0.369E-01 0.848E-06 0.151E-06 -.120E-05

0.695E+01 -.447E+03 -.198E+03 -.696E+01 0.448E+03 0.198E+03 0.948E-02 -.112E+01 0.882E-01 0.193E-05 -.129E-07 -.209E-05

-.454E+00 -.451E+03 0.204E+03 0.455E+00 0.452E+03 -.204E+03 -.212E-02 -.108E+01 -.112E+00 0.198E-05 -.140E-05 0.570E-06

0.172E+01 -.203E+03 0.269E+03 -.171E+01 0.203E+03 -.269E+03 -.483E-02 -.927E-01 -.320E-01 0.615E-06 0.292E-06 0.148E-05

-.207E+01 -.338E+03 -.222E+03 0.212E+01 0.338E+03 0.222E+03 -.443E-01 -.604E+00 0.538E-01 0.194E-05 -.921E-06 -.209E-05

0.219E+01 -.136E+03 0.282E+03 -.219E+01 0.136E+03 -.282E+03 -.638E-02 -.126E+00 -.944E-02 0.458E-06 0.463E-06 0.141E-05

0.673E+01 -.339E+03 0.238E+03 -.671E+01 0.340E+03 -.238E+03 -.128E-01 -.462E+00 -.460E-01 0.432E-06 0.116E-05 0.249E-05

0.680E+01 -.193E+03 -.258E+03 -.682E+01 0.193E+03 0.258E+03 0.112E-01 -.146E+00 0.634E-01 0.142E-06 0.125E-05 -.187E-05

0.313E+02 -.427E+03 -.198E+03 -.314E+02 0.428E+03 0.197E+03 0.725E-01 -.971E+00 0.135E+00 -.154E-05 -.148E-06 -.305E-05

0.546E+01 -.449E+03 0.209E+03 -.546E+01 0.450E+03 -.209E+03 0.529E-03 -.108E+01 -.798E-01 0.122E-05 0.962E-06 0.254E-05

0.369E+01 -.201E+03 0.272E+03 -.369E+01 0.201E+03 -.272E+03 -.762E-03 -.977E-01 -

.306E-01 0.400E-06 0.620E-06 0.176E-05

0.124E+02 -.332E+03 -.223E+03 -.125E+02 0.332E+03 0.223E+03 0.120E+00 -.535E+00 0.315E-01 0.800E-07 0.380E-06 -.223E-05

0.219E+01 -.133E+03 0.283E+03 -.220E+01 0.133E+03 -.283E+03 0.524E-03 -.128E+00 -.444E-02 0.263E-06 0.379E-06 0.113E-05

0.493E+01 -.332E+03 0.245E+03 -.489E+01 0.332E+03 -.245E+03 -.319E-01 -.476E+00 -.376E-01 -.243E-06 0.856E-06 0.155E-05

0.112E+02 -.182E+03 -.258E+03 -.113E+02 0.182E+03 0.258E+03 0.476E-01 -.992E-01 -.105E+00 0.140E-05 -.171E-06 -.219E-05

0.318E+02 -.399E+03 -.175E+03 -.321E+02 0.400E+03 0.174E+03 0.297E+00 -.142E+01 0.133E+01 0.131E-05 -.525E-05 -.382E-05

0.931E+01 -.443E+03 0.219E+03 -.931E+01 0.444E+03 -.219E+03 -.571E-02 -.109E+01 -.483E-01 -.306E-08 0.114E-05 0.210E-05

0.169E+01 -.196E+03 0.273E+03 -.170E+01 0.197E+03 -.273E+03 0.549E-02 -.109E+00 -.511E-01 -.619E-07 0.531E-06 0.129E-05

0.172E+02 -.310E+03 -.216E+03 -.176E+02 0.310E+03 0.216E+03 0.325E+00 -.220E+00 0.123E+00 0.230E-06 -.788E-06 -.309E-05

-.104E+01 -.132E+03 0.281E+03 0.103E+01 0.132E+03 -.281E+03 0.103E-01 -.127E+00 0.147E-03 -.335E-06 0.444E-06 0.778E-06

-.514E+01 -.332E+03 0.239E+03 0.513E+01 0.332E+03 -.239E+03 0.893E-02 -.494E+00 -.419E-01 -.128E-05 -.242E-06 0.481E-06

0.155E+01 -.170E+03 -.261E+03 -.167E+01 0.169E+03 0.261E+03 0.119E+00 0.375E+00 -

.930E-01 -.187E-05 0.198E-05 -.261E-05

-.684E+01 -.301E+03 -.189E+03 0.638E+01 0.296E+03 0.185E+03 0.505E+00 0.504E+01

0.404E+01 -.405E-05 -.142E-05 -.192E-05

-.628E+00 -.436E+03 0.227E+03 0.625E+00 0.437E+03 -.227E+03 0.173E-02 -.120E+01 -

.484E-01 -.107E-05 -.552E-07 0.660E-06

-.303E+01 -.197E+03 0.268E+03 0.302E+01 0.197E+03 -.268E+03 0.146E-01 -.112E+00 -

.428E-01 -.689E-06 0.370E-06 0.736E-06

0.327E+01 -.280E+03 -.215E+03 -.520E+01 0.280E+03 0.214E+03 0.192E+01 0.651E+00

0.825E+00 0.803E-06 0.142E-07 -.244E-05

-.275E+01 -.134E+03 0.277E+03 0.275E+01 0.134E+03 -.277E+03 0.252E-02 -.123E+00 -

.185E-01 -.520E-06 0.347E-06 0.404E-06

-.602E+01 -.338E+03 0.230E+03 0.602E+01 0.339E+03 -.230E+03 0.113E-01 -.494E+00 -

.460E-01 -.663E-06 -.162E-05 -.241E-06

-.654E+01 -.171E+03 -.257E+03 0.661E+01 0.170E+03 0.257E+03 -.755E-01 0.481E+00

0.177E-01 -.250E-06 -.102E-05 -.301E-05

-.442E+02 -.422E+03 -.184E+03 0.447E+02 0.424E+03 0.183E+03 -.562E+00 -.109E+01

0.635E+00 -.239E-05 -.309E-05 -.344E-05

-.870E+01 -.441E+03 0.211E+03 0.869E+01 0.442E+03 -.211E+03 0.145E-01 -.111E+01 -

.754E-01 -.176E-05 -.199E-05 -.702E-06

-.294E+01 -.201E+03 0.265E+03 0.295E+01 0.201E+03 -.265E+03 -.914E-02 -.110E+00 -

.204E-01 -.471E-06 -.124E-06 0.323E-06

-.146E+02 -.290E+03 -.209E+03 0.165E+02 0.289E+03 0.209E+03 -.197E+01 0.595E+00

0.783E+00 -.222E-05 0.910E-06 -.273E-05

-.139E+01 -.136E+03 0.277E+03 0.140E+01 0.136E+03 -.277E+03 -.102E-01 -.125E+00 -.239E-01 -.210E-06 0.505E-07 0.669E-06

-.279E+01 -.343E+03 0.230E+03 0.276E+01 0.343E+03 -.230E+03 0.235E-01 -.473E+00 -.593E-01 0.315E-06 -.145E-05 0.261E-06

-.104E+02 -.189E+03 -.258E+03 0.104E+02 0.189E+03 0.258E+03 -.770E-01 -.138E+00 -.529E-01 -.264E-06 -.290E-05 -.272E-05

-.149E+02 -.446E+03 -.196E+03 0.150E+02 0.447E+03 0.196E+03 -.698E-01 -.112E+01 0.101E+00 0.415E-05 -.399E-05 -.386E-05

-.550E+01 -.448E+03 0.204E+03 0.551E+01 0.449E+03 -.203E+03 -.483E-02 -.109E+01 -.125E+00 -.220E-06 -.321E-05 -.771E-06

-.911E+00 -.203E+03 0.267E+03 0.920E+00 0.203E+03 -.267E+03 -.911E-02 -.102E+00 -.317E-01 0.182E-06 -.319E-06 0.796E-06

-.163E+02 -.329E+03 -.218E+03 0.166E+02 0.329E+03 0.218E+03 -.360E+00 -.479E+00 0.435E-01 0.784E-07 -.276E-05 -.422E-05

-.643E+01 -.256E+03 -.193E+03 0.548E+01 0.248E+03 0.189E+03 0.870E+00 0.781E+01 0.490E+01 0.267E-05 -.280E-04 -.197E-04

0.533E+02 -.518E+03 -.136E+03 -.543E+02 0.522E+03 0.140E+03 0.105E+01 -.396E+01 -.383E+01 -.656E-05 -.766E-05 -.818E-05

-.444E+02 -.586E+03 -.447E+03 0.495E+02 0.637E+03 0.481E+03 -.503E+01 -.511E+02 -.344E+02 0.343E-04 -.263E-04 -.186E-04

0.359E+01 0.279E+02 0.224E+02 -.327E-12 -.125E-11 0.136E-11 -.364E+01 -.279E+02 -.225E+02 0.302E-04 -.646E-04 -.110E-03

POSITION			TOTAL-FORCE (eV/Angst)		
1.24575	4.02870	5.43979	0.000053	0.001005	-0.000407
1.21024	4.07581	8.43726	-0.000972	0.002594	-0.001143
3.70862	4.02890	5.43965	0.000319	0.001877	-0.001092
3.67998	4.07733	8.43690	-0.004023	-0.000437	-0.002906
6.17157	4.02854	5.43942	0.000002	-0.000151	-0.001750
6.14482	4.08292	8.43295	-0.002824	-0.003321	-0.003193
8.63513	4.02801	5.43869	0.000786	-0.000456	-0.001999
8.60339	4.08732	8.43089	-0.000127	-0.001192	-0.002214
11.09928	4.02784	5.43885	0.000882	0.001957	-0.002713
11.06021	4.08619	8.43099	-0.001738	0.000686	-0.000653
13.56311	4.02807	5.43972	0.000343	0.001607	-0.001619
13.52141	4.08047	8.43349	0.000413	-0.002271	0.000286
2.44241	15.48073	8.85224	-0.000585	-0.005229	0.002326
0.01714	15.44624	5.32469	0.000363	0.001530	-0.001198
4.86040	15.47728	8.86623	0.001163	0.000175	-0.000399
2.48016	15.44854	5.27562	0.000382	-0.001217	-0.000503

4.94382	15.44925	5.24869	0.001813	-0.003038	0.000343
12.31531	15.48242	9.00211	-0.004826	0.003148	0.002638
9.86772	15.44556	5.34176	0.000417	-0.001131	0.000924
14.76279	15.48245	8.89951	-0.006032	-0.000369	0.005539
12.33384	15.44510	5.36128	0.001370	-0.003219	-0.001294
7.40743	15.44616	5.26463	0.002370	0.001468	0.001472
6.44846	16.34427	7.40648	-0.002249	-0.001836	0.002065
8.60064	16.47644	7.89249	0.005162	0.002045	0.005451
1.24544	5.11881	5.35500	0.000962	0.000155	-0.002464
2.44348	5.83889	8.62292	0.002413	-0.004450	0.001217
0.01380	5.79530	5.28573	0.002083	-0.002473	0.000472
1.21063	5.16420	8.54151	0.000273	-0.000522	-0.001882
2.44351	7.27931	8.74832	-0.000073	-0.001267	-0.000122
3.70866	5.11896	5.35390	-0.000410	-0.001640	0.000331
4.90800	5.84315	8.62123	-0.001050	0.003818	-0.000749
2.47701	5.79561	5.28397	0.001454	-0.000614	-0.002607
3.67679	5.16572	8.54000	-0.000105	0.001629	-0.000036
4.90764	7.28398	8.74777	0.000704	-0.000594	0.001041
6.17184	5.11860	5.35433	0.001488	0.000373	0.000895
7.37096	5.84929	8.62094	-0.000584	0.007051	-0.002462
4.94029	5.79548	5.28340	0.000608	-0.002703	-0.001175
6.14080	5.17108	8.53715	-0.002537	0.002523	0.002469

7.37071	7.28983	8.75132	-0.001939	0.001587	0.000132
8.63543	5.11820	5.35521	0.001251	0.001342	-0.001078
9.83233	5.85166	8.62337	0.002743	0.000612	-0.001099
7.40374	5.79498	5.28512	0.003465	-0.002700	-0.001337
8.60194	5.17528	8.53759	-0.001869	-0.000437	-0.000195
9.83204	7.29110	8.75719	-0.001928	-0.002585	-0.002431
11.09930	5.11814	5.35578	-0.000857	-0.003350	-0.001368
12.29449	5.84673	8.62385	0.000068	0.005709	-0.002191
9.86750	5.79468	5.28678	-0.000742	-0.000736	0.001551
11.06261	5.17409	8.53894	0.002668	0.002729	-0.000384
12.29428	7.28729	8.75533	-0.004485	0.001213	-0.001512
13.56278	5.11829	5.35605	0.002667	0.000533	-0.001992
14.75895	5.83988	8.62434	-0.000201	-0.002699	-0.002207
12.33118	5.79480	5.28692	-0.004496	-0.001494	0.002593
13.52535	5.16844	8.54022	-0.003510	0.003805	-0.001413
14.75917	7.28012	8.75179	0.000948	0.002496	-0.000705
0.01434	7.23830	5.19017	0.000100	-0.000221	0.000077
1.24689	9.38061	5.13160	0.000556	-0.001872	-0.000002
1.21085	7.98059	8.79588	-0.000913	-0.000498	0.001561
2.44214	10.12243	8.87141	-0.000926	0.003252	-0.005016
0.01532	10.08686	5.14049	-0.002033	-0.000147	-0.002398
1.24606	7.94244	5.15775	0.002015	-0.002618	0.000831

1.21082	9.41592	8.85782	-0.000724	0.004424	0.000190
2.44072	11.55513	8.88414	-0.006223	-0.002805	0.001653
2.47747	7.23842	5.18585	0.002804	0.002865	0.001311
3.70997	9.38055	5.12566	-0.001068	-0.003024	0.000046
3.67534	7.98360	8.79349	-0.000528	0.001015	0.000940
4.90487	10.12925	8.87518	0.000242	-0.000314	0.000057
2.47867	10.08713	5.12695	-0.002265	0.001491	0.000767
3.70939	7.94242	5.15441	0.000824	-0.004021	-0.001697
3.67589	9.41970	8.85445	-0.001411	0.001925	-0.000136
4.90263	11.56506	8.89086	-0.000568	0.001438	0.000900
4.94085	7.23830	5.18552	-0.004688	0.002238	0.000829
6.17318	9.38002	5.13173	0.002049	0.002075	0.001834
6.13864	7.99044	8.79647	0.002471	-0.000342	-0.001652
7.36780	10.13760	8.89473	-0.000153	0.002973	0.000366
4.94196	10.08682	5.12700	0.004135	0.001472	-0.001155
6.17284	7.94199	5.15766	-0.000047	0.000543	0.003035
6.13939	9.42660	8.86164	0.000685	-0.000306	-0.002209
7.36410	11.57721	8.92935	-0.000865	-0.001383	0.003500
7.40426	7.23794	5.19012	0.002161	0.001747	0.001072
8.63700	9.37970	5.14543	-0.000523	0.002934	0.000946
8.60086	7.99568	8.80617	0.001146	-0.000654	-0.001047
9.83068	10.14286	8.92842	-0.002472	0.002424	-0.000740

7.40553	10.08627	5.14064	0.001205	-0.003598	0.003144
8.63637	7.94166	5.16555	0.002615	0.001764	-0.001406
8.60077	9.43254	8.88532	-0.006081	0.002460	-0.001240
9.82927	11.58244	9.00096	0.000789	0.003503	0.001025
9.86805	7.23787	5.19489	-0.000362	0.000085	-0.000215
11.10106	9.37979	5.15156	-0.003816	-0.001047	0.000664
11.06331	7.99411	8.80818	-0.000251	-0.001625	0.000109
12.29815	10.12943	8.90340	-0.000196	-0.000978	0.001530
9.86930	10.08593	5.15631	-0.005448	-0.001480	0.001410
11.10021	7.94175	5.16862	-0.000596	-0.003090	0.001392
11.06206	9.43062	8.88839	0.004577	0.001819	0.002035
12.30255	11.56557	8.94694	0.002554	-0.001811	-0.000804
12.33169	7.23799	5.19447	-0.001013	0.000230	-0.001755
13.56437	9.38021	5.14435	0.000730	0.001634	-0.000577
13.52754	7.98555	8.80171	-0.000720	-0.002576	-0.003128
14.76233	10.12320	8.88285	-0.005207	0.000883	-0.001651
12.33257	10.08637	5.15511	0.002651	0.000512	-0.001540
13.56350	7.94214	5.16485	-0.000079	-0.000908	-0.000371
13.52731	9.42040	8.86925	-0.000246	0.002990	-0.000495
14.76430	11.55727	8.90646	-0.002200	-0.000617	0.001631
0.01611	11.52516	5.16621	-0.001067	-0.002566	0.000391
1.24770	13.67535	5.22209	0.001877	-0.002286	-0.002480

1.21217	12.26335	8.89409	0.000769	-0.000357	0.001193
2.43998	14.38728	8.86748	-0.002755	0.000706	0.000835
0.01699	14.35408	5.27295	-0.000453	-0.000743	-0.001988
1.24794	12.22963	5.17275	0.001058	0.000840	-0.001363
1.21434	13.70818	8.88771	0.002137	0.002540	0.003739
2.47958	11.52580	5.14547	-0.001607	-0.000213	-0.001485
3.71218	13.67636	5.19535	0.004660	0.000577	0.001074
3.66932	12.26248	8.88184	-0.001936	-0.000024	-0.000651
4.89370	14.38589	8.86075	0.004013	-0.001948	-0.002141
2.48000	14.35596	5.23149	0.001283	-0.001226	0.001679
3.71150	12.23022	5.15602	0.000898	-0.004525	0.001012
3.66212	13.70366	8.87117	-0.004927	0.004235	-0.000666
4.94290	11.52542	5.14351	-0.000043	-0.001804	-0.001600
6.17627	13.67505	5.20032	0.000879	0.000600	0.000056
6.13145	12.27911	8.90591	0.005010	0.006980	0.004585
7.36614	14.42967	8.88203	-0.000206	0.001336	0.000068
4.94347	14.35627	5.21375	0.000127	-0.001864	0.001054
6.17493	12.22917	5.16623	-0.001413	-0.001055	0.001574
6.11879	13.72336	8.87765	0.004413	0.000659	0.000197
7.40625	11.52413	5.16368	0.000930	-0.003364	0.000355
8.63876	13.67323	5.24377	0.001816	0.002119	-0.001349
8.58939	12.29067	9.00208	0.002146	-0.000450	0.000268

9.83855	14.39048	9.30305	0.048271	-0.006428	-0.001556
7.40672	14.35386	5.23530	-0.001102	-0.000346	-0.000848
8.63820	12.22778	5.19800	0.000318	-0.001264	0.001077
8.55571	13.73596	9.04598	-0.002847	0.001398	0.006292
9.86985	11.52338	5.18893	0.001761	-0.001982	-0.000108
11.10099	13.67352	5.27669	0.003172	-0.000824	-0.000973
11.07378	12.27333	9.00891	0.000136	0.004809	-0.003649
12.30694	14.38896	9.00333	-0.001071	-0.001814	0.002405
9.86934	14.35300	5.29564	0.002933	-0.000037	-0.000092
11.10161	12.22804	5.21650	-0.001108	-0.002745	0.001050
11.11464	13.70636	9.07877	-0.006419	-0.005577	-0.001449
12.33326	11.52411	5.18815	-0.000912	0.000283	0.000534
13.56430	13.67399	5.25995	0.001599	0.000036	0.000087
13.53626	12.26601	8.93587	-0.002345	0.004277	0.001971
14.76266	14.38906	8.90426	-0.003715	0.000720	0.003706
12.33397	14.35288	5.30710	0.002773	-0.001996	-0.001779
13.56505	12.22870	5.20105	0.000100	0.000075	-0.001141
13.54921	13.70690	8.94399	0.000068	-0.002642	0.002264
9.91126	15.53185	9.99472	-0.076450	-0.096496	-0.059789
7.28864	16.40884	8.69813	-0.004569	-0.003028	-0.006059
10.01026	16.50365	10.64498	0.047636	0.101111	0.070827

---

total drift: -0.045794 0.026756 -0.022987

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

---

free energy TOTEN = -1209.38888859 eV

energy without entropy= -1209.38888859 energy(sigma->0) = -1209.38888859

d Force = 0.2810612E-04[-0.143E-02, 0.149E-02] d Energy =-0.3732707E-04 0.654E-04

d Force =-0.1572762E+01[-0.148E+01,-0.166E+01] d Ewald =-0.1573120E+01 0.358E-03

POTLOK: cpu time 0.1740: real time 0.1749

---

stress matrix after NEB project (eV)

-17.73381 -0.25487 0.06422

-0.25487 -15.17868 0.52340

0.06422 0.52340 -19.00161

FORCES: max atom, RMS 0.136861 0.015701

FORCE total and by dimension 0.190368 0.101111

Stress total and by dimension 30.110256 19.001608

Finite differences progress:

Degree of freedom: 4/ 6

Displacement: 2/ 2

Total: 8/ 12

LATTYP: Found a simple orthorhombic cell.

ALAT = 14.7806000000

B/A-ratio = 1.2466138046

C/A-ratio = 1.4433717170

Lattice vectors:

A1 = (-14.7806000000, 0.0000000000, 0.0000000000)

A2 = (0.0000000000, 0.0000000000, -18.4257000000)

A3 = (0.0000000000, -21.3339000000, 0.0000000000)

Analysis of symmetry for initial positions (statically):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The static configuration has the point symmetry C_1 .

Analysis of symmetry for dynamics (positions and initial velocities):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The dynamic configuration has the point symmetry C_1 .

Analysis of constrained symmetry for selective dynamics:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The constrained configuration has the point symmetry C_1 .

Analysis of structural, dynamic, and magnetic symmetry:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The magnetic configuration has the point symmetry C_1 .

Subroutine INISYM returns: Found 1 space group operations

(whereof 1 operations are pure point group operations),

and found 1 'primitive' translations

KPOINTS: KPT-Resolved Value to Generate K-Mesh: 0

Automatic generation of k-mesh.

Space group operators:

irot det(A) alpha n_x n_y n_z tau_x tau_y tau_z

1 1.000000 0.000000 1.000000 0.000000 0.000000 0.000000

0.000000 0.000000

Subroutine IBZKPT returns following result:

==========

Found 1 irreducible k-points:

Following reciprocal coordinates:

Coordinates Weight

0.000000 0.000000 0.000000 1.000000

Following cartesian coordinates:

Coordinates Weight

0.000000 0.000000 0.000000 1.000000

WAVPRE: cpu time 0.1304: real time 0.1547

FEWALD: cpu time 0.0027: real time 0.0027

ORTHCH: cpu time 1.0077: real time 1.0109

LOOP+: cpu time 158.5040: real time 159.3373

---------- Iteration 10(1) ----------

POTLOK: cpu time 0.1699: real time 0.1828

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9276: real time 1.9345

RMM-DIIS: cpu time 7.0888: real time 7.1283

ORTHCH: cpu time 0.3516: real time 0.3527

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5256: real time 0.5273

MIXING: cpu time 0.0044: real time 0.0045

LOOP: cpu time 10.0783: real time 10.1403

eigenvalue-minimisations : 1926

total energy-change (2. order) :-0.2971737E-03 (-0.2515046E+00)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7277963 magnetization 0.0542749

Broyden mixing:

rms(total) = 0.34046E-01 rms(broyden)= 0.33764E-01

rms(prec) = 0.34835E-01

weight for this iteration 100.00

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107327.84416934

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.74701209

PAW double counting = 52179.15613595 -52242.07641762

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.30569316

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77140659 eV

energy without entropy = -1202.77140659 energy(sigma->0) = -1202.77140659

---------- Iteration 10(2) ----------

POTLOK: cpu time 0.1668: real time 0.1688

SETDIJ: cpu time 0.0103: real time 0.0103

EDDIAG: cpu time 1.9190: real time 1.9258

RMM-DIIS: cpu time 7.2519: real time 7.2880

ORTHCH: cpu time 0.3512: real time 0.3523

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5251: real time 0.5269

MIXING: cpu time 0.0044: real time 0.0044

LOOP: cpu time 10.2290: real time 10.2768

eigenvalue-minimisations : 1936

total energy-change (2. order) : 0.6303020E-02 (-0.2068360E-02)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7328676 magnetization 0.0542633

Broyden mixing:

rms(total) = 0.20429E-01 rms(broyden)= 0.20387E-01

rms(prec) = 0.21678E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 0.9658

0.9658

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107327.17912229

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.71584306

PAW double counting = 52170.70488606 -52233.61153832

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.94689756

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76510357 eV

energy without entropy = -1202.76510357 energy(sigma->0) = -1202.76510357

---------- Iteration 10(3) ----------

POTLOK: cpu time 0.1668: real time 0.1788

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9215: real time 1.9279

RMM-DIIS: cpu time 7.2249: real time 7.2640

ORTHCH: cpu time 0.3516: real time 0.3529

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5254: real time 0.5271

MIXING: cpu time 0.0049: real time 0.0050

LOOP: cpu time 10.2056: real time 10.2662

eigenvalue-minimisations : 1942

total energy-change (2. order) : 0.7352045E-03 (-0.6130571E-04)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7314905 magnetization 0.0542670

Broyden mixing:

rms(total) = 0.11971E-01 rms(broyden)= 0.11963E-01

rms(prec) = 0.12373E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4878

0.6986 2.2770

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107326.82644566

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.71988100

PAW double counting = 52165.84725792 -52228.75383079

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.30295631

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76436837 eV

energy without entropy = -1202.76436837 energy(sigma->0) = -1202.76436837

---------- Iteration 10(4) ----------

POTLOK: cpu time 0.1659: real time 0.1925

SETDIJ: cpu time 0.0100: real time 0.0101

```
      EDDIAG:  cpu time        1.9216: real time        1.9279
    RMM-DIIS:  cpu time        7.2853: real time        7.3118
      ORTHCH:  cpu time        0.3514: real time        0.3525
         DOS:  cpu time        0.0004: real time        0.0004
      CHARGE:  cpu time        0.5255: real time        0.5274
      MIXING:  cpu time        0.0051: real time        0.0051
      ------------------------------------------
        LOOP:  cpu time       10.2652: real time       10.3278

 eigenvalue-minimisations  :  1937
 total energy-change (2. order) : 0.1337269E-04  (-0.5378449E-04)
 number of electron       518.9999702 magnetization             0.9999998
 augmentation part         11.7309957 magnetization             0.0542750

 Broyden mixing:
  rms(total) = 0.51700E-02        rms(broyden)= 0.51642E-02
  rms(prec ) = 0.55558E-02
  weight for this iteration         100.00

 eigenvalues of (default mixing * dielectric matrix)
  average eigenvalue GAMMA=      1.3852
  2.2412    0.9572    0.9572
```

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107326.20384288

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.71342338

PAW double counting = 52157.40812167 -52220.31206816

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.92171448

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76435500 eV

energy without entropy = -1202.76435500 energy(sigma->0) = -1202.76435500

-- Iteration 10(5) --

POTLOK: cpu time 0.1720: real time 0.1849

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9218: real time 1.9282

RMM-DIIS: cpu time 7.0035: real time 7.0271

ORTHCH: cpu time 0.3507: real time 0.3518

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5256: real time 0.5275

MIXING: cpu time 0.0053: real time 0.0053

LOOP: cpu time 9.9894: real time 10.0354

eigenvalue-minimisations : 1913

total energy-change (2. order) : 0.2074007E-04 (-0.1306249E-04)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7318008 magnetization 0.0542747

Broyden mixing:

rms(total) = 0.15110E-02 rms(broyden)= 0.15052E-02

rms(prec) = 0.17044E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4501

2.0630 2.0630 0.8373 0.8373

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107326.10115538

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.71003350

PAW double counting = 52156.69148190 -52219.59476051

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.02165924

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76433426 eV

energy without entropy = -1202.76433426 energy(sigma->0) = -1202.76433426

---------- Iteration 10(6) ----------

POTLOK: cpu time 0.1665: real time 0.1680

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9197: real time 1.9263

RMM-DIIS: cpu time 7.1489: real time 7.1881

ORTHCH: cpu time 0.3541: real time 0.3554

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5248: real time 0.5267

MIXING: cpu time 0.0057: real time 0.0056

LOOP: cpu time 10.1302: real time 10.1808

eigenvalue-minimisations : 1912

total energy-change (2. order) :-0.1846050E-04 (-0.7981115E-06)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7316836 magnetization 0.0542767

Broyden mixing:

rms(total) = 0.56481E-03 rms(broyden)= 0.56449E-03

rms(prec) = 0.74747E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4238

2.4879 1.8807 0.8758 0.8758 0.9988

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107326.00840405

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.71117864

PAW double counting = 52156.14806443 -52219.05215532

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.11476190

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76435272 eV

energy without entropy = -1202.76435272 energy(sigma->0) = -1202.76435272

---------- Iteration 10(7) ----------

POTLOK: cpu time 0.1660: real time 0.1971

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9194: real time 1.9265

RMM-DIIS: cpu time 6.2275: real time 6.2826

ORTHCH: cpu time 0.3513: real time 0.3524

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5255: real time 0.5272

MIXING: cpu time 0.0056: real time 0.0056

LOOP: cpu time 9.2059: real time 9.3020

eigenvalue-minimisations : 1708

total energy-change (2. order) :-0.1540860E-04 (-0.1759286E-06)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7316010 magnetization 0.0542771

Broyden mixing:

rms(total) = 0.28915E-03 rms(broyden)= 0.28864E-03

rms(prec) = 0.44410E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3933

2.5515 1.6688 1.6688 0.8784 0.8784 0.7137

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107325.92888458

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.71094607

PAW double counting = 52155.94145097 -52218.84560957

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.19399650

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76436813 eV

energy without entropy = -1202.76436813 energy(sigma->0) = -1202.76436813

---------- Iteration 10(8) ----------

POTLOK: cpu time 0.1671: real time 0.1731

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9225: real time 1.9284

RMM-DIIS: cpu time 6.0438: real time 6.0772

ORTHCH: cpu time 0.3524: real time 0.3533

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5246: real time 0.5261

MIXING: cpu time 0.0059: real time 0.0059

LOOP: cpu time 9.0266: real time 9.0745

eigenvalue-minimisations : 1636

total energy-change (2. order) :-0.1935178E-04 (-0.9853450E-07)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7316145 magnetization 0.0542773

Broyden mixing:

rms(total) = 0.16548E-03 rms(broyden)= 0.16542E-03

rms(prec) = 0.30802E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4360

2.4927 2.4927 1.6429 1.0010 0.8770 0.8770 0.6688

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107325.86393928

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.71042429

PAW double counting = 52156.00614932 -52218.91022745

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.25851984

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76438748 eV

energy without entropy = -1202.76438748 energy(sigma->0) = -1202.76438748

---------- Iteration 10(9) ----------

POTLOK: cpu time 0.1674: real time 0.1705

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9209: real time 1.9275

RMM-DIIS: cpu time 6.1095: real time 6.1376

ORTHCH: cpu time 0.3526: real time 0.3539

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5255: real time 0.5274

MIXING: cpu time 0.0062: real time 0.0062

LOOP: cpu time 9.0925: real time 9.1334

eigenvalue-minimisations : 1653

total energy-change (2. order) :-0.2536154E-04 (-0.1456948E-06)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7316249 magnetization 0.0542776

Broyden mixing:

rms(total) = 0.12063E-03 rms(broyden)= 0.12057E-03

rms(prec) = 0.20687E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4711

2.9324 2.6041 1.6868 1.1414 0.8962 0.8962 0.9580 0.6537

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107325.77995669

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.70990977

PAW double counting = 52156.10974517 -52219.01376910

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.34206746

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76441284 eV

energy without entropy = -1202.76441284 energy(sigma->0) = -1202.76441284

---------- Iteration 10(10) ----------

POTLOK: cpu time 0.1650: real time 0.1827

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9217: real time 1.9279

RMM-DIIS: cpu time 5.9997: real time 6.0351

ORTHCH: cpu time 0.3521: real time 0.3532

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5269: real time 0.5284

MIXING: cpu time 0.0066: real time 0.0067

LOOP: cpu time 8.9823: real time 9.0443

eigenvalue-minimisations : 1619

total energy-change (2. order) :-0.1927689E-04 (-0.9570528E-07)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7316102 magnetization 0.0542779

Broyden mixing:

rms(total) = 0.60827E-04 rms(broyden)= 0.60723E-04

rms(prec) = 0.11105E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5826

3.9614 2.5797 1.9855 1.3829 1.1559 0.8810 0.8810 0.7712 0.6443

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107325.71466375

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.70962375

PAW double counting = 52156.15930614 -52219.06330216

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.40712158

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76443212 eV

energy without entropy = -1202.76443212 energy(sigma->0) = -1202.76443212

---------- Iteration 10(11) ----------

POTLOK: cpu time 0.1683: real time 0.1882

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9196: real time 1.9264

RMM-DIIS: cpu time 5.7967: real time 5.8290

ORTHCH: cpu time 0.3510: real time 0.3521

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5254: real time 0.5273

MIXING: cpu time 0.0071: real time 0.0072

LOOP: cpu time 8.7786: real time 8.8408

eigenvalue-minimisations : 1568

total energy-change (2. order) :-0.1145449E-04 (-0.5505809E-07)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7316021 magnetization 0.0542782

Broyden mixing:

rms(total) = 0.50139E-04 rms(broyden)= 0.50071E-04

rms(prec) = 0.72407E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6542

5.0456 2.5796 2.0862 1.6217 1.1284 0.9061 0.9061 0.9277 0.7055 0.6352

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107325.66981805

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.70943150

PAW double counting = 52156.17405541 -52219.07803509

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.45180282

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76444357 eV

energy without entropy = -1202.76444357 energy(sigma->0) = -1202.76444357

---------- Iteration 10(12) ----------

POTLOK: cpu time 0.1650: real time 0.1674

SETDIJ: cpu time 0.0102: real time 0.0103

EDDIAG: cpu time 1.9252: real time 1.9321

RMM-DIIS: cpu time 5.2116: real time 5.2291

ORTHCH: cpu time 0.3560: real time 0.3570

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5257: real time 0.5275

MIXING: cpu time 0.0077: real time 0.0077

LOOP: cpu time 8.2018: real time 8.2314

eigenvalue-minimisations : 1406

total energy-change (2. order) :-0.4808222E-05 (-0.1453725E-07)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7316040 magnetization 0.0542782

Broyden mixing:

rms(total) = 0.27747E-04 rms(broyden)= 0.27736E-04

rms(prec) = 0.46030E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7605

6.0773 2.6650 2.3286 1.8483 1.3352 1.0815 0.8993 0.8993 0.9229 0.6792

0.6291

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107325.65564142

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.70936493

PAW double counting = 52156.17070234 -52219.07467802

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.46592168

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76444838 eV

energy without entropy = -1202.76444838 energy(sigma->0) = -1202.76444838

---------- Iteration 10(13) ----------

POTLOK: cpu time 0.1644: real time 0.1655

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9203: real time 1.9267

RMM-DIIS: cpu time 5.3282: real time 5.3574

ORTHCH: cpu time 0.3507: real time 0.3518

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5251: real time 0.5270

MIXING: cpu time 0.0081: real time 0.0082

LOOP: cpu time 8.3072: real time 8.3471

eigenvalue-minimisations : 1453

total energy-change (2. order) :-0.5264308E-05 (-0.1765159E-07)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7316075 magnetization 0.0542781

Broyden mixing:

rms(total) = 0.18207E-04 rms(broyden)= 0.18188E-04

rms(prec) = 0.27367E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7888

6.5878 2.9902 2.4734 1.7132 1.7132 1.0251 1.0251 0.9093 0.9093 0.8235

0.6680 0.6270

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107325.64411601

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.70931566

PAW double counting = 52156.16382134 -52219.06779351

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.47740660

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76445364 eV

energy without entropy = -1202.76445364 energy(sigma->0) = -1202.76445364

---------- Iteration 10(14) ----------

POTLOK: cpu time 0.1629: real time 0.1640

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9221: real time 1.9293

RMM-DIIS: cpu time 4.8527: real time 4.9316

ORTHCH: cpu time 0.3507: real time 0.3520

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5258: real time 0.5277

MIXING: cpu time 0.0085: real time 0.0085

LOOP: cpu time 7.8329: real time 7.9235

eigenvalue-minimisations : 1322

total energy-change (2. order) :-0.2259716E-05 (-0.5333169E-08)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7316069 magnetization 0.0542781

Broyden mixing:

rms(total) = 0.11908E-04 rms(broyden)= 0.11905E-04

rms(prec) = 0.17028E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8681

7.0879 3.6364 2.5034 2.1028 1.8070 1.3174 0.8994 0.8994 1.0608 0.9581

0.7310 0.6567 0.6254

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107325.64047641

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.70931639

PAW double counting = 52156.16336097 -52219.06733438

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.48104796

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76445590 eV

energy without entropy = -1202.76445590 energy(sigma->0) = -1202.76445590

---------- Iteration 10(15) ----------

POTLOK: cpu time 0.1668: real time 0.1897

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9220: real time 1.9286

RMM-DIIS: cpu time 4.8534: real time 4.8690

ORTHCH: cpu time 0.3539: real time 0.3550

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5248: real time 0.5267

MIXING: cpu time 0.0088: real time 0.0088

LOOP: cpu time 7.8402: real time 7.8884

eigenvalue-minimisations : 1324

total energy-change (2. order) :-0.1461369E-05 (-0.2735595E-08)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7316060 magnetization 0.0542782

Broyden mixing:

rms(total) = 0.53293E-05 rms(broyden)= 0.53235E-05

rms(prec) = 0.87072E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9103

7.6150 4.1998 2.5803 2.4116 1.6246 1.6246 1.0315 1.0315 0.8917 0.8917

0.8726 0.7007 0.6457 0.6234

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107325.63920133

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.70933082

PAW double counting = 52156.16472978 -52219.06870773

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.48233439

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76445736 eV

energy without entropy = -1202.76445736 energy(sigma->0) = -1202.76445736

---------- Iteration 10(16) ----------

POTLOK: cpu time 0.1667: real time 0.1719

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9210: real time 1.9276

RMM-DIIS: cpu time 4.6455: real time 4.6684

ORTHCH: cpu time 0.3509: real time 0.3519

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5252: real time 0.5267

MIXING: cpu time 0.0092: real time 0.0092

LOOP: cpu time 7.6289: real time 7.6661

eigenvalue-minimisations : 1220

total energy-change (2. order) :-0.8158968E-06 (-0.8466658E-09)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7316059 magnetization 0.0542782

Broyden mixing:

rms(total) = 0.36824E-05 rms(broyden)= 0.36812E-05

rms(prec) = 0.59177E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9184

7.8607 4.5713 2.6667 2.4035 1.7425 1.6520 1.1407 1.1407 0.8969 0.8969

1.0072 0.8482 0.6867 0.6401 0.6222

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107325.63876468

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.70933577

PAW double counting = 52156.16565357 -52219.06963256

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.48277576

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76445818 eV

energy without entropy = -1202.76445818 energy(sigma->0) = -1202.76445818

---------- Iteration 10(17) ----------

POTLOK: cpu time 0.1701: real time 0.1723

SETDIJ: cpu time 0.0198: real time 0.0200

EDDIAG: cpu time 1.9276: real time 1.9341

RMM-DIIS: cpu time 4.6640: real time 4.6775

ORTHCH: cpu time 0.3515: real time 0.3524

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5250: real time 0.5265

MIXING: cpu time 0.0095: real time 0.0095

LOOP: cpu time 7.6680: real time 7.6927

eigenvalue-minimisations : 1235

total energy-change (2. order) :-0.7201379E-06 (-0.3859668E-09)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7316059 magnetization 0.0542781

Broyden mixing:

rms(total) = 0.21313E-05 rms(broyden)= 0.21302E-05

rms(prec) = 0.36267E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9553

8.0131 5.0613 2.7941 2.5083 2.2329 1.5764 1.5764 1.0632 1.0632 0.8939

0.8939 0.8881 0.7815 0.6792 0.6368 0.6224

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107325.63831621

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.70933443

PAW double counting = 52156.16659234 -52219.07056963

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.48322531

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76445890 eV

energy without entropy = -1202.76445890 energy(sigma->0) = -1202.76445890

---------- Iteration 10(18) ----------

POTLOK: cpu time 0.1667: real time 0.1806

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9242: real time 1.9306

RMM-DIIS: cpu time 4.4554: real time 4.4808

ORTHCH: cpu time 0.3505: real time 0.3515

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5248: real time 0.5264

MIXING: cpu time 0.0095: real time 0.0095

LOOP: cpu time 7.4415: real time 7.4899

eigenvalue-minimisations : 1135

total energy-change (2. order) :-0.2813831E-06 (-0.2184004E-09)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7316059 magnetization 0.0542781

Broyden mixing:

rms(total) = 0.15589E-05 rms(broyden)= 0.15577E-05

rms(prec) = 0.23097E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9800

8.2552 5.5602 3.1942 2.6087 2.2053 1.6378 1.6378 1.1304 1.1304 0.8995

0.8995 0.9286 0.9286 0.7081 0.6753 0.6236 0.6361

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107325.63812638

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.70933623

PAW double counting = 52156.16739553 -52219.07137261

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.48341744

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76445918 eV

energy without entropy = -1202.76445918 energy(sigma->0) = -1202.76445918

---------- Iteration 10(19) ----------

POTLOK: cpu time 0.1666: real time 0.1918

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9217: real time 1.9285

RMM-DIIS: cpu time 4.1372: real time 4.1606

ORTHCH: cpu time 0.3523: real time 0.3534

DOS: cpu time 0.0003: real time 0.0003

LOOP: cpu time 6.5882: real time 6.6448

eigenvalue-minimisations : 978

total energy-change (2. order) :-0.4837057E-07 (-0.1165077E-09)

number of electron 518.9999702 magnetization 0.9999998

augmentation part 11.7316059 magnetization 0.0542781

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91319.72103868

-Hartree energ DENC = -107325.63810344

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.70933848

PAW double counting = 52156.16731242 -52219.07129005

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.48344211

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76445923 eV

energy without entropy = -1202.76445923 energy(sigma->0) = -1202.76445923

---

average (electrostatic) potential at core

the test charge radii are 0.5201 0.6991 1.0621 0.7215

(the norm of the test charge is 1.0000)

1 -40.7556	2 -40.7536	3 -40.7549	4 -40.7537	5 -40.7555
6 -40.7578	7 -40.7551	8 -40.7630	9 -40.7548	10 -40.7624
11 -40.7563	12 -40.7583	13 -40.6550	14 -40.6994	15 -40.7742
16 -40.7016	17 -40.6951	18 -40.8607	19 -40.6820	20 -40.6717

21 -40.6916	22 -40.6641	23 -40.0813	24 -40.1237	25 -57.4619
26 -57.6733	27 -57.6600	28 -57.4721	29 -57.6674	30 -57.4619
31 -57.6731	32 -57.6596	33 -57.4700	34 -57.6723	35 -57.4627
36 -57.6749	37 -57.6596	38 -57.4722	39 -57.6781	40 -57.4618
41 -57.6789	42 -57.6597	43 -57.4770	44 -57.6924	45 -57.4617
46 -57.6779	47 -57.6605	48 -57.4772	49 -57.6838	50 -57.4629
51 -57.6746	52 -57.6603	53 -57.4749	54 -57.6702	55 -57.6399
56 -57.6661	57 -57.6909	58 -57.6879	59 -57.6698	60 -57.6725
61 -57.6945	62 -57.6794	63 -57.6402	64 -57.6655	65 -57.6930
66 -57.6991	67 -57.6681	68 -57.6723	69 -57.6982	70 -57.7058
71 -57.6396	72 -57.6669	73 -57.7006	74 -57.7258	75 -57.6689
76 -57.6729	77 -57.7102	78 -57.7561	79 -57.6398	80 -57.6695
81 -57.7142	82 -57.7560	83 -57.6722	84 -57.6744	85 -57.7415
86 -57.8453	87 -57.6423	88 -57.6702	89 -57.7161	90 -57.7212
91 -57.6769	92 -57.6746	93 -57.7461	94 -57.7644	95 -57.6406
96 -57.6684	97 -57.6999	98 -57.6950	99 -57.6742	100 -57.6734
101 -57.7121	102 -57.6906	103 -57.6637	104 -57.6346	105 -57.6505
106 -57.2962	107 -57.3918	108 -57.6347	109 -57.6031	110 -57.6627
111 -57.6345	112 -57.6471	113 -57.3156	114 -57.3976	115 -57.6339
116 -57.6049	117 -57.6618	118 -57.6261	119 -57.7029	120 -57.6909
121 -57.3911	122 -57.6327	123 -57.7145	124 -57.6628	125 -57.6288
126 -57.8378	127 -58.3445	128 -57.3643	129 -57.6379	130 -58.1485

131 -57.6707	132 -57.6381	133 -57.8051	134 -57.4239	135 -57.3756
136 -57.6419	137 -58.0831	138 -57.6672	139 -57.6339	140 -57.6761
141 -57.3060	142 -57.3818	143 -57.6373	144 -57.6529	145 -60.8136
146 -57.3118	147 -81.1768			

E-fermi : -2.3370 XC(G=0): -2.7343 alpha+bet : -2.2521

spin component 1

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-26.7564	1.00000
2	-21.5727	1.00000
3	-21.4751	1.00000
4	-21.1040	1.00000
5	-21.0727	1.00000
6	-21.0187	1.00000
7	-20.9823	1.00000
8	-20.9805	1.00000

9	-20.8947	1.00000
10	-20.5621	1.00000
11	-20.5075	1.00000
12	-20.4152	1.00000
13	-20.4017	1.00000
14	-20.1305	1.00000
15	-19.9793	1.00000
16	-19.7076	1.00000
17	-19.6318	1.00000
18	-19.6036	1.00000
19	-19.5881	1.00000
20	-19.5323	1.00000
21	-19.5305	1.00000
22	-19.5022	1.00000
23	-19.4848	1.00000
24	-19.1162	1.00000
25	-19.0796	1.00000
26	-18.9820	1.00000
27	-18.9685	1.00000
28	-18.9045	1.00000
29	-18.7370	1.00000
30	-18.5088	1.00000

31	-18.3632	1.00000
32	-18.2789	1.00000
33	-18.2558	1.00000
34	-18.1878	1.00000
35	-18.1857	1.00000
36	-18.0834	1.00000
37	-18.0797	1.00000
38	-17.5653	1.00000
39	-17.3170	1.00000
40	-17.2919	1.00000
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spin component 2

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200	-7.1488	1.00000
201	-7.0591	1.00000
202	-7.0393	1.00000
203	-7.0182	1.00000
204	-6.9886	1.00000
205	-6.9811	1.00000

206	-6.9759	1.00000
207	-6.9443	1.00000
208	-6.8654	1.00000
209	-6.8196	1.00000
210	-6.7985	1.00000
211	-6.7911	1.00000
212	-6.7285	1.00000
213	-6.6796	1.00000
214	-6.4716	1.00000
215	-6.3984	1.00000
216	-6.3863	1.00000
217	-6.3817	1.00000
218	-6.3668	1.00000
219	-6.3421	1.00000
220	-6.3069	1.00000
221	-6.2793	1.00000
222	-6.2327	1.00000
223	-6.2313	1.00000
224	-6.2257	1.00000
225	-6.0504	1.00000
226	-6.0125	1.00000
227	-5.7594	1.00000

228	-5.7149	1.00000
229	-5.6963	1.00000
230	-5.6390	1.00000
231	-5.6263	1.00000
232	-5.5474	1.00000
233	-5.5266	1.00000
234	-5.4448	1.00000
235	-5.4154	1.00000
236	-5.1450	1.00000
237	-5.0636	1.00000
238	-5.0298	1.00000
239	-5.0261	1.00000
240	-4.9633	1.00000
241	-4.8811	1.00000
242	-4.8579	1.00000
243	-4.8068	1.00000
244	-4.7816	1.00000
245	-4.6525	1.00000
246	-4.5824	1.00000
247	-4.5793	1.00000
248	-4.4796	1.00000
249	-4.4248	1.00000

250	-4.3987	1.00000
251	-4.2999	1.00000
252	-4.2310	1.00000
253	-4.1788	1.00000
254	-3.5413	1.00000
255	-3.3129	1.00000
256	-3.1474	1.00000
257	-2.9473	1.00000
258	-2.8030	1.00000
259	-2.7443	1.00000
260	-2.0654	0.00000
261	-1.9176	0.00000
262	-1.7274	0.00000
263	-1.6836	0.00000
264	-1.3306	0.00000
265	-1.2890	0.00000
266	-1.1675	0.00000
267	-0.7359	0.00000
268	-0.5878	0.00000
269	-0.5150	0.00000
270	-0.2843	0.00000
271	-0.2813	0.00000

272	-0.2636	0.00000
273	-0.1608	0.00000
274	-0.0621	0.00000
275	-0.0522	0.00000
276	0.0085	0.00000
277	0.0362	0.00000
278	0.0746	0.00000
279	0.2048	0.00000
280	0.2518	0.00000
281	0.2761	0.00000
282	0.4297	0.00000
283	0.4469	0.00000
284	0.4796	0.00000
285	0.6034	0.00000
286	0.6865	0.00000
287	0.8213	0.00000
288	0.8817	0.00000
289	1.0550	0.00000
290	1.1024	0.00000
291	1.1384	0.00000
292	1.1754	0.00000
293	1.2308	0.00000

294	1.2496	0.00000
295	1.3071	0.00000
296	1.3189	0.00000
297	1.3584	0.00000
298	1.4288	0.00000
299	1.4791	0.00000
300	1.4981	0.00000
301	1.5752	0.00000
302	1.6017	0.00000
303	1.6477	0.00000
304	1.6854	0.00000
305	1.7568	0.00000
306	1.7714	0.00000
307	1.8782	0.00000
308	1.8985	0.00000
309	1.9054	0.00000
310	1.9192	0.00000
311	2.1381	0.00000
312	2.1992	0.00000
313	2.2188	0.00000
314	2.2507	0.00000
315	2.2881	0.00000

316	2.2955	0.00000
317	2.3363	0.00000
318	2.3593	0.00000
319	2.3809	0.00000
320	2.4057	0.00000
321	2.4265	0.00000
322	2.4339	0.00000
323	2.4485	0.00000
324	2.4575	0.00000
325	2.4665	0.00000
326	2.5283	0.00000
327	2.5458	0.00000
328	2.7061	0.00000
329	2.7348	0.00000
330	2.7519	0.00000
331	2.7582	0.00000
332	2.7735	0.00000
333	2.8265	0.00000
334	2.8449	0.00000
335	2.8684	0.00000
336	2.9020	0.00000
337	2.9323	0.00000

338	2.9550	0.00000
339	2.9826	0.00000
340	3.0058	0.00000
341	3.0373	0.00000
342	3.0496	0.00000
343	3.0715	0.00000
344	3.0912	0.00000
345	3.1535	0.00000
346	3.1707	0.00000
347	3.1878	0.00000
348	3.1991	0.00000
349	3.3073	0.00000
350	3.3287	0.00000
351	3.3611	0.00000
352	3.3716	0.00000
353	3.3930	0.00000
354	3.4390	0.00000
355	3.4824	0.00000
356	3.4898	0.00000
357	3.4915	0.00000
358	3.5021	0.00000
359	3.6399	0.00000

360	3.6765	0.00000
361	3.7003	0.00000
362	3.7369	0.00000
363	3.7528	0.00000
364	3.7592	0.00000
365	3.7769	0.00000
366	3.7974	0.00000
367	3.8131	0.00000
368	3.8388	0.00000
369	3.8459	0.00000
370	3.8646	0.00000
371	3.8788	0.00000
372	3.8913	0.00000
373	3.9202	0.00000
374	3.9334	0.00000
375	3.9468	0.00000
376	3.9587	0.00000
377	3.9824	0.00000
378	3.9868	0.00000
379	4.0216	0.00000
380	4.0778	0.00000
381	4.1707	0.00000

382	4.2582	0.00000
383	4.2622	0.00000
384	4.2688	0.00000
385	4.2927	0.00000
386	4.3208	0.00000
387	4.3344	0.00000
388	4.3499	0.00000
389	4.3797	0.00000
390	4.3843	0.00000
391	4.4234	0.00000
392	4.4485	0.00000
393	4.4749	0.00000
394	4.4828	0.00000
395	4.4898	0.00000
396	4.4992	0.00000
397	4.5213	0.00000
398	4.5540	0.00000
399	4.5914	0.00000
400	4.6102	0.00000
401	4.6279	0.00000
402	4.6455	0.00000
403	4.6591	0.00000

404	4.6846	0.00000
405	4.7082	0.00000
406	4.7362	0.00000
407	4.7511	0.00000
408	4.7703	0.00000
409	4.7856	0.00000
410	4.7875	0.00000
411	4.8024	0.00000
412	4.8324	0.00000
413	4.8646	0.00000
414	4.8841	0.00000
415	4.9013	0.00000
416	4.9417	0.00000
417	4.9926	0.00000
418	5.0092	0.00000
419	5.0125	0.00000
420	5.0374	0.00000
421	5.0439	0.00000
422	5.0674	0.00000
423	5.0855	0.00000
424	5.1177	0.00000
425	5.1210	0.00000

426	5.1405	0.00000
427	5.1440	0.00000
428	5.1686	0.00000
429	5.1790	0.00000
430	5.1879	0.00000
431	5.1925	0.00000
432	5.2217	0.00000
433	5.2360	0.00000
434	5.2448	0.00000
435	5.2614	0.00000
436	5.2965	0.00000
437	5.3011	0.00000
438	5.3109	0.00000
439	5.3357	0.00000
440	5.3519	0.00000
441	5.3696	0.00000
442	5.3791	0.00000
443	5.3935	0.00000
444	5.4281	0.00000
445	5.4589	0.00000
446	5.4679	0.00000
447	5.4863	0.00000

448	5.4985	0.00000
449	5.5231	0.00000
450	5.5671	0.00000
451	5.5715	0.00000
452	5.5933	0.00000
453	5.6071	0.00000
454	5.6225	0.00000
455	5.6674	0.00000
456	5.6910	0.00000
457	5.7170	0.00000
458	5.7266	0.00000
459	5.7484	0.00000
460	5.7624	0.00000
461	5.7885	0.00000
462	5.7906	0.00000
463	5.7968	0.00000
464	5.8031	0.00000
465	5.8195	0.00000
466	5.8251	0.00000
467	5.8537	0.00000
468	5.8605	0.00000
469	5.8795	0.00000

470	5.8847	0.00000
471	5.8891	0.00000
472	5.9050	0.00000
473	5.9199	0.00000
474	5.9449	0.00000
475	5.9510	0.00000
476	5.9684	0.00000
477	5.9753	0.00000
478	5.9899	0.00000
479	6.0102	0.00000
480	6.0436	0.00000

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soft charge-density along one line, spin component 1

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

soft charge-density along one line, spin component 2

0 1 2 3 4 5 6 7

8 9

total charge-density along one line

pseudopotential strength for first ion, spin component: 1

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

pseudopotential strength for first ion, spin component: 2

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

total augmentation occupancy for first ion, spin component: 1

3.579 -0.646 0.444 -0.034 -0.000

-0.646 0.130 -0.082 0.006 0.000

0.444 -0.082 0.056 -0.003 -0.000

-0.034 0.006 -0.003 0.011 0.000

-0.000 0.000 -0.000 0.000 0.007

total augmentation occupancy for first ion, spin component: 2

-0.000	0.000	-0.000	0.000	0.000
0.000	-0.000	0.000	-0.000	-0.000
-0.000	0.000	-0.000	-0.000	-0.000
0.000	-0.000	-0.000	-0.000	-0.000
0.000	-0.000	-0.000	-0.000	-0.000

---------- aborting loop because EDIFF is reached ----------

total charge

# of ion	s	p	d	tot
1	0.646	0.043	0.000	0.690
2	0.646	0.043	0.000	0.690
3	0.646	0.043	0.000	0.690
4	0.646	0.043	0.000	0.690

5	0.646	0.043	0.000	0.690
6	0.646	0.043	0.000	0.690
7	0.646	0.043	0.000	0.690
8	0.646	0.043	0.000	0.690
9	0.646	0.043	0.000	0.690
10	0.646	0.043	0.000	0.690
11	0.646	0.043	0.000	0.690
12	0.646	0.043	0.000	0.690
13	0.646	0.043	0.000	0.689
14	0.646	0.043	0.000	0.689
15	0.648	0.045	0.000	0.693
16	0.646	0.043	0.000	0.689
17	0.646	0.043	0.000	0.689
18	0.646	0.043	0.000	0.689
19	0.646	0.043	0.000	0.689
20	0.646	0.043	0.000	0.689
21	0.646	0.043	0.000	0.689
22	0.646	0.044	0.000	0.690
23	0.542	0.015	0.000	0.557
24	0.541	0.015	0.000	0.556
25	0.870	1.763	0.000	2.633
26	0.867	1.785	0.000	2.653

27	0.867	1.786	0.000	2.653
28	0.870	1.762	0.000	2.632
29	0.865	1.783	0.000	2.648
30	0.870	1.763	0.000	2.633
31	0.867	1.786	0.000	2.653
32	0.867	1.786	0.000	2.653
33	0.870	1.762	0.000	2.632
34	0.865	1.783	0.000	2.648
35	0.870	1.763	0.000	2.633
36	0.868	1.787	0.000	2.654
37	0.867	1.786	0.000	2.653
38	0.870	1.763	0.000	2.633
39	0.865	1.784	0.000	2.649
40	0.870	1.763	0.000	2.633
41	0.868	1.787	0.000	2.655
42	0.867	1.786	0.000	2.653
43	0.871	1.764	0.000	2.634
44	0.865	1.783	0.000	2.648
45	0.870	1.763	0.000	2.633
46	0.867	1.786	0.000	2.653
47	0.867	1.786	0.000	2.653
48	0.871	1.763	0.000	2.634

49	0.865	1.783	0.000	2.648
50	0.870	1.763	0.000	2.633
51	0.867	1.786	0.000	2.653
52	0.867	1.786	0.000	2.653
53	0.870	1.762	0.000	2.632
54	0.865	1.784	0.000	2.648
55	0.865	1.784	0.000	2.649
56	0.865	1.786	0.000	2.651
57	0.866	1.787	0.000	2.653
58	0.866	1.790	0.000	2.656
59	0.865	1.786	0.000	2.651
60	0.866	1.786	0.000	2.651
61	0.866	1.788	0.000	2.654
62	0.867	1.791	0.000	2.658
63	0.865	1.784	0.000	2.649
64	0.865	1.786	0.000	2.651
65	0.866	1.787	0.000	2.652
66	0.865	1.788	0.000	2.653
67	0.865	1.786	0.000	2.651
68	0.866	1.785	0.000	2.651
69	0.865	1.787	0.000	2.652
70	0.866	1.787	0.000	2.653

71	0.865	1.784	0.000	2.649
72	0.865	1.786	0.000	2.651
73	0.866	1.786	0.000	2.652
74	0.864	1.785	0.000	2.649
75	0.865	1.786	0.000	2.651
76	0.866	1.786	0.000	2.651
77	0.865	1.786	0.000	2.651
78	0.865	1.784	0.000	2.649
79	0.865	1.784	0.000	2.649
80	0.865	1.786	0.000	2.651
81	0.865	1.785	0.000	2.650
82	0.863	1.782	0.000	2.645
83	0.865	1.786	0.000	2.651
84	0.866	1.786	0.000	2.651
85	0.865	1.784	0.000	2.648
86	0.862	1.774	0.000	2.636
87	0.865	1.784	0.000	2.649
88	0.865	1.787	0.000	2.652
89	0.865	1.785	0.000	2.650
90	0.865	1.788	0.000	2.653
91	0.865	1.786	0.000	2.651
92	0.866	1.786	0.000	2.651

93	0.864	1.783	0.000	2.647
94	0.866	1.785	0.000	2.651
95	0.865	1.784	0.000	2.649
96	0.865	1.786	0.000	2.651
97	0.866	1.787	0.000	2.653
98	0.866	1.789	0.000	2.655
99	0.865	1.786	0.000	2.651
100	0.866	1.786	0.000	2.651
101	0.865	1.787	0.000	2.652
102	0.867	1.790	0.000	2.657
103	0.865	1.786	0.000	2.651
104	0.867	1.785	0.000	2.653
105	0.866	1.786	0.000	2.652
106	0.870	1.778	0.000	2.648
107	0.869	1.765	0.000	2.635
108	0.865	1.783	0.000	2.648
109	0.869	1.789	0.000	2.658
110	0.865	1.786	0.000	2.651
111	0.867	1.785	0.000	2.653
112	0.867	1.789	0.000	2.655
113	0.871	1.782	0.000	2.653
114	0.869	1.765	0.000	2.634

115	0.865	1.783	0.000	2.648
116	0.870	1.791	0.000	2.661
117	0.865	1.786	0.000	2.651
118	0.867	1.786	0.000	2.653
119	0.865	1.782	0.000	2.647
120	0.858	1.706	0.000	2.564
121	0.869	1.765	0.000	2.634
122	0.865	1.783	0.000	2.648
123	0.866	1.778	0.000	2.644
124	0.866	1.786	0.000	2.652
125	0.868	1.785	0.000	2.653
126	0.862	1.776	0.000	2.638
127	0.849	1.829	0.000	2.679
128	0.870	1.767	0.000	2.637
129	0.865	1.783	0.000	2.648
130	0.860	1.757	0.000	2.617
131	0.866	1.786	0.000	2.652
132	0.867	1.784	0.000	2.652
133	0.864	1.787	0.000	2.651
134	0.869	1.789	0.000	2.659
135	0.869	1.767	0.000	2.636
136	0.865	1.783	0.000	2.648

137	0.866	1.772	0.000	2.638
138	0.866	1.786	0.000	2.652
139	0.867	1.785	0.000	2.652
140	0.866	1.788	0.000	2.654
141	0.870	1.779	0.000	2.649
142	0.869	1.766	0.000	2.635
143	0.865	1.783	0.000	2.648
144	0.869	1.790	0.000	2.659
145	0.936	1.701	0.000	2.637
146	1.240	1.545	0.075	2.860
147	1.631	3.508	0.000	5.140
tot	123.055	221.511	0.075	344.641

magnetization (x)

# of ion	s	p	d	tot
1	0.000	-0.000	0.000	0.000
2	-0.000	0.000	0.000	-0.000

3	0.000	-0.000	0.000	0.000
4	-0.000	0.000	0.000	-0.000
5	0.000	-0.000	0.000	0.000
6	-0.000	0.000	0.000	-0.000
7	0.000	-0.000	0.000	0.000
8	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	0.000
10	-0.000	0.000	0.000	-0.000
11	0.000	-0.000	0.000	0.000
12	-0.000	0.000	0.000	-0.000
13	0.000	-0.000	0.000	0.000
14	-0.004	0.002	0.000	-0.002
15	0.000	-0.000	0.000	0.000
16	-0.004	0.002	0.000	-0.002
17	-0.004	0.002	0.000	-0.002
18	0.000	-0.000	0.000	0.000
19	-0.003	0.001	0.000	-0.002
20	0.000	-0.000	0.000	0.000
21	-0.003	0.002	0.000	-0.002
22	-0.003	0.002	0.000	-0.002
23	-0.000	0.000	0.000	-0.000
24	-0.000	0.000	0.000	-0.000

25	-0.000	-0.007	0.000	-0.008
26	-0.000	-0.002	0.000	-0.002
27	0.000	0.003	0.000	0.003
28	0.000	0.005	0.000	0.005
29	0.000	0.003	0.000	0.003
30	-0.000	-0.007	0.000	-0.008
31	-0.000	-0.002	0.000	-0.002
32	0.000	0.003	0.000	0.003
33	0.000	0.005	0.000	0.005
34	0.000	0.002	0.000	0.002
35	-0.000	-0.007	0.000	-0.008
36	-0.000	-0.002	0.000	-0.002
37	0.000	0.003	0.000	0.003
38	0.000	0.006	0.000	0.007
39	0.000	0.002	0.000	0.002
40	-0.000	-0.007	0.000	-0.008
41	-0.000	-0.002	0.000	-0.002
42	0.000	0.002	0.000	0.003
43	0.000	0.005	0.000	0.006
44	0.000	0.004	0.000	0.004
45	-0.000	-0.007	0.000	-0.008
46	-0.000	-0.002	0.000	-0.002

47	0.000	0.003	0.000	0.003
48	0.000	0.005	0.000	0.006
49	0.000	0.001	0.000	0.002
50	-0.000	-0.007	0.000	-0.008
51	-0.000	-0.002	0.000	-0.002
52	0.000	0.002	0.000	0.003
53	0.000	0.006	0.000	0.007
54	0.000	0.002	0.000	0.002
55	-0.000	-0.005	0.000	-0.006
56	-0.000	-0.007	0.000	-0.007
57	-0.000	-0.001	0.000	-0.001
58	-0.000	-0.001	0.000	-0.001
59	0.000	0.006	0.000	0.007
60	0.000	0.003	0.000	0.003
61	0.000	0.001	0.000	0.001
62	0.000	0.003	0.000	0.003
63	-0.000	-0.005	0.000	-0.006
64	-0.000	-0.007	0.000	-0.007
65	-0.000	-0.001	0.000	-0.001
66	-0.000	-0.001	0.000	-0.001
67	0.000	0.006	0.000	0.006
68	0.000	0.003	0.000	0.003

69	0.000	0.001	0.000	0.001
70	0.000	0.002	0.000	0.002
71	-0.000	-0.005	0.000	-0.006
72	-0.000	-0.007	0.000	-0.007
73	-0.000	-0.001	0.000	-0.001
74	-0.000	-0.002	0.000	-0.002
75	0.000	0.006	0.000	0.007
76	0.000	0.003	0.000	0.004
77	0.000	0.003	0.000	0.003
78	0.000	0.001	0.000	0.001
79	-0.000	-0.005	0.000	-0.006
80	-0.000	-0.007	0.000	-0.007
81	-0.000	-0.001	0.000	-0.002
82	-0.000	-0.002	0.000	-0.002
83	0.001	0.007	0.000	0.008
84	0.000	0.003	0.000	0.003
85	0.000	0.002	0.000	0.002
86	0.000	0.005	0.000	0.006
87	-0.000	-0.005	0.000	-0.005
88	-0.000	-0.007	0.000	-0.007
89	-0.000	-0.001	0.000	-0.002
90	-0.000	-0.002	0.000	-0.002

91	0.001	0.008	0.000	0.008
92	0.000	0.003	0.000	0.003
93	0.000	0.002	0.000	0.003
94	0.000	0.001	0.000	0.001
95	-0.000	-0.005	0.000	-0.006
96	-0.000	-0.007	0.000	-0.007
97	-0.000	-0.001	0.000	-0.001
98	-0.000	-0.001	0.000	-0.001
99	0.001	0.007	0.000	0.007
100	0.000	0.003	0.000	0.004
101	0.000	0.003	0.000	0.003
102	0.000	0.002	0.000	0.002
103	-0.001	-0.010	0.000	-0.011
104	-0.003	-0.028	0.000	-0.031
105	-0.000	-0.001	0.000	-0.002
106	-0.000	-0.004	0.000	-0.005
107	0.007	0.116	0.000	0.122
108	0.001	0.010	0.000	0.011
109	0.000	0.001	0.000	0.001
110	-0.001	-0.010	0.000	-0.011
111	-0.003	-0.028	0.000	-0.031
112	-0.000	-0.001	0.000	-0.002

113	-0.000	-0.004	0.000	-0.004
114	0.007	0.120	0.000	0.127
115	0.001	0.010	0.000	0.011
116	0.000	0.001	0.000	0.002
117	-0.001	-0.010	0.000	-0.011
118	-0.003	-0.026	0.000	-0.029
119	-0.000	-0.002	0.000	-0.002
120	-0.000	-0.002	0.000	-0.002
121	0.007	0.115	0.000	0.122
122	0.001	0.010	0.000	0.010
123	0.000	0.003	0.000	0.003
124	-0.001	-0.010	0.000	-0.011
125	-0.003	-0.024	0.000	-0.027
126	-0.000	-0.002	0.000	-0.002
127	-0.000	0.001	0.000	0.000
128	0.006	0.105	0.000	0.111
129	0.001	0.009	0.000	0.010
130	0.000	0.004	0.000	0.004
131	-0.001	-0.009	0.000	-0.010
132	-0.003	-0.024	0.000	-0.027
133	-0.000	-0.002	0.000	-0.002
134	-0.000	-0.002	0.000	-0.002

135	0.006	0.097	0.000	0.102
136	0.001	0.009	0.000	0.010
137	0.000	0.004	0.000	0.005
138	-0.001	-0.010	0.000	-0.011
139	-0.003	-0.026	0.000	-0.029
140	-0.000	-0.002	0.000	-0.002
141	-0.000	-0.004	0.000	-0.004
142	0.006	0.105	0.000	0.111
143	0.001	0.010	0.000	0.010
144	0.000	0.002	0.000	0.003
145	0.000	0.005	0.000	0.006
146	-0.000	0.000	-0.000	0.000
147	0.000	0.004	0.000	0.005
tot	0.001	0.513	-0.000	0.514

CHARGE: cpu time 0.5237: real time 0.5254

FORLOC: cpu time 0.0198: real time 0.0199

FORNL : cpu time 2.0611: real time 2.0719

STRESS: cpu time 6.2028: real time 6.2251

FORCOR: cpu time 0.1432: real time 0.1450

FORHAR: cpu time 0.0335: real time 0.0336

MIXING: cpu time 0.0107: real time 0.0107

OFIELD: cpu time 0.0001: real time 0.0001

DFTD3 V3.0 Rev 1

Edisp (eV) -6.61765

E6 (eV) : -3.9312

E8 (eV) : -2.6864

% E8 : 40.59

FORVDW: cpu time 1.8463: real time 1.8746

FORCE on cell =-STRESS in cart. coord. units (eV):

Direction	XX	YY	ZZ	XY	YZ	ZX
Alpha Z	233.50077	233.50077	233.50077			
Ewald	107573.21105	23482.34343	-39735.96351	9.79010	3450.08921	128.02553
Hartree	106088.71144	25038.36984	-23801.44325	-6.34576	2945.19293	93.15110
E(xc)	-1914.14560	-1916.49392	-1979.81554	0.13094	1.81702	0.12932
Local	**********	-53969.66323	57030.80920	-0.19394	-6353.95095	-217.85569
n-local	-472.54018	-482.28974	-439.37095	-0.66261	-0.58629	-0.30663

augment	-38.30599	-38.59417	-34.29594	0.01271	-0.96620	0.00370
Kinetic	7634.65338	7638.10556	8713.70951	-3.08850	-41.68273	-3.17305
Fock	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
vdW	-2.64194	-1.49192	-6.59298	0.00137	-0.07436	0.01163

Total	-17.77782	-16.21338	-19.46268	-0.35568	-0.16135	-0.01408
in kB	-4.90233	-4.47093	-5.36694	-0.09808	-0.04449	-0.00388

external pressure = -4.91 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

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energy-cutoff : 400.00

volume of cell : 5810.14

direct lattice vectors			reciprocal lattice vectors		
14.780600000	0.000000000	0.000000000	0.067656252	0.000000000	0.000000000
0.000000000	21.333900000	0.000000000	0.000000000	0.046873755	0.000000000
0.000000000	0.000000000	18.425700000	0.000000000	0.000000000	0.054272022

length of vectors

14.780600000	21.333900000	18.425700000	0.067656252	0.046873755	0.054272022

FORCES acting on ions

electron-ion (+dipol) ewald-force non-local-force convergence-correction

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0.441E-02 0.154E+03 0.361E+02 -.292E-02 -.160E+03 -.357E+02 -.179E-02 0.566E+01 -.438E+00 0.971E-07 -.120E-06 -.594E-06

-.189E-01 0.155E+03 -.340E+02 0.165E-01 -.160E+03 0.335E+02 0.116E-02 0.565E+01 0.541E+00 0.941E-06 0.487E-06 0.731E-07

0.184E+00 0.154E+03 0.360E+02 -.184E+00 -.160E+03 -.356E+02 0.515E-05 0.565E+01 -.443E+00 0.125E-06 -.439E-06 -.194E-06

0.112E+00 0.155E+03 -.341E+02 -.991E-01 -.160E+03 0.336E+02 -.175E-01 0.565E+01 0.535E+00 0.124E-06 -.732E-07 0.445E-06

0.172E+00 0.154E+03 0.362E+02 -.173E+00 -.160E+03 -.357E+02 0.116E-02 0.566E+01 -.440E+00 0.733E-07 -.375E-06 -.483E-06

0.127E+00 0.154E+03 -.340E+02 -.109E+00 -.160E+03 0.334E+02 -.211E-01 0.565E+01 0.541E+00 -.706E-06 -.535E-07 -.747E-07

-.190E-01 0.154E+03 0.363E+02 0.179E-01 -.160E+03 -.359E+02 0.158E-02 0.566E+01 -.431E+00 -.108E-07 -.953E-07 -.112E-05

-.124E-01 0.154E+03 -.338E+02 0.193E-01 -.160E+03 0.332E+02 -.721E-02 0.565E+01 0.555E+00 -.793E-06 0.520E-06 -.947E-06

-.182E+00 0.154E+03 0.363E+02 0.182E+00 -.160E+03 -.359E+02 0.259E-03 0.566E+01 -

.429E+00 -.167E-06 0.171E-06 -.150E-05

-.128E+00 0.155E+03 -.337E+02 0.115E+00 -.160E+03 0.331E+02 0.109E-01 0.565E+01 0.561E+00 -.208E-06 0.992E-06 -.129E-05

-.174E+00 0.154E+03 0.362E+02 0.176E+00 -.160E+03 -.358E+02 -.176E-02 0.566E+01 -.432E+00 -.119E-06 0.180E-06 -.126E-05

-.116E+00 0.155E+03 -.338E+02 0.965E-01 -.160E+03 0.332E+02 0.192E-01 0.565E+01 0.555E+00 0.651E-06 0.105E-05 -.792E-06

0.228E+01 -.150E+03 -.387E+02 -.227E+01 0.156E+03 0.386E+02 -.103E-01 -.566E+01 0.766E-01 -.512E-06 0.250E-06 -.880E-07

-.415E+00 -.151E+03 0.388E+02 0.416E+00 0.157E+03 -.386E+02 -.126E-02 -.567E+01 -.269E+00 -.131E-07 0.259E-06 -.164E-07

0.136E+02 -.146E+03 -.413E+02 -.138E+02 0.151E+03 0.413E+02 0.257E+00 -.567E+01 -.349E-01 -.127E-06 0.256E-06 0.137E-06

0.162E+01 -.151E+03 0.402E+02 -.162E+01 0.156E+03 -.400E+02 -.101E-02 -.567E+01 -.229E+00 -.247E-06 -.774E-08 -.611E-06

0.352E+01 -.149E+03 0.443E+02 -.352E+01 0.155E+03 -.441E+02 -.207E-02 -.567E+01 -.180E+00 -.359E-06 0.629E-07 -.615E-06

-.148E+02 -.146E+03 -.330E+02 0.149E+02 0.151E+03 0.330E+02 -.943E-01 -.566E+01 0.477E-01 0.118E-05 0.112E-06 -.869E-06

-.297E+01 -.149E+03 0.432E+02 0.296E+01 0.155E+03 -.430E+02 0.115E-01 -.567E+01 -.241E+00 0.297E-06 0.381E-06 0.214E-06

-.379E+01 -.150E+03 -.385E+02 0.379E+01 0.155E+03 0.385E+02 -.601E-02 -.566E+01

0.238E-01 0.238E-06 0.356E-06 -.292E-06

-.207E+01 -.151E+03 0.395E+02 0.207E+01 0.156E+03 -.392E+02 0.155E-02 -.566E+01 -.282E+00 0.421E-06 0.415E-06 0.316E-06

0.383E-03 -.148E+03 0.486E+02 0.723E-02 0.154E+03 -.484E+02 -.552E-02 -.570E+01 -.158E+00 -.122E-06 0.264E-06 -.780E-07

0.196E+02 -.103E+03 0.222E+02 -.212E+02 0.103E+03 -.246E+02 0.153E+01 0.138E+00 0.238E+01 -.716E-07 0.811E-06 -.527E-06

-.192E+02 -.103E+03 0.153E+02 0.216E+02 0.103E+03 -.168E+02 -.241E+01 -.120E+00 0.151E+01 -.249E-06 0.129E-05 -.101E-05

0.709E-01 0.461E+03 0.202E+03 -.742E-01 -.462E+03 -.201E+03 0.385E-02 0.102E+01 -.219E+00 -.315E-06 0.366E-07 -.129E-05

0.212E+00 0.353E+03 -.234E+03 -.212E+00 -.353E+03 0.234E+03 0.260E-02 0.443E+00 -.371E-01 0.920E-06 -.803E-06 0.217E-05

-.249E-01 0.351E+03 0.240E+03 0.235E-01 -.351E+03 -.241E+03 0.318E-02 0.408E+00 0.565E-01 -.894E-06 0.110E-05 -.197E-05

-.174E+00 0.462E+03 -.195E+03 0.180E+00 -.463E+03 0.195E+03 -.659E-02 0.105E+01 0.233E+00 0.254E-05 0.990E-06 0.115E-05

-.620E-01 0.210E+03 -.272E+03 0.661E-01 -.210E+03 0.272E+03 -.448E-02 0.944E-01 0.560E-01 0.146E-06 -.106E-05 0.143E-05

0.562E+00 0.461E+03 0.202E+03 -.565E+00 -.462E+03 -.201E+03 0.200E-02 0.102E+01 -.214E+00 0.288E-06 -.724E-06 -.320E-07

0.106E+01 0.352E+03 -.234E+03 -.107E+01 -.353E+03 0.234E+03 0.159E-01 0.449E+00 -

.425E-01 -.994E-06 -.112E-05 0.167E-05

0.413E+00 0.351E+03 0.240E+03 -.415E+00 -.351E+03 -.240E+03 0.303E-02 0.408E+00 0.493E-01 -.219E-06 0.558E-06 -.477E-07

0.579E+00 0.462E+03 -.195E+03 -.584E+00 -.463E+03 0.195E+03 0.475E-02 0.105E+01 0.235E+00 -.667E-07 -.135E-05 0.227E-05

0.688E+00 0.210E+03 -.272E+03 -.693E+00 -.210E+03 0.272E+03 0.594E-02 0.920E-01 0.617E-01 -.469E-06 -.993E-06 0.104E-05

0.426E+00 0.461E+03 0.202E+03 -.429E+00 -.462E+03 -.202E+03 0.381E-02 0.102E+01 -.213E+00 0.782E-06 -.590E-06 -.131E-05

0.939E+00 0.352E+03 -.233E+03 -.955E+00 -.352E+03 0.233E+03 0.150E-01 0.442E+00 -.377E-01 -.142E-05 0.876E-06 -.834E-06

0.478E+00 0.351E+03 0.241E+03 -.480E+00 -.351E+03 -.241E+03 0.247E-02 0.406E+00 0.513E-01 0.620E-06 0.327E-06 -.176E-06

0.706E+00 0.462E+03 -.194E+03 -.716E+00 -.463E+03 0.194E+03 0.777E-02 0.106E+01 0.242E+00 -.192E-05 -.350E-06 0.305E-06

0.723E+00 0.210E+03 -.271E+03 -.731E+00 -.210E+03 0.271E+03 0.634E-02 0.918E-01 0.592E-01 -.291E-06 0.468E-06 -.361E-06

-.181E+00 0.461E+03 0.202E+03 0.178E+00 -.462E+03 -.202E+03 0.446E-02 0.102E+01 -.218E+00 0.502E-06 0.181E-06 -.366E-05

-.294E+00 0.352E+03 -.233E+03 0.298E+00 -.352E+03 0.233E+03 -.207E-02 0.441E+00 -.300E-01 -.968E-06 0.342E-05 -.273E-05

0.404E-01 0.351E+03 0.241E+03 -.394E-01 -.351E+03 -.241E+03 0.220E-02 0.410E+00

0.559E-01 0.907E-06 0.515E-06 -.207E-05

0.509E-01 0.462E+03 -.194E+03 -.570E-01 -.463E+03 0.194E+03 0.390E-02 0.106E+01 0.232E+00 -.210E-05 0.288E-05 -.272E-05

-.479E-01 0.210E+03 -.271E+03 0.460E-01 -.210E+03 0.271E+03 -.221E-03 0.939E-01 0.323E-01 -.449E-06 0.190E-05 -.133E-05

-.552E+00 0.461E+03 0.202E+03 0.550E+00 -.462E+03 -.202E+03 0.787E-03 0.102E+01 -.219E+00 -.423E-06 0.895E-06 -.484E-05

-.119E+01 0.352E+03 -.233E+03 0.120E+01 -.353E+03 0.233E+03 -.162E-01 0.448E+00 -.331E-01 0.781E-06 0.366E-05 -.224E-05

-.352E+00 0.351E+03 0.241E+03 0.349E+00 -.351E+03 -.241E+03 0.207E-02 0.414E+00 0.625E-01 0.341E-06 0.859E-06 -.380E-05

-.412E+00 0.462E+03 -.194E+03 0.426E+00 -.463E+03 0.194E+03 -.114E-01 0.106E+01 0.230E+00 -.400E-06 0.486E-05 -.369E-05

-.559E+00 0.210E+03 -.271E+03 0.563E+00 -.210E+03 0.271E+03 -.922E-02 0.922E-01 0.525E-01 0.459E-06 0.204E-05 -.991E-06

-.476E+00 0.461E+03 0.202E+03 0.475E+00 -.462E+03 -.202E+03 0.310E-02 0.102E+01 -.220E+00 -.836E-06 0.929E-06 -.378E-05

-.805E+00 0.353E+03 -.234E+03 0.820E+00 -.353E+03 0.234E+03 -.148E-01 0.448E+00 -.393E-01 0.171E-05 0.180E-05 0.120E-06

-.374E+00 0.351E+03 0.241E+03 0.368E+00 -.351E+03 -.241E+03 0.100E-02 0.411E+00 0.627E-01 -.759E-06 0.122E-05 -.385E-05

-.595E+00 0.462E+03 -.194E+03 0.608E+00 -.463E+03 0.194E+03 -.169E-01 0.105E+01

0.234E+00 0.199E-05 0.413E-05 -.188E-05

-.586E+00 0.210E+03 -.272E+03 0.597E+00 -.210E+03 0.272E+03 -.101E-01 0.100E+00 0.567E-01 0.698E-06 0.665E-06 0.339E-06

-.797E-02 0.206E+03 0.279E+03 0.113E-01 -.206E+03 -.279E+03 -.358E-02 0.690E-01 -.410E-01 -.940E-06 0.869E-06 -.101E-05

0.670E+00 0.302E+02 0.296E+03 -.665E+00 -.302E+02 -.296E+03 -.467E-02 -.407E-01 0.774E-02 -.444E-06 0.106E-05 -.435E-06

-.844E+00 0.144E+03 -.282E+03 0.846E+00 -.144E+03 0.282E+03 -.317E-02 0.138E+00 0.286E-01 0.136E-07 -.413E-06 0.610E-06

0.535E+00 -.215E+02 -.285E+03 -.535E+00 0.214E+02 0.285E+03 -.791E-03 0.394E-01 0.185E-01 -.602E-06 0.120E-06 -.942E-06

0.502E+00 -.294E+02 0.293E+03 -.499E+00 0.294E+02 -.293E+03 -.551E-02 0.256E-01 -.301E-01 0.185E-07 0.638E-06 -.485E-06

0.525E+00 0.139E+03 0.289E+03 -.525E+00 -.139E+03 -.289E+03 0.180E-02 0.104E+00 -.246E-01 -.721E-06 0.102E-05 -.146E-06

-.126E+01 0.364E+02 -.287E+03 0.126E+01 -.364E+02 0.287E+03 0.127E-03 -.672E-02 0.137E-01 -.560E-06 -.199E-06 -.474E-06

0.167E+01 -.130E+03 -.271E+03 -.169E+01 0.130E+03 0.271E+03 0.106E-01 -.872E-01 0.371E-01 -.665E-06 0.368E-06 -.150E-05

0.397E+00 0.207E+03 0.280E+03 -.395E+00 -.207E+03 -.280E+03 0.699E-03 0.698E-01 -.369E-01 -.432E-06 0.103E-05 0.341E-06

0.918E+00 0.312E+02 0.296E+03 -.922E+00 -.311E+02 -.296E+03 0.221E-02 -.408E-01

0.124E-01 -.247E-06 0.120E-05 -.148E-06

0.133E+01 0.144E+03 -.282E+03 -.133E+01 -.144E+03 0.282E+03 0.499E-02 0.127E+00 0.279E-01 -.235E-06 -.115E-05 0.830E-06

0.341E+01 -.200E+02 -.285E+03 -.342E+01 0.199E+02 0.285E+03 0.132E-01 0.421E-01 0.134E-01 0.501E-06 -.779E-07 -.748E-06

0.139E+01 -.287E+02 0.294E+03 -.139E+01 0.287E+02 -.294E+03 -.350E-02 0.255E-01 -.305E-01 -.377E-06 0.117E-05 -.649E-06

0.677E+00 0.139E+03 0.290E+03 -.677E+00 -.139E+03 -.290E+03 0.589E-03 0.103E+00 -.293E-01 -.489E-07 0.101E-05 0.439E-06

0.160E+01 0.367E+02 -.287E+03 -.159E+01 -.366E+02 0.287E+03 -.130E-01 -.197E-01 0.128E-01 -.133E-06 -.601E-06 -.413E-06

0.610E+01 -.125E+03 -.271E+03 -.612E+01 0.125E+03 0.271E+03 0.216E-01 -.888E-01 0.145E-01 0.263E-06 0.773E-07 -.976E-06

0.366E+00 0.207E+03 0.280E+03 -.371E+00 -.207E+03 -.280E+03 0.706E-04 0.687E-01 -.363E-01 0.546E-06 0.681E-06 0.232E-06

-.408E-01 0.319E+02 0.296E+03 0.322E-01 -.318E+02 -.296E+03 0.105E-01 -.360E-01 0.141E-01 0.244E-06 0.364E-06 0.106E-06

0.209E+01 0.144E+03 -.281E+03 -.210E+01 -.144E+03 0.281E+03 0.120E-01 0.121E+00 0.239E-01 -.590E-07 -.835E-07 0.151E-06

0.302E+01 -.172E+02 -.283E+03 -.304E+01 0.171E+02 0.283E+03 0.242E-01 0.881E-01 0.600E-01 0.458E-06 0.191E-06 -.468E-06

0.105E+01 -.272E+02 0.294E+03 -.105E+01 0.272E+02 -.294E+03 0.283E-02 0.245E-01 -

.373E-01 -.386E-06 0.692E-06 -.258E-06

0.948E-01 0.140E+03 0.290E+03 -.964E-01 -.140E+03 -.290E+03 0.127E-02 0.107E+00 -.230E-01 0.755E-06 0.340E-06 -.821E-07

0.276E+01 0.387E+02 -.286E+03 -.276E+01 -.387E+02 0.286E+03 0.892E-03 -.102E-01 0.291E-01 0.549E-06 -.117E-06 -.388E-06

0.593E+01 -.115E+03 -.267E+03 -.608E+01 0.115E+03 0.267E+03 0.154E+00 0.271E-02 0.128E+00 0.485E-06 -.189E-06 -.358E-06

-.243E+00 0.207E+03 0.280E+03 0.241E+00 -.207E+03 -.280E+03 0.436E-02 0.720E-01 -.385E-01 0.958E-06 0.207E-06 -.101E-05

-.115E+01 0.314E+02 0.294E+03 0.114E+01 -.314E+02 -.294E+03 0.917E-02 -.309E-01 0.563E-02 0.405E-06 -.537E-06 0.324E-07

0.592E+00 0.144E+03 -.281E+03 -.609E+00 -.144E+03 0.281E+03 0.175E-01 0.126E+00 0.437E-01 0.251E-06 0.794E-06 -.765E-06

-.941E+00 -.159E+02 -.286E+03 0.933E+00 0.158E+02 0.286E+03 0.602E-02 0.910E-01 0.798E-01 0.502E-06 0.979E-07 -.536E-06

-.647E+00 -.265E+02 0.293E+03 0.644E+00 0.265E+02 -.293E+03 0.489E-02 0.236E-01 -.268E-01 0.917E-07 -.346E-06 0.361E-06

-.535E+00 0.139E+03 0.289E+03 0.531E+00 -.139E+03 -.289E+03 0.655E-02 0.114E+00 -.212E-01 0.687E-06 -.236E-06 -.106E-05

0.772E+00 0.407E+02 -.287E+03 -.784E+00 -.407E+02 0.287E+03 0.487E-02 0.234E-02 -.193E-01 0.712E-06 0.540E-06 -.546E-06

-.463E+00 -.113E+03 -.276E+03 0.429E+00 0.113E+03 0.277E+03 0.348E-01 0.608E-01 -

.269E+00 0.291E-06 0.370E-06 -.963E-06

-.572E+00 0.206E+03 0.279E+03 0.570E+00 -.206E+03 -.279E+03 0.116E-02 0.724E-01 -.454E-01 0.441E-06 -.212E-07 -.222E-05

-.782E+00 0.304E+02 0.294E+03 0.785E+00 -.304E+02 -.294E+03 -.751E-02 -.306E-01 -.118E-02 0.265E-06 -.572E-06 -.291E-06

-.123E+01 0.144E+03 -.281E+03 0.124E+01 -.144E+03 0.281E+03 -.155E-01 0.123E+00 0.504E-01 -.171E-06 0.169E-05 -.937E-06

-.365E+01 -.174E+02 -.283E+03 0.368E+01 0.173E+02 0.283E+03 -.306E-01 0.118E+00 0.579E-01 0.129E-06 0.846E-06 -.494E-06

-.130E+01 -.277E+02 0.291E+03 0.129E+01 0.277E+02 -.291E+03 -.130E-02 0.342E-01 -.217E-01 0.363E-06 -.946E-06 0.486E-06

-.347E+00 0.139E+03 0.289E+03 0.346E+00 -.139E+03 -.289E+03 0.339E-04 0.112E+00 -.145E-01 0.318E-07 -.316E-06 -.168E-05

-.825E+00 0.400E+02 -.287E+03 0.817E+00 -.400E+02 0.287E+03 0.129E-01 -.721E-02 -.185E-01 -.316E-06 0.973E-06 -.545E-06

-.783E+01 -.119E+03 -.267E+03 0.802E+01 0.119E+03 0.267E+03 -.190E+00 0.442E-02 0.328E-01 0.617E-06 0.194E-06 -.632E-06

-.408E+00 0.206E+03 0.279E+03 0.409E+00 -.206E+03 -.279E+03 -.277E-02 0.719E-01 -.463E-01 -.585E-06 0.300E-06 -.227E-05

-.601E-01 0.300E+02 0.294E+03 0.699E-01 -.299E+02 -.294E+03 -.944E-02 -.345E-01 0.144E-02 -.207E-06 0.215E-06 -.471E-06

-.206E+01 0.145E+03 -.282E+03 0.207E+01 -.145E+03 0.282E+03 -.189E-01 0.133E+00

0.256E-01 0.195E-06 0.132E-05 -.333E-06

-.256E+01 -.209E+02 -.285E+03 0.258E+01 0.208E+02 0.285E+03 -.288E-01 0.416E-01 0.316E-01 -.101E-05 0.687E-06 -.726E-06

-.549E+00 -.290E+02 0.291E+03 0.553E+00 0.290E+02 -.291E+03 -.281E-02 0.294E-01 -.249E-01 0.252E-06 -.367E-06 0.861E-07

0.606E-01 0.139E+03 0.289E+03 -.607E-01 -.139E+03 -.289E+03 -.305E-03 0.109E+00 -.206E-01 -.694E-06 0.287E-06 -.123E-05

-.289E+01 0.377E+02 -.286E+03 0.290E+01 -.377E+02 0.286E+03 -.145E-01 -.302E-02 0.208E-01 -.167E-06 0.645E-06 -.457E-06

-.512E+01 -.128E+03 -.271E+03 0.517E+01 0.128E+03 0.271E+03 -.461E-01 -.855E-01 0.375E-01 -.100E-05 0.402E-06 -.963E-06

0.404E+00 -.137E+03 0.280E+03 -.397E+00 0.137E+03 -.280E+03 -.964E-02 -.127E+00 -.153E-01 0.494E-06 0.441E-06 -.485E-06

0.194E+01 -.343E+03 0.233E+03 -.195E+01 0.344E+03 -.233E+03 0.915E-02 -.460E+00 -.541E-01 0.141E-06 -.190E-06 -.166E-05

-.252E+01 -.197E+03 -.259E+03 0.253E+01 0.197E+03 0.259E+03 -.952E-02 -.196E+00 0.367E-01 -.113E-05 0.945E-06 -.131E-05

0.691E+01 -.447E+03 -.198E+03 -.693E+01 0.448E+03 0.198E+03 0.948E-02 -.112E+01 0.874E-01 -.148E-05 -.689E-06 -.748E-06

-.458E+00 -.451E+03 0.204E+03 0.459E+00 0.452E+03 -.204E+03 -.192E-02 -.108E+01 -.112E+00 0.491E-06 0.684E-06 -.415E-06

0.171E+01 -.203E+03 0.269E+03 -.171E+01 0.203E+03 -.269E+03 -.479E-02 -.924E-01 -

.316E-01 0.874E-07 0.597E-06 -.135E-05

-.209E+01 -.338E+03 -.222E+03 0.214E+01 0.338E+03 0.222E+03 -.444E-01 -.603E+00 0.535E-01 -.759E-06 -.844E-07 -.800E-06

0.219E+01 -.136E+03 0.282E+03 -.218E+01 0.136E+03 -.282E+03 -.639E-02 -.126E+00 -.910E-02 -.392E-06 0.809E-06 -.141E-05

0.672E+01 -.339E+03 0.238E+03 -.670E+01 0.340E+03 -.238E+03 -.129E-01 -.461E+00 -.455E-01 -.116E-05 -.460E-06 -.232E-05

0.678E+01 -.193E+03 -.259E+03 -.679E+01 0.193E+03 0.258E+03 0.111E-01 -.144E+00 0.632E-01 -.420E-06 0.727E-06 -.132E-05

0.312E+02 -.427E+03 -.198E+03 -.313E+02 0.428E+03 0.197E+03 0.721E-01 -.974E+00 0.138E+00 0.515E-07 -.172E-05 0.370E-07

0.544E+01 -.449E+03 0.209E+03 -.545E+01 0.450E+03 -.209E+03 0.532E-03 -.108E+01 -.794E-01 -.707E-06 -.176E-06 -.240E-05

0.368E+01 -.201E+03 0.272E+03 -.368E+01 0.201E+03 -.272E+03 -.810E-03 -.974E-01 -.302E-01 -.875E-06 0.400E-06 -.167E-05

0.124E+02 -.332E+03 -.223E+03 -.125E+02 0.332E+03 0.223E+03 0.121E+00 -.534E+00 0.313E-01 -.113E-05 -.994E-06 -.751E-06

0.219E+01 -.133E+03 0.283E+03 -.219E+01 0.133E+03 -.283E+03 0.448E-03 -.128E+00 -.413E-02 -.877E-06 0.280E-06 -.822E-06

0.492E+01 -.332E+03 0.245E+03 -.488E+01 0.332E+03 -.245E+03 -.321E-01 -.476E+00 -.372E-01 -.118E-05 -.811E-06 -.558E-06

0.112E+02 -.182E+03 -.258E+03 -.112E+02 0.182E+03 0.258E+03 0.470E-01 -.989E-01 -

.105E+00 0.639E-06 0.843E-07 -.454E-06

0.317E+02 -.399E+03 -.175E+03 -.319E+02 0.401E+03 0.174E+03 0.297E+00 -.143E+01 0.132E+01 -.244E-05 -.347E-05 -.116E-05

0.930E+01 -.443E+03 0.219E+03 -.929E+01 0.444E+03 -.219E+03 -.595E-02 -.110E+01 -.481E-01 -.157E-05 -.586E-06 -.200E-05

0.168E+01 -.196E+03 0.273E+03 -.169E+01 0.197E+03 -.273E+03 0.542E-02 -.109E+00 -.507E-01 -.915E-06 -.421E-06 -.194E-06

0.172E+02 -.310E+03 -.216E+03 -.175E+02 0.310E+03 0.216E+03 0.325E+00 -.219E+00 0.122E+00 -.129E-06 -.147E-05 -.278E-06

-.104E+01 -.132E+03 0.281E+03 0.103E+01 0.132E+03 -.281E+03 0.102E-01 -.127E+00 0.439E-03 -.433E-06 -.625E-06 0.732E-06

-.513E+01 -.332E+03 0.239E+03 0.512E+01 0.332E+03 -.239E+03 0.890E-02 -.495E+00 -.415E-01 -.581E-07 -.911E-06 0.157E-05

0.154E+01 -.170E+03 -.261E+03 -.166E+01 0.169E+03 0.261E+03 0.118E+00 0.374E+00 -.900E-01 0.932E-06 -.335E-06 -.105E-05

-.659E+01 -.301E+03 -.189E+03 0.612E+01 0.296E+03 0.185E+03 0.475E+00 0.498E+01 0.407E+01 -.158E-05 -.839E-05 -.252E-05

-.631E+00 -.436E+03 0.227E+03 0.628E+00 0.437E+03 -.227E+03 0.164E-02 -.120E+01 -.481E-01 -.814E-06 -.534E-06 0.329E-06

-.303E+01 -.197E+03 0.268E+03 0.301E+01 0.197E+03 -.268E+03 0.146E-01 -.112E+00 -.425E-01 -.155E-06 -.946E-06 0.157E-05

0.319E+01 -.281E+03 -.215E+03 -.513E+01 0.280E+03 0.214E+03 0.192E+01 0.643E+00

0.820E+00 -.176E-05 -.628E-05 -.195E-05

-.274E+01 -.134E+03 0.277E+03 0.274E+01 0.134E+03 -.277E+03 0.251E-02 -.123E+00 -.182E-01 0.341E-06 -.983E-06 0.155E-05

-.600E+01 -.338E+03 0.230E+03 0.600E+01 0.339E+03 -.230E+03 0.113E-01 -.494E+00 -.455E-01 0.117E-05 -.303E-06 0.202E-05

-.647E+01 -.171E+03 -.257E+03 0.655E+01 0.170E+03 0.257E+03 -.778E-01 0.486E+00 0.218E-01 0.382E-06 0.846E-06 -.146E-05

-.441E+02 -.422E+03 -.184E+03 0.446E+02 0.423E+03 0.183E+03 -.562E+00 -.111E+01 0.618E+00 0.343E-05 -.483E-05 -.324E-05

-.867E+01 -.441E+03 0.211E+03 0.867E+01 0.442E+03 -.211E+03 0.145E-01 -.112E+01 -.747E-01 0.870E-06 0.797E-07 0.160E-05

-.292E+01 -.201E+03 0.265E+03 0.293E+01 0.201E+03 -.265E+03 -.911E-02 -.110E+00 -.201E-01 0.939E-06 -.759E-06 0.182E-05

-.144E+02 -.290E+03 -.209E+03 0.164E+02 0.289E+03 0.209E+03 -.198E+01 0.604E+00 0.787E+00 0.411E-05 -.812E-05 -.406E-05

-.138E+01 -.136E+03 0.277E+03 0.139E+01 0.136E+03 -.277E+03 -.101E-01 -.125E+00 -.236E-01 0.821E-06 -.460E-06 0.970E-06

-.278E+01 -.343E+03 0.230E+03 0.276E+01 0.343E+03 -.230E+03 0.236E-01 -.473E+00 -.588E-01 0.105E-05 0.157E-06 0.662E-06

-.103E+02 -.189E+03 -.258E+03 0.104E+02 0.189E+03 0.258E+03 -.769E-01 -.139E+00 -.527E-01 -.300E-06 0.350E-06 -.762E-06

-.149E+02 -.446E+03 -.196E+03 0.150E+02 0.447E+03 0.196E+03 -.692E-01 -.113E+01

0.100E+00 -.665E-07 -.757E-06 -.689E-06

-.548E+01 -.448E+03 0.204E+03 0.549E+01 0.449E+03 -.203E+03 -.467E-02 -.109E+01 -.125E+00 0.162E-05 0.899E-06 0.150E-05

-.905E+00 -.203E+03 0.267E+03 0.914E+00 0.203E+03 -.267E+03 -.903E-02 -.102E+00 -.313E-01 0.899E-06 0.531E-08 0.422E-06

-.162E+02 -.329E+03 -.218E+03 0.166E+02 0.329E+03 0.218E+03 -.359E+00 -.480E+00 0.423E-01 0.671E-06 -.138E-05 -.135E-05

-.400E+01 -.259E+03 -.198E+03 0.312E+01 0.252E+03 0.193E+03 0.973E+00 0.785E+01 0.479E+01 -.193E-05 0.556E-05 0.317E-05

0.531E+02 -.518E+03 -.137E+03 -.541E+02 0.522E+03 0.141E+03 0.106E+01 -.396E+01 -.382E+01 -.259E-05 0.519E-05 -.679E-06

-.461E+02 -.582E+03 -.442E+03 0.517E+02 0.632E+03 0.475E+03 -.571E+01 -.505E+02 -.334E+02 0.193E-05 0.310E-04 0.127E-04

0.420E+01 0.274E+02 0.216E+02 -.327E-12 -.784E-11 0.153E-11 -.425E+01 -.273E+02 -.216E+02 -.315E-05 0.506E-04 -.774E-04

POSITION TOTAL-FORCE (eV/Angst)

1.24575	4.02870	5.43979	0.000054	0.001064	-0.000442
1.21024	4.07581	8.43726	-0.000976	0.002690	-0.001097

3.70862	4.02890	5.43965	0.000326	0.001936	-0.001128
3.67998	4.07733	8.43690	-0.004014	-0.000341	-0.002856
6.17157	4.02854	5.43942	0.000016	-0.000090	-0.001783
6.14482	4.08292	8.43295	-0.002808	-0.003224	-0.003132
8.63513	4.02801	5.43869	0.000799	-0.000392	-0.002029
8.60339	4.08732	8.43089	-0.000112	-0.001102	-0.002138
11.09928	4.02784	5.43885	0.000888	0.002023	-0.002739
11.06021	4.08619	8.43099	-0.001729	0.000779	-0.000567
13.56311	4.02807	5.43972	0.000342	0.001670	-0.001648
13.52141	4.08047	8.43349	0.000408	-0.002176	0.000359
2.44241	15.48073	8.85224	-0.000604	-0.005358	0.002449
0.01714	15.44624	5.32469	0.000337	0.001532	-0.001250
4.86040	15.47728	8.86623	0.001458	0.000030	-0.000590
2.48016	15.44854	5.27562	0.000385	-0.001203	-0.000575
4.94382	15.44925	5.24869	0.001863	-0.003060	0.000347
12.31531	15.48242	9.00211	-0.006101	0.000954	0.005977
9.86772	15.44556	5.34176	0.000436	-0.001164	0.000950
14.76279	15.48245	8.89951	-0.006310	-0.000633	0.005587
12.33384	15.44510	5.36128	0.001337	-0.003256	-0.001275
7.40743	15.44616	5.26463	0.002388	0.001393	0.001484
6.44846	16.34427	7.40648	-0.003266	-0.003381	0.000178
8.60064	16.47644	7.89249	0.002228	0.002676	0.006198

1.24544	5.11881	5.35500	0.000951	0.000036	-0.002397
2.44348	5.83889	8.62292	0.002436	-0.004353	0.001228
0.01380	5.79530	5.28573	0.002098	-0.002337	0.000461
1.21063	5.16420	8.54151	0.000281	-0.000506	-0.001974
2.44351	7.27931	8.74832	-0.000028	-0.001285	-0.000145
3.70866	5.11896	5.35390	-0.000408	-0.001749	0.000390
4.90800	5.84315	8.62123	-0.001057	0.003877	-0.000723
2.47701	5.79561	5.28397	0.001472	-0.000488	-0.002618
3.67679	5.16572	8.54000	-0.000102	0.001660	-0.000116
4.90764	7.28398	8.74777	0.000602	-0.000651	0.000992
6.17184	5.11860	5.35433	0.001493	0.000243	0.000960
7.37096	5.84929	8.62094	-0.000608	0.007170	-0.002452
4.94029	5.79548	5.28340	0.000623	-0.002569	-0.001186
6.14080	5.17108	8.53715	-0.002494	0.002481	0.002371
7.37071	7.28983	8.75132	-0.002045	0.001528	0.000108
8.63543	5.11820	5.35521	0.001245	0.001178	-0.000998
9.83233	5.85166	8.62337	0.002821	0.001050	-0.001078
7.40374	5.79498	5.28512	0.003490	-0.002552	-0.001348
8.60194	5.17528	8.53759	-0.001910	-0.000566	-0.000322
9.83204	7.29110	8.75719	-0.001775	-0.003001	-0.002480
11.09930	5.11814	5.35578	-0.000855	-0.003519	-0.001295
12.29449	5.84673	8.62385	0.000020	0.005855	-0.002201

9.86750	5.79468	5.28678	-0.000723	-0.000571	0.001543
11.06261	5.17409	8.53894	0.002699	0.002554	-0.000506
12.29428	7.28729	8.75533	-0.004463	0.001088	-0.001550
13.56278	5.11829	5.35605	0.002666	0.000386	-0.001918
14.75895	5.83988	8.62434	-0.000259	-0.002618	-0.002161
12.33118	5.79480	5.28692	-0.004495	-0.001332	0.002584
13.52535	5.16844	8.54022	-0.003446	0.003731	-0.001526
14.75917	7.28012	8.75179	0.001065	0.002519	-0.000732
0.01434	7.23830	5.19017	0.000095	-0.000211	0.000084
1.24689	9.38061	5.13160	0.000568	-0.001877	0.000007
1.21085	7.98059	8.79588	-0.000940	-0.000442	0.001554
2.44214	10.12243	8.87141	-0.000798	0.003823	-0.005009
0.01532	10.08686	5.14049	-0.002031	-0.000114	-0.002402
1.24606	7.94244	5.15775	0.002024	-0.002576	0.000822
1.21082	9.41592	8.85782	-0.000957	0.004204	0.000150
2.44072	11.55513	8.88414	-0.006034	-0.003278	0.001543
2.47747	7.23842	5.18585	0.002808	0.002867	0.001319
3.70997	9.38055	5.12566	-0.001076	-0.003026	0.000051
3.67534	7.98360	8.79349	-0.000578	0.001053	0.000965
4.90487	10.12925	8.87518	0.000130	0.000284	0.000049
2.47867	10.08713	5.12695	-0.002250	0.001509	0.000766
3.70939	7.94242	5.15441	0.000851	-0.003988	-0.001706

3.67589	9.41970	8.85445	-0.001399	0.001795	-0.000177
4.90263	11.56506	8.89086	-0.000329	0.000588	0.000956
4.94085	7.23830	5.18552	-0.004695	0.002240	0.000838
6.17318	9.38002	5.13173	0.002010	0.002059	0.001841
6.13864	7.99044	8.79647	0.002546	-0.000071	-0.001678
7.36780	10.13760	8.89473	-0.000670	0.003572	0.000342
4.94196	10.08682	5.12700	0.004172	0.001490	-0.001161
6.17284	7.94199	5.15766	-0.000026	0.000592	0.003029
6.13939	9.42660	8.86164	0.001004	-0.000536	-0.002311
7.36410	11.57721	8.92935	-0.001110	-0.002819	0.004119
7.40426	7.23794	5.19012	0.002153	0.001750	0.001085
8.63700	9.37970	5.14543	-0.000559	0.002910	0.000966
8.60086	7.99568	8.80617	0.001097	-0.000002	-0.000972
9.83068	10.14286	8.92842	-0.002250	0.003839	-0.000957
7.40553	10.08627	5.14064	0.001256	-0.003522	0.003137
8.63637	7.94166	5.16555	0.002625	0.001834	-0.001413
8.60077	9.43254	8.88532	-0.005967	0.001695	-0.001265
9.82927	11.58244	9.00096	0.001265	0.000808	0.000727
9.86805	7.23787	5.19489	-0.000360	0.000083	-0.000194
11.10106	9.37979	5.15156	-0.003814	-0.001061	0.000676
11.06331	7.99411	8.80818	-0.000282	-0.001181	0.000219
12.29815	10.12943	8.90340	-0.000881	-0.000743	0.001088

9.86930	10.08593	5.15631	-0.005420	-0.001383	0.001408
11.10021	7.94175	5.16862	-0.000564	-0.003034	0.001385
11.06206	9.43062	8.88839	0.004636	0.001263	0.002069
12.30255	11.56557	8.94694	0.003740	-0.001427	-0.000067
12.33169	7.23799	5.19447	-0.001029	0.000236	-0.001742
13.56437	9.38021	5.14435	0.000760	0.001620	-0.000567
13.52754	7.98555	8.80171	-0.000761	-0.002331	-0.003116
14.76233	10.12320	8.88285	-0.005075	0.001216	-0.001615
12.33257	10.08637	5.15511	0.002642	0.000585	-0.001544
13.56350	7.94214	5.16485	-0.000061	-0.000861	-0.000376
13.52731	9.42040	8.86925	-0.000225	0.003021	-0.000681
14.76430	11.55727	8.90646	-0.002336	-0.001253	0.001857
0.01611	11.52516	5.16621	-0.001071	-0.002604	0.000396
1.24770	13.67535	5.22209	0.001764	-0.002661	-0.002501
1.21217	12.26335	8.89409	0.000370	-0.000081	0.001221
2.43998	14.38728	8.86748	-0.003075	0.002563	0.000766
0.01699	14.35408	5.27295	-0.000327	-0.000205	-0.001892
1.24794	12.22963	5.17275	0.001089	0.000813	-0.001370
1.21434	13.70818	8.88771	0.003016	0.000706	0.003948
2.47958	11.52580	5.14547	-0.001602	-0.000223	-0.001472
3.71218	13.67636	5.19535	0.004752	0.000206	0.001024
3.66932	12.26248	8.88184	-0.001991	0.000140	-0.000612

4.89370	14.38589	8.86075	0.004629	0.000135	-0.002309
2.48000	14.35596	5.23149	0.001321	-0.000743	0.001756
3.71150	12.23022	5.15602	0.000923	-0.004580	0.001008
3.66212	13.70366	8.87117	-0.004951	0.002529	-0.000159
4.94290	11.52542	5.14351	-0.000062	-0.001823	-0.001597
6.17627	13.67505	5.20032	0.000946	0.000125	0.000001
6.13145	12.27911	8.90591	0.005518	0.006837	0.004811
7.36614	14.42967	8.88203	0.004343	0.002736	-0.000856
4.94347	14.35627	5.21375	0.000062	-0.001370	0.001063
6.17493	12.22917	5.16623	-0.001421	-0.001040	0.001582
6.11879	13.72336	8.87765	0.004383	-0.003029	-0.001538
7.40625	11.52413	5.16368	0.000919	-0.003457	0.000360
8.63876	13.67323	5.24377	0.001786	0.001504	-0.001394
8.58939	12.29067	9.00208	0.000966	0.003110	0.001504
9.83855	14.39048	9.30305	0.011745	0.046510	0.038929
7.40672	14.35386	5.23530	-0.001154	0.000368	-0.000818
8.63820	12.22778	5.19800	0.000325	-0.001217	0.001077
8.55571	13.73596	9.04598	-0.014064	-0.018215	-0.000888
9.86985	11.52338	5.18893	0.001757	-0.002097	-0.000106
11.10099	13.67352	5.27669	0.003260	-0.001411	-0.001015
11.07378	12.27333	9.00891	-0.004762	0.005929	-0.000204
12.30694	14.38896	9.00333	-0.005162	0.003234	-0.000182

9.86934	14.35300	5.29564	0.002913	0.000733	0.000195
11.10161	12.22804	5.21650	-0.001083	-0.002710	0.001054
11.11464	13.70636	9.07877	0.015910	-0.012863	-0.004565
12.33326	11.52411	5.18815	-0.000921	0.000202	0.000536
13.56430	13.67399	5.25995	0.001447	-0.000435	0.000049
13.53626	12.26601	8.93587	-0.002470	0.004370	0.002403
14.76266	14.38906	8.90426	-0.005339	0.003387	0.003598
12.33397	14.35288	5.30710	0.002854	-0.001286	-0.001722
13.56505	12.22870	5.20105	0.000149	0.000070	-0.001140
13.54921	13.70690	8.94399	0.000343	-0.007058	-0.000819
9.91126	15.53185	9.99472	0.097751	0.912785	0.572189
7.28864	16.40884	8.69813	0.005422	0.000410	-0.000024
10.02526	16.51865	10.64498	-0.101751	-0.940125	-0.597577

---

total drift:	-0.046789	0.023688	-0.022830

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

---

free energy TOTEN = -1209.38210678 eV

energy without entropy= -1209.38210678 energy(sigma->0) = -1209.38210678

d Force =-0.6698464E-02[-0.156E-01, 0.223E-02] d Energy =-0.6781810E-02 0.833E-04

d Force = 0.1027351E+02[0.102E+02, 0.103E+02] d Ewald = 0.1027376E+02-0.258E-03

POTLOK: cpu time 0.1766: real time 0.1829

---

stress matrix after NEB project (eV)

-17.77782	-0.35568	-0.01408
-0.35568	-16.21338	-0.16135
-0.01408	-0.16135	-19.46268

FORCES: max atom, RMS 1.118609 0.128344

FORCE total and by dimension 1.556090 0.940125

Stress total and by dimension 30.951989 19.462677

Finite differences progress:

Degree of freedom: 5/ 6

Displacement: 1/ 2

Total: 9/ 12

LATTYP: Found a simple orthorhombic cell.

ALAT = 14.7806000000

B/A-ratio = 1.2466138046

C/A-ratio = 1.4433717170

Lattice vectors:

A1 = (-14.7806000000, 0.0000000000, 0.0000000000)

A2 = (0.0000000000, 0.0000000000, -18.4257000000)

A3 = (0.0000000000, -21.3339000000, 0.0000000000)

Analysis of symmetry for initial positions (statically):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The static configuration has the point symmetry C_1 .

Analysis of symmetry for dynamics (positions and initial velocities):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The dynamic configuration has the point symmetry C_1 .

Analysis of constrained symmetry for selective dynamics:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The constrained configuration has the point symmetry C_1 .

Analysis of structural, dynamic, and magnetic symmetry:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The magnetic configuration has the point symmetry C_1 .

Subroutine INISYM returns: Found 1 space group operations

(whereof 1 operations are pure point group operations),

and found 1 'primitive' translations

KPOINTS: KPT-Resolved Value to Generate K-Mesh: 0

Automatic generation of k-mesh.

Space group operators:

irot	det(A)	alpha	n_x	n_y	n_z	tau_x	tau_y	tau_z
1	1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Subroutine IBZKPT returns following result:

==========

Found 1 irreducible k-points:

Following reciprocal coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

Following cartesian coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

WAVPRE: cpu time 0.1207: real time 0.1323

FEWALD: cpu time 0.0026: real time 0.0026

ORTHCH: cpu time 0.9996: real time 1.0027

LOOP+: cpu time 179.6916: real time 180.7948

---------- Iteration 11(1) ----------

POTLOK: cpu time 0.1698: real time 0.1828

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9281: real time 1.9333

RMM-DIIS: cpu time 7.0760: real time 7.1233

ORTHCH: cpu time 0.3535: real time 0.3542

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5243: real time 0.5261

MIXING: cpu time 0.0044: real time 0.0044

LOOP: cpu time 10.0665: real time 10.1347

eigenvalue-minimisations : 1928

total energy-change (2. order) :-0.1396035E-01 (-0.5072594E+00)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7419922 magnetization 0.0542933

Broyden mixing:

rms(total) = 0.46752E-01 rms(broyden)= 0.46237E-01

rms(prec) = 0.47795E-01

weight for this iteration 100.00

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107342.19431339

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81410388

PAW double counting = 52156.16678093 -52219.07075889

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5818.13637168

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77841954 eV

energy without entropy = -1202.77841954 energy(sigma->0) = -1202.77841954

---------- Iteration 11(2) ----------

POTLOK: cpu time 0.1644: real time 0.1733

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9264: real time 1.9332

RMM-DIIS: cpu time 7.2731: real time 7.3094

ORTHCH: cpu time 0.3545: real time 0.3557

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5261: real time 0.5278

MIXING: cpu time 0.0047: real time 0.0047

LOOP: cpu time 10.2596: real time 10.3146

eigenvalue-minimisations : 1940

total energy-change (2. order) : 0.1327565E-01 (-0.4068605E-02)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7454916 magnetization 0.0542806

Broyden mixing:

rms(total) = 0.34650E-01 rms(broyden)= 0.34616E-01

rms(prec) = 0.35838E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4081

1.4081

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107343.35362768

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.83937945

PAW double counting = 52171.18075999 -52234.09583378

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.97796147

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76514388 eV

energy without entropy = -1202.76514388 energy(sigma->0) = -1202.76514388

---------- Iteration 11(3) ----------

POTLOK: cpu time 0.1678: real time 0.1916

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9286: real time 1.9345

RMM-DIIS: cpu time 7.0819: real time 7.1057

ORTHCH: cpu time 0.3520: real time 0.3529

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5260: real time 0.5277

MIXING: cpu time 0.0051: real time 0.0051

LOOP: cpu time 10.0719: real time 10.1280

eigenvalue-minimisations : 1925

total energy-change (2. order) : 0.1119737E-02 (-0.5804014E-03)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7413595 magnetization 0.0542823

Broyden mixing:

rms(total) = 0.16260E-01 rms(broyden)= 0.16244E-01

rms(prec) = 0.17263E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4369

2.2705 0.6033

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107344.46902143

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88042326

PAW double counting = 52184.61219969 -52247.54391286

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.88585243

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76402414 eV

energy without entropy = -1202.76402414 energy(sigma->0) = -1202.76402414

---------- Iteration 11(4) ----------

POTLOK: cpu time 0.1634: real time 0.1643

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9256: real time 1.9314

RMM-DIIS: cpu time 7.2795: real time 7.3003

ORTHCH: cpu time 0.3523: real time 0.3532

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5255: real time 0.5270

MIXING: cpu time 0.0053: real time 0.0053

LOOP: cpu time 10.2621: real time 10.2921

eigenvalue-minimisations : 1939

total energy-change (2. order) : 0.2091509E-03 (-0.8233286E-04)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7415959 magnetization 0.0542785

Broyden mixing:

rms(total) = 0.79721E-02 rms(broyden)= 0.79692E-02

rms(prec) = 0.87431E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3907

2.3223 1.0869 0.7629

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107345.28810157

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.89099110

PAW double counting = 52195.69279534 -52258.63030835

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.07133114

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76381499 eV

energy without entropy = -1202.76381499 energy(sigma->0) = -1202.76381499

---------- Iteration 11(5) ----------

POTLOK: cpu time 0.1647: real time 0.1864

SETDIJ: cpu time 0.0102: real time 0.0103

EDDIAG: cpu time 1.9262: real time 1.9328

RMM-DIIS: cpu time 7.0458: real time 7.0768

ORTHCH: cpu time 0.3531: real time 0.3543

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5255: real time 0.5270

MIXING: cpu time 0.0055: real time 0.0055

LOOP: cpu time 10.0315: real time 10.0935

eigenvalue-minimisations : 1921

total energy-change (2. order) : 0.1471304E-03 (-0.2243945E-04)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7427033 magnetization 0.0542733

Broyden mixing:

rms(total) = 0.23511E-02 rms(broyden)= 0.23392E-02

rms(prec) = 0.26228E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4601

2.3840 1.8259 0.8154 0.8154

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107345.41749542

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88283543

PAW double counting = 52197.34640408 -52260.28113960

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.93641198

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76366786 eV

energy without entropy = -1202.76366786 energy(sigma->0) = -1202.76366786

---------- Iteration 11(6) ----------

POTLOK: cpu time 0.1648: real time 0.1888

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9233: real time 1.9296

RMM-DIIS: cpu time 7.1971: real time 7.2230

ORTHCH: cpu time 0.3541: real time 0.3552

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5262: real time 0.5276

MIXING: cpu time 0.0060: real time 0.0060

LOOP: cpu time 10.1820: real time 10.2407

eigenvalue-minimisations : 1932

total energy-change (2. order) :-0.1485787E-04 (-0.2425109E-05)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7429305 magnetization 0.0542711

Broyden mixing:

rms(total) = 0.13297E-02 rms(broyden)= 0.13269E-02

rms(prec) = 0.15576E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4399

2.4881 1.9303 0.7652 1.0079 1.0079

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107345.59018517

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88093227

PAW double counting = 52198.50929870 -52261.44314738

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.76272076

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76368272 eV

energy without entropy = -1202.76368272 energy(sigma->0) = -1202.76368272

---------- Iteration 11(7) ----------

POTLOK: cpu time 0.1655: real time 0.1680

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9258: real time 1.9324

RMM-DIIS: cpu time 6.9335: real time 7.0087

ORTHCH: cpu time 0.3532: real time 0.3543

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5252: real time 0.5272

MIXING: cpu time 0.0060: real time 0.0061

LOOP: cpu time 9.9196: real time 10.0071

eigenvalue-minimisations : 1885

total energy-change (2. order) :-0.2120497E-04 (-0.9287926E-06)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7427965 magnetization 0.0542701

Broyden mixing:

rms(total) = 0.40458E-03 rms(broyden)= 0.40416E-03

rms(prec) = 0.69916E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4023

2.5156 2.0749 1.3369 0.8687 0.8687 0.7490

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107345.73088395

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88267934

PAW double counting = 52198.70692097 -52261.64116216

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.62339776

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76370393 eV

energy without entropy = -1202.76370393 energy(sigma->0) = -1202.76370393

---------- Iteration 11(8) ----------

POTLOK: cpu time 0.1646: real time 0.1656

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9271: real time 1.9339

RMM-DIIS: cpu time 6.3877: real time 6.4126

ORTHCH: cpu time 0.3561: real time 0.3574

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5255: real time 0.5273

MIXING: cpu time 0.0064: real time 0.0064

LOOP: cpu time 9.3779: real time 9.4137

eigenvalue-minimisations : 1748

total energy-change (2. order) :-0.2816728E-04 (-0.1962897E-06)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7427740 magnetization 0.0542702

Broyden mixing:

rms(total) = 0.27933E-03 rms(broyden)= 0.27914E-03

rms(prec) = 0.51649E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4507

2.5923 2.5923 1.4959 1.0139 1.0139 0.7842 0.6622

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107345.85170468

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88345817

PAW double counting = 52198.61144659 -52261.54581402

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.50325778

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76373209 eV

energy without entropy = -1202.76373209 energy(sigma->0) = -1202.76373209

---------- Iteration 11(9) ----------

POTLOK: cpu time 0.1654: real time 0.1677

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9242: real time 1.9311

RMM-DIIS: cpu time 6.2380: real time 6.2600

ORTHCH: cpu time 0.3520: real time 0.3531

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5251: real time 0.5268

MIXING: cpu time 0.0068: real time 0.0068

LOOP: cpu time 9.2219: real time 9.2559

eigenvalue-minimisations : 1700

total energy-change (2. order) :-0.3519969E-04 (-0.1238403E-06)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7427993 magnetization 0.0542695

Broyden mixing:

rms(total) = 0.15916E-03 rms(broyden)= 0.15893E-03

rms(prec) = 0.31052E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4811

3.0128 2.6688 1.6522 1.1730 0.9650 0.9650 0.7702 0.6419

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107345.98807195

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88399131

PAW double counting = 52198.45359690 -52261.38802211

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.36740105

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76376729 eV

energy without entropy = -1202.76376729 energy(sigma->0) = -1202.76376729

---------- Iteration 11(10) ----------

POTLOK: cpu time 0.1651: real time 0.1858

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9267: real time 1.9332

RMM-DIIS: cpu time 6.0965: real time 6.1170

ORTHCH: cpu time 0.3550: real time 0.3560

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5249: real time 0.5267

MIXING: cpu time 0.0070: real time 0.0070

LOOP: cpu time 9.0857: real time 9.1362

eigenvalue-minimisations : 1658

total energy-change (2. order) :-0.3321566E-04 (-0.1087072E-06)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7428102 magnetization 0.0542689

Broyden mixing:

rms(total) = 0.10453E-03 rms(broyden)= 0.10441E-03

rms(prec) = 0.18397E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5840

4.0125 2.5898 2.0114 1.3371 1.0611 1.0611 0.7765 0.7765 0.6304

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107346.09727616

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88448736

PAW double counting = 52198.35956270 -52261.29406630

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.25864772

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76380051 eV

energy without entropy = -1202.76380051 energy(sigma->0) = -1202.76380051

---------- Iteration 11(11) ----------

POTLOK: cpu time 0.1662: real time 0.1682

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9257: real time 1.9322

RMM-DIIS: cpu time 6.0363: real time 6.0559

ORTHCH: cpu time 0.3557: real time 0.3567

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5263: real time 0.5280

MIXING: cpu time 0.0075: real time 0.0075

LOOP: cpu time 9.0281: real time 9.0589

eigenvalue-minimisations : 1629

total energy-change (2. order) :-0.2539483E-04 (-0.7765237E-07)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7428097 magnetization 0.0542686

Broyden mixing:

rms(total) = 0.66788E-04 rms(broyden)= 0.66740E-04

rms(prec) = 0.10746E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6499

5.0363 2.5759 2.2235 1.5165 1.1106 0.9762 0.9762 0.7772 0.6868 0.6197

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107346.17030457

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88479468

PAW double counting = 52198.32833234 -52261.26287256

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.18591540

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76382590 eV

energy without entropy = -1202.76382590 energy(sigma->0) = -1202.76382590

---------- Iteration 11(12) ----------

POTLOK: cpu time 0.1634: real time 0.1747

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9279: real time 1.9347

RMM-DIIS: cpu time 5.2972: real time 5.3224

ORTHCH: cpu time 0.3527: real time 0.3538

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5251: real time 0.5270

MIXING: cpu time 0.0079: real time 0.0080

LOOP: cpu time 8.2847: real time 8.3310

eigenvalue-minimisations : 1454

total energy-change (2. order) :-0.1046715E-04 (-0.1462887E-07)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7428109 magnetization 0.0542686

Broyden mixing:

rms(total) = 0.44219E-04 rms(broyden)= 0.44202E-04

rms(prec) = 0.76021E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7613

5.9916 2.6741 2.3536 1.8731 1.4048 1.0594 1.0594 0.8774 0.7970 0.6689

0.6153

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107346.19085949

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88483695

PAW double counting = 52198.33080479 -52261.26533561

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.16542264

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76383637 eV

energy without entropy = -1202.76383637 energy(sigma->0) = -1202.76383637

---------- Iteration 11(13) ----------

POTLOK: cpu time 0.1647: real time 0.1755

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9335: real time 1.9397

RMM-DIIS: cpu time 5.4597: real time 5.4895

ORTHCH: cpu time 0.3534: real time 0.3542

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5254: real time 0.5269

MIXING: cpu time 0.0080: real time 0.0081

LOOP: cpu time 8.4553: real time 8.5046

eigenvalue-minimisations : 1485

total energy-change (2. order) :-0.1391149E-04 (-0.1981914E-07)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7428136 magnetization 0.0542686

Broyden mixing:

rms(total) = 0.23425E-04 rms(broyden)= 0.23399E-04

rms(prec) = 0.40337E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7984

6.6416 2.9876 2.5065 2.0272 1.4194 1.0377 1.0377 1.0256 0.8088 0.8088

0.6639 0.6159

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107346.20835083

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88482680

PAW double counting = 52198.34549301 -52261.28000050

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.14795839

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76385028 eV

energy without entropy = -1202.76385028 energy(sigma->0) = -1202.76385028

---------- Iteration 11(14) ----------

POTLOK: cpu time 0.1649: real time 0.1908

SETDIJ: cpu time 0.0099: real time 0.0100

EDDIAG: cpu time 1.9294: real time 1.9363

RMM-DIIS: cpu time 5.0386: real time 5.0636

ORTHCH: cpu time 0.3521: real time 0.3532

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5247: real time 0.5263

MIXING: cpu time 0.0086: real time 0.0086

LOOP: cpu time 8.0285: real time 8.0891

eigenvalue-minimisations : 1391

total energy-change (2. order) :-0.5827682E-05 (-0.5813103E-08)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7428130 magnetization 0.0542687

Broyden mixing:

rms(total) = 0.15236E-04 rms(broyden)= 0.15230E-04

rms(prec) = 0.25468E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8367

7.0154 3.3926 2.5447 2.0986 1.5123 1.5123 1.0535 1.0535 0.8571 0.8084

0.7550 0.6573 0.6170

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107346.21358133

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88482436

PAW double counting = 52198.35153769 -52261.28604533

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.14273112

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76385611 eV

energy without entropy = -1202.76385611 energy(sigma->0) = -1202.76385611

---------- Iteration 11(15) ----------

POTLOK: cpu time 0.1708: real time 0.1822

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9263: real time 1.9329

RMM-DIIS: cpu time 4.8679: real time 4.8973

ORTHCH: cpu time 0.3536: real time 0.3548

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5246: real time 0.5266

MIXING: cpu time 0.0091: real time 0.0092

LOOP: cpu time 7.8628: real time 7.9133

eigenvalue-minimisations : 1354

total energy-change (2. order) :-0.4189937E-05 (-0.3424280E-08)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7428135 magnetization 0.0542686

Broyden mixing:

rms(total) = 0.96529E-05 rms(broyden)= 0.96480E-05

rms(prec) = 0.15181E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9253

7.6011 4.2629 2.5833 2.4548 1.8607 1.4751 1.0742 1.0742 0.9151 0.9151

0.7860 0.6908 0.6182 0.6428

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107346.21569737

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88481343

PAW double counting = 52198.34920844 -52261.28372019

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.14060423

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76386030 eV

energy without entropy = -1202.76386030 energy(sigma->0) = -1202.76386030

---------- Iteration 11(16) ----------

POTLOK: cpu time 0.1677: real time 0.1694

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9250: real time 1.9315

RMM-DIIS: cpu time 4.7480: real time 4.7700

ORTHCH: cpu time 0.3533: real time 0.3544

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5250: real time 0.5269

MIXING: cpu time 0.0093: real time 0.0094

LOOP: cpu time 7.7386: real time 7.7721

eigenvalue-minimisations : 1286

total energy-change (2. order) :-0.1734195E-05 (-0.1400021E-08)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7428137 magnetization 0.0542686

Broyden mixing:

rms(total) = 0.60669E-05 rms(broyden)= 0.60648E-05

rms(prec) = 0.96114E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9276

7.8365 4.6311 2.5968 2.5968 1.9427 1.2998 1.2998 1.0709 1.0709 0.9689

0.8519 0.8098 0.6835 0.6182 0.6358

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107346.21639739

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88480903

PAW double counting = 52198.34571316 -52261.28022835

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.13989811

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76386203 eV

energy without entropy = -1202.76386203 energy(sigma->0) = -1202.76386203

---------- Iteration 11(17) ----------

POTLOK: cpu time 0.1638: real time 0.1662

SETDIJ: cpu time 0.0101: real time 0.0101

```
      EDDIAG:  cpu time        1.9289: real time        1.9352
 RMM-DIIS:  cpu time        4.5340: real time        4.5553
     ORTHCH:  cpu time        0.3514: real time        0.3523
        DOS:  cpu time        0.0004: real time        0.0005
     CHARGE:  cpu time        0.5246: real time        0.5266
     MIXING:  cpu time        0.0098: real time        0.0098
     ----------------------------------------------
       LOOP:  cpu time        7.5230: real time        7.5560

eigenvalue-minimisations  :  1165
total energy-change (2. order) :-0.7511626E-06  (-0.5996803E-09)
number of electron       518.9999727 magnetization             0.9999998
augmentation part         11.7428131 magnetization             0.0542686

Broyden mixing:
 rms(total) = 0.36348E-05        rms(broyden)= 0.36315E-05
 rms(prec ) = 0.58046E-05
 weight for this iteration         100.00

eigenvalues of (default mixing * dielectric matrix)
 average eigenvalue GAMMA=      1.9674
 8.0288   5.1237   2.8682   2.6198   2.1472   1.5912   1.5912   1.0892   1.0892   0.9260
```

0.9260 0.7777 0.7777 0.6754 0.6172 0.6306

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107346.21653567

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88481058

PAW double counting = 52198.34310019 -52261.27761840

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.13975911

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76386279 eV

energy without entropy = -1202.76386279 energy(sigma->0) = -1202.76386279

---------- Iteration 11(18) ----------

POTLOK: cpu time 0.1686: real time 0.1881

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9395: real time 1.9462

RMM-DIIS: cpu time 4.3667: real time 4.3882

ORTHCH: cpu time 0.3532: real time 0.3544

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5241: real time 0.5258

MIXING: cpu time 0.0103: real time 0.0104

LOOP: cpu time 7.3728: real time 7.4235

eigenvalue-minimisations : 1100

total energy-change (2. order) :-0.2899615E-06 (-0.2724443E-09)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7428130 magnetization 0.0542686

Broyden mixing:

rms(total) = 0.31070E-05 rms(broyden)= 0.31062E-05

rms(prec) = 0.41861E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9947

8.2133 5.5869 3.2747 2.6180 2.3170 1.8909 1.3075 1.1911 1.1911 1.0145

1.0145 0.8309 0.8309 0.7168 0.6664 0.6168 0.6286

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107346.21658219

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88480505

PAW double counting = 52198.34280228 -52261.27732005

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.13970778

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76386308 eV

energy without entropy = -1202.76386308 energy(sigma->0) = -1202.76386308

---------- Iteration 11(19) ----------

POTLOK: cpu time 0.1678: real time 0.1699

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9317: real time 1.9373

RMM-DIIS: cpu time 4.1706: real time 4.1963

ORTHCH: cpu time 0.3512: real time 0.3523

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5241: real time 0.5257

MIXING: cpu time 0.0110: real time 0.0110

LOOP: cpu time 7.1668: real time 7.2030

eigenvalue-minimisations : 987

total energy-change (2. order) :-0.1001972E-06 (-0.1413989E-09)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7428133 magnetization 0.0542686

Broyden mixing:

rms(total) = 0.13195E-05 rms(broyden)= 0.13177E-05

rms(prec) = 0.20795E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0119

8.4292 5.8293 3.6691 2.6084 2.3082 2.1372 1.4434 1.4434 1.0968 1.0968

0.9581 0.9581 0.8215 0.8215 0.6854 0.6618 0.6183 0.6282

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107346.21655662

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88479746

PAW double counting = 52198.34374142 -52261.27825743

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.13972762

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76386318 eV

energy without entropy = -1202.76386318 energy(sigma->0) = -1202.76386318

---------- Iteration 11(20) ----------

POTLOK: cpu time 0.1700: real time 0.1859

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9256: real time 1.9316

RMM-DIIS: cpu time 4.0968: real time 4.1086

ORTHCH: cpu time 0.3506: real time 0.3516

DOS: cpu time 0.0003: real time 0.0003

LOOP: cpu time 6.5534: real time 6.5881

eigenvalue-minimisations : 921

total energy-change (2. order) :-0.4108006E-07 (-0.6682921E-10)

number of electron 518.9999727 magnetization 0.9999998

augmentation part 11.7428133 magnetization 0.0542686

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91338.81145283

-Hartree energ DENC = -107346.21650784

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.88479400

PAW double counting = 52198.34451526 -52261.27903049

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.13977377

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76386322 eV

energy without entropy = -1202.76386322 energy(sigma->0) = -1202.76386322

---

average (electrostatic) potential at core

the test charge radii are 0.5201 0.6991 1.0621 0.7215

(the norm of the test charge is 1.0000)

1 -40.7500	2 -40.7478	3 -40.7493	4 -40.7478	5 -40.7501
6 -40.7522	7 -40.7498	8 -40.7576	9 -40.7494	10 -40.7571
11 -40.7508	12 -40.7528	13 -40.6453	14 -40.6927	15 -40.7657
16 -40.6948	17 -40.6890	18 -40.8605	19 -40.6765	20 -40.6625

21 -40.6857	22 -40.6590	23 -40.0890	24 -40.1322	25 -57.4558
26 -57.6667	27 -57.6539	28 -57.4655	29 -57.6598	30 -57.4558
31 -57.6665	32 -57.6534	33 -57.4635	34 -57.6646	35 -57.4567
36 -57.6684	37 -57.6535	38 -57.4658	39 -57.6705	40 -57.4557
41 -57.6725	42 -57.6537	43 -57.4707	44 -57.6853	45 -57.4557
46 -57.6714	47 -57.6545	48 -57.4709	49 -57.6762	50 -57.4569
51 -57.6680	52 -57.6542	53 -57.4685	54 -57.6625	55 -57.6335
56 -57.6595	57 -57.6833	58 -57.6789	59 -57.6631	60 -57.6661
61 -57.6858	62 -57.6703	63 -57.6338	64 -57.6589	65 -57.6854
66 -57.6906	67 -57.6614	68 -57.6659	69 -57.6896	70 -57.6967
71 -57.6333	72 -57.6604	73 -57.6931	74 -57.7179	75 -57.6623
76 -57.6665	77 -57.7021	78 -57.7469	79 -57.6335	80 -57.6629
81 -57.7070	82 -57.7486	83 -57.6656	84 -57.6680	85 -57.7338
86 -57.8382	87 -57.6359	88 -57.6636	89 -57.7089	90 -57.7132
91 -57.6703	92 -57.6683	93 -57.7384	94 -57.7552	95 -57.6343
96 -57.6618	97 -57.6924	98 -57.6865	99 -57.6675	100 -57.6670
101 -57.7039	102 -57.6815	103 -57.6568	104 -57.6273	105 -57.6408
106 -57.2839	107 -57.3843	108 -57.6278	109 -57.5921	110 -57.6558
111 -57.6273	112 -57.6375	113 -57.3025	114 -57.3899	115 -57.6270
116 -57.5941	117 -57.6550	118 -57.6192	119 -57.6936	120 -57.6756
121 -57.3837	122 -57.6259	123 -57.7044	124 -57.6560	125 -57.6219
126 -57.8291	127 -58.3131	128 -57.3572	129 -57.6312	130 -58.1390

131 -57.6640	132 -57.6311	133 -57.7966	134 -57.4091	135 -57.3683
136 -57.6351	137 -58.0735	138 -57.6604	139 -57.6268	140 -57.6667
141 -57.2926	142 -57.3745	143 -57.6304	144 -57.6427	145 -60.8816
146 -57.3171	147 -81.3687			

E-fermi : -2.3242 XC(G=0): -2.7341 alpha+bet : -2.2521

spin component 1

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-27.2189	1.00000
2	-21.5646	1.00000
3	-21.4682	1.00000
4	-21.0956	1.00000
5	-21.0648	1.00000
6	-21.0110	1.00000
7	-20.9754	1.00000
8	-20.9733	1.00000

9	-20.8878	1.00000
10	-20.5538	1.00000
11	-20.4995	1.00000
12	-20.4084	1.00000
13	-20.3947	1.00000
14	-20.1226	1.00000
15	-19.9726	1.00000
16	-19.6993	1.00000
17	-19.6236	1.00000
18	-19.5959	1.00000
19	-19.5802	1.00000
20	-19.5254	1.00000
21	-19.5236	1.00000
22	-19.4954	1.00000
23	-19.4777	1.00000
24	-19.1081	1.00000
25	-19.0714	1.00000
26	-18.9754	1.00000
27	-18.9616	1.00000
28	-18.8970	1.00000
29	-18.7304	1.00000
30	-18.5010	1.00000

31	-18.3554	1.00000
32	-18.2722	1.00000
33	-18.2489	1.00000
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spin component 2

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193	-7.5512	1.00000
194	-7.5365	1.00000
195	-7.4693	1.00000
196	-7.4691	1.00000
197	-7.4242	1.00000
198	-7.3197	1.00000
199	-7.2327	1.00000
200	-7.1589	1.00000
201	-7.0521	1.00000
202	-7.0333	1.00000
203	-7.0131	1.00000
204	-6.9820	1.00000
205	-6.9738	1.00000

206	-6.9687	1.00000
207	-6.9376	1.00000
208	-6.8599	1.00000
209	-6.8131	1.00000
210	-6.7922	1.00000
211	-6.7847	1.00000
212	-6.7219	1.00000
213	-6.6752	1.00000
214	-6.4636	1.00000
215	-6.3917	1.00000
216	-6.3793	1.00000
217	-6.3750	1.00000
218	-6.3592	1.00000
219	-6.3348	1.00000
220	-6.2998	1.00000
221	-6.2721	1.00000
222	-6.2262	1.00000
223	-6.2248	1.00000
224	-6.2192	1.00000
225	-6.0434	1.00000
226	-6.0054	1.00000
227	-5.7531	1.00000

228	-5.7079	1.00000
229	-5.6880	1.00000
230	-5.6324	1.00000
231	-5.6193	1.00000
232	-5.5406	1.00000
233	-5.5199	1.00000
234	-5.4377	1.00000
235	-5.4080	1.00000
236	-5.1419	1.00000
237	-5.0566	1.00000
238	-5.0225	1.00000
239	-5.0187	1.00000
240	-4.9555	1.00000
241	-4.8742	1.00000
242	-4.8508	1.00000
243	-4.7986	1.00000
244	-4.7738	1.00000
245	-4.6489	1.00000
246	-4.5750	1.00000
247	-4.5720	1.00000
248	-4.4716	1.00000
249	-4.4178	1.00000

250	-4.3910	1.00000
251	-4.2933	1.00000
252	-4.2227	1.00000
253	-4.1716	1.00000
254	-3.5235	1.00000
255	-3.3053	1.00000
256	-3.1353	1.00000
257	-2.9411	1.00000
258	-2.7954	1.00000
259	-2.7358	1.00000
260	-2.0559	0.00000
261	-1.9115	0.00000
262	-1.7178	0.00000
263	-1.6744	0.00000
264	-1.2798	0.00000
265	-1.2469	0.00000
266	-1.1411	0.00000
267	-0.7105	0.00000
268	-0.5800	0.00000
269	-0.5035	0.00000
270	-0.2772	0.00000
271	-0.2740	0.00000

272	-0.2562	0.00000
273	-0.1519	0.00000
274	-0.0532	0.00000
275	-0.0441	0.00000
276	0.0183	0.00000
277	0.0440	0.00000
278	0.0841	0.00000
279	0.2115	0.00000
280	0.2594	0.00000
281	0.2833	0.00000
282	0.4385	0.00000
283	0.4571	0.00000
284	0.4864	0.00000
285	0.6013	0.00000
286	0.7038	0.00000
287	0.8219	0.00000
288	0.8782	0.00000
289	1.0567	0.00000
290	1.1083	0.00000
291	1.1462	0.00000
292	1.1787	0.00000
293	1.2330	0.00000

294	1.2510	0.00000
295	1.3103	0.00000
296	1.3206	0.00000
297	1.3617	0.00000
298	1.4326	0.00000
299	1.4776	0.00000
300	1.5033	0.00000
301	1.5796	0.00000
302	1.6044	0.00000
303	1.6584	0.00000
304	1.6874	0.00000
305	1.7594	0.00000
306	1.7751	0.00000
307	1.8771	0.00000
308	1.9015	0.00000
309	1.9106	0.00000
310	1.9239	0.00000
311	2.1408	0.00000
312	2.1969	0.00000
313	2.2213	0.00000
314	2.2565	0.00000
315	2.2904	0.00000

316	2.2975	0.00000
317	2.3371	0.00000
318	2.3627	0.00000
319	2.3847	0.00000
320	2.4102	0.00000
321	2.4301	0.00000
322	2.4365	0.00000
323	2.4525	0.00000
324	2.4595	0.00000
325	2.4682	0.00000
326	2.5251	0.00000
327	2.5431	0.00000
328	2.7062	0.00000
329	2.7344	0.00000
330	2.7546	0.00000
331	2.7603	0.00000
332	2.7739	0.00000
333	2.8313	0.00000
334	2.8491	0.00000
335	2.8758	0.00000
336	2.9027	0.00000
337	2.9327	0.00000

338	2.9565	0.00000
339	2.9841	0.00000
340	3.0076	0.00000
341	3.0386	0.00000
342	3.0520	0.00000
343	3.0719	0.00000
344	3.0935	0.00000
345	3.1516	0.00000
346	3.1716	0.00000
347	3.1891	0.00000
348	3.2007	0.00000
349	3.3070	0.00000
350	3.3259	0.00000
351	3.3604	0.00000
352	3.3704	0.00000
353	3.3927	0.00000
354	3.4375	0.00000
355	3.4807	0.00000
356	3.4918	0.00000
357	3.4979	0.00000
358	3.5078	0.00000
359	3.6389	0.00000

360	3.6772	0.00000
361	3.6981	0.00000
362	3.7393	0.00000
363	3.7572	0.00000
364	3.7618	0.00000
365	3.7774	0.00000
366	3.7993	0.00000
367	3.8161	0.00000
368	3.8429	0.00000
369	3.8490	0.00000
370	3.8674	0.00000
371	3.8818	0.00000
372	3.8947	0.00000
373	3.9215	0.00000
374	3.9378	0.00000
375	3.9499	0.00000
376	3.9598	0.00000
377	3.9828	0.00000
378	3.9867	0.00000
379	4.0223	0.00000
380	4.0786	0.00000
381	4.1710	0.00000

382	4.2598	0.00000
383	4.2623	0.00000
384	4.2700	0.00000
385	4.2933	0.00000
386	4.3220	0.00000
387	4.3348	0.00000
388	4.3511	0.00000
389	4.3823	0.00000
390	4.3872	0.00000
391	4.4230	0.00000
392	4.4488	0.00000
393	4.4733	0.00000
394	4.4834	0.00000
395	4.4952	0.00000
396	4.4996	0.00000
397	4.5202	0.00000
398	4.5561	0.00000
399	4.5953	0.00000
400	4.6110	0.00000
401	4.6296	0.00000
402	4.6468	0.00000
403	4.6604	0.00000

404	4.6862	0.00000
405	4.7092	0.00000
406	4.7382	0.00000
407	4.7514	0.00000
408	4.7704	0.00000
409	4.7874	0.00000
410	4.7909	0.00000
411	4.8033	0.00000
412	4.8338	0.00000
413	4.8717	0.00000
414	4.8857	0.00000
415	4.9048	0.00000
416	4.9423	0.00000
417	4.9937	0.00000
418	5.0100	0.00000
419	5.0136	0.00000
420	5.0391	0.00000
421	5.0444	0.00000
422	5.0704	0.00000
423	5.0862	0.00000
424	5.1174	0.00000
425	5.1221	0.00000

426	5.1414	0.00000
427	5.1444	0.00000
428	5.1718	0.00000
429	5.1802	0.00000
430	5.1895	0.00000
431	5.1937	0.00000
432	5.2203	0.00000
433	5.2395	0.00000
434	5.2439	0.00000
435	5.2617	0.00000
436	5.2995	0.00000
437	5.3043	0.00000
438	5.3131	0.00000
439	5.3364	0.00000
440	5.3541	0.00000
441	5.3722	0.00000
442	5.3829	0.00000
443	5.3972	0.00000
444	5.4303	0.00000
445	5.4600	0.00000
446	5.4717	0.00000
447	5.4876	0.00000

448	5.4993	0.00000
449	5.5282	0.00000
450	5.5685	0.00000
451	5.5757	0.00000
452	5.5958	0.00000
453	5.6082	0.00000
454	5.6273	0.00000
455	5.6725	0.00000
456	5.6928	0.00000
457	5.7202	0.00000
458	5.7279	0.00000
459	5.7478	0.00000
460	5.7625	0.00000
461	5.7903	0.00000
462	5.7942	0.00000
463	5.7991	0.00000
464	5.8049	0.00000
465	5.8209	0.00000
466	5.8259	0.00000
467	5.8558	0.00000
468	5.8616	0.00000
469	5.8846	0.00000

470	5.8882	0.00000
471	5.8928	0.00000
472	5.9106	0.00000
473	5.9222	0.00000
474	5.9509	0.00000
475	5.9548	0.00000
476	5.9713	0.00000
477	5.9773	0.00000
478	5.9910	0.00000
479	6.0142	0.00000
480	6.0439	0.00000

---

soft charge-density along one line, spin component 1

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

soft charge-density along one line, spin component 2

0 1 2 3 4 5 6 7

8 9

total charge-density along one line

pseudopotential strength for first ion, spin component: 1

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

pseudopotential strength for first ion, spin component: 2

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

total augmentation occupancy for first ion, spin component: 1

3.579 -0.646 0.444 -0.034 -0.000

-0.646 0.130 -0.082 0.006 0.000

0.444 -0.082 0.056 -0.003 -0.000

-0.034 0.006 -0.003 0.011 0.000

-0.000 0.000 -0.000 0.000 0.007

total augmentation occupancy for first ion, spin component: 2

-0.000	0.000	-0.000	0.000	0.000
0.000	-0.000	0.000	-0.000	-0.000
-0.000	0.000	-0.000	-0.000	-0.000
0.000	-0.000	-0.000	-0.000	-0.000
0.000	-0.000	-0.000	-0.000	-0.000

---------- aborting loop because EDIFF is reached ----------

total charge

# of ion	s	p	d	tot
1	0.646	0.043	0.000	0.690
2	0.646	0.043	0.000	0.690
3	0.646	0.043	0.000	0.690
4	0.646	0.043	0.000	0.690

5	0.646	0.043	0.000	0.690
6	0.646	0.043	0.000	0.690
7	0.646	0.043	0.000	0.690
8	0.646	0.043	0.000	0.690
9	0.646	0.043	0.000	0.690
10	0.646	0.043	0.000	0.690
11	0.646	0.043	0.000	0.690
12	0.646	0.043	0.000	0.690
13	0.646	0.043	0.000	0.689
14	0.646	0.043	0.000	0.689
15	0.649	0.045	0.000	0.693
16	0.646	0.043	0.000	0.689
17	0.646	0.043	0.000	0.689
18	0.646	0.043	0.000	0.689
19	0.646	0.043	0.000	0.689
20	0.646	0.043	0.000	0.689
21	0.646	0.043	0.000	0.689
22	0.646	0.044	0.000	0.690
23	0.541	0.015	0.000	0.556
24	0.541	0.015	0.000	0.556
25	0.870	1.763	0.000	2.633
26	0.867	1.785	0.000	2.653

27	0.867	1.786	0.000	2.653
28	0.870	1.762	0.000	2.632
29	0.865	1.783	0.000	2.648
30	0.870	1.763	0.000	2.633
31	0.867	1.786	0.000	2.653
32	0.867	1.786	0.000	2.653
33	0.870	1.762	0.000	2.632
34	0.865	1.783	0.000	2.648
35	0.870	1.763	0.000	2.633
36	0.868	1.787	0.000	2.654
37	0.867	1.786	0.000	2.653
38	0.870	1.763	0.000	2.633
39	0.865	1.784	0.000	2.649
40	0.870	1.763	0.000	2.633
41	0.868	1.787	0.000	2.655
42	0.867	1.786	0.000	2.653
43	0.871	1.764	0.000	2.634
44	0.865	1.783	0.000	2.648
45	0.870	1.763	0.000	2.633
46	0.867	1.786	0.000	2.653
47	0.867	1.786	0.000	2.653
48	0.871	1.763	0.000	2.634

49	0.865	1.783	0.000	2.648
50	0.870	1.763	0.000	2.633
51	0.867	1.786	0.000	2.653
52	0.867	1.786	0.000	2.653
53	0.870	1.762	0.000	2.632
54	0.865	1.784	0.000	2.648
55	0.865	1.784	0.000	2.649
56	0.865	1.786	0.000	2.651
57	0.866	1.787	0.000	2.653
58	0.866	1.790	0.000	2.656
59	0.865	1.786	0.000	2.651
60	0.866	1.786	0.000	2.651
61	0.866	1.788	0.000	2.654
62	0.867	1.791	0.000	2.658
63	0.865	1.784	0.000	2.649
64	0.865	1.786	0.000	2.651
65	0.866	1.787	0.000	2.652
66	0.865	1.788	0.000	2.653
67	0.865	1.786	0.000	2.651
68	0.866	1.785	0.000	2.651
69	0.865	1.787	0.000	2.652
70	0.866	1.787	0.000	2.653

71	0.865	1.784	0.000	2.649
72	0.865	1.786	0.000	2.651
73	0.866	1.786	0.000	2.652
74	0.864	1.785	0.000	2.649
75	0.865	1.786	0.000	2.651
76	0.866	1.786	0.000	2.651
77	0.865	1.786	0.000	2.651
78	0.865	1.784	0.000	2.649
79	0.865	1.784	0.000	2.649
80	0.865	1.786	0.000	2.651
81	0.865	1.785	0.000	2.650
82	0.863	1.782	0.000	2.645
83	0.865	1.786	0.000	2.651
84	0.866	1.786	0.000	2.651
85	0.865	1.784	0.000	2.648
86	0.862	1.774	0.000	2.636
87	0.865	1.784	0.000	2.649
88	0.865	1.787	0.000	2.652
89	0.865	1.785	0.000	2.650
90	0.865	1.788	0.000	2.653
91	0.865	1.786	0.000	2.651
92	0.866	1.786	0.000	2.651

93	0.864	1.783	0.000	2.647
94	0.866	1.785	0.000	2.651
95	0.865	1.784	0.000	2.649
96	0.865	1.786	0.000	2.651
97	0.866	1.787	0.000	2.653
98	0.866	1.789	0.000	2.655
99	0.865	1.786	0.000	2.651
100	0.866	1.786	0.000	2.651
101	0.865	1.787	0.000	2.652
102	0.867	1.790	0.000	2.657
103	0.865	1.786	0.000	2.651
104	0.867	1.785	0.000	2.653
105	0.866	1.786	0.000	2.652
106	0.870	1.778	0.000	2.648
107	0.869	1.765	0.000	2.635
108	0.865	1.783	0.000	2.648
109	0.869	1.789	0.000	2.658
110	0.865	1.786	0.000	2.651
111	0.867	1.785	0.000	2.653
112	0.867	1.789	0.000	2.655
113	0.871	1.782	0.000	2.653
114	0.869	1.765	0.000	2.634

115	0.865	1.783	0.000	2.648
116	0.870	1.791	0.000	2.661
117	0.865	1.786	0.000	2.651
118	0.867	1.786	0.000	2.653
119	0.865	1.782	0.000	2.647
120	0.857	1.707	0.000	2.564
121	0.869	1.765	0.000	2.634
122	0.865	1.783	0.000	2.648
123	0.866	1.778	0.000	2.644
124	0.866	1.786	0.000	2.652
125	0.867	1.785	0.000	2.653
126	0.862	1.776	0.000	2.638
127	0.848	1.832	0.000	2.680
128	0.870	1.767	0.000	2.637
129	0.865	1.783	0.000	2.648
130	0.860	1.757	0.000	2.617
131	0.866	1.786	0.000	2.652
132	0.867	1.784	0.000	2.652
133	0.864	1.787	0.000	2.651
134	0.869	1.790	0.000	2.659
135	0.869	1.767	0.000	2.636
136	0.865	1.783	0.000	2.648

137	0.866	1.772	0.000	2.637
138	0.866	1.786	0.000	2.652
139	0.867	1.785	0.000	2.652
140	0.866	1.788	0.000	2.654
141	0.870	1.779	0.000	2.649
142	0.869	1.766	0.000	2.635
143	0.865	1.783	0.000	2.648
144	0.869	1.790	0.000	2.659
145	0.948	1.736	0.000	2.684
146	1.240	1.546	0.074	2.860
147	1.636	3.544	0.000	5.180
tot	123.070	221.586	0.074	344.731

magnetization (x)

# of ion	s	p	d	tot
1	0.000	-0.000	0.000	0.000
2	-0.000	0.000	0.000	-0.000

3	0.000	-0.000	0.000	0.000
4	-0.000	0.000	0.000	-0.000
5	0.000	-0.000	0.000	0.000
6	-0.000	0.000	0.000	-0.000
7	0.000	-0.000	0.000	0.000
8	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	0.000
10	-0.000	0.000	0.000	-0.000
11	0.000	-0.000	0.000	0.000
12	-0.000	0.000	0.000	-0.000
13	0.000	-0.000	0.000	0.000
14	-0.004	0.002	0.000	-0.002
15	0.000	-0.000	0.000	0.000
16	-0.004	0.002	0.000	-0.002
17	-0.004	0.002	0.000	-0.002
18	0.000	-0.000	0.000	0.000
19	-0.003	0.001	0.000	-0.002
20	0.000	-0.000	0.000	0.000
21	-0.003	0.002	0.000	-0.002
22	-0.003	0.002	0.000	-0.002
23	-0.000	0.000	0.000	-0.000
24	-0.000	0.000	0.000	-0.000

25	-0.000	-0.007	0.000	-0.008
26	-0.000	-0.002	0.000	-0.002
27	0.000	0.003	0.000	0.003
28	0.000	0.005	0.000	0.005
29	0.000	0.003	0.000	0.003
30	-0.000	-0.007	0.000	-0.008
31	-0.000	-0.002	0.000	-0.002
32	0.000	0.003	0.000	0.003
33	0.000	0.005	0.000	0.005
34	0.000	0.002	0.000	0.002
35	-0.000	-0.007	0.000	-0.008
36	-0.000	-0.002	0.000	-0.002
37	0.000	0.003	0.000	0.003
38	0.000	0.006	0.000	0.007
39	0.000	0.002	0.000	0.002
40	-0.000	-0.007	0.000	-0.008
41	-0.000	-0.002	0.000	-0.002
42	0.000	0.002	0.000	0.003
43	0.000	0.005	0.000	0.005
44	0.000	0.004	0.000	0.004
45	-0.000	-0.007	0.000	-0.008
46	-0.000	-0.002	0.000	-0.002

47	0.000	0.002	0.000	0.003
48	0.000	0.005	0.000	0.006
49	0.000	0.001	0.000	0.001
50	-0.000	-0.007	0.000	-0.008
51	-0.000	-0.002	0.000	-0.002
52	0.000	0.002	0.000	0.003
53	0.000	0.006	0.000	0.007
54	0.000	0.002	0.000	0.002
55	-0.000	-0.005	0.000	-0.006
56	-0.000	-0.007	0.000	-0.007
57	-0.000	-0.001	0.000	-0.001
58	-0.000	-0.001	0.000	-0.001
59	0.000	0.006	0.000	0.007
60	0.000	0.003	0.000	0.003
61	0.000	0.001	0.000	0.001
62	0.000	0.003	0.000	0.003
63	-0.000	-0.005	0.000	-0.006
64	-0.000	-0.007	0.000	-0.007
65	-0.000	-0.001	0.000	-0.001
66	-0.000	-0.001	0.000	-0.001
67	0.000	0.006	0.000	0.006
68	0.000	0.003	0.000	0.003

69	0.000	0.001	0.000	0.001
70	0.000	0.002	0.000	0.002
71	-0.000	-0.005	0.000	-0.006
72	-0.000	-0.007	0.000	-0.007
73	-0.000	-0.001	0.000	-0.001
74	-0.000	-0.002	0.000	-0.002
75	0.000	0.006	0.000	0.007
76	0.000	0.003	0.000	0.004
77	0.000	0.003	0.000	0.003
78	0.000	0.001	0.000	0.001
79	-0.000	-0.005	0.000	-0.006
80	-0.000	-0.007	0.000	-0.007
81	-0.000	-0.001	0.000	-0.002
82	-0.000	-0.002	0.000	-0.002
83	0.001	0.007	0.000	0.008
84	0.000	0.003	0.000	0.003
85	0.000	0.002	0.000	0.002
86	0.000	0.005	0.000	0.006
87	-0.000	-0.005	0.000	-0.005
88	-0.000	-0.007	0.000	-0.007
89	-0.000	-0.001	0.000	-0.002
90	-0.000	-0.002	0.000	-0.002

91	0.001	0.008	0.000	0.008
92	0.000	0.003	0.000	0.003
93	0.000	0.002	0.000	0.003
94	0.000	0.001	0.000	0.001
95	-0.000	-0.005	0.000	-0.006
96	-0.000	-0.007	0.000	-0.007
97	-0.000	-0.001	0.000	-0.001
98	-0.000	-0.001	0.000	-0.001
99	0.001	0.007	0.000	0.007
100	0.000	0.003	0.000	0.004
101	0.000	0.003	0.000	0.003
102	0.000	0.002	0.000	0.002
103	-0.001	-0.010	0.000	-0.011
104	-0.003	-0.028	0.000	-0.031
105	-0.000	-0.001	0.000	-0.002
106	-0.000	-0.004	0.000	-0.004
107	0.007	0.116	0.000	0.122
108	0.001	0.010	0.000	0.011
109	0.000	0.001	0.000	0.001
110	-0.001	-0.010	0.000	-0.011
111	-0.003	-0.028	0.000	-0.031
112	-0.000	-0.001	0.000	-0.002

113	-0.000	-0.003	0.000	-0.004
114	0.007	0.120	0.000	0.127
115	0.001	0.010	0.000	0.011
116	0.000	0.001	0.000	0.002
117	-0.001	-0.010	0.000	-0.011
118	-0.003	-0.026	0.000	-0.029
119	-0.000	-0.002	0.000	-0.002
120	-0.000	-0.002	0.000	-0.002
121	0.007	0.115	0.000	0.122
122	0.001	0.010	0.000	0.010
123	0.000	0.003	0.000	0.003
124	-0.001	-0.010	0.000	-0.011
125	-0.003	-0.024	0.000	-0.027
126	-0.000	-0.002	0.000	-0.002
127	-0.000	0.001	0.000	0.001
128	0.006	0.105	0.000	0.111
129	0.001	0.009	0.000	0.010
130	0.000	0.004	0.000	0.004
131	-0.001	-0.009	0.000	-0.010
132	-0.003	-0.024	0.000	-0.027
133	-0.000	-0.002	0.000	-0.002
134	-0.000	-0.002	0.000	-0.002

135	0.006	0.097	0.000	0.102
136	0.001	0.009	0.000	0.010
137	0.000	0.004	0.000	0.004
138	-0.001	-0.010	0.000	-0.011
139	-0.003	-0.026	0.000	-0.029
140	-0.000	-0.002	0.000	-0.002
141	-0.000	-0.003	0.000	-0.004
142	0.006	0.105	0.000	0.111
143	0.001	0.010	0.000	0.010
144	0.000	0.002	0.000	0.003
145	0.000	0.005	0.000	0.005
146	-0.000	0.000	-0.000	0.000
147	0.000	0.004	0.000	0.004
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tot	0.001	0.513	-0.000	0.514

CHARGE: cpu time 0.5213: real time 0.5231

FORLOC: cpu time 0.0200: real time 0.0200

FORNL : cpu time 2.0451: real time 2.0522

STRESS: cpu time 6.1179: real time 6.1385

FORCOR: cpu time 0.1407: real time 0.1487

FORHAR: cpu time 0.0333: real time 0.0334

MIXING: cpu time 0.0111: real time 0.0112

OFIELD: cpu time 0.0001: real time 0.0001

DFTD3 V3.0 Rev 1

Edisp (eV) -6.61794

E6 (eV) : -3.9313

E8 (eV) : -2.6866

% E8 : 40.60

FORVDW: cpu time 1.7724: real time 1.8358

FORCE on cell =-STRESS in cart. coord. units (eV):

Direction	XX	YY	ZZ	XY	YZ	ZX
Alpha Z	233.50077	233.50077	233.50077			
Ewald	107586.10535	23471.65693	-39719.08093	9.67943	3459.76939	128.99994
Hartree	106106.84662	25026.80297	-23787.43331	-7.10968	2949.10747	93.23067
E(xc)	-1914.33054	-1916.68505	-1979.98148	0.13278	1.82732	0.13091
Local	**********	-53946.35858	57000.77949	0.94083	-6366.18410	-218.70006
n-local	-472.76948	-482.64124	-439.72523	-0.69852	-0.82130	-0.33079

augment	-38.26579	-38.59209	-34.32072	0.00606	-0.99933	-0.00373
Kinetic	7635.66571	7639.50130	8714.25750	-3.08442	-41.50146	-3.20755
Fock	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
vdW	-2.64203	-1.49238	-6.59328	0.00141	-0.07458	0.01172

Total	-17.70877	-14.30736	-18.59719	-0.13210	1.12340	0.13110
in kB	-4.88329	-3.94533	-5.12828	-0.03643	0.30978	0.03615

external pressure = -4.65 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

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energy-cutoff : 400.00

volume of cell : 5810.14

direct lattice vectors			reciprocal lattice vectors		
14.780600000	0.000000000	0.000000000	0.067656252	0.000000000	0.000000000
0.000000000	21.333900000	0.000000000	0.000000000	0.046873755	0.000000000
0.000000000	0.000000000	18.425700000	0.000000000	0.000000000	0.054272022

length of vectors

14.780600000	21.333900000	18.425700000	0.067656252	0.046873755	0.054272022

FORCES acting on ions

electron-ion (+dipol) ewald-force non-local-force convergence-correction

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0.480E-02 0.154E+03 0.361E+02 -.329E-02 -.160E+03 -.356E+02 -.180E-02 0.566E+01 -.438E+00 0.692E-07 0.278E-06 0.698E-06

-.182E-01 0.155E+03 -.340E+02 0.158E-01 -.160E+03 0.335E+02 0.114E-02 0.565E+01 0.541E+00 -.505E-06 -.324E-06 -.127E-06

0.184E+00 0.154E+03 0.360E+02 -.184E+00 -.160E+03 -.356E+02 0.114E-04 0.565E+01 -.443E+00 -.244E-06 0.447E-06 0.484E-06

0.112E+00 0.155E+03 -.341E+02 -.985E-01 -.160E+03 0.336E+02 -.174E-01 0.565E+01 0.535E+00 -.110E-06 0.473E-07 -.359E-06

0.171E+00 0.154E+03 0.362E+02 -.173E+00 -.160E+03 -.357E+02 0.117E-02 0.566E+01 -.440E+00 -.328E-06 0.533E-06 0.680E-06

0.126E+00 0.154E+03 -.340E+02 -.107E+00 -.160E+03 0.334E+02 -.211E-01 0.565E+01 0.541E+00 0.381E-06 0.258E-06 0.301E-06

-.195E-01 0.154E+03 0.363E+02 0.183E-01 -.160E+03 -.359E+02 0.159E-02 0.566E+01 -.431E+00 -.120E-06 0.490E-06 0.111E-05

-.133E-01 0.154E+03 -.338E+02 0.201E-01 -.160E+03 0.332E+02 -.719E-02 0.565E+01 0.555E+00 0.431E-06 0.609E-07 0.112E-05

-.182E+00 0.154E+03 0.363E+02 0.182E+00 -.160E+03 -.359E+02 0.252E-03 0.565E+01 -

.429E+00 0.260E-06 0.354E-06 0.130E-05

-.128E+00 0.155E+03 -.337E+02 0.114E+00 -.160E+03 0.331E+02 0.109E-01 0.565E+01 0.561E+00 0.126E-06 -.226E-06 0.134E-05

-.173E+00 0.154E+03 0.362E+02 0.175E+00 -.160E+03 -.358E+02 -.178E-02 0.566E+01 -.432E+00 0.363E-06 0.188E-06 0.111E-05

-.114E+00 0.155E+03 -.338E+02 0.951E-01 -.160E+03 0.332E+02 0.192E-01 0.565E+01 0.555E+00 -.327E-06 -.309E-06 0.731E-06

0.228E+01 -.150E+03 -.386E+02 -.227E+01 0.156E+03 0.386E+02 -.103E-01 -.566E+01 0.767E-01 0.407E-06 -.689E-06 0.493E-08

-.416E+00 -.151E+03 0.388E+02 0.418E+00 0.157E+03 -.386E+02 -.131E-02 -.567E+01 -.269E+00 -.135E-06 -.785E-06 0.119E-06

0.136E+02 -.146E+03 -.413E+02 -.138E+02 0.151E+03 0.413E+02 0.257E+00 -.567E+01 -.347E-01 -.948E-07 -.404E-06 -.116E-06

0.162E+01 -.151E+03 0.402E+02 -.162E+01 0.156E+03 -.400E+02 -.996E-03 -.567E+01 -.229E+00 0.319E-06 -.559E-06 0.693E-06

0.352E+01 -.149E+03 0.443E+02 -.352E+01 0.155E+03 -.441E+02 -.192E-02 -.567E+01 -.180E+00 0.395E-06 -.453E-06 0.501E-06

-.149E+02 -.146E+03 -.329E+02 0.150E+02 0.151E+03 0.329E+02 -.972E-01 -.566E+01 0.497E-01 0.672E-06 -.495E-06 -.108E-06

-.297E+01 -.149E+03 0.432E+02 0.296E+01 0.155E+03 -.430E+02 0.115E-01 -.567E+01 -.241E+00 -.193E-06 -.637E-06 -.737E-06

-.380E+01 -.150E+03 -.385E+02 0.380E+01 0.156E+03 0.385E+02 -.639E-02 -.566E+01

0.241E-01 -.592E-07 -.800E-06 0.213E-06

-.208E+01 -.151E+03 0.395E+02 0.208E+01 0.156E+03 -.392E+02 0.147E-02 -.566E+01 -.282E+00 -.465E-06 -.833E-06 -.482E-06

0.285E-02 -.148E+03 0.486E+02 0.479E-02 0.154E+03 -.484E+02 -.555E-02 -.569E+01 -.158E+00 0.123E-06 -.556E-06 -.435E-06

0.196E+02 -.103E+03 0.222E+02 -.212E+02 0.103E+03 -.246E+02 0.154E+01 0.139E+00 0.238E+01 -.754E-06 -.732E-06 0.214E-07

-.192E+02 -.103E+03 0.153E+02 0.216E+02 0.103E+03 -.168E+02 -.241E+01 -.118E+00 0.152E+01 -.844E-07 -.765E-06 -.374E-06

0.716E-01 0.461E+03 0.202E+03 -.748E-01 -.462E+03 -.201E+03 0.381E-02 0.102E+01 -.219E+00 0.626E-06 0.584E-06 0.153E-05

0.212E+00 0.353E+03 -.234E+03 -.212E+00 -.353E+03 0.234E+03 0.260E-02 0.442E+00 -.370E-01 -.472E-06 -.658E-06 -.229E-05

-.248E-01 0.351E+03 0.240E+03 0.235E-01 -.351E+03 -.241E+03 0.312E-02 0.407E+00 0.562E-01 0.140E-05 0.919E-07 0.187E-05

-.173E+00 0.462E+03 -.195E+03 0.179E+00 -.463E+03 0.195E+03 -.669E-02 0.105E+01 0.233E+00 -.159E-05 -.166E-05 -.136E-05

-.624E-01 0.210E+03 -.272E+03 0.665E-01 -.210E+03 0.272E+03 -.449E-02 0.928E-01 0.560E-01 -.214E-06 0.830E-06 -.168E-05

0.562E+00 0.461E+03 0.202E+03 -.564E+00 -.462E+03 -.201E+03 0.204E-02 0.102E+01 -.214E+00 -.777E-06 0.113E-05 0.807E-06

0.106E+01 0.352E+03 -.234E+03 -.107E+01 -.353E+03 0.234E+03 0.161E-01 0.447E+00 -

.424E-01 0.713E-06 -.641E-06 -.135E-05

0.413E+00 0.351E+03 0.240E+03 -.415E+00 -.351E+03 -.240E+03 0.302E-02 0.407E+00 0.490E-01 0.584E-07 0.261E-06 0.368E-06

0.578E+00 0.462E+03 -.195E+03 -.583E+00 -.463E+03 0.195E+03 0.483E-02 0.105E+01 0.235E+00 0.558E-07 -.438E-06 -.217E-05

0.691E+00 0.210E+03 -.272E+03 -.697E+00 -.210E+03 0.272E+03 0.613E-02 0.905E-01 0.615E-01 0.471E-06 0.792E-06 -.991E-06

0.425E+00 0.461E+03 0.202E+03 -.428E+00 -.462E+03 -.202E+03 0.389E-02 0.102E+01 -.214E+00 -.138E-05 0.123E-05 0.200E-05

0.939E+00 0.352E+03 -.233E+03 -.955E+00 -.352E+03 0.233E+03 0.152E-01 0.440E+00 -.376E-01 0.981E-06 -.171E-05 0.150E-05

0.478E+00 0.351E+03 0.241E+03 -.480E+00 -.351E+03 -.241E+03 0.253E-02 0.405E+00 0.510E-01 -.126E-05 0.616E-06 0.738E-06

0.704E+00 0.462E+03 -.194E+03 -.714E+00 -.463E+03 0.194E+03 0.796E-02 0.106E+01 0.242E+00 0.143E-05 -.961E-06 0.469E-06

0.727E+00 0.210E+03 -.271E+03 -.736E+00 -.210E+03 0.271E+03 0.674E-02 0.903E-01 0.593E-01 0.614E-06 -.176E-06 0.665E-06

-.182E+00 0.461E+03 0.202E+03 0.178E+00 -.462E+03 -.202E+03 0.451E-02 0.102E+01 -.218E+00 -.658E-06 0.121E-05 0.405E-05

-.294E+00 0.352E+03 -.233E+03 0.298E+00 -.352E+03 0.233E+03 -.207E-02 0.439E+00 -.298E-01 0.648E-06 -.246E-05 0.336E-05

0.403E-01 0.351E+03 0.241E+03 -.393E-01 -.351E+03 -.241E+03 0.227E-02 0.409E+00

0.556E-01 -.123E-05 0.827E-06 0.257E-05

0.496E-01 0.462E+03 -.194E+03 -.558E-01 -.463E+03 0.194E+03 0.405E-02 0.106E+01 0.232E+00 0.137E-05 -.238E-05 0.342E-05

-.476E-01 0.210E+03 -.271E+03 0.455E-01 -.210E+03 0.271E+03 -.268E-03 0.927E-01 0.325E-01 0.417E-06 -.957E-06 0.165E-05

-.551E+00 0.461E+03 0.202E+03 0.549E+00 -.462E+03 -.202E+03 0.747E-03 0.102E+01 -.220E+00 0.770E-06 0.763E-06 0.475E-05

-.119E+01 0.352E+03 -.233E+03 0.120E+01 -.353E+03 0.233E+03 -.163E-01 0.446E+00 -.329E-01 -.494E-06 -.287E-05 0.247E-05

-.352E+00 0.351E+03 0.241E+03 0.349E+00 -.351E+03 -.241E+03 0.206E-02 0.413E+00 0.622E-01 -.830E-07 0.731E-06 0.412E-05

-.411E+00 0.462E+03 -.194E+03 0.425E+00 -.463E+03 0.194E+03 -.116E-01 0.106E+01 0.231E+00 0.104E-06 -.320E-05 0.414E-05

-.563E+00 0.210E+03 -.271E+03 0.567E+00 -.210E+03 0.271E+03 -.962E-02 0.907E-01 0.525E-01 -.478E-06 -.834E-06 0.103E-05

-.474E+00 0.461E+03 0.202E+03 0.474E+00 -.462E+03 -.202E+03 0.302E-02 0.102E+01 -.221E+00 0.142E-05 0.312E-06 0.351E-05

-.805E+00 0.353E+03 -.234E+03 0.820E+00 -.353E+03 0.234E+03 -.150E-01 0.446E+00 -.393E-01 -.138E-05 -.207E-05 -.361E-06

-.374E+00 0.351E+03 0.241E+03 0.368E+00 -.351E+03 -.241E+03 0.919E-03 0.410E+00 0.625E-01 0.110E-05 0.324E-06 0.373E-05

-.593E+00 0.462E+03 -.194E+03 0.606E+00 -.463E+03 0.194E+03 -.171E-01 0.105E+01

0.234E+00 -.140E-05 -.316E-05 0.186E-05

-.590E+00 0.210E+03 -.272E+03 0.601E+00 -.210E+03 0.272E+03 -.103E-01 0.984E-01 0.566E-01 -.805E-06 0.112E-06 -.623E-06

-.966E-02 0.206E+03 0.279E+03 0.130E-01 -.206E+03 -.279E+03 -.363E-02 0.684E-01 -.413E-01 0.124E-05 0.259E-09 0.999E-06

0.667E+00 0.303E+02 0.296E+03 -.662E+00 -.302E+02 -.296E+03 -.469E-02 -.412E-01 0.730E-02 0.355E-06 -.682E-06 0.569E-06

-.848E+00 0.144E+03 -.282E+03 0.850E+00 -.144E+03 0.282E+03 -.318E-02 0.136E+00 0.286E-01 -.473E-06 0.844E-06 -.928E-06

0.533E+00 -.214E+02 -.285E+03 -.534E+00 0.214E+02 0.285E+03 -.783E-03 0.380E-01 0.186E-01 -.644E-07 0.176E-05 0.682E-06

0.496E+00 -.294E+02 0.293E+03 -.493E+00 0.294E+02 -.293E+03 -.555E-02 0.252E-01 -.306E-01 0.268E-07 -.858E-07 0.929E-06

0.523E+00 0.139E+03 0.289E+03 -.524E+00 -.139E+03 -.289E+03 0.177E-02 0.103E+00 -.250E-01 0.633E-06 -.458E-06 0.230E-06

-.127E+01 0.365E+02 -.287E+03 0.127E+01 -.364E+02 0.287E+03 -.220E-03 -.838E-02 0.139E-01 -.526E-06 0.145E-05 0.130E-06

0.167E+01 -.130E+03 -.271E+03 -.168E+01 0.130E+03 0.271E+03 0.106E-01 -.885E-01 0.373E-01 0.843E-07 0.107E-05 0.113E-05

0.397E+00 0.207E+03 0.280E+03 -.395E+00 -.207E+03 -.280E+03 0.717E-03 0.692E-01 -.372E-01 0.219E-06 -.351E-06 -.190E-06

0.921E+00 0.312E+02 0.296E+03 -.924E+00 -.311E+02 -.296E+03 0.229E-02 -.412E-01

0.120E-01 0.490E-07 -.661E-06 0.234E-06

0.133E+01 0.144E+03 -.282E+03 -.133E+01 -.144E+03 0.282E+03 0.501E-02 0.125E+00 0.279E-01 0.181E-06 0.106E-05 -.994E-06

0.342E+01 -.199E+02 -.285E+03 -.344E+01 0.199E+02 0.285E+03 0.139E-01 0.407E-01 0.138E-01 0.393E-06 0.175E-05 0.328E-06

0.139E+01 -.287E+02 0.294E+03 -.139E+01 0.287E+02 -.294E+03 -.347E-02 0.251E-01 -.310E-01 0.208E-06 -.683E-06 0.876E-06

0.678E+00 0.139E+03 0.290E+03 -.679E+00 -.139E+03 -.290E+03 0.646E-03 0.103E+00 -.297E-01 -.291E-06 -.467E-06 -.235E-06

0.160E+01 0.367E+02 -.287E+03 -.159E+01 -.367E+02 0.287E+03 -.126E-01 -.213E-01 0.129E-01 0.366E-06 0.149E-05 0.150E-06

0.613E+01 -.125E+03 -.271E+03 -.615E+01 0.125E+03 0.271E+03 0.222E-01 -.899E-01 0.148E-01 0.330E-06 0.118E-05 0.481E-06

0.368E+00 0.207E+03 0.280E+03 -.373E+00 -.207E+03 -.280E+03 0.141E-03 0.681E-01 -.367E-01 -.106E-05 0.111E-06 0.124E-06

-.350E-01 0.319E+02 0.296E+03 0.264E-01 -.319E+02 -.296E+03 0.106E-01 -.364E-01 0.137E-01 -.342E-06 0.407E-06 0.124E-06

0.210E+01 0.144E+03 -.281E+03 -.211E+01 -.144E+03 0.281E+03 0.122E-01 0.120E+00 0.241E-01 0.366E-06 0.958E-06 -.973E-07

0.304E+01 -.171E+02 -.283E+03 -.307E+01 0.170E+02 0.283E+03 0.247E-01 0.861E-01 0.615E-01 -.595E-07 0.183E-05 0.198E-06

0.106E+01 -.272E+02 0.294E+03 -.106E+01 0.272E+02 -.294E+03 0.292E-02 0.242E-01 -

.378E-01 0.153E-06 0.159E-07 0.412E-06

0.979E-01 0.140E+03 0.290E+03 -.995E-01 -.140E+03 -.290E+03 0.133E-02 0.107E+00 -.233E-01 -.893E-06 0.393E-06 0.469E-06

0.277E+01 0.387E+02 -.286E+03 -.278E+01 -.387E+02 0.286E+03 0.144E-02 -.115E-01 0.294E-01 0.305E-06 0.150E-05 0.111E-06

0.598E+01 -.115E+03 -.267E+03 -.614E+01 0.115E+03 0.267E+03 0.153E+00 0.276E-03 0.131E+00 0.110E-05 0.146E-05 0.231E-06

-.241E+00 0.207E+03 0.280E+03 0.239E+00 -.207E+03 -.280E+03 0.440E-02 0.714E-01 -.388E-01 -.112E-05 0.854E-06 0.149E-05

-.114E+01 0.314E+02 0.294E+03 0.113E+01 -.314E+02 -.294E+03 0.919E-02 -.313E-01 0.525E-02 -.413E-06 0.127E-05 0.380E-06

0.597E+00 0.144E+03 -.281E+03 -.614E+00 -.144E+03 0.281E+03 0.180E-01 0.125E+00 0.438E-01 0.629E-06 -.121E-06 0.892E-06

-.938E+00 -.159E+02 -.286E+03 0.930E+00 0.158E+02 0.285E+03 0.598E-02 0.906E-01 0.807E-01 0.483E-06 0.263E-05 0.165E-06

-.640E+00 -.265E+02 0.293E+03 0.637E+00 0.265E+02 -.293E+03 0.492E-02 0.233E-01 -.272E-01 -.147E-06 0.112E-05 -.840E-07

-.533E+00 0.139E+03 0.289E+03 0.529E+00 -.139E+03 -.289E+03 0.655E-02 0.114E+00 -.215E-01 -.670E-06 0.113E-05 0.158E-05

0.783E+00 0.408E+02 -.287E+03 -.796E+00 -.408E+02 0.287E+03 0.543E-02 0.186E-02 -.188E-01 0.339E-06 0.149E-05 0.287E-06

-.456E+00 -.113E+03 -.276E+03 0.422E+00 0.113E+03 0.276E+03 0.348E-01 0.596E-01 -

.268E+00 0.271E-06 -.705E-06 -.505E-07

-.572E+00 0.206E+03 0.279E+03 0.570E+00 -.206E+03 -.279E+03 0.115E-02 0.717E-01 -.457E-01 -.168E-06 0.112E-05 0.272E-05

-.785E+00 0.304E+02 0.294E+03 0.788E+00 -.304E+02 -.294E+03 -.759E-02 -.310E-01 -.157E-02 0.286E-07 0.126E-05 0.793E-06

-.123E+01 0.144E+03 -.281E+03 0.125E+01 -.145E+03 0.281E+03 -.160E-01 0.122E+00 0.504E-01 -.166E-06 -.225E-06 0.947E-06

-.367E+01 -.174E+02 -.283E+03 0.370E+01 0.173E+02 0.283E+03 -.311E-01 0.115E+00 0.596E-01 -.256E-06 0.209E-05 0.189E-06

-.130E+01 -.277E+02 0.291E+03 0.129E+01 0.277E+02 -.291E+03 -.134E-02 0.339E-01 -.221E-01 -.184E-06 0.159E-05 0.183E-07

-.348E+00 0.139E+03 0.289E+03 0.347E+00 -.139E+03 -.289E+03 -.837E-06 0.111E+00 -.148E-01 0.270E-06 0.112E-05 0.211E-05

-.833E+00 0.400E+02 -.287E+03 0.826E+00 -.400E+02 0.287E+03 0.122E-01 -.775E-02 -.180E-01 0.509E-07 0.163E-05 0.286E-06

-.788E+01 -.119E+03 -.267E+03 0.808E+01 0.119E+03 0.267E+03 -.190E+00 0.205E-02 0.363E-01 -.116E-05 0.117E-05 0.222E-06

-.410E+00 0.206E+03 0.279E+03 0.411E+00 -.206E+03 -.279E+03 -.283E-02 0.712E-01 -.466E-01 0.878E-06 0.733E-06 0.244E-05

-.661E-01 0.300E+02 0.294E+03 0.758E-01 -.299E+02 -.294E+03 -.952E-02 -.349E-01 0.101E-02 0.335E-06 0.415E-06 0.855E-06

-.206E+01 0.145E+03 -.282E+03 0.208E+01 -.145E+03 0.282E+03 -.190E-01 0.131E+00

0.257E-01 -.597E-06 0.347E-06 0.105E-06

-.257E+01 -.208E+02 -.285E+03 0.260E+01 0.208E+02 0.285E+03 -.294E-01 0.402E-01 0.320E-01 -.461E-06 0.169E-05 0.396E-06

-.555E+00 -.290E+02 0.291E+03 0.560E+00 0.290E+02 -.291E+03 -.289E-02 0.291E-01 -.253E-01 -.509E-07 0.109E-05 0.503E-06

0.575E-01 0.139E+03 0.289E+03 -.576E-01 -.139E+03 -.289E+03 -.376E-03 0.109E+00 -.210E-01 0.952E-06 0.380E-06 0.139E-05

-.290E+01 0.378E+02 -.286E+03 0.292E+01 -.378E+02 0.286E+03 -.150E-01 -.435E-02 0.211E-01 -.572E-06 0.150E-05 0.179E-06

-.515E+01 -.128E+03 -.271E+03 0.520E+01 0.128E+03 0.271E+03 -.466E-01 -.869E-01 0.381E-01 -.636E-06 0.837E-06 0.590E-06

0.395E+00 -.137E+03 0.280E+03 -.387E+00 0.137E+03 -.280E+03 -.975E-02 -.128E+00 -.159E-01 -.549E-06 -.133E-06 0.138E-05

0.193E+01 -.343E+03 0.233E+03 -.194E+01 0.344E+03 -.233E+03 0.907E-02 -.461E+00 -.551E-01 -.176E-06 -.152E-05 0.243E-05

-.254E+01 -.197E+03 -.259E+03 0.255E+01 0.197E+03 0.259E+03 -.943E-02 -.199E+00 0.370E-01 -.195E-06 0.483E-07 0.925E-06

0.691E+01 -.447E+03 -.198E+03 -.693E+01 0.448E+03 0.198E+03 0.983E-02 -.112E+01 0.889E-01 0.775E-06 -.131E-05 0.314E-06

-.469E+00 -.451E+03 0.204E+03 0.470E+00 0.452E+03 -.204E+03 -.223E-02 -.108E+01 -.113E+00 -.845E-06 -.277E-05 0.104E-05

0.171E+01 -.203E+03 0.269E+03 -.170E+01 0.203E+03 -.269E+03 -.483E-02 -.929E-01 -

.323E-01 -.230E-06 -.709E-06 0.222E-05

-.212E+01 -.338E+03 -.222E+03 0.216E+01 0.338E+03 0.222E+03 -.440E-01 -.605E+00

0.540E-01 0.199E-06 -.177E-05 0.531E-06

0.218E+01 -.136E+03 0.282E+03 -.218E+01 0.136E+03 -.282E+03 -.632E-02 -.126E+00 -

.973E-02 0.302E-06 -.541E-06 0.203E-05

0.672E+01 -.339E+03 0.238E+03 -.670E+01 0.340E+03 -.238E+03 -.125E-01 -.462E+00 -

.464E-01 0.109E-05 -.996E-06 0.276E-05

0.679E+01 -.193E+03 -.258E+03 -.680E+01 0.193E+03 0.258E+03 0.112E-01 -.146E+00

0.635E-01 0.365E-06 0.281E-06 0.851E-06

0.313E+02 -.427E+03 -.198E+03 -.314E+02 0.428E+03 0.197E+03 0.730E-01 -.966E+00

0.132E+00 0.420E-06 -.131E-05 -.201E-06

0.544E+01 -.449E+03 0.209E+03 -.544E+01 0.451E+03 -.209E+03 0.671E-03 -.108E+01 -

.802E-01 0.832E-06 -.205E-05 0.298E-05

0.369E+01 -.201E+03 0.272E+03 -.368E+01 0.201E+03 -.272E+03 -.661E-03 -.978E-01 -

.309E-01 0.830E-06 -.467E-06 0.217E-05

0.124E+02 -.332E+03 -.223E+03 -.125E+02 0.332E+03 0.223E+03 0.120E+00 -.536E+00

0.316E-01 0.422E-06 -.933E-06 0.271E-06

0.219E+01 -.133E+03 0.283E+03 -.219E+01 0.133E+03 -.283E+03 0.637E-03 -.128E+00 -

.472E-02 0.709E-06 0.631E-07 0.109E-05

0.493E+01 -.332E+03 0.245E+03 -.490E+01 0.332E+03 -.245E+03 -.318E-01 -.476E+00 -

.378E-01 0.104E-05 -.512E-06 0.146E-06

0.113E+02 -.182E+03 -.258E+03 -.113E+02 0.182E+03 0.258E+03 0.475E-01 -.989E-01 -

.104E+00 -.631E-08 0.106E-05 0.197E-06

0.319E+02 -.399E+03 -.175E+03 -.322E+02 0.401E+03 0.174E+03 0.295E+00 -.140E+01 0.133E+01 -.141E-05 -.443E-05 0.102E-05

0.931E+01 -.443E+03 0.219E+03 -.930E+01 0.444E+03 -.219E+03 -.528E-02 -.109E+01 -.485E-01 0.147E-05 -.118E-05 0.187E-05

0.169E+01 -.196E+03 0.273E+03 -.170E+01 0.197E+03 -.273E+03 0.557E-02 -.109E+00 -.514E-01 0.817E-06 0.305E-06 0.291E-06

0.172E+02 -.310E+03 -.216E+03 -.176E+02 0.310E+03 0.216E+03 0.325E+00 -.219E+00 0.124E+00 -.116E-05 -.243E-05 0.386E-06

-.103E+01 -.132E+03 0.281E+03 0.102E+01 0.132E+03 -.281E+03 0.103E-01 -.127E+00 -.136E-03 0.366E-06 0.963E-06 -.527E-06

-.512E+01 -.332E+03 0.239E+03 0.511E+01 0.332E+03 -.239E+03 0.876E-02 -.494E+00 -.423E-01 0.171E-06 -.457E-06 -.250E-05

0.161E+01 -.169E+03 -.261E+03 -.173E+01 0.169E+03 0.261E+03 0.117E+00 0.371E+00 -.967E-01 -.154E-05 -.219E-05 -.854E-07

-.648E+01 -.301E+03 -.188E+03 0.600E+01 0.296E+03 0.184E+03 0.470E+00 0.509E+01 0.400E+01 -.576E-06 -.479E-05 -.433E-05

-.615E+00 -.436E+03 0.227E+03 0.613E+00 0.437E+03 -.227E+03 0.164E-02 -.120E+01 -.480E-01 0.709E-06 -.109E-05 -.167E-05

-.302E+01 -.197E+03 0.268E+03 0.301E+01 0.197E+03 -.268E+03 0.146E-01 -.112E+00 -.431E-01 0.119E-06 0.888E-06 -.151E-05

0.347E+01 -.280E+03 -.215E+03 -.537E+01 0.280E+03 0.214E+03 0.191E+01 0.643E+00

0.821E+00 -.521E-05 -.442E-05 -.656E-06

-.274E+01 -.134E+03 0.277E+03 0.274E+01 0.134E+03 -.277E+03 0.244E-02 -.124E+00 -.187E-01 -.189E-06 0.138E-05 -.111E-05

-.601E+01 -.338E+03 0.230E+03 0.601E+01 0.339E+03 -.230E+03 0.112E-01 -.494E+00 -.464E-01 -.730E-06 -.802E-06 -.239E-05

-.653E+01 -.171E+03 -.257E+03 0.661E+01 0.170E+03 0.257E+03 -.771E-01 0.485E+00 0.145E-01 0.197E-05 -.258E-05 -.655E-07

-.443E+02 -.422E+03 -.184E+03 0.449E+02 0.423E+03 0.183E+03 -.564E+00 -.108E+01 0.637E+00 0.845E-06 -.465E-05 0.522E-06

-.867E+01 -.441E+03 0.211E+03 0.866E+01 0.443E+03 -.211E+03 0.143E-01 -.111E+01 -.758E-01 -.453E-06 -.140E-05 -.303E-05

-.293E+01 -.201E+03 0.265E+03 0.294E+01 0.201E+03 -.265E+03 -.922E-02 -.110E+00 -.207E-01 -.529E-06 0.793E-06 -.132E-05

-.146E+02 -.290E+03 -.209E+03 0.166E+02 0.289E+03 0.208E+03 -.198E+01 0.605E+00 0.781E+00 0.505E-05 -.517E-05 -.655E-06

-.139E+01 -.136E+03 0.277E+03 0.140E+01 0.136E+03 -.277E+03 -.103E-01 -.125E+00 -.242E-01 -.599E-06 0.884E-06 -.132E-06

-.280E+01 -.343E+03 0.230E+03 0.277E+01 0.343E+03 -.230E+03 0.233E-01 -.473E+00 -.597E-01 -.130E-05 -.156E-05 -.587E-07

-.104E+02 -.189E+03 -.258E+03 0.105E+02 0.189E+03 0.258E+03 -.774E-01 -.139E+00 -.524E-01 -.597E-06 0.137E-06 0.292E-06

-.150E+02 -.446E+03 -.196E+03 0.150E+02 0.447E+03 0.196E+03 -.695E-01 -.112E+01

0.992E-01 -.547E-06 -.286E-05 0.446E-06

-.550E+01 -.448E+03 0.204E+03 0.551E+01 0.449E+03 -.204E+03 -.503E-02 -.108E+01 -.125E+00 -.155E-05 -.243E-05 -.173E-05

-.919E+00 -.203E+03 0.267E+03 0.927E+00 0.203E+03 -.267E+03 -.918E-02 -.102E+00 -.320E-01 -.964E-06 -.861E-08 0.530E-06

-.163E+02 -.329E+03 -.218E+03 0.167E+02 0.329E+03 0.218E+03 -.360E+00 -.480E+00 0.435E-01 0.976E-06 -.325E-05 0.573E-06

-.267E+01 -.254E+03 -.190E+03 0.158E+01 0.245E+03 0.185E+03 0.986E+00 0.775E+01 0.499E+01 -.313E-05 -.217E-04 -.190E-04

0.531E+02 -.518E+03 -.137E+03 -.542E+02 0.522E+03 0.141E+03 0.105E+01 -.395E+01 -.382E+01 -.347E-05 -.322E-05 -.259E-07

-.471E+02 -.589E+03 -.451E+03 0.532E+02 0.641E+03 0.487E+03 -.602E+01 -.514E+02 -.351E+02 -.188E-05 0.138E-04 -.794E-06

0.453E+01 0.282E+02 0.232E+02 -.334E-12 -.705E-11 0.125E-11 -.457E+01 -.282E+02 -.232E+02 -.833E-05 -.470E-04 0.574E-04

POSITION TOTAL-FORCE (eV/Angst)

1.24575	4.02870	5.43979	0.000040	0.000961	-0.000382
1.21024	4.07581	8.43726	-0.000982	0.002516	-0.001189

3.70862	4.02890	5.43965	0.000300	0.001833	-0.001067
3.67998	4.07733	8.43690	-0.004044	-0.000515	-0.002945
6.17157	4.02854	5.43942	-0.000019	-0.000197	-0.001728
6.14482	4.08292	8.43295	-0.002850	-0.003398	-0.003251
8.63513	4.02801	5.43869	0.000767	-0.000504	-0.001981
8.60339	4.08732	8.43089	-0.000145	-0.001264	-0.002287
11.09928	4.02784	5.43885	0.000870	0.001910	-0.002693
11.06021	4.08619	8.43099	-0.001750	0.000617	-0.000723
13.56311	4.02807	5.43972	0.000333	0.001561	-0.001597
13.52141	4.08047	8.43349	0.000408	-0.002350	0.000229
2.44241	15.48073	8.85224	-0.000629	-0.005202	0.002196
0.01714	15.44624	5.32469	0.000366	0.001519	-0.001147
4.86040	15.47728	8.86623	0.000741	0.000383	-0.000117
2.48016	15.44854	5.27562	0.000353	-0.001226	-0.000449
4.94382	15.44925	5.24869	0.001709	-0.002959	0.000263
12.31531	15.48242	9.00211	-0.002464	0.002248	0.002313
9.86772	15.44556	5.34176	0.000430	-0.001072	0.000863
14.76279	15.48245	8.89951	-0.005935	-0.000327	0.005445
12.33384	15.44510	5.36128	0.001396	-0.003195	-0.001291
7.40743	15.44616	5.26463	0.002366	0.001678	0.001293
6.44846	16.34427	7.40648	-0.002118	0.001026	0.003873
8.60064	16.47644	7.89249	0.008003	0.001499	0.004011

1.24544	5.11881	5.35500	0.000953	0.000264	-0.002519
2.44348	5.83889	8.62292	0.002415	-0.004528	0.001205
0.01380	5.79530	5.28573	0.002064	-0.002594	0.000476
1.21063	5.16420	8.54151	0.000246	-0.000546	-0.001819
2.44351	7.27931	8.74832	-0.000117	-0.001246	-0.000109
3.70866	5.11896	5.35390	-0.000433	-0.001528	0.000274
4.90800	5.84315	8.62123	-0.001089	0.003763	-0.000792
2.47701	5.79561	5.28397	0.001438	-0.000731	-0.002602
3.67679	5.16572	8.54000	-0.000135	0.001597	0.000028
4.90764	7.28398	8.74777	0.000811	-0.000593	0.001066
6.17184	5.11860	5.35433	0.001472	0.000516	0.000826
7.37096	5.84929	8.62094	-0.000630	0.006986	-0.002458
4.94029	5.79548	5.28340	0.000594	-0.002829	-0.001170
6.14080	5.17108	8.53715	-0.002532	0.002570	0.002552
7.37071	7.28983	8.75132	-0.001929	0.001657	0.000159
8.63543	5.11820	5.35521	0.001247	0.001503	-0.001147
9.83233	5.85166	8.62337	0.002767	0.000237	-0.001127
7.40374	5.79498	5.28512	0.003434	-0.002846	-0.001334
8.60194	5.17528	8.53759	-0.001853	-0.000302	-0.000108
9.83204	7.29110	8.75719	-0.001883	-0.002219	-0.002395
11.09930	5.11814	5.35578	-0.000873	-0.003192	-0.001438
12.29449	5.84673	8.62385	0.000049	0.005621	-0.002205

9.86750	5.79468	5.28678	-0.000762	-0.000885	0.001553
11.06261	5.17409	8.53894	0.002624	0.002805	-0.000295
12.29428	7.28729	8.75533	-0.004578	0.001262	-0.001495
13.56278	5.11829	5.35605	0.002658	0.000662	-0.002055
14.75895	5.83988	8.62434	-0.000194	-0.002721	-0.002235
12.33118	5.79480	5.28692	-0.004503	-0.001626	0.002596
13.52535	5.16844	8.54022	-0.003551	0.003842	-0.001336
14.75917	7.28012	8.75179	0.000830	0.002535	-0.000673
0.01434	7.23830	5.19017	0.000086	-0.000226	0.000067
1.24689	9.38061	5.13160	0.000530	-0.001866	-0.000012
1.21085	7.98059	8.79588	-0.000912	-0.000537	0.001530
2.44214	10.12243	8.87141	-0.000994	0.002724	-0.005019
0.01532	10.08686	5.14049	-0.002039	-0.000177	-0.002397
1.24606	7.94244	5.15775	0.002006	-0.002647	0.000834
1.21082	9.41592	8.85782	-0.000549	0.004550	0.000215
2.44072	11.55513	8.88414	-0.006230	-0.002340	0.001723
2.47747	7.23842	5.18585	0.002794	0.002867	0.001301
3.70997	9.38055	5.12566	-0.001081	-0.003016	0.000035
3.67534	7.98360	8.79349	-0.000544	0.001027	0.000931
4.90487	10.12925	8.87518	0.000392	-0.000827	0.000009
2.47867	10.08713	5.12695	-0.002276	0.001473	0.000760
3.70939	7.94242	5.15441	0.000799	-0.004054	-0.001694

3.67589	9.41970	8.85445	-0.001520	0.002045	-0.000120
4.90263	11.56506	8.89086	-0.000440	0.002283	0.000862
4.94085	7.23830	5.18552	-0.004703	0.002240	0.000818
6.17318	9.38002	5.13173	0.002053	0.002104	0.001821
6.13864	7.99044	8.79647	0.002386	-0.000577	-0.001666
7.36780	10.13760	8.89473	-0.000608	0.002755	0.000798
4.94196	10.08682	5.12700	0.004109	0.001446	-0.001152
6.17284	7.94199	5.15766	-0.000069	0.000498	0.003032
6.13939	9.42660	8.86164	0.000529	-0.000304	-0.002065
7.36410	11.57721	8.92935	-0.000206	-0.001550	0.002906
7.40426	7.23794	5.19012	0.002142	0.001753	0.001059
8.63700	9.37970	5.14543	-0.000513	0.002955	0.000932
8.60086	7.99568	8.80617	0.001130	-0.001095	-0.001168
9.83068	10.14286	8.92842	-0.002245	0.001155	-0.000466
7.40553	10.08627	5.14064	0.001163	-0.003651	0.003151
8.63637	7.94166	5.16555	0.002612	0.001715	-0.001406
8.60077	9.43254	8.88532	-0.006135	0.003031	-0.001271
9.82927	11.58244	9.00096	0.000934	0.005799	0.001260
9.86805	7.23787	5.19489	-0.000367	0.000094	-0.000240
11.10106	9.37979	5.15156	-0.003840	-0.001028	0.000643
11.06331	7.99411	8.80818	-0.000256	-0.002094	0.000014
12.29815	10.12943	8.90340	-0.000751	-0.001429	0.001654

9.86930	10.08593	5.15631	-0.005473	-0.001560	0.001406
11.10021	7.94175	5.16862	-0.000630	-0.003142	0.001393
11.06206	9.43062	8.88839	0.004594	0.002359	0.002056
12.30255	11.56557	8.94694	0.002895	-0.000281	-0.001513
12.33169	7.23799	5.19447	-0.001021	0.000227	-0.001768
13.56437	9.38021	5.14435	0.000701	0.001647	-0.000588
13.52754	7.98555	8.80171	-0.000756	-0.002819	-0.003117
14.76233	10.12320	8.88285	-0.005341	0.000570	-0.001618
12.33257	10.08637	5.15511	0.002652	0.000463	-0.001538
13.56350	7.94214	5.16485	-0.000099	-0.000945	-0.000371
13.52731	9.42040	8.86925	-0.000069	0.003242	-0.000399
14.76430	11.55727	8.90646	-0.002134	-0.000206	0.001653
0.01611	11.52516	5.16621	-0.001075	-0.002547	0.000383
1.24770	13.67535	5.22209	0.001921	-0.002006	-0.002467
1.21217	12.26335	8.89409	0.000887	-0.000555	0.001135
2.43998	14.38728	8.86748	-0.002283	-0.000852	0.000848
0.01699	14.35408	5.27295	-0.000545	-0.001144	-0.002052
1.24794	12.22963	5.17275	0.001030	0.000870	-0.001358
1.21434	13.70818	8.88771	0.001120	0.003978	0.003594
2.47958	11.52580	5.14547	-0.001619	-0.000197	-0.001496
3.71218	13.67636	5.19535	0.004522	0.000939	0.001105
3.66932	12.26248	8.88184	-0.002238	-0.000101	-0.000638

4.89370	14.38589	8.86075	0.003369	-0.003130	-0.002607
2.48000	14.35596	5.23149	0.001256	-0.001629	0.001615
3.71150	12.23022	5.15602	0.000890	-0.004506	0.001006
3.66212	13.70366	8.87117	-0.005461	0.005799	-0.001151
4.94290	11.52542	5.14351	-0.000068	-0.001752	-0.001610
6.17627	13.67505	5.20032	0.000772	0.001053	0.000118
6.13145	12.27911	8.90591	0.004951	0.006201	0.004424
7.36614	14.42967	8.88203	-0.004883	-0.003577	0.001393
4.94347	14.35627	5.21375	0.000161	-0.002444	0.001068
6.17493	12.22917	5.16623	-0.001411	-0.001075	0.001523
6.11879	13.72336	8.87765	0.006247	0.005478	0.001799
7.40625	11.52413	5.16368	0.000912	-0.003271	0.000344
8.63876	13.67323	5.24377	0.001933	0.002678	-0.001258
8.58939	12.29067	9.00208	-0.001906	-0.001854	-0.003216
9.83855	14.39048	9.30305	-0.002778	-0.052174	-0.037009
7.40672	14.35386	5.23530	-0.001120	-0.001105	-0.000686
8.63820	12.22778	5.19800	0.000306	-0.001284	0.001035
8.55571	13.73596	9.04598	0.016652	0.008718	0.009212
9.86985	11.52338	5.18893	0.001754	-0.001876	-0.000117
11.10099	13.67352	5.27669	0.003113	-0.000331	-0.000955
11.07378	12.27333	9.00891	-0.002232	0.001797	-0.005321
12.30694	14.38896	9.00333	0.002991	-0.005413	0.003066

9.86934	14.35300	5.29564	0.002947	-0.000721	-0.000282
11.10161	12.22804	5.21650	-0.001135	-0.002759	0.001056
11.11464	13.70636	9.07877	-0.012867	0.013702	0.004524
12.33326	11.52411	5.18815	-0.000918	0.000338	0.000531
13.56430	13.67399	5.25995	0.001688	0.000379	0.000112
13.53626	12.26601	8.93587	-0.002069	0.004089	0.001802
14.76266	14.38906	8.90426	-0.002128	-0.000993	0.003661
12.33397	14.35288	5.30710	0.002706	-0.002529	-0.001805
13.56505	12.22870	5.20105	0.000064	0.000096	-0.001138
13.54921	13.70690	8.94399	-0.001570	-0.000121	0.002943
9.91126	15.53185	9.99472	-0.104427	-0.974621	-0.624107
7.28864	16.40884	8.69813	-0.005533	-0.009035	-0.005534
10.02526	16.48865	10.64498	0.117680	1.009862	0.664171

---

total drift:	-0.043520	0.029164	-0.022399

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

---

free energy TOTEN = -1209.38180214 eV

energy without entropy= -1209.38180214 energy(sigma->0) = -1209.38180214

d Force =-0.1046049E-02[-0.303E-01, 0.282E-01] d Energy =-0.3046485E-03-0.741E-03

d Force =-0.1909082E+02[-0.192E+02,-0.189E+02] d Ewald =-0.1909041E+02-0.409E-03

POTLOK: cpu time 0.1746: real time 0.1827

---

stress matrix after NEB project (eV)

-17.70877	-0.13210	0.13110
-0.13210	-14.30736	1.12340
0.13110	1.12340	-18.59719

FORCES: max atom, RMS 1.214410 0.138630

FORCE total and by dimension 1.680802 1.009862

Stress total and by dimension 29.440616 18.597192

Finite differences progress:

Degree of freedom: 5/ 6

Displacement: 2/ 2

Total: 10/ 12

LATTYP: Found a simple orthorhombic cell.

ALAT = 14.7806000000

B/A-ratio = 1.2466138046

C/A-ratio = 1.4433717170

Lattice vectors:

A1 = (-14.7806000000, 0.0000000000, 0.0000000000)

A2 = (0.0000000000, 0.0000000000, -18.4257000000)

A3 = (0.0000000000, -21.3339000000, 0.0000000000)

Analysis of symmetry for initial positions (statically):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The static configuration has the point symmetry C_1 .

Analysis of symmetry for dynamics (positions and initial velocities):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The dynamic configuration has the point symmetry C_1 .

Analysis of constrained symmetry for selective dynamics:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The constrained configuration has the point symmetry C_1 .

Analysis of structural, dynamic, and magnetic symmetry:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The magnetic configuration has the point symmetry C_1 .

Subroutine INISYM returns: Found 1 space group operations

(whereof 1 operations are pure point group operations),

and found 1 'primitive' translations

KPOINTS: KPT-Resolved Value to Generate K-Mesh: 0

Automatic generation of k-mesh.

Space group operators:

irot	det(A)	alpha	n_x	n_y	n_z	tau_x	tau_y	tau_z
1	1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Subroutine IBZKPT returns following result:

==========

Found 1 irreducible k-points:

Following reciprocal coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

Following cartesian coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

WAVPRE: cpu time 0.1206: real time 0.1492

FEWALD: cpu time 0.0026: real time 0.0026

ORTHCH: cpu time 1.0093: real time 1.0129

LOOP+: cpu time 188.5243: real time 189.6346

---------- Iteration 12(1) ----------

POTLOK: cpu time 0.1762: real time 0.1882

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9257: real time 1.9315

RMM-DIIS: cpu time 7.0840: real time 7.1174

ORTHCH: cpu time 0.3513: real time 0.3522

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5260: real time 0.5273

MIXING: cpu time 0.0045: real time 0.0045

LOOP: cpu time 10.0782: real time 10.1316

eigenvalue-minimisations : 1928

total energy-change (2. order) :-0.9440617E-02 (-0.2524042E+00)

number of electron 518.9999718 magnetization 0.9999998

augmentation part 11.7291160 magnetization 0.0542734

Broyden mixing:

rms(total) = 0.43171E-01 rms(broyden)= 0.42953E-01

rms(prec) = 0.44302E-01

weight for this iteration 100.00

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107331.53261606

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.79450979

PAW double counting = 52198.34475733 -52261.27927310

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5811.95017134

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.77330379 eV

energy without entropy = -1202.77330379 energy(sigma->0) = -1202.77330379

---------- Iteration 12(2) ----------

POTLOK: cpu time 0.1659: real time 0.1748

SETDIJ: cpu time 0.0102: real time 0.0103

```
      EDDIAG:    cpu time        1.9203: real time        1.9267
    RMM-DIIS:    cpu time        7.2865: real time        7.3165
      ORTHCH:    cpu time        0.3567: real time        0.3578
         DOS:    cpu time        0.0004: real time        0.0004
      CHARGE:    cpu time        0.5247: real time        0.5265
      MIXING:    cpu time        0.0044: real time        0.0044
      ----------------------------------------------
        LOOP:    cpu time       10.2689: real time       10.3172

eigenvalue-minimisations    :    1939
total energy-change (2. order) : 0.4125926E-02    (-0.2521665E-02)
number of electron          518.9999719 magnetization             0.9999998
augmentation part             11.7342518 magnetization             0.0542615

Broyden mixing:
  rms(total) = 0.24552E-01        rms(broyden)= 0.24512E-01
  rms(prec ) = 0.25848E-01
  weight for this iteration          100.00

eigenvalues of (default mixing * dielectric matrix)
  average eigenvalue GAMMA=       1.1569
  1.1569
```

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107330.49244881

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.75262805

PAW double counting = 52185.18566009 -52248.10174920

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5812.96275758

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76917787 eV

energy without entropy = -1202.76917787 energy(sigma->0) = -1202.76917787

---------- Iteration 12(3) ----------

POTLOK: cpu time 0.1670: real time 0.1750

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9174: real time 1.9236

RMM-DIIS: cpu time 7.3526: real time 7.3768

ORTHCH: cpu time 0.3569: real time 0.3578

DOS: cpu time 0.0003: real time 0.0003

CHARGE: cpu time 0.5238: real time 0.5255

MIXING: cpu time 0.0052: real time 0.0052

LOOP: cpu time 10.3335: real time 10.3745

eigenvalue-minimisations : 1959

total energy-change (2. order) : 0.1017449E-02 (-0.1022643E-03)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7329353 magnetization 0.0542644

Broyden mixing:

rms(total) = 0.14670E-01 rms(broyden)= 0.14659E-01

rms(prec) = 0.15121E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5216

0.7254 2.3178

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107329.80519785

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.75103550

PAW double counting = 52176.00927517 -52238.92224002

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5813.65052281

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76816042 eV

energy without entropy = -1202.76816042 energy(sigma->0) = -1202.76816042

---------- Iteration 12(4) ----------

POTLOK: cpu time 0.1641: real time 0.1880

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9198: real time 1.9261

RMM-DIIS: cpu time 7.2843: real time 7.3102

ORTHCH: cpu time 0.3539: real time 0.3549

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5228: real time 0.5248

MIXING: cpu time 0.0054: real time 0.0054

LOOP: cpu time 10.2608: real time 10.3197

eigenvalue-minimisations : 1940

total energy-change (2. order) : 0.1631238E-03 (-0.6483231E-04)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7330367 magnetization 0.0542731

Broyden mixing:

rms(total) = 0.46941E-02 rms(broyden)= 0.46894E-02

rms(prec) = 0.50848E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4548

2.2857 1.2434 0.8354

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.93906318

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73883165

PAW double counting = 52164.42501333 -52227.33271664

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.50955204

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76799729 eV

energy without entropy = -1202.76799729 energy(sigma->0) = -1202.76799729

---------- Iteration 12(5) ----------

POTLOK: cpu time 0.1653: real time 0.1676

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9225: real time 1.9289

RMM-DIIS: cpu time 7.0807: real time 7.1202

ORTHCH: cpu time 0.3530: real time 0.3540

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5240: real time 0.5260

MIXING: cpu time 0.0055: real time 0.0055

LOOP: cpu time 10.0615: real time 10.1128

eigenvalue-minimisations : 1925

total energy-change (2. order) :-0.1314357E-04 (-0.1232601E-04)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7336697 magnetization 0.0542753

Broyden mixing:

rms(total) = 0.19032E-02 rms(broyden)= 0.18993E-02

rms(prec) = 0.21851E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4931

2.2462 2.0093 0.8584 0.8584

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.79126129

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73737350

PAW double counting = 52163.25566901 -52226.16359741

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.65568384

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76801044 eV

energy without entropy = -1202.76801044 energy(sigma->0) = -1202.76801044

---------- Iteration 12(6) ----------

POTLOK: cpu time 0.1671: real time 0.1771

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9218: real time 1.9286

RMM-DIIS: cpu time 7.2013: real time 7.2586

ORTHCH: cpu time 0.3522: real time 0.3533

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5235: real time 0.5253

MIXING: cpu time 0.0059: real time 0.0060

LOOP: cpu time 10.1824: real time 10.2594

eigenvalue-minimisations : 1931

total energy-change (2. order) :-0.3279449E-04 (-0.1274355E-05)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7334254 magnetization 0.0542774

Broyden mixing:

rms(total) = 0.60806E-03 rms(broyden)= 0.60715E-03

rms(prec) = 0.87089E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4623

2.5188 1.8617 0.8699 0.8699 1.1913

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.65603555

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73912859

PAW double counting = 52162.56059279 -52225.46959484

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.79162382

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76804323 eV

energy without entropy = -1202.76804323 energy(sigma->0) = -1202.76804323

---------- Iteration 12(7) ----------

POTLOK: cpu time 0.1665: real time 0.1917

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9190: real time 1.9257

RMM-DIIS: cpu time 6.5087: real time 6.5387

ORTHCH: cpu time 0.3520: real time 0.3533

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5234: real time 0.5249

MIXING: cpu time 0.0060: real time 0.0060

LOOP: cpu time 9.4858: real time 9.5508

eigenvalue-minimisations : 1772

total energy-change (2. order) :-0.3137431E-04 (-0.3039900E-06)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7333903 magnetization 0.0542779

Broyden mixing:

rms(total) = 0.36607E-03 rms(broyden)= 0.36583E-03

rms(prec) = 0.59502E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4373

2.5367 1.8843 1.6823 0.8924 0.8924 0.7360

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.53773429

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73828212

PAW double counting = 52162.43095586 -52225.33984589

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.90922199

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76807461 eV

energy without entropy = -1202.76807461 energy(sigma->0) = -1202.76807461

---------- Iteration 12(8) ----------

POTLOK: cpu time 0.1632: real time 0.1667

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9203: real time 1.9271

RMM-DIIS: cpu time 6.2808: real time 6.3157

ORTHCH: cpu time 0.3507: real time 0.3521

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5227: real time 0.5246

MIXING: cpu time 0.0063: real time 0.0063

LOOP: cpu time 9.2545: real time 9.3029

eigenvalue-minimisations : 1720

total energy-change (2. order) :-0.3744439E-04 (-0.2224000E-06)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7334066 magnetization 0.0542778

Broyden mixing:

rms(total) = 0.20505E-03 rms(broyden)= 0.20497E-03

rms(prec) = 0.39770E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4587

2.5949 2.5949 1.4519 1.1368 0.8776 0.8776 0.6774

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.42699182

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73757414

PAW double counting = 52162.56398330 -52225.47280300

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.01936426

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76811205 eV

energy without entropy = -1202.76811205 energy(sigma->0) = -1202.76811205

---------- Iteration 12(9) ----------

POTLOK: cpu time 0.1620: real time 0.1633

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9183: real time 1.9252

RMM-DIIS: cpu time 6.1617: real time 6.2000

ORTHCH: cpu time 0.3504: real time 0.3519

DOS: cpu time 0.0003: real time 0.0003

CHARGE: cpu time 0.5227: real time 0.5246

MIXING: cpu time 0.0069: real time 0.0069

LOOP: cpu time 9.1323: real time 9.1823

eigenvalue-minimisations : 1682

total energy-change (2. order) :-0.3909832E-04 (-0.2166312E-06)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7334065 magnetization 0.0542785

Broyden mixing:

rms(total) = 0.14515E-03 rms(broyden)= 0.14508E-03

rms(prec) = 0.26573E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.5254

3.0812 2.6213 1.8146 1.1142 1.1142 0.9010 0.9010 0.6562

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.31751354

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73699289

PAW double counting = 52162.69171869 -52225.60047768

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.12836110

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76815115 eV

energy without entropy = -1202.76815115 energy(sigma->0) = -1202.76815115

---------- Iteration 12(10) ----------

POTLOK: cpu time 0.1638: real time 0.1661

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9212: real time 1.9278

RMM-DIIS: cpu time 6.1855: real time 6.2183

ORTHCH: cpu time 0.3501: real time 0.3514

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5226: real time 0.5242

MIXING: cpu time 0.0069: real time 0.0069

LOOP: cpu time 9.1607: real time 9.2053

eigenvalue-minimisations : 1692

total energy-change (2. order) :-0.3812843E-04 (-0.2611983E-06)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7333975 magnetization 0.0542789

Broyden mixing:

rms(total) = 0.73886E-04 rms(broyden)= 0.73779E-04

rms(prec) = 0.13536E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6351

4.2653 2.5967 2.1399 1.2620 1.2620 0.8851 0.8851 0.7771 0.6430

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.20708543

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73636290

PAW double counting = 52162.77660397 -52225.68524400

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.23831631

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76818928 eV

energy without entropy = -1202.76818928 energy(sigma->0) = -1202.76818928

---------- Iteration 12(11) ----------

POTLOK: cpu time 0.1662: real time 0.1878

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9212: real time 1.9277

RMM-DIIS: cpu time 5.8924: real time 5.9192

ORTHCH: cpu time 0.3525: real time 0.3537

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5232: real time 0.5251

MIXING: cpu time 0.0075: real time 0.0075

LOOP: cpu time 8.8735: real time 8.9316

eigenvalue-minimisations : 1595

total energy-change (2. order) :-0.1533494E-04 (-0.7861592E-07)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7333912 magnetization 0.0542792

Broyden mixing:

rms(total) = 0.56059E-04 rms(broyden)= 0.56005E-04

rms(prec) = 0.89655E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6863

5.1847 2.5924 2.0647 1.6900 1.1228 0.9216 0.9216 1.0113 0.7184 0.6350

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.15656903

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73616743

PAW double counting = 52162.78564190 -52225.69427911

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.28865539

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76820461 eV

energy without entropy = -1202.76820461 energy(sigma->0) = -1202.76820461

---------- Iteration 12(12) ----------

POTLOK: cpu time 0.1653: real time 0.1717

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9239: real time 1.9304

RMM-DIIS: cpu time 5.4357: real time 5.4615

ORTHCH: cpu time 0.3510: real time 0.3522

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5221: real time 0.5238

MIXING: cpu time 0.0077: real time 0.0077

LOOP: cpu time 8.4162: real time 8.4577

eigenvalue-minimisations : 1476

total energy-change (2. order) :-0.8026072E-05 (-0.2431843E-07)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7333914 magnetization 0.0542792

Broyden mixing:

rms(total) = 0.33505E-04 rms(broyden)= 0.33490E-04

rms(prec) = 0.58712E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8164

6.3059 2.7869 2.3870 2.0160 1.2849 0.8975 0.8975 1.1035 0.9876 0.6848

0.6287

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.13874723

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73613434

PAW double counting = 52162.77081228 -52225.67947032

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.30643129

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76821264 eV

energy without entropy = -1202.76821264 energy(sigma->0) = -1202.76821264

---------- Iteration 12(13) ----------

POTLOK: cpu time 0.1666: real time 0.1804

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9119: real time 1.9399

RMM-DIIS: cpu time 5.5377: real time 5.5562

ORTHCH: cpu time 0.3515: real time 0.3527

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5238: real time 0.5256

MIXING: cpu time 0.0079: real time 0.0079

LOOP: cpu time 8.5097: real time 8.5732

eigenvalue-minimisations : 1492

total energy-change (2. order) :-0.7553095E-05 (-0.2671113E-07)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7333944 magnetization 0.0542791

Broyden mixing:

rms(total) = 0.22873E-04 rms(broyden)= 0.22856E-04

rms(prec) = 0.35081E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8354

6.7359 3.1271 2.4819 1.8401 1.6963 1.0738 1.0738 0.9109 0.9109 0.8717

0.6747 0.6276

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.12348063

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73608478

PAW double counting = 52162.75837590 -52225.66703608

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.32165375

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76822019 eV

energy without entropy = -1202.76822019 energy(sigma->0) = -1202.76822019

---------- Iteration 12(14) ----------

POTLOK: cpu time 0.1652: real time 0.1804

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9263: real time 1.9330

RMM-DIIS: cpu time 5.0539: real time 5.0754

ORTHCH: cpu time 0.3532: real time 0.3544

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5236: real time 0.5254

MIXING: cpu time 0.0082: real time 0.0082

LOOP: cpu time 8.0408: real time 8.0872

eigenvalue-minimisations : 1387

total energy-change (2. order) :-0.3269808E-05 (-0.8480622E-08)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7333941 magnetization 0.0542792

Broyden mixing:

rms(total) = 0.14436E-04 rms(broyden)= 0.14429E-04

rms(prec) = 0.21010E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9295

7.3403 3.8227 2.5323 2.2887 1.8798 1.3475 1.0261 1.0261 0.8915 0.8915

0.7459 0.6639 0.6270

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.11842564

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73607288

PAW double counting = 52162.76145527 -52225.67010941

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.32670615

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76822346 eV

energy without entropy = -1202.76822346 energy(sigma->0) = -1202.76822346

-- Iteration 12(15) --

POTLOK: cpu time 0.1698: real time 0.1867

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9197: real time 1.9260

RMM-DIIS: cpu time 4.9270: real time 4.9612

ORTHCH: cpu time 0.3510: real time 0.3520

DOS: cpu time 0.0003: real time 0.0003

CHARGE: cpu time 0.5232: real time 0.5250

MIXING: cpu time 0.0087: real time 0.0088

LOOP: cpu time 7.9099: real time 7.9701

eigenvalue-minimisations : 1351

total energy-change (2. order) :-0.1773478E-05 (-0.3489837E-08)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7333925 magnetization 0.0542792

Broyden mixing:

rms(total) = 0.69782E-05 rms(broyden)= 0.69695E-05

rms(prec) = 0.11178E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9531

7.7598 4.3464 2.6453 2.4390 1.6705 1.6705 1.0618 1.0618 0.8933 0.8933

0.9141 0.7076 0.6527 0.6268

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.11687854

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73609375

PAW double counting = 52162.76479761 -52225.67345662

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.32827102

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76822523 eV

energy without entropy = -1202.76822523 energy(sigma->0) = -1202.76822523

---------- Iteration 12(16) ----------

POTLOK: cpu time 0.1691: real time 0.1732

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9193: real time 1.9255

RMM-DIIS: cpu time 4.7120: real time 4.7275

ORTHCH: cpu time 0.3512: real time 0.3522

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5239: real time 0.5259

MIXING: cpu time 0.0092: real time 0.0092

LOOP: cpu time 7.6951: real time 7.7241

eigenvalue-minimisations : 1233

total energy-change (2. order) :-0.8491006E-06 (-0.9388001E-09)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7333923 magnetization 0.0542792

Broyden mixing:

rms(total) = 0.54499E-05 rms(broyden)= 0.54482E-05

rms(prec) = 0.81842E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9641

7.8798 4.7549 2.7009 2.4137 2.0636 1.4976 1.4602 1.0400 1.0400 0.8888

0.8888 0.8672 0.6930 0.6460 0.6267

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.11633591

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73610080

PAW double counting = 52162.76617485 -52225.67483475

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.32882066

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76822608 eV

energy without entropy = -1202.76822608 energy(sigma->0) = -1202.76822608

---------- Iteration 12(17) ----------

POTLOK: cpu time 0.1638: real time 0.1733

SETDIJ: cpu time 0.0100: real time 0.0101

```
      EDDIAG:    cpu time        1.9277: real time        1.9345
    RMM-DIIS:    cpu time        4.7188: real time        4.7450
      ORTHCH:    cpu time        0.3527: real time        0.3539
         DOS:    cpu time        0.0004: real time        0.0004
      CHARGE:    cpu time        0.5223: real time        0.5239
      MIXING:    cpu time        0.0096: real time        0.0097
      ------------------------------------------
        LOOP:    cpu time        7.7052: real time        7.7507

eigenvalue-minimisations    :    1278
total energy-change (2. order) :-0.1024862E-05    (-0.5486465E-09)
number of electron          518.9999719 magnetization             0.9999998
augmentation part            11.7333928 magnetization             0.0542791

Broyden mixing:
  rms(total) = 0.27119E-05        rms(broyden)= 0.27092E-05
  rms(prec ) = 0.44782E-05
  weight for this iteration          100.00

eigenvalues of (default mixing * dielectric matrix)
  average eigenvalue GAMMA=      2.0006
  8.0710    5.3197    2.9453    2.5749    2.2901    1.6138    1.6138    1.0798    1.0798    0.8918
```

0.8918 0.9183 0.7743 0.6791 0.6265 0.6389

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.11567748

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73609757

PAW double counting = 52162.76771280 -52225.67636942

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.32948017

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76822711 eV

energy without entropy = -1202.76822711 energy(sigma->0) = -1202.76822711

---------- Iteration 12(18) ----------

POTLOK: cpu time 0.1644: real time 0.1665

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9223: real time 1.9292

RMM-DIIS: cpu time 4.5016: real time 4.5286

ORTHCH: cpu time 0.3518: real time 0.3530

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5223: real time 0.5240

MIXING: cpu time 0.0100: real time 0.0101

LOOP: cpu time 7.4828: real time 7.5217

eigenvalue-minimisations : 1160

total energy-change (2. order) :-0.4529466E-06 (-0.2723475E-09)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7333928 magnetization 0.0542792

Broyden mixing:

rms(total) = 0.17672E-05 rms(broyden)= 0.17661E-05

rms(prec) = 0.28336E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 2.0044

8.2981 5.6218 3.2566 2.6213 2.0847 1.9393 1.5230 1.2528 1.0471 1.0471

0.8921 0.8921 0.9414 0.7214 0.6734 0.6263 0.6354

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.11551638

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73610189

PAW double counting = 52162.76810422 -52225.67676157

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.32964532

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76822756 eV

energy without entropy = -1202.76822756 energy(sigma->0) = -1202.76822756

---------- Iteration 12(19) ----------

POTLOK: cpu time 0.1688: real time 0.1891

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9202: real time 1.9267

RMM-DIIS: cpu time 4.2597: real time 4.2754

ORTHCH: cpu time 0.3525: real time 0.3538

DOS: cpu time 0.0004: real time 0.0004

LOOP: cpu time 6.7116: real time 6.7553

eigenvalue-minimisations : 1024

total energy-change (2. order) :-0.9591895E-07 (-0.8834711E-10)

number of electron 518.9999719 magnetization 0.9999998

augmentation part 11.7333928 magnetization 0.0542792

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91322.01880280

-Hartree energ DENC = -107328.11549627

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.73610714

PAW double counting = 52162.76730472 -52225.67596369

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.32966915

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76822766 eV

energy without entropy = -1202.76822766 energy(sigma->0) = -1202.76822766

---

average (electrostatic) potential at core

the test charge radii are 0.5201 0.6991 1.0621 0.7215

(the norm of the test charge is 1.0000)

1 -40.7548	2 -40.7528	3 -40.7540	4 -40.7528	5 -40.7547
6 -40.7570	7 -40.7544	8 -40.7622	9 -40.7540	10 -40.7617
11 -40.7555	12 -40.7575	13 -40.6533	14 -40.6983	15 -40.7728
16 -40.7005	17 -40.6941	18 -40.8611	19 -40.6813	20 -40.6701
21 -40.6907	22 -40.6634	23 -40.0834	24 -40.1276	25 -57.4610
26 -57.6723	27 -57.6590	28 -57.4711	29 -57.6662	30 -57.4610
31 -57.6721	32 -57.6586	33 -57.4690	34 -57.6711	35 -57.4618
36 -57.6740	37 -57.6586	38 -57.4712	39 -57.6770	40 -57.4609
41 -57.6780	42 -57.6588	43 -57.4761	44 -57.6914	45 -57.4609
46 -57.6769	47 -57.6596	48 -57.4763	49 -57.6827	50 -57.4620
51 -57.6737	52 -57.6594	53 -57.4740	54 -57.6690	55 -57.6389
56 -57.6651	57 -57.6897	58 -57.6864	59 -57.6688	60 -57.6715

61 -57.6931	62 -57.6779	63 -57.6392	64 -57.6645	65 -57.6918
66 -57.6978	67 -57.6670	68 -57.6713	69 -57.6969	70 -57.7044
71 -57.6387	72 -57.6659	73 -57.6995	74 -57.7248	75 -57.6679
76 -57.6719	77 -57.7090	78 -57.7551	79 -57.6388	80 -57.6685
81 -57.7132	82 -57.7551	83 -57.6711	84 -57.6734	85 -57.7405
86 -57.8448	87 -57.6413	88 -57.6692	89 -57.7151	90 -57.7201
91 -57.6759	92 -57.6736	93 -57.7451	94 -57.7634	95 -57.6396
96 -57.6674	97 -57.6988	98 -57.6937	99 -57.6731	100 -57.6724
101 -57.7109	102 -57.6892	103 -57.6626	104 -57.6334	105 -57.6489
106 -57.2940	107 -57.3906	108 -57.6336	109 -57.6012	110 -57.6615
111 -57.6333	112 -57.6455	113 -57.3134	114 -57.3963	115 -57.6328
116 -57.6031	117 -57.6608	118 -57.6250	119 -57.7015	120 -57.6884
121 -57.3899	122 -57.6316	123 -57.7129	124 -57.6617	125 -57.6277
126 -57.8377	127 -58.3414	128 -57.3631	129 -57.6369	130 -58.1486
131 -57.6697	132 -57.6370	133 -57.8049	134 -57.4215	135 -57.3745
136 -57.6408	137 -58.0829	138 -57.6661	139 -57.6328	140 -57.6747
141 -57.3035	142 -57.3806	143 -57.6362	144 -57.6512	145 -60.8251
146 -57.3138	147 -81.2072			

E-fermi : -2.2972 XC(G=0): -2.7342 alpha+bet : -2.2521

spin component 1

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-26.8307	1.00000
2	-21.5716	1.00000
3	-21.4741	1.00000
4	-21.1030	1.00000
5	-21.0716	1.00000
6	-21.0176	1.00000
7	-20.9813	1.00000
8	-20.9794	1.00000
9	-20.8936	1.00000
10	-20.5610	1.00000
11	-20.5063	1.00000
12	-20.4141	1.00000
13	-20.4007	1.00000
14	-20.1295	1.00000
15	-19.9783	1.00000
16	-19.7065	1.00000

17	-19.6306	1.00000
18	-19.6025	1.00000
19	-19.5869	1.00000
20	-19.5312	1.00000
21	-19.5295	1.00000
22	-19.5011	1.00000
23	-19.4837	1.00000
24	-19.1150	1.00000
25	-19.0785	1.00000
26	-18.9810	1.00000
27	-18.9674	1.00000
28	-18.9036	1.00000
29	-18.7360	1.00000
30	-18.5077	1.00000
31	-18.3621	1.00000
32	-18.2778	1.00000
33	-18.2547	1.00000
34	-18.1866	1.00000
35	-18.1845	1.00000
36	-18.0824	1.00000
37	-18.0786	1.00000
38	-17.5646	1.00000

39	-17.3159	1.00000
40	-17.2908	1.00000
41	-17.2856	1.00000
42	-17.2125	1.00000
43	-17.2061	1.00000
44	-17.1798	1.00000
45	-17.0258	1.00000
46	-16.9532	1.00000
47	-16.9355	1.00000
48	-16.8958	1.00000
49	-16.8940	1.00000
50	-16.8527	1.00000
51	-16.8444	1.00000
52	-16.8244	1.00000
53	-16.8218	1.00000
54	-16.7319	1.00000
55	-16.7288	1.00000
56	-16.1806	1.00000
57	-15.7322	1.00000
58	-15.6947	1.00000
59	-15.6632	1.00000
60	-15.6403	1.00000

61	-15.6187	1.00000
62	-15.5563	1.00000
63	-15.5523	1.00000
64	-15.1785	1.00000
65	-14.8121	1.00000
66	-14.6116	1.00000
67	-14.5805	1.00000
68	-14.5374	1.00000
69	-14.5009	1.00000
70	-14.4713	1.00000
71	-14.4455	1.00000
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spin component 2

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231	-5.6254	1.00000
232	-5.5465	1.00000
233	-5.5257	1.00000
234	-5.4438	1.00000
235	-5.4144	1.00000

236	-5.1450	1.00000
237	-5.0625	1.00000
238	-5.0287	1.00000
239	-5.0250	1.00000
240	-4.9622	1.00000
241	-4.8802	1.00000
242	-4.8569	1.00000
243	-4.8056	1.00000
244	-4.7804	1.00000
245	-4.6523	1.00000
246	-4.5813	1.00000
247	-4.5782	1.00000
248	-4.4784	1.00000
249	-4.4237	1.00000
250	-4.3976	1.00000
251	-4.2989	1.00000
252	-4.2298	1.00000
253	-4.1777	1.00000
254	-3.5382	1.00000
255	-3.3117	1.00000
256	-3.1454	1.00000
257	-2.9464	1.00000

258	-2.8018	1.00000
259	-2.7430	1.00000
260	-2.0636	0.00000
261	-1.9167	0.00000
262	-1.7256	0.00000
263	-1.6821	0.00000
264	-1.3177	0.00000
265	-1.2865	0.00000
266	-1.1648	0.00000
267	-0.7293	0.00000
268	-0.5865	0.00000
269	-0.5135	0.00000
270	-0.2832	0.00000
271	-0.2802	0.00000
272	-0.2625	0.00000
273	-0.1592	0.00000
274	-0.0610	0.00000
275	-0.0511	0.00000
276	0.0105	0.00000
277	0.0376	0.00000
278	0.0759	0.00000
279	0.2058	0.00000

280	0.2532	0.00000
281	0.2772	0.00000
282	0.4315	0.00000
283	0.4491	0.00000
284	0.4807	0.00000
285	0.6015	0.00000
286	0.6873	0.00000
287	0.8211	0.00000
288	0.8781	0.00000
289	1.0558	0.00000
290	1.1035	0.00000
291	1.1388	0.00000
292	1.1747	0.00000
293	1.2311	0.00000
294	1.2494	0.00000
295	1.3073	0.00000
296	1.3189	0.00000
297	1.3589	0.00000
298	1.4289	0.00000
299	1.4769	0.00000
300	1.4997	0.00000
301	1.5759	0.00000

302	1.6018	0.00000
303	1.6482	0.00000
304	1.6854	0.00000
305	1.7571	0.00000
306	1.7719	0.00000
307	1.8767	0.00000
308	1.8971	0.00000
309	1.9058	0.00000
310	1.9174	0.00000
311	2.1404	0.00000
312	2.1989	0.00000
313	2.2188	0.00000
314	2.2511	0.00000
315	2.2881	0.00000
316	2.2959	0.00000
317	2.3363	0.00000
318	2.3599	0.00000
319	2.3814	0.00000
320	2.4063	0.00000
321	2.4256	0.00000
322	2.4344	0.00000
323	2.4454	0.00000

324	2.4579	0.00000
325	2.4662	0.00000
326	2.5286	0.00000
327	2.5459	0.00000
328	2.7056	0.00000
329	2.7348	0.00000
330	2.7521	0.00000
331	2.7584	0.00000
332	2.7737	0.00000
333	2.8253	0.00000
334	2.8450	0.00000
335	2.8726	0.00000
336	2.9020	0.00000
337	2.9317	0.00000
338	2.9545	0.00000
339	2.9827	0.00000
340	3.0059	0.00000
341	3.0372	0.00000
342	3.0490	0.00000
343	3.0714	0.00000
344	3.0915	0.00000
345	3.1530	0.00000

346	3.1699	0.00000
347	3.1879	0.00000
348	3.2001	0.00000
349	3.3075	0.00000
350	3.3282	0.00000
351	3.3613	0.00000
352	3.3717	0.00000
353	3.3927	0.00000
354	3.4398	0.00000
355	3.4818	0.00000
356	3.4904	0.00000
357	3.4923	0.00000
358	3.5029	0.00000
359	3.6398	0.00000
360	3.6767	0.00000
361	3.6998	0.00000
362	3.7381	0.00000
363	3.7534	0.00000
364	3.7595	0.00000
365	3.7766	0.00000
366	3.7973	0.00000
367	3.8134	0.00000

368	3.8398	0.00000
369	3.8466	0.00000
370	3.8649	0.00000
371	3.8792	0.00000
372	3.8919	0.00000
373	3.9200	0.00000
374	3.9344	0.00000
375	3.9471	0.00000
376	3.9588	0.00000
377	3.9827	0.00000
378	3.9869	0.00000
379	4.0215	0.00000
380	4.0774	0.00000
381	4.1710	0.00000
382	4.2595	0.00000
383	4.2621	0.00000
384	4.2695	0.00000
385	4.2931	0.00000
386	4.3217	0.00000
387	4.3348	0.00000
388	4.3505	0.00000
389	4.3802	0.00000

390	4.3849	0.00000
391	4.4232	0.00000
392	4.4487	0.00000
393	4.4747	0.00000
394	4.4832	0.00000
395	4.4919	0.00000
396	4.4995	0.00000
397	4.5216	0.00000
398	4.5545	0.00000
399	4.5925	0.00000
400	4.6106	0.00000
401	4.6282	0.00000
402	4.6459	0.00000
403	4.6595	0.00000
404	4.6849	0.00000
405	4.7082	0.00000
406	4.7367	0.00000
407	4.7512	0.00000
408	4.7705	0.00000
409	4.7859	0.00000
410	4.7884	0.00000
411	4.8024	0.00000

412	4.8332	0.00000
413	4.8671	0.00000
414	4.8843	0.00000
415	4.9023	0.00000
416	4.9420	0.00000
417	4.9929	0.00000
418	5.0094	0.00000
419	5.0127	0.00000
420	5.0378	0.00000
421	5.0440	0.00000
422	5.0678	0.00000
423	5.0857	0.00000
424	5.1181	0.00000
425	5.1212	0.00000
426	5.1409	0.00000
427	5.1441	0.00000
428	5.1691	0.00000
429	5.1793	0.00000
430	5.1882	0.00000
431	5.1929	0.00000
432	5.2221	0.00000
433	5.2369	0.00000

434	5.2452	0.00000
435	5.2616	0.00000
436	5.2970	0.00000
437	5.3017	0.00000
438	5.3113	0.00000
439	5.3359	0.00000
440	5.3525	0.00000
441	5.3702	0.00000
442	5.3800	0.00000
443	5.3940	0.00000
444	5.4289	0.00000
445	5.4591	0.00000
446	5.4684	0.00000
447	5.4866	0.00000
448	5.4990	0.00000
449	5.5238	0.00000
450	5.5670	0.00000
451	5.5722	0.00000
452	5.5936	0.00000
453	5.6077	0.00000
454	5.6233	0.00000
455	5.6691	0.00000

456	5.6909	0.00000
457	5.7180	0.00000
458	5.7271	0.00000
459	5.7484	0.00000
460	5.7626	0.00000
461	5.7889	0.00000
462	5.7914	0.00000
463	5.7971	0.00000
464	5.8035	0.00000
465	5.8197	0.00000
466	5.8253	0.00000
467	5.8540	0.00000
468	5.8610	0.00000
469	5.8801	0.00000
470	5.8853	0.00000
471	5.8897	0.00000
472	5.9060	0.00000
473	5.9203	0.00000
474	5.9468	0.00000
475	5.9514	0.00000
476	5.9690	0.00000
477	5.9755	0.00000

478 5.9883 0.00000

479 6.0092 0.00000

480 6.0414 0.00000

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soft charge-density along one line, spin component 1

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

soft charge-density along one line, spin component 2

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

pseudopotential strength for first ion, spin component: 1

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

pseudopotential strength for first ion, spin component: 2

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

total augmentation occupancy for first ion, spin component: 1

3.579 -0.646 0.444 -0.034 -0.000

-0.646 0.130 -0.082 0.006 0.000

0.444 -0.082 0.056 -0.003 -0.000

-0.034 0.006 -0.003 0.011 0.000

-0.000 0.000 -0.000 0.000 0.007

total augmentation occupancy for first ion, spin component: 2

-0.000 0.000 -0.000 0.000 0.000

0.000 -0.000 0.000 -0.000 -0.000

-0.000 0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

0.000 -0.000 -0.000 -0.000 -0.000

---------- aborting loop because EDIFF is reached ----------

total charge

# of ion	s	p	d	tot
1	0.646	0.043	0.000	0.690
2	0.646	0.043	0.000	0.690
3	0.646	0.043	0.000	0.690
4	0.646	0.043	0.000	0.690
5	0.646	0.043	0.000	0.690
6	0.646	0.043	0.000	0.690
7	0.646	0.043	0.000	0.690
8	0.646	0.043	0.000	0.690
9	0.646	0.043	0.000	0.690
10	0.646	0.043	0.000	0.690
11	0.646	0.043	0.000	0.690
12	0.646	0.043	0.000	0.690

13	0.646	0.043	0.000	0.689
14	0.646	0.043	0.000	0.689
15	0.648	0.045	0.000	0.693
16	0.646	0.043	0.000	0.689
17	0.646	0.043	0.000	0.689
18	0.646	0.043	0.000	0.689
19	0.646	0.043	0.000	0.689
20	0.646	0.043	0.000	0.689
21	0.646	0.043	0.000	0.689
22	0.646	0.044	0.000	0.690
23	0.542	0.015	0.000	0.557
24	0.541	0.015	0.000	0.556
25	0.870	1.763	0.000	2.633
26	0.867	1.785	0.000	2.653
27	0.867	1.786	0.000	2.653
28	0.870	1.762	0.000	2.632
29	0.865	1.783	0.000	2.648
30	0.870	1.763	0.000	2.633
31	0.867	1.786	0.000	2.653
32	0.867	1.786	0.000	2.653
33	0.870	1.762	0.000	2.632
34	0.865	1.783	0.000	2.648

35	0.870	1.763	0.000	2.633
36	0.868	1.787	0.000	2.654
37	0.867	1.786	0.000	2.653
38	0.870	1.763	0.000	2.633
39	0.865	1.784	0.000	2.649
40	0.870	1.763	0.000	2.633
41	0.868	1.787	0.000	2.655
42	0.867	1.786	0.000	2.653
43	0.871	1.764	0.000	2.634
44	0.865	1.783	0.000	2.648
45	0.870	1.763	0.000	2.633
46	0.867	1.786	0.000	2.653
47	0.867	1.786	0.000	2.653
48	0.871	1.763	0.000	2.634
49	0.865	1.783	0.000	2.648
50	0.870	1.763	0.000	2.633
51	0.867	1.786	0.000	2.653
52	0.867	1.786	0.000	2.653
53	0.870	1.762	0.000	2.632
54	0.865	1.784	0.000	2.648
55	0.865	1.784	0.000	2.649
56	0.865	1.786	0.000	2.651

57	0.866	1.787	0.000	2.653
58	0.866	1.790	0.000	2.656
59	0.865	1.786	0.000	2.651
60	0.866	1.786	0.000	2.651
61	0.866	1.788	0.000	2.654
62	0.867	1.791	0.000	2.658
63	0.865	1.784	0.000	2.649
64	0.865	1.786	0.000	2.651
65	0.866	1.787	0.000	2.652
66	0.865	1.788	0.000	2.653
67	0.865	1.786	0.000	2.651
68	0.866	1.785	0.000	2.651
69	0.865	1.787	0.000	2.652
70	0.866	1.787	0.000	2.653
71	0.865	1.784	0.000	2.649
72	0.865	1.786	0.000	2.651
73	0.866	1.786	0.000	2.652
74	0.864	1.785	0.000	2.649
75	0.865	1.786	0.000	2.651
76	0.866	1.786	0.000	2.651
77	0.865	1.786	0.000	2.651
78	0.865	1.784	0.000	2.649

79	0.865	1.784	0.000	2.649
80	0.865	1.786	0.000	2.651
81	0.865	1.785	0.000	2.650
82	0.863	1.782	0.000	2.645
83	0.865	1.786	0.000	2.651
84	0.866	1.786	0.000	2.651
85	0.865	1.784	0.000	2.648
86	0.862	1.774	0.000	2.636
87	0.865	1.784	0.000	2.649
88	0.865	1.787	0.000	2.652
89	0.865	1.785	0.000	2.650
90	0.865	1.788	0.000	2.653
91	0.865	1.786	0.000	2.651
92	0.866	1.786	0.000	2.651
93	0.864	1.783	0.000	2.647
94	0.866	1.785	0.000	2.651
95	0.865	1.784	0.000	2.649
96	0.865	1.786	0.000	2.651
97	0.866	1.787	0.000	2.653
98	0.866	1.789	0.000	2.655
99	0.865	1.786	0.000	2.651
100	0.866	1.786	0.000	2.651

101	0.865	1.787	0.000	2.652
102	0.867	1.790	0.000	2.657
103	0.865	1.786	0.000	2.651
104	0.867	1.785	0.000	2.653
105	0.866	1.786	0.000	2.652
106	0.870	1.778	0.000	2.648
107	0.869	1.765	0.000	2.635
108	0.865	1.783	0.000	2.648
109	0.869	1.789	0.000	2.658
110	0.865	1.786	0.000	2.651
111	0.867	1.785	0.000	2.653
112	0.867	1.789	0.000	2.655
113	0.871	1.782	0.000	2.653
114	0.869	1.765	0.000	2.634
115	0.865	1.783	0.000	2.648
116	0.870	1.791	0.000	2.661
117	0.865	1.786	0.000	2.651
118	0.867	1.786	0.000	2.653
119	0.865	1.782	0.000	2.647
120	0.858	1.707	0.000	2.564
121	0.869	1.765	0.000	2.634
122	0.865	1.783	0.000	2.648

123	0.866	1.778	0.000	2.644
124	0.866	1.786	0.000	2.652
125	0.868	1.785	0.000	2.653
126	0.862	1.776	0.000	2.638
127	0.849	1.830	0.000	2.679
128	0.870	1.767	0.000	2.637
129	0.865	1.783	0.000	2.648
130	0.860	1.757	0.000	2.617
131	0.866	1.786	0.000	2.652
132	0.867	1.784	0.000	2.652
133	0.864	1.787	0.000	2.651
134	0.869	1.789	0.000	2.659
135	0.869	1.767	0.000	2.636
136	0.865	1.783	0.000	2.648
137	0.866	1.772	0.000	2.638
138	0.866	1.786	0.000	2.652
139	0.867	1.785	0.000	2.652
140	0.866	1.788	0.000	2.654
141	0.870	1.779	0.000	2.649
142	0.869	1.766	0.000	2.635
143	0.865	1.783	0.000	2.648
144	0.869	1.790	0.000	2.659

145	0.938	1.707	0.000	2.645
146	1.240	1.546	0.074	2.860
147	1.632	3.514	0.000	5.146
tot	123.057	221.523	0.074	344.655

magnetization (x)

# of ion	s	p	d	tot
1	0.000	-0.000	0.000	0.000
2	-0.000	0.000	0.000	-0.000
3	0.000	-0.000	0.000	0.000
4	-0.000	0.000	0.000	-0.000
5	0.000	-0.000	0.000	0.000
6	-0.000	0.000	0.000	-0.000
7	0.000	-0.000	0.000	0.000
8	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	0.000
10	-0.000	0.000	0.000	-0.000

11	0.000	-0.000	0.000	0.000
12	-0.000	0.000	0.000	-0.000
13	0.000	-0.000	0.000	0.000
14	-0.004	0.002	0.000	-0.002
15	0.000	-0.000	0.000	0.000
16	-0.004	0.002	0.000	-0.002
17	-0.004	0.002	0.000	-0.002
18	0.000	-0.000	0.000	0.000
19	-0.003	0.001	0.000	-0.002
20	0.000	-0.000	0.000	0.000
21	-0.003	0.002	0.000	-0.002
22	-0.003	0.002	0.000	-0.002
23	-0.000	0.000	0.000	-0.000
24	-0.000	0.000	0.000	-0.000
25	-0.000	-0.007	0.000	-0.008
26	-0.000	-0.002	0.000	-0.002
27	0.000	0.003	0.000	0.003
28	0.000	0.005	0.000	0.005
29	0.000	0.003	0.000	0.003
30	-0.000	-0.007	0.000	-0.008
31	-0.000	-0.002	0.000	-0.002
32	0.000	0.003	0.000	0.003

33	0.000	0.005	0.000	0.005
34	0.000	0.002	0.000	0.002
35	-0.000	-0.007	0.000	-0.008
36	-0.000	-0.002	0.000	-0.002
37	0.000	0.003	0.000	0.003
38	0.000	0.006	0.000	0.007
39	0.000	0.002	0.000	0.002
40	-0.000	-0.007	0.000	-0.008
41	-0.000	-0.002	0.000	-0.002
42	0.000	0.002	0.000	0.003
43	0.000	0.005	0.000	0.006
44	0.000	0.004	0.000	0.004
45	-0.000	-0.007	0.000	-0.008
46	-0.000	-0.002	0.000	-0.002
47	0.000	0.003	0.000	0.003
48	0.000	0.005	0.000	0.006
49	0.000	0.001	0.000	0.002
50	-0.000	-0.007	0.000	-0.008
51	-0.000	-0.002	0.000	-0.002
52	0.000	0.002	0.000	0.003
53	0.000	0.006	0.000	0.007
54	0.000	0.002	0.000	0.002

55	-0.000	-0.005	0.000	-0.006
56	-0.000	-0.007	0.000	-0.007
57	-0.000	-0.001	0.000	-0.001
58	-0.000	-0.001	0.000	-0.001
59	0.000	0.006	0.000	0.007
60	0.000	0.003	0.000	0.003
61	0.000	0.001	0.000	0.001
62	0.000	0.003	0.000	0.003
63	-0.000	-0.005	0.000	-0.006
64	-0.000	-0.007	0.000	-0.007
65	-0.000	-0.001	0.000	-0.001
66	-0.000	-0.001	0.000	-0.001
67	0.000	0.006	0.000	0.006
68	0.000	0.003	0.000	0.003
69	0.000	0.001	0.000	0.001
70	0.000	0.002	0.000	0.002
71	-0.000	-0.005	0.000	-0.006
72	-0.000	-0.007	0.000	-0.007
73	-0.000	-0.001	0.000	-0.001
74	-0.000	-0.002	0.000	-0.002
75	0.000	0.006	0.000	0.007
76	0.000	0.003	0.000	0.004

77	0.000	0.003	0.000	0.003
78	0.000	0.001	0.000	0.001
79	-0.000	-0.005	0.000	-0.006
80	-0.000	-0.007	0.000	-0.007
81	-0.000	-0.001	0.000	-0.002
82	-0.000	-0.002	0.000	-0.002
83	0.001	0.007	0.000	0.008
84	0.000	0.003	0.000	0.003
85	0.000	0.002	0.000	0.002
86	0.000	0.005	0.000	0.006
87	-0.000	-0.005	0.000	-0.005
88	-0.000	-0.007	0.000	-0.007
89	-0.000	-0.001	0.000	-0.002
90	-0.000	-0.002	0.000	-0.002
91	0.001	0.008	0.000	0.008
92	0.000	0.003	0.000	0.003
93	0.000	0.002	0.000	0.003
94	0.000	0.001	0.000	0.001
95	-0.000	-0.005	0.000	-0.006
96	-0.000	-0.007	0.000	-0.007
97	-0.000	-0.001	0.000	-0.001
98	-0.000	-0.001	0.000	-0.001

99	0.001	0.007	0.000	0.007
100	0.000	0.003	0.000	0.004
101	0.000	0.003	0.000	0.003
102	0.000	0.002	0.000	0.002
103	-0.001	-0.010	0.000	-0.011
104	-0.003	-0.028	0.000	-0.031
105	-0.000	-0.001	0.000	-0.002
106	-0.000	-0.004	0.000	-0.005
107	0.007	0.116	0.000	0.122
108	0.001	0.010	0.000	0.011
109	0.000	0.001	0.000	0.001
110	-0.001	-0.010	0.000	-0.011
111	-0.003	-0.028	0.000	-0.031
112	-0.000	-0.001	0.000	-0.002
113	-0.000	-0.003	0.000	-0.004
114	0.007	0.120	0.000	0.127
115	0.001	0.010	0.000	0.011
116	0.000	0.001	0.000	0.002
117	-0.001	-0.010	0.000	-0.011
118	-0.003	-0.026	0.000	-0.029
119	-0.000	-0.002	0.000	-0.002
120	-0.000	-0.002	0.000	-0.002

121	0.007	0.115	0.000	0.122
122	0.001	0.010	0.000	0.010
123	0.000	0.003	0.000	0.003
124	-0.001	-0.010	0.000	-0.011
125	-0.003	-0.024	0.000	-0.027
126	-0.000	-0.002	0.000	-0.002
127	-0.000	0.001	0.000	0.001
128	0.006	0.105	0.000	0.111
129	0.001	0.009	0.000	0.010
130	0.000	0.004	0.000	0.004
131	-0.001	-0.009	0.000	-0.010
132	-0.003	-0.024	0.000	-0.027
133	-0.000	-0.002	0.000	-0.002
134	-0.000	-0.002	0.000	-0.002
135	0.006	0.097	0.000	0.102
136	0.001	0.009	0.000	0.010
137	0.000	0.004	0.000	0.005
138	-0.001	-0.010	0.000	-0.011
139	-0.003	-0.026	0.000	-0.029
140	-0.000	-0.002	0.000	-0.002
141	-0.000	-0.003	0.000	-0.004
142	0.006	0.105	0.000	0.111

143	0.001	0.010	0.000	0.010
144	0.000	0.002	0.000	0.003
145	0.000	0.005	0.000	0.006
146	-0.000	0.000	-0.000	0.000
147	0.000	0.004	0.000	0.004

---

tot	0.001	0.513	-0.000	0.514

CHARGE: cpu time 0.5240: real time 0.5257

FORLOC: cpu time 0.0201: real time 0.0201

FORNL : cpu time 2.0621: real time 2.0695

STRESS: cpu time 6.1906: real time 6.2234

FORCOR: cpu time 0.1444: real time 0.1467

FORHAR: cpu time 0.0332: real time 0.0332

MIXING: cpu time 0.0109: real time 0.0109

OFIELD: cpu time 0.0001: real time 0.0001

DFTD3 V3.0 Rev 1

Edisp (eV) -6.61762

E6 (eV) : -3.9313

E8 (eV) : -2.6864

% E8 : 40.59

FORVDW: cpu time 1.8462: real time 1.8740

FORCE on cell =-STRESS in cart. coord. units (eV):

Direction	XX	YY	ZZ	XY	YZ	ZX
Alpha Z	233.50077	233.50077	233.50077			
Ewald	107573.96915	23465.01840	-39717.09885	9.24782	3455.95470	128.35758
Hartree	106090.43772	25023.78292	-23786.10531	-6.78414	2948.89587	93.17815
E(xc)	-1914.17382	-1916.53750	-1979.82649	0.13016	1.82426	0.13045
Local	**********	-53938.08770	56997.24171	0.79545	-6363.11138	-218.13863
n-local	-472.57980	-482.30124	-439.47598	-0.66641	-0.64403	-0.31312
augment	-38.29967	-38.56659	-34.32470	0.01357	-0.97993	0.00008
Kinetic	7634.81071	7638.77469	8713.33513	-3.06305	-41.83229	-3.22353
Fock	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
vdW	-2.64272	-1.49191	-6.59373	0.00135	-0.07445	0.01110
Total	-17.77497	-15.90815	-19.34745	-0.32523	0.03276	0.00209
in kB	-4.90155	-4.38676	-5.33517	-0.08968	0.00903	0.00058

external pressure = -4.87 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

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energy-cutoff : 400.00

volume of cell : 5810.14

direct lattice vectors			reciprocal lattice vectors		
14.780600000	0.000000000	0.000000000	0.067656252	0.000000000	0.000000000
0.000000000	21.333900000	0.000000000	0.000000000	0.046873755	0.000000000
0.000000000	0.000000000	18.425700000	0.000000000	0.000000000	0.054272022

length of vectors

14.780600000	21.333900000	18.425700000	0.067656252	0.046873755	0.054272022

FORCES acting on ions

electron-ion (+dipol)			ewald-force			non-local-force			convergence-correction
0.474E-02	0.154E+03	0.361E+02	-.324E-02	-.160E+03	-.357E+02	-.180E-02	0.566E+01	-.438E+00	0.203E-07 -.442E-06 -.639E-06
-.184E-01	0.155E+03	-.340E+02	0.160E-01	-.160E+03	0.335E+02	0.116E-02	0.565E+01		

0.541E+00 0.804E-06 0.275E-06 0.267E-06

0.184E+00 0.154E+03 0.360E+02 -.184E+00 -.160E+03 -.356E+02 0.690E-05 0.565E+01 -.443E+00 0.205E-06 -.652E-06 -.359E-06

0.112E+00 0.155E+03 -.341E+02 -.987E-01 -.160E+03 0.336E+02 -.175E-01 0.565E+01 0.535E+00 -.457E-09 -.698E-07 0.494E-06

0.171E+00 0.154E+03 0.362E+02 -.173E+00 -.160E+03 -.357E+02 0.116E-02 0.566E+01 -.440E+00 0.252E-06 -.639E-06 -.777E-06

0.126E+00 0.154E+03 -.340E+02 -.108E+00 -.160E+03 0.334E+02 -.211E-01 0.565E+01 0.541E+00 -.745E-06 -.137E-07 -.302E-06

-.194E-01 0.154E+03 0.363E+02 0.183E-01 -.160E+03 -.359E+02 0.159E-02 0.566E+01 -.431E+00 0.529E-07 -.477E-06 -.146E-05

-.130E-01 0.154E+03 -.338E+02 0.198E-01 -.160E+03 0.332E+02 -.721E-02 0.565E+01 0.555E+00 -.688E-06 0.561E-06 -.132E-05

-.182E+00 0.154E+03 0.363E+02 0.182E+00 -.160E+03 -.359E+02 0.257E-03 0.566E+01 -.429E+00 -.248E-06 -.340E-06 -.174E-05

-.128E+00 0.155E+03 -.337E+02 0.115E+00 -.160E+03 0.331E+02 0.109E-01 0.565E+01 0.561E+00 -.353E-07 0.793E-06 -.153E-05

-.174E+00 0.154E+03 0.362E+02 0.175E+00 -.160E+03 -.358E+02 -.176E-02 0.566E+01 -.432E+00 -.279E-06 -.270E-06 -.132E-05

-.115E+00 0.155E+03 -.338E+02 0.956E-01 -.160E+03 0.332E+02 0.192E-01 0.565E+01 0.555E+00 0.679E-06 0.762E-06 -.762E-06

0.228E+01 -.150E+03 -.386E+02 -.227E+01 0.156E+03 0.386E+02 -.103E-01 -.566E+01

0.766E-01 -.491E-06 0.307E-06 -.154E-06

-.412E+00 -.151E+03 0.388E+02 0.413E+00 0.157E+03 -.386E+02 -.127E-02 -.567E+01 -.269E+00 0.172E-06 0.547E-06 -.844E-07

0.136E+02 -.146E+03 -.413E+02 -.138E+02 0.151E+03 0.413E+02 0.257E+00 -.567E+01 -.348E-01 -.754E-07 0.169E-06 0.100E-06

0.162E+01 -.151E+03 0.402E+02 -.162E+01 0.156E+03 -.399E+02 -.101E-02 -.567E+01 -.229E+00 -.305E-06 0.273E-06 -.834E-06

0.352E+01 -.149E+03 0.443E+02 -.352E+01 0.155E+03 -.441E+02 -.204E-02 -.567E+01 -.180E+00 -.540E-06 0.228E-06 -.601E-06

-.148E+02 -.146E+03 -.330E+02 0.149E+02 0.151E+03 0.329E+02 -.950E-01 -.566E+01 0.476E-01 0.519E-06 0.451E-06 -.721E-06

-.297E+01 -.149E+03 0.432E+02 0.296E+01 0.155E+03 -.430E+02 0.115E-01 -.567E+01 -.241E+00 0.294E-06 0.463E-06 0.855E-06

-.379E+01 -.150E+03 -.385E+02 0.379E+01 0.156E+03 0.385E+02 -.610E-02 -.566E+01 0.239E-01 0.137E-06 0.647E-06 -.350E-06

-.207E+01 -.151E+03 0.395E+02 0.207E+01 0.156E+03 -.392E+02 0.153E-02 -.566E+01 -.282E+00 0.555E-06 0.692E-06 0.674E-06

-.444E-02 -.148E+03 0.486E+02 0.120E-01 0.154E+03 -.484E+02 -.551E-02 -.570E+01 -.158E+00 -.223E-06 0.316E-06 0.408E-06

0.196E+02 -.103E+03 0.222E+02 -.212E+02 0.103E+03 -.246E+02 0.153E+01 0.138E+00 0.238E+01 0.309E-06 0.868E-06 -.393E-06

-.192E+02 -.103E+03 0.153E+02 0.216E+02 0.103E+03 -.168E+02 -.241E+01 -.119E+00

0.151E+01 -.127E-06 0.130E-05 -.800E-06

0.717E-01 0.461E+03 0.202E+03 -.749E-01 -.462E+03 -.201E+03 0.384E-02 0.102E+01 -.219E+00 -.417E-06 -.169E-06 -.123E-05

0.212E+00 0.353E+03 -.234E+03 -.212E+00 -.353E+03 0.234E+03 0.260E-02 0.443E+00 -.371E-01 0.875E-06 0.732E-07 0.306E-05

-.243E-01 0.351E+03 0.240E+03 0.229E-01 -.351E+03 -.241E+03 0.316E-02 0.408E+00 0.565E-01 -.106E-05 0.111E-05 -.181E-05

-.173E+00 0.462E+03 -.195E+03 0.179E+00 -.463E+03 0.195E+03 -.662E-02 0.105E+01 0.233E+00 0.219E-05 0.102E-05 0.216E-05

-.622E-01 0.210E+03 -.272E+03 0.662E-01 -.210E+03 0.272E+03 -.448E-02 0.941E-01 0.560E-01 0.321E-06 -.506E-06 0.205E-05

0.562E+00 0.461E+03 0.202E+03 -.564E+00 -.462E+03 -.201E+03 0.201E-02 0.102E+01 -.214E+00 0.643E-06 -.800E-06 -.346E-06

0.106E+01 0.352E+03 -.234E+03 -.107E+01 -.353E+03 0.234E+03 0.159E-01 0.449E+00 -.425E-01 -.120E-05 0.102E-06 0.184E-05

0.413E+00 0.351E+03 0.240E+03 -.415E+00 -.351E+03 -.240E+03 0.303E-02 0.408E+00 0.492E-01 0.655E-08 0.823E-06 0.128E-07

0.578E+00 0.462E+03 -.195E+03 -.583E+00 -.463E+03 0.195E+03 0.478E-02 0.105E+01 0.235E+00 -.154E-06 -.485E-06 0.281E-05

0.689E+00 0.210E+03 -.272E+03 -.694E+00 -.210E+03 0.272E+03 0.604E-02 0.918E-01 0.616E-01 -.631E-06 -.351E-06 0.120E-05

0.425E+00 0.461E+03 0.202E+03 -.428E+00 -.462E+03 -.202E+03 0.383E-02 0.102E+01 -

.213E+00 0.136E-05 -.789E-06 -.216E-05

0.938E+00 0.352E+03 -.233E+03 -.954E+00 -.352E+03 0.233E+03 0.151E-01 0.442E+00 -.377E-01 -.134E-05 0.217E-05 -.139E-05

0.478E+00 0.351E+03 0.241E+03 -.480E+00 -.351E+03 -.241E+03 0.249E-02 0.406E+00 0.513E-01 0.112E-05 0.592E-06 -.526E-06

0.704E+00 0.462E+03 -.194E+03 -.715E+00 -.463E+03 0.194E+03 0.783E-02 0.106E+01 0.242E+00 -.216E-05 0.109E-05 -.140E-06

0.724E+00 0.210E+03 -.271E+03 -.733E+00 -.210E+03 0.271E+03 0.647E-02 0.916E-01 0.592E-01 -.489E-06 0.102E-05 -.686E-06

-.182E+00 0.461E+03 0.202E+03 0.178E+00 -.462E+03 -.202E+03 0.448E-02 0.102E+01 -.218E+00 0.539E-06 -.442E-06 -.489E-05

-.294E+00 0.352E+03 -.233E+03 0.298E+00 -.352E+03 0.233E+03 -.209E-02 0.441E+00 -.300E-01 -.100E-05 0.402E-05 -.343E-05

0.398E-01 0.351E+03 0.241E+03 -.387E-01 -.351E+03 -.241E+03 0.222E-02 0.409E+00 0.559E-01 0.121E-05 0.452E-06 -.294E-05

0.499E-01 0.462E+03 -.194E+03 -.560E-01 -.463E+03 0.194E+03 0.395E-02 0.106E+01 0.232E+00 -.194E-05 0.386E-05 -.373E-05

-.478E-01 0.210E+03 -.271E+03 0.458E-01 -.210E+03 0.271E+03 -.240E-03 0.938E-01 0.324E-01 -.580E-06 0.234E-05 -.176E-05

-.551E+00 0.461E+03 0.202E+03 0.549E+00 -.462E+03 -.202E+03 0.775E-03 0.102E+01 -.220E+00 -.827E-06 -.646E-08 -.580E-05

-.119E+01 0.352E+03 -.233E+03 0.120E+01 -.353E+03 0.233E+03 -.162E-01 0.448E+00 -

.330E-01 0.102E-05 0.386E-05 -.222E-05

-.353E+00 0.351E+03 0.241E+03 0.349E+00 -.351E+03 -.241E+03 0.207E-02 0.414E+00 0.625E-01 -.939E-07 0.623E-06 -.485E-05

-.411E+00 0.462E+03 -.194E+03 0.425E+00 -.463E+03 0.194E+03 -.115E-01 0.106E+01 0.230E+00 0.422E-07 0.521E-05 -.428E-05

-.560E+00 0.210E+03 -.271E+03 0.565E+00 -.210E+03 0.271E+03 -.935E-02 0.920E-01 0.525E-01 0.602E-06 0.214E-05 -.883E-06

-.474E+00 0.461E+03 0.202E+03 0.473E+00 -.462E+03 -.202E+03 0.308E-02 0.102E+01 -.220E+00 -.130E-05 0.172E-06 -.392E-05

-.805E+00 0.353E+03 -.234E+03 0.819E+00 -.353E+03 0.234E+03 -.149E-01 0.448E+00 -.393E-01 0.161E-05 0.218E-05 0.971E-06

-.373E+00 0.351E+03 0.241E+03 0.367E+00 -.351E+03 -.241E+03 0.979E-03 0.411E+00 0.627E-01 -.117E-05 0.994E-06 -.428E-05

-.594E+00 0.462E+03 -.194E+03 0.607E+00 -.463E+03 0.194E+03 -.170E-01 0.105E+01 0.234E+00 0.211E-05 0.393E-05 -.152E-05

-.587E+00 0.210E+03 -.272E+03 0.598E+00 -.210E+03 0.272E+03 -.102E-01 0.997E-01 0.567E-01 0.763E-06 0.853E-06 0.967E-06

-.805E-02 0.206E+03 0.279E+03 0.114E-01 -.206E+03 -.279E+03 -.360E-02 0.689E-01 -.411E-01 -.968E-06 0.136E-05 -.746E-06

0.669E+00 0.303E+02 0.296E+03 -.664E+00 -.302E+02 -.296E+03 -.468E-02 -.408E-01 0.768E-02 -.252E-06 0.153E-05 -.618E-06

-.845E+00 0.144E+03 -.282E+03 0.847E+00 -.144E+03 0.282E+03 -.319E-02 0.137E+00

0.286E-01 0.194E-06 -.159E-06 0.109E-05

0.534E+00 -.215E+02 -.285E+03 -.534E+00 0.214E+02 0.285E+03 -.791E-03 0.391E-01 0.185E-01 -.227E-06 -.538E-06 -.114E-05

0.502E+00 -.294E+02 0.293E+03 -.499E+00 0.294E+02 -.293E+03 -.553E-02 0.255E-01 -.302E-01 0.229E-06 0.739E-06 -.769E-06

0.525E+00 0.139E+03 0.289E+03 -.525E+00 -.139E+03 -.289E+03 0.179E-02 0.104E+00 -.247E-01 -.573E-06 0.161E-05 0.456E-08

-.126E+01 0.364E+02 -.287E+03 0.126E+01 -.364E+02 0.287E+03 0.239E-04 -.703E-02 0.138E-01 -.251E-06 -.494E-06 -.413E-06

0.167E+01 -.130E+03 -.271E+03 -.169E+01 0.130E+03 0.271E+03 0.106E-01 -.875E-01 0.371E-01 -.311E-06 -.450E-06 -.185E-05

0.397E+00 0.207E+03 0.280E+03 -.395E+00 -.207E+03 -.280E+03 0.703E-03 0.697E-01 -.369E-01 -.230E-06 0.160E-05 0.471E-06

0.919E+00 0.312E+02 0.296E+03 -.922E+00 -.311E+02 -.296E+03 0.223E-02 -.409E-01 0.124E-01 -.945E-07 0.154E-05 -.350E-06

0.133E+01 0.144E+03 -.282E+03 -.133E+01 -.144E+03 0.282E+03 0.502E-02 0.127E+00 0.279E-01 -.195E-06 -.699E-06 0.109E-05

0.341E+01 -.199E+02 -.285E+03 -.343E+01 0.199E+02 0.285E+03 0.134E-01 0.418E-01 0.134E-01 0.228E-06 -.710E-06 -.879E-06

0.139E+01 -.287E+02 0.294E+03 -.139E+01 0.287E+02 -.294E+03 -.349E-02 0.254E-01 -.306E-01 -.192E-06 0.143E-05 -.108E-05

0.677E+00 0.139E+03 0.290E+03 -.678E+00 -.139E+03 -.290E+03 0.605E-03 0.103E+00 -

.294E-01 0.315E-06 0.160E-05 0.412E-06

0.160E+01 0.367E+02 -.287E+03 -.159E+01 -.366E+02 0.287E+03 -.129E-01 -.200E-01 0.128E-01 -.115E-06 -.771E-06 -.517E-06

0.611E+01 -.125E+03 -.271E+03 -.613E+01 0.125E+03 0.271E+03 0.219E-01 -.889E-01 0.146E-01 0.181E-06 -.594E-06 -.103E-05

0.366E+00 0.207E+03 0.280E+03 -.371E+00 -.207E+03 -.280E+03 0.925E-04 0.686E-01 -.364E-01 0.983E-06 0.117E-05 0.149E-06

-.401E-01 0.319E+02 0.296E+03 0.314E-01 -.318E+02 -.296E+03 0.105E-01 -.361E-01 0.140E-01 0.173E-06 0.275E-06 0.713E-07

0.210E+01 0.144E+03 -.281E+03 -.211E+01 -.144E+03 0.281E+03 0.121E-01 0.121E+00 0.239E-01 -.337E-06 0.239E-06 0.684E-09

0.303E+01 -.172E+02 -.283E+03 -.305E+01 0.171E+02 0.283E+03 0.246E-01 0.885E-01 0.601E-01 0.229E-06 -.543E-06 -.578E-06

0.105E+01 -.272E+02 0.294E+03 -.105E+01 0.272E+02 -.294E+03 0.287E-02 0.244E-01 -.374E-01 -.379E-06 0.736E-06 -.387E-06

0.952E-01 0.140E+03 0.290E+03 -.968E-01 -.140E+03 -.290E+03 0.129E-02 0.107E+00 -.230E-01 0.890E-06 0.626E-06 -.273E-06

0.276E+01 0.387E+02 -.286E+03 -.277E+01 -.387E+02 0.286E+03 0.129E-02 -.102E-01 0.290E-01 0.148E-06 -.384E-06 -.562E-06

0.594E+01 -.115E+03 -.267E+03 -.610E+01 0.115E+03 0.267E+03 0.155E+00 0.364E-02 0.129E+00 0.305E-06 -.493E-06 -.437E-06

-.243E+00 0.207E+03 0.280E+03 0.241E+00 -.207E+03 -.280E+03 0.437E-02 0.719E-01 -

.385E-01 0.111E-05 0.354E-06 -.147E-05

-.115E+01 0.314E+02 0.294E+03 0.114E+01 -.314E+02 -.294E+03 0.918E-02 -.310E-01 0.560E-02 0.196E-06 -.872E-06 0.147E-06

0.594E+00 0.144E+03 -.281E+03 -.611E+00 -.144E+03 0.281E+03 0.177E-01 0.126E+00 0.437E-01 -.117E-06 0.110E-05 -.111E-05

-.940E+00 -.159E+02 -.286E+03 0.932E+00 0.158E+02 0.285E+03 0.597E-02 0.916E-01 0.799E-01 0.322E-07 -.703E-06 -.580E-06

-.647E+00 -.265E+02 0.293E+03 0.643E+00 0.265E+02 -.293E+03 0.491E-02 0.235E-01 -.269E-01 -.119E-06 -.739E-06 0.590E-06

-.535E+00 0.139E+03 0.289E+03 0.531E+00 -.139E+03 -.289E+03 0.655E-02 0.114E+00 -.212E-01 0.521E-06 -.259E-06 -.141E-05

0.776E+00 0.408E+02 -.287E+03 -.788E+00 -.408E+02 0.287E+03 0.504E-02 0.255E-02 -.192E-01 0.343E-06 0.181E-06 -.706E-06

-.461E+00 -.113E+03 -.276E+03 0.427E+00 0.113E+03 0.276E+03 0.347E-01 0.615E-01 -.269E+00 -.156E-06 0.164E-05 -.793E-06

-.572E+00 0.206E+03 0.279E+03 0.570E+00 -.206E+03 -.279E+03 0.115E-02 0.723E-01 -.454E-01 0.311E-07 -.255E-07 -.276E-05

-.782E+00 0.304E+02 0.294E+03 0.786E+00 -.304E+02 -.294E+03 -.753E-02 -.307E-01 -.122E-02 0.853E-07 -.795E-06 -.156E-06

-.123E+01 0.144E+03 -.281E+03 0.124E+01 -.145E+03 0.281E+03 -.156E-01 0.123E+00 0.504E-01 -.125E-06 0.165E-05 -.114E-05

-.365E+01 -.174E+02 -.283E+03 0.369E+01 0.173E+02 0.283E+03 -.310E-01 0.118E+00

0.580E-01 0.101E-06 -.411E-06 -.638E-06

-.130E+01 -.277E+02 0.291E+03 0.129E+01 0.277E+02 -.291E+03 -.131E-02 0.342E-01 -.217E-01 0.821E-07 -.123E-05 0.880E-06

-.347E+00 0.139E+03 0.289E+03 0.346E+00 -.139E+03 -.289E+03 0.211E-04 0.112E+00 -.145E-01 -.276E-06 -.261E-06 -.187E-05

-.828E+00 0.400E+02 -.287E+03 0.820E+00 -.400E+02 0.287E+03 0.126E-01 -.703E-02 -.184E-01 -.312E-06 0.474E-06 -.719E-06

-.785E+01 -.119E+03 -.267E+03 0.804E+01 0.119E+03 0.267E+03 -.191E+00 0.510E-02 0.338E-01 0.195E-06 -.549E-06 -.760E-06

-.408E+00 0.206E+03 0.279E+03 0.410E+00 -.206E+03 -.279E+03 -.279E-02 0.718E-01 -.463E-01 -.919E-06 0.515E-06 -.242E-05

-.609E-01 0.300E+02 0.294E+03 0.706E-01 -.299E+02 -.294E+03 -.947E-02 -.346E-01 0.138E-02 -.143E-06 0.351E-06 -.508E-06

-.206E+01 0.145E+03 -.282E+03 0.208E+01 -.145E+03 0.282E+03 -.190E-01 0.133E+00 0.256E-01 0.646E-06 0.124E-05 -.131E-07

-.256E+01 -.208E+02 -.285E+03 0.259E+01 0.208E+02 0.285E+03 -.290E-01 0.413E-01 0.317E-01 -.432E-06 -.374E-06 -.835E-06

-.549E+00 -.290E+02 0.291E+03 0.554E+00 0.290E+02 -.291E+03 -.284E-02 0.293E-01 -.249E-01 0.385E-06 -.543E-06 0.167E-06

0.602E-01 0.139E+03 0.289E+03 -.603E-01 -.139E+03 -.289E+03 -.327E-03 0.109E+00 -.207E-01 -.899E-06 0.745E-06 -.115E-05

-.289E+01 0.378E+02 -.286E+03 0.291E+01 -.377E+02 0.286E+03 -.148E-01 -.306E-02

0.208E-01 0.271E-06 -.637E-07 -.481E-06

-.513E+01 -.128E+03 -.271E+03 0.518E+01 0.128E+03 0.271E+03 -.464E-01 -.858E-01 0.375E-01 -.312E-06 -.490E-06 -.121E-05

0.405E+00 -.137E+03 0.280E+03 -.397E+00 0.137E+03 -.280E+03 -.968E-02 -.127E+00 -.154E-01 0.806E-06 0.303E-06 -.107E-05

0.194E+01 -.343E+03 0.233E+03 -.195E+01 0.344E+03 -.233E+03 0.913E-02 -.460E+00 -.543E-01 0.429E-06 0.472E-06 -.256E-05

-.252E+01 -.197E+03 -.259E+03 0.253E+01 0.197E+03 0.259E+03 -.954E-02 -.197E+00 0.367E-01 -.410E-06 0.151E-06 -.161E-05

0.691E+01 -.447E+03 -.198E+03 -.693E+01 0.448E+03 0.198E+03 0.965E-02 -.112E+01 0.875E-01 -.111E-05 -.176E-06 -.965E-06

-.451E+00 -.451E+03 0.204E+03 0.452E+00 0.452E+03 -.204E+03 -.201E-02 -.108E+01 -.112E+00 0.119E-05 0.167E-05 -.931E-06

0.172E+01 -.203E+03 0.269E+03 -.171E+01 0.203E+03 -.269E+03 -.480E-02 -.925E-01 -.317E-01 0.489E-06 0.538E-06 -.222E-05

-.210E+01 -.338E+03 -.222E+03 0.214E+01 0.338E+03 0.222E+03 -.444E-01 -.604E+00 0.536E-01 -.212E-06 0.638E-06 -.107E-05

0.219E+01 -.136E+03 0.282E+03 -.218E+01 0.136E+03 -.282E+03 -.638E-02 -.126E+00 -.920E-02 -.246E-06 0.811E-06 -.220E-05

0.671E+01 -.339E+03 0.238E+03 -.670E+01 0.340E+03 -.238E+03 -.128E-01 -.461E+00 -.456E-01 -.143E-05 -.156E-06 -.299E-05

0.678E+01 -.193E+03 -.258E+03 -.679E+01 0.193E+03 0.258E+03 0.112E-01 -.145E+00

0.633E-01 -.298E-06 -.538E-07 -.146E-05

0.312E+02 -.427E+03 -.198E+03 -.313E+02 0.428E+03 0.197E+03 0.725E-01 -.972E+00 0.135E+00 -.235E-06 -.920E-06 0.818E-07

0.544E+01 -.449E+03 0.209E+03 -.545E+01 0.450E+03 -.209E+03 0.549E-03 -.108E+01 -.795E-01 -.822E-06 0.825E-06 -.341E-05

0.368E+01 -.201E+03 0.272E+03 -.368E+01 0.201E+03 -.272E+03 -.771E-03 -.975E-01 -.303E-01 -.962E-06 0.232E-06 -.230E-05

0.124E+02 -.332E+03 -.223E+03 -.125E+02 0.332E+03 0.223E+03 0.121E+00 -.534E+00 0.313E-01 -.896E-06 -.313E-06 -.761E-06

0.219E+01 -.133E+03 0.283E+03 -.219E+01 0.133E+03 -.283E+03 0.506E-03 -.128E+00 -.421E-02 -.102E-05 0.776E-07 -.976E-06

0.491E+01 -.332E+03 0.245E+03 -.488E+01 0.332E+03 -.245E+03 -.320E-01 -.476E+00 -.372E-01 -.154E-05 -.785E-06 0.211E-06

0.112E+02 -.182E+03 -.258E+03 -.113E+02 0.182E+03 0.258E+03 0.475E-01 -.991E-01 -.104E+00 0.399E-06 -.664E-06 -.479E-06

0.317E+02 -.399E+03 -.175E+03 -.320E+02 0.401E+03 0.174E+03 0.300E+00 -.143E+01 0.131E+01 -.119E-05 -.232E-05 -.263E-05

0.929E+01 -.443E+03 0.219E+03 -.929E+01 0.444E+03 -.219E+03 -.578E-02 -.110E+01 -.483E-01 -.203E-05 -.827E-07 -.203E-05

0.168E+01 -.196E+03 0.273E+03 -.169E+01 0.197E+03 -.273E+03 0.549E-02 -.109E+00 -.508E-01 -.136E-05 -.812E-06 0.249E-06

0.172E+02 -.310E+03 -.216E+03 -.175E+02 0.310E+03 0.216E+03 0.326E+00 -.219E+00

0.122E+00 0.105E-05 -.862E-07 -.595E-06

-.104E+01 -.132E+03 0.281E+03 0.103E+01 0.132E+03 -.281E+03 0.103E-01 -.127E+00 0.383E-03 -.770E-06 -.103E-05 0.138E-05

-.513E+01 -.332E+03 0.239E+03 0.513E+01 0.332E+03 -.239E+03 0.890E-02 -.494E+00 -.415E-01 -.323E-06 -.816E-06 0.355E-05

0.156E+01 -.170E+03 -.261E+03 -.168E+01 0.169E+03 0.261E+03 0.119E+00 0.379E+00 -.888E-01 0.206E-05 0.196E-05 -.106E-05

-.657E+01 -.302E+03 -.189E+03 0.610E+01 0.297E+03 0.185E+03 0.477E+00 0.506E+01 0.395E+01 0.359E-06 -.828E-05 -.409E-05

-.642E+00 -.436E+03 0.227E+03 0.639E+00 0.437E+03 -.227E+03 0.171E-02 -.120E+01 -.478E-01 -.114E-05 -.319E-06 0.208E-05

-.303E+01 -.197E+03 0.268E+03 0.302E+01 0.197E+03 -.268E+03 0.146E-01 -.112E+00 -.426E-01 -.316E-06 -.145E-05 0.282E-05

0.325E+01 -.281E+03 -.215E+03 -.518E+01 0.280E+03 0.214E+03 0.192E+01 0.647E+00 0.817E+00 0.168E-05 -.498E-05 -.333E-05

-.274E+01 -.134E+03 0.277E+03 0.274E+01 0.134E+03 -.277E+03 0.249E-02 -.123E+00 -.183E-01 0.155E-06 -.147E-05 0.251E-05

-.600E+01 -.338E+03 0.230E+03 0.599E+01 0.339E+03 -.230E+03 0.113E-01 -.494E+00 -.456E-01 0.101E-05 -.277E-06 0.362E-05

-.649E+01 -.171E+03 -.257E+03 0.656E+01 0.170E+03 0.257E+03 -.789E-01 0.491E+00 0.229E-01 -.191E-05 0.181E-05 -.140E-05

-.441E+02 -.422E+03 -.184E+03 0.447E+02 0.424E+03 0.183E+03 -.563E+00 -.111E+01

0.624E+00 0.185E-05 -.828E-06 -.303E-05

-.868E+01 -.441E+03 0.211E+03 0.867E+01 0.443E+03 -.211E+03 0.144E-01 -.112E+01 -.748E-01 0.649E-06 0.280E-06 0.398E-05

-.292E+01 -.201E+03 0.265E+03 0.293E+01 0.201E+03 -.265E+03 -.915E-02 -.110E+00 -.201E-01 0.806E-06 -.127E-05 0.275E-05

-.144E+02 -.290E+03 -.209E+03 0.164E+02 0.289E+03 0.208E+03 -.198E+01 0.607E+00 0.782E+00 -.189E-05 -.398E-05 -.392E-05

-.138E+01 -.136E+03 0.277E+03 0.139E+01 0.136E+03 -.277E+03 -.102E-01 -.125E+00 -.237E-01 0.102E-05 -.852E-06 0.116E-05

-.278E+01 -.343E+03 0.230E+03 0.275E+01 0.343E+03 -.230E+03 0.235E-01 -.473E+00 -.589E-01 0.176E-05 0.444E-06 0.662E-06

-.104E+02 -.189E+03 -.258E+03 0.104E+02 0.189E+03 0.258E+03 -.774E-01 -.139E+00 -.530E-01 0.240E-06 -.324E-06 -.923E-06

-.149E+02 -.446E+03 -.196E+03 0.150E+02 0.447E+03 0.196E+03 -.695E-01 -.113E+01 0.101E+00 0.342E-06 0.817E-06 -.852E-06

-.547E+01 -.448E+03 0.204E+03 0.548E+01 0.449E+03 -.203E+03 -.481E-02 -.109E+01 -.125E+00 0.196E-05 0.158E-05 0.259E-05

-.904E+00 -.203E+03 0.267E+03 0.912E+00 0.203E+03 -.267E+03 -.909E-02 -.102E+00 -.314E-01 0.131E-05 -.300E-06 0.185E-06

-.163E+02 -.329E+03 -.218E+03 0.166E+02 0.329E+03 0.218E+03 -.360E+00 -.480E+00 0.430E-01 0.831E-07 0.465E-06 -.134E-05

-.378E+01 -.260E+03 -.193E+03 0.287E+01 0.253E+03 0.189E+03 0.969E+00 0.771E+01

0.500E+01 0.233E-05 0.152E-04 0.667E-05

0.528E+02 -.518E+03 -.137E+03 -.539E+02 0.522E+03 0.141E+03 0.106E+01 -.396E+01 -.382E+01 -.104E-05 0.475E-05 -.208E-05

-.460E+02 -.581E+03 -.447E+03 0.517E+02 0.630E+03 0.481E+03 -.576E+01 -.501E+02 -.345E+02 0.303E-05 0.313E-05 -.964E-05

0.426E+01 0.270E+02 0.226E+02 -.256E-12 -.227E-12 0.182E-11 -.430E+01 -.270E+02 -.226E+02 0.409E-05 0.540E-04 -.104E-03

POSITION			TOTAL-FORCE (eV/Angst)		
1.24575	4.02870	5.43979	0.000042	0.001038	-0.000406
1.21024	4.07581	8.43726	-0.000988	0.002654	-0.001084
3.70862	4.02890	5.43965	0.000311	0.001910	-0.001092
3.67998	4.07733	8.43690	-0.004029	-0.000377	-0.002843
6.17157	4.02854	5.43942	-0.000002	-0.000118	-0.001747
6.14482	4.08292	8.43295	-0.002826	-0.003260	-0.003126
8.63513	4.02801	5.43869	0.000782	-0.000421	-0.001996
8.60339	4.08732	8.43089	-0.000128	-0.001139	-0.002136
11.09928	4.02784	5.43885	0.000875	0.001994	-0.002705
11.06021	4.08619	8.43099	-0.001744	0.000742	-0.000566

13.56311	4.02807	5.43972	0.000331	0.001642	-0.001613
13.52141	4.08047	8.43349	0.000398	-0.002213	0.000363
2.44241	15.48073	8.85224	-0.000618	-0.005349	0.002417
0.01714	15.44624	5.32469	0.000336	0.001520	-0.001206
4.86040	15.47728	8.86623	0.001317	0.000074	-0.000238
2.48016	15.44854	5.27562	0.000370	-0.001216	-0.000526
4.94382	15.44925	5.24869	0.001821	-0.003061	0.000368
12.31531	15.48242	9.00211	-0.005930	0.001144	0.003558
9.86772	15.44556	5.34176	0.000429	-0.001152	0.000930
14.76279	15.48245	8.89951	-0.006240	-0.000606	0.005662
12.33384	15.44510	5.36128	0.001345	-0.003247	-0.001267
7.40743	15.44616	5.26463	0.002349	0.001457	0.001436
6.44846	16.34427	7.40648	-0.003873	-0.002024	0.000195
8.60064	16.47644	7.89249	0.004852	0.002679	0.006040
1.24544	5.11881	5.35500	0.000944	0.000065	-0.002392
2.44348	5.83889	8.62292	0.002422	-0.004404	0.001247
0.01380	5.79530	5.28573	0.002081	-0.002386	0.000491
1.21063	5.16420	8.54151	0.000274	-0.000510	-0.001919
2.44351	7.27931	8.74832	-0.000067	-0.001273	-0.000104
3.70866	5.11896	5.35390	-0.000426	-0.001723	0.000398
4.90800	5.84315	8.62123	-0.001055	0.003834	-0.000706
2.47701	5.79561	5.28397	0.001455	-0.000536	-0.002589

3.67679	5.16572	8.54000	-0.000129	0.001649	-0.000064
4.90764	7.28398	8.74777	0.000663	-0.000628	0.001025
6.17184	5.11860	5.35433	0.001474	0.000286	0.000962
7.37096	5.84929	8.62094	-0.000643	0.007121	-0.002425
4.94029	5.79548	5.28340	0.000611	-0.002620	-0.001155
6.14080	5.17108	8.53715	-0.002512	0.002511	0.002436
7.37071	7.28983	8.75132	-0.002038	0.001556	0.000150
8.63543	5.11820	5.35521	0.001237	0.001234	-0.000998
9.83233	5.85166	8.62337	0.002798	0.000802	-0.001074
7.40374	5.79498	5.28512	0.003470	-0.002611	-0.001317
8.60194	5.17528	8.53759	-0.001878	-0.000480	-0.000249
9.83204	7.29110	8.75719	-0.001806	-0.002740	-0.002421
11.09930	5.11814	5.35578	-0.000871	-0.003462	-0.001292
12.29449	5.84673	8.62385	0.000028	0.005783	-0.002174
9.86750	5.79468	5.28678	-0.000741	-0.000641	0.001573
11.06261	5.17409	8.53894	0.002652	0.002627	-0.000435
12.29428	7.28729	8.75533	-0.004481	0.001129	-0.001508
13.56278	5.11829	5.35605	0.002655	0.000429	-0.001917
14.75895	5.83988	8.62434	-0.000271	-0.002647	-0.002146
12.33118	5.79480	5.28692	-0.004503	-0.001391	0.002615
13.52535	5.16844	8.54022	-0.003478	0.003763	-0.001457
14.75917	7.28012	8.75179	0.000992	0.002524	-0.000702

0.01434	7.23830	5.19017	0.000079	-0.000221	0.000108
1.24689	9.38061	5.13160	0.000549	-0.001881	0.000030
1.21085	7.98059	8.79588	-0.000921	-0.000468	0.001584
2.44214	10.12243	8.87141	-0.000881	0.003580	-0.004996
0.01532	10.08686	5.14049	-0.002038	-0.000131	-0.002373
1.24606	7.94244	5.15775	0.002016	-0.002596	0.000852
1.21082	9.41592	8.85782	-0.000818	0.004255	0.000207
2.44072	11.55513	8.88414	-0.006083	-0.003086	0.001638
2.47747	7.23842	5.18585	0.002792	0.002863	0.001341
3.70997	9.38055	5.12566	-0.001093	-0.003033	0.000076
3.67534	7.98360	8.79349	-0.000602	0.001066	0.000987
4.90487	10.12925	8.87518	0.000224	-0.000038	0.000095
2.47867	10.08713	5.12695	-0.002262	0.001496	0.000790
3.70939	7.94242	5.15441	0.000833	-0.004006	-0.001676
3.67589	9.41970	8.85445	-0.001419	0.001815	-0.000137
4.90263	11.56506	8.89086	-0.000220	0.000986	0.000954
4.94085	7.23830	5.18552	-0.004708	0.002237	0.000859
6.17318	9.38002	5.13173	0.002006	0.002063	0.001863
6.13864	7.99044	8.79647	0.002528	-0.000204	-0.001673
7.36780	10.13760	8.89473	-0.000359	0.003394	0.000521
4.94196	10.08682	5.12700	0.004149	0.001481	-0.001131
6.17284	7.94199	5.15766	-0.000045	0.000564	0.003056

6.13939	9.42660	8.86164	0.000774	-0.000354	-0.002254
7.36410	11.57721	8.92935	-0.001507	-0.001768	0.004493
7.40426	7.23794	5.19012	0.002137	0.001745	0.001108
8.63700	9.37970	5.14543	-0.000553	0.002917	0.000986
8.60086	7.99568	8.80617	0.001137	-0.000328	-0.000962
9.83068	10.14286	8.92842	-0.002238	0.002991	-0.000972
7.40553	10.08627	5.14064	0.001228	-0.003555	0.003168
8.63637	7.94166	5.16555	0.002619	0.001798	-0.001382
8.60077	9.43254	8.88532	-0.005993	0.002095	-0.001233
9.82927	11.58244	9.00096	0.001122	0.002105	0.000597
9.86805	7.23787	5.19489	-0.000373	0.000087	-0.000180
11.10106	9.37979	5.15156	-0.003834	-0.001060	0.000697
11.06331	7.99411	8.80818	-0.000338	-0.001438	0.000224
12.29815	10.12943	8.90340	-0.001123	-0.000891	0.001279
9.86930	10.08593	5.15631	-0.005442	-0.001442	0.001433
11.10021	7.94175	5.16862	-0.000589	-0.003066	0.001415
11.06206	9.43062	8.88839	0.004577	0.001593	0.002108
12.30255	11.56557	8.94694	0.003994	-0.000634	0.000289
12.33169	7.23799	5.19447	-0.001034	0.000229	-0.001719
13.56437	9.38021	5.14435	0.000735	0.001622	-0.000544
13.52754	7.98555	8.80171	-0.000796	-0.002456	-0.003107
14.76233	10.12320	8.88285	-0.005198	0.001111	-0.001575

12.33257	10.08637	5.15511	0.002642	0.000550	-0.001515
13.56350	7.94214	5.16485	-0.000077	-0.000889	-0.000348
13.52731	9.42040	8.86925	-0.000131	0.003171	-0.000635
14.76430	11.55727	8.90646	-0.002300	-0.001099	0.001668
0.01611	11.52516	5.16621	-0.001079	-0.002602	0.000421
1.24770	13.67535	5.22209	0.001809	-0.002531	-0.002466
1.21217	12.26335	8.89409	0.000489	-0.000177	0.001245
2.43998	14.38728	8.86748	-0.002703	0.001790	0.000834
0.01699	14.35408	5.27295	-0.000405	-0.000409	-0.001914
1.24794	12.22963	5.17275	0.001067	0.000825	-0.001339
1.21434	13.70818	8.88771	0.002454	0.001379	0.003900
2.47958	11.52580	5.14547	-0.001612	-0.000231	-0.001447
3.71218	13.67636	5.19535	0.004718	0.000353	0.001060
3.66932	12.26248	8.88184	-0.002101	0.000149	-0.000587
4.89370	14.38589	8.86075	0.004611	-0.000078	-0.002615
2.48000	14.35596	5.23149	0.001279	-0.000925	0.001742
3.71150	12.23022	5.15602	0.000906	-0.004571	0.001037
3.66212	13.70366	8.87117	-0.005459	0.003161	-0.000483
4.94290	11.52542	5.14351	-0.000082	-0.001821	-0.001573
6.17627	13.67505	5.20032	0.000833	0.000302	0.000058
6.13145	12.27911	8.90591	0.005283	0.006493	0.004749
7.36614	14.42967	8.88203	0.001889	0.002006	0.001017

4.94347	14.35627	5.21375	0.000058	-0.001628	0.001036
6.17493	12.22917	5.16623	-0.001432	-0.001037	0.001593
6.11879	13.72336	8.87765	0.005322	-0.000938	-0.000933
7.40625	11.52413	5.16368	0.000899	-0.003427	0.000384
8.63876	13.67323	5.24377	0.001799	0.001762	-0.001320
8.58939	12.29067	9.00208	0.003018	0.001315	0.000437
9.83855	14.39048	9.30305	0.010542	0.023828	0.011970
7.40672	14.35386	5.23530	-0.001151	0.000085	-0.000729
8.63820	12.22778	5.19800	0.000322	-0.001253	0.001098
8.55571	13.73596	9.04598	-0.006941	-0.005033	-0.004440
9.86985	11.52338	5.18893	0.001736	-0.002047	-0.000080
11.10099	13.67352	5.27669	0.003244	-0.001170	-0.000965
11.07378	12.27333	9.00891	-0.006340	0.004426	-0.001442
12.30694	14.38896	9.00333	-0.002357	0.001734	0.001819
9.86934	14.35300	5.29564	0.002897	0.000388	0.000110
11.10161	12.22804	5.21650	-0.001101	-0.002726	0.001082
11.11464	13.70636	9.07877	0.008449	-0.001120	-0.007297
12.33326	11.52411	5.18815	-0.000922	0.000226	0.000562
13.56430	13.67399	5.25995	0.001525	-0.000267	0.000094
13.53626	12.26601	8.93587	-0.002328	0.004320	0.002312
14.76266	14.38906	8.90426	-0.004719	0.002418	0.003508
12.33397	14.35288	5.30710	0.002803	-0.001564	-0.001706

13.56505	12.22870	5.20105	0.000125	0.000077	-0.001114
13.54921	13.70690	8.94399	0.000062	-0.005679	0.001233
9.91126	15.53185	9.99472	0.067955	0.586669	0.455603
7.28864	16.40884	8.69813	0.003703	-0.002215	0.001549
10.02526	16.50365	10.65998	-0.070271	-0.613357	-0.454288

---

total drift:	-0.044688	0.025694	-0.026853

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

---

free energy TOTEN = -1209.38584555 eV

energy without entropy= -1209.38584555 energy(sigma->0) = -1209.38584555

d Force = 0.4547907E-02[-0.160E-01, 0.251E-01] d Energy = 0.4043418E-02 0.504E-03

d Force = 0.1679345E+02[0.167E+02, 0.169E+02] d Ewald = 0.1679265E+02 0.800E-03

POTLOK: cpu time 0.1764: real time 0.1768

---

stress matrix after NEB project (eV)

-17.77497 -0.32523 0.00209

-0.32523 -15.90815 0.03276

0.00209 0.03276 -19.34745

FORCES: max atom, RMS 0.766500 0.088213

FORCE total and by dimension 1.069530 0.613357

Stress total and by dimension 30.717366 19.347454

Finite differences progress:

Degree of freedom: 6/ 6

Displacement: 1/ 2

Total: 11/ 12

LATTYP: Found a simple orthorhombic cell.

ALAT = 14.7806000000

B/A-ratio = 1.2466138046

C/A-ratio = 1.4433717170

Lattice vectors:

A1 = (-14.7806000000, 0.0000000000, 0.0000000000)

A2 = (0.0000000000, 0.0000000000, -18.4257000000)

A3 = (0.0000000000, -21.3339000000, 0.0000000000)

Analysis of symmetry for initial positions (statically):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The static configuration has the point symmetry C_1 .

Analysis of symmetry for dynamics (positions and initial velocities):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The dynamic configuration has the point symmetry C_1 .

Analysis of constrained symmetry for selective dynamics:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The constrained configuration has the point symmetry C_1 .

Analysis of structural, dynamic, and magnetic symmetry:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The magnetic configuration has the point symmetry C_1 .

Subroutine INISYM returns: Found 1 space group operations

(whereof 1 operations are pure point group operations),

and found 1 'primitive' translations

KPOINTS: KPT-Resolved Value to Generate K-Mesh: 0

Automatic generation of k-mesh.

Space group operators:

irot	det(A)	alpha	n_x	n_y	n_z	tau_x	tau_y	tau_z
1	1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Subroutine IBZKPT returns following result:

==========

Found 1 irreducible k-points:

Following reciprocal coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

Following cartesian coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

WAVPRE: cpu time 0.1227: real time 0.1371

FEWALD: cpu time 0.0026: real time 0.0027

ORTHCH: cpu time 0.9980: real time 1.0013

LOOP+: cpu time 181.7522: real time 182.8113

---------- Iteration 13(1) ----------

POTLOK: cpu time 0.1650: real time 0.1785

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9284: real time 1.9354

RMM-DIIS: cpu time 7.1161: real time 7.1416

ORTHCH: cpu time 0.3539: real time 0.3550

DOS: cpu time 0.0003: real time 0.0003

CHARGE: cpu time 0.5249: real time 0.5265

MIXING: cpu time 0.0045: real time 0.0045

LOOP: cpu time 10.1031: real time 10.1519

eigenvalue-minimisations : 1928

total energy-change (2. order) :-0.2280951E-01 (-0.5169459E+00)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7385970 magnetization 0.0542874

Broyden mixing:

rms(total) = 0.36749E-01 rms(broyden)= 0.36176E-01

rms(prec) = 0.37597E-01

weight for this iteration 100.00

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107340.82083503

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.80795069

PAW double counting = 52162.76655977 -52225.67521870

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5817.13522346

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.79103707 eV

energy without entropy = -1202.79103707 energy(sigma->0) = -1202.79103707

---------- Iteration 13(2) ----------

POTLOK: cpu time 0.1648: real time 0.1699

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9247: real time 1.9319

RMM-DIIS: cpu time 7.3124: real time 7.3360

ORTHCH: cpu time 0.3534: real time 0.3545

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5253: real time 0.5271

MIXING: cpu time 0.0047: real time 0.0046

LOOP: cpu time 10.2959: real time 10.3344

eigenvalue-minimisations : 1943

total energy-change (2. order) : 0.2224865E-01 (-0.3774268E-02)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7439406 magnetization 0.0542722

Broyden mixing:

rms(total) = 0.30390E-01 rms(broyden)= 0.30353E-01

rms(prec) = 0.31688E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 0.7551

0.7551

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107341.63854682

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.81691003

PAW double counting = 52172.71634441 -52235.62927431

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5816.29995141

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76878842 eV

energy without entropy = -1202.76878842 energy(sigma->0) = -1202.76878842

---------- Iteration 13(3) ----------

POTLOK: cpu time 0.1662: real time 0.1843

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9261: real time 1.9321

RMM-DIIS: cpu time 7.0829: real time 7.1026

ORTHCH: cpu time 0.3526: real time 0.3535

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5247: real time 0.5262

MIXING: cpu time 0.0048: real time 0.0049

LOOP: cpu time 10.0677: real time 10.1142

eigenvalue-minimisations : 1926

total energy-change (2. order) : 0.1010947E-02 (-0.2040965E-03)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7413801 magnetization 0.0542751

Broyden mixing:

rms(total) = 0.16849E-01 rms(broyden)= 0.16844E-01

rms(prec) = 0.17414E-01

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3850

2.1279 0.6421

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107342.07331397

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.83870421

PAW double counting = 52177.74382866 -52240.66498885

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.87773720

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76777748 eV

energy without entropy = -1202.76777748 energy(sigma->0) = -1202.76777748

---------- Iteration 13(4) ----------

POTLOK: cpu time 0.1628: real time 0.1682

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9271: real time 1.9334

RMM-DIIS: cpu time 7.1870: real time 7.2155

ORTHCH: cpu time 0.3535: real time 0.3546

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5260: real time 0.5278

MIXING: cpu time 0.0054: real time 0.0054

LOOP: cpu time 10.1723: real time 10.2155

eigenvalue-minimisations : 1932

total energy-change (2. order) :-0.8858703E-04 (-0.2035647E-03)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7397596 magnetization 0.0542758

Broyden mixing:

rms(total) = 0.74847E-02 rms(broyden)= 0.74760E-02

rms(prec) = 0.82135E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3282

2.3186 0.8331 0.8331

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107342.93953291

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.86138850

PAW double counting = 52188.93113613 -52251.86206993

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5815.02451752

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76786606 eV

energy without entropy = -1202.76786606 energy(sigma->0) = -1202.76786606

---------- Iteration 13(5) ----------

POTLOK: cpu time 0.1687: real time 0.1737

SETDIJ: cpu time 0.0102: real time 0.0103

EDDIAG: cpu time 1.9290: real time 1.9344

RMM-DIIS: cpu time 7.0893: real time 7.1162

ORTHCH: cpu time 0.3528: real time 0.3537

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5256: real time 0.5272

MIXING: cpu time 0.0057: real time 0.0057

LOOP: cpu time 10.0817: real time 10.1216

eigenvalue-minimisations : 1913

total energy-change (2. order) : 0.1309032E-03 (-0.9830713E-05)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7405381 magnetization 0.0542717

Broyden mixing:

rms(total) = 0.24648E-02 rms(broyden)= 0.24610E-02

rms(prec) = 0.27390E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3987

2.3302 1.6396 0.8125 0.8125

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107343.07295804

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.85659030

PAW double counting = 52190.39499756 -52253.32466643

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.88742823

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76773516 eV

energy without entropy = -1202.76773516 energy(sigma->0) = -1202.76773516

---------- Iteration 13(6) ----------

POTLOK: cpu time 0.1674: real time 0.1930

SETDIJ: cpu time 0.0102: real time 0.0102

EDDIAG: cpu time 1.9260: real time 1.9325

RMM-DIIS: cpu time 6.9437: real time 6.9905

ORTHCH: cpu time 0.3541: real time 0.3552

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5256: real time 0.5274

MIXING: cpu time 0.0059: real time 0.0059

LOOP: cpu time 9.9333: real time 10.0152

eigenvalue-minimisations : 1896

total energy-change (2. order) :-0.6196409E-05 (-0.5490530E-05)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7410478 magnetization 0.0542703

Broyden mixing:

rms(total) = 0.14212E-02 rms(broyden)= 0.14157E-02

rms(prec) = 0.15801E-02

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4100

2.4873 1.8847 0.7550 0.9616 0.9616

Free energy of the ion-electron system (eV)

```
  ----------------------------------------------------

  alpha Z        PSCENC =            233.50077011

  Ewald energy   TEWEN  =          91336.43504288

  -Hartree energ DENC   =       -107343.18426981

  -exchange      EXHF   =             0.00000000

  -V(xc)+E(xc)   XCENC  =           1743.85316818

  PAW double counting   =          52191.05269600     -52253.98126648

  entropy T*S    EENTRO =             -0.00000000

  eigenvalues    EBANDS =          -5814.77379892

  atomic energy  EATOM  =          18704.32991668

  Solvation  Ediel_sol  =             0.00000000

  ----------------------------------------------------

  free energy    TOTEN  =         -1202.76774136 eV


  energy without entropy =       -1202.76774136  energy(sigma->0) =       -1202.76774136


-----------------------------------------------------------------------------------------------
```

---------- Iteration 13(7) ----------

POTLOK: cpu time 0.1659: real time 0.1815

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9258: real time 1.9325

RMM-DIIS: cpu time 6.8997: real time 6.9239

ORTHCH: cpu time 0.3528: real time 0.3539

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5251: real time 0.5268

MIXING: cpu time 0.0061: real time 0.0061

LOOP: cpu time 9.8857: real time 9.9351

eigenvalue-minimisations : 1855

total energy-change (2. order) :-0.1259329E-04 (-0.7936526E-06)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7409116 magnetization 0.0542692

Broyden mixing:

rms(total) = 0.35718E-03 rms(broyden)= 0.35693E-03

rms(prec) = 0.54343E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3500

2.5410 1.9619 1.0312 1.0312 0.8021 0.7324

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107343.29376789

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.85460588

PAW double counting = 52191.35246590 -52254.28140743

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.66538008

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76775395 eV

energy without entropy = -1202.76775395 energy(sigma->0) = -1202.76775395

---------- Iteration 13(8) ----------

POTLOK: cpu time 0.1645: real time 0.1737

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9280: real time 1.9342

RMM-DIIS: cpu time 6.1593: real time 6.1863

ORTHCH: cpu time 0.3531: real time 0.3541

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5254: real time 0.5268

MIXING: cpu time 0.0063: real time 0.0064

LOOP: cpu time 9.1470: real time 9.1919

eigenvalue-minimisations : 1682

total energy-change (2. order) :-0.1539907E-04 (-0.1631728E-06)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7408683 magnetization 0.0542690

Broyden mixing:

rms(total) = 0.22773E-03 rms(broyden)= 0.22744E-03

rms(prec) = 0.40539E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.3888

2.4539 2.4539 1.3577 1.0066 1.0066 0.7778 0.6653

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107343.36769588

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.85521855

PAW double counting = 52191.31740740 -52254.24647293

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.59195616

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76776935 eV

energy without entropy = -1202.76776935 energy(sigma->0) = -1202.76776935

---------- Iteration 13(9) ----------

POTLOK: cpu time 0.1652: real time 0.1723

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9251: real time 1.9311

RMM-DIIS: cpu time 6.0520: real time 6.0792

ORTHCH: cpu time 0.3537: real time 0.3546

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5260: real time 0.5277

MIXING: cpu time 0.0066: real time 0.0066

LOOP: cpu time 9.0390: real time 9.0821

eigenvalue-minimisations : 1627

total energy-change (2. order) :-0.2325241E-04 (-0.7171427E-07)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7408887 magnetization 0.0542689

Broyden mixing:

rms(total) = 0.11626E-03 rms(broyden)= 0.11612E-03

rms(prec) = 0.24075E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4589

2.9930 2.6377 1.6582 0.9898 0.9898 0.9838 0.7750 0.6441

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107343.47149478

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.85561782

PAW double counting = 52191.19614696 -52254.12525014

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.48854214

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76779260 eV

energy without entropy = -1202.76779260 energy(sigma->0) = -1202.76779260

---------- Iteration 13(10) ----------

POTLOK: cpu time 0.1677: real time 0.1870

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9291: real time 1.9341

RMM-DIIS: cpu time 5.9106: real time 5.9245

ORTHCH: cpu time 0.3554: real time 0.3563

DOS: cpu time 0.0005: real time 0.0005

CHARGE: cpu time 0.5255: real time 0.5269

MIXING: cpu time 0.0072: real time 0.0072

LOOP: cpu time 8.9061: real time 8.9466

eigenvalue-minimisations : 1596

total energy-change (2. order) :-0.2080721E-04 (-0.6742736E-07)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7408968 magnetization 0.0542684

Broyden mixing:

rms(total) = 0.85608E-04 rms(broyden)= 0.85505E-04

rms(prec) = 0.14853E-03

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.4868

3.5399 2.5775 1.8275 1.0583 1.0583 1.1257 0.7795 0.7795 0.6348

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107343.56108892

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.85604322

PAW double counting = 52191.12219619 -52254.05135600

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.39933757

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76781341 eV

energy without entropy = -1202.76781341 energy(sigma->0) = -1202.76781341

---------- Iteration 13(11) ----------

POTLOK: cpu time 0.1666: real time 0.1751

SETDIJ: cpu time 0.0100: real time 0.0100

EDDIAG: cpu time 1.9260: real time 1.9327

RMM-DIIS: cpu time 5.7583: real time 5.7769

ORTHCH: cpu time 0.3560: real time 0.3572

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5252: real time 0.5270

MIXING: cpu time 0.0074: real time 0.0074

LOOP: cpu time 8.7498: real time 8.7866

eigenvalue-minimisations : 1559

total energy-change (2. order) :-0.1581067E-04 (-0.4273747E-07)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7408926 magnetization 0.0542683

Broyden mixing:

rms(total) = 0.60856E-04 rms(broyden)= 0.60825E-04

rms(prec) = 0.94224E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6089

4.7295 2.5694 2.1304 1.5695 1.0049 1.0049 0.9965 0.7724 0.6889 0.6221

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107343.61562200

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.85630386

PAW double counting = 52191.10348316 -52254.03266969

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.34505423

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76782922 eV

energy without entropy = -1202.76782922 energy(sigma->0) = -1202.76782922

---------- Iteration 13(12) ----------

POTLOK: cpu time 0.1645: real time 0.1685

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9276: real time 1.9342

RMM-DIIS: cpu time 5.2182: real time 5.2384

ORTHCH: cpu time 0.3534: real time 0.3547

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5249: real time 0.5266

MIXING: cpu time 0.0078: real time 0.0078

LOOP: cpu time 8.2070: real time 8.2408

eigenvalue-minimisations : 1443

total energy-change (2. order) :-0.8936768E-05 (-0.1385461E-07)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7408960 magnetization 0.0542681

Broyden mixing:

rms(total) = 0.36893E-04 rms(broyden)= 0.36874E-04

rms(prec) = 0.59680E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.6640

5.6027 2.5978 2.2181 1.6736 1.0524 1.0524 1.1203 0.9136 0.7860 0.6712

0.6164

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107343.64325912

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.85637820

PAW double counting = 52191.09715666 -52254.02633571

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.31750786

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76783816 eV

energy without entropy = -1202.76783816 energy(sigma->0) = -1202.76783816

---------- Iteration 13(13) ----------

POTLOK: cpu time 0.1655: real time 0.1740

SETDIJ: cpu time 0.0100: real time 0.0101

EDDIAG: cpu time 1.9235: real time 1.9429

RMM-DIIS: cpu time 4.9823: real time 5.0115

ORTHCH: cpu time 0.3529: real time 0.3540

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5257: real time 0.5275

MIXING: cpu time 0.0083: real time 0.0084

LOOP: cpu time 7.9687: real time 8.0288

eigenvalue-minimisations : 1369

total energy-change (2. order) :-0.6661565E-05 (-0.6117372E-08)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7409002 magnetization 0.0542681

Broyden mixing:

rms(total) = 0.21850E-04 rms(broyden)= 0.21818E-04

rms(prec) = 0.38145E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7582

6.4859 2.8032 2.4754 1.9120 1.4388 1.0203 1.0203 1.0445 0.8094 0.8094

0.6640 0.6155

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107343.65507710

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.85637435

PAW double counting = 52191.10020984 -52254.02937476

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.30570682

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76784482 eV

energy without entropy = -1202.76784482 energy(sigma->0) = -1202.76784482

---------- Iteration 13(14) ----------

POTLOK: cpu time 0.1783: real time 0.1946

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9277: real time 1.9340

RMM-DIIS: cpu time 5.0018: real time 5.0305

ORTHCH: cpu time 0.3525: real time 0.3538

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5252: real time 0.5268

MIXING: cpu time 0.0084: real time 0.0084

LOOP: cpu time 8.0045: real time 8.0586

eigenvalue-minimisations : 1402

total energy-change (2. order) :-0.6393933E-05 (-0.6102247E-08)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7408987 magnetization 0.0542681

Broyden mixing:

rms(total) = 0.12301E-04 rms(broyden)= 0.12295E-04

rms(prec) = 0.20521E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.7638

6.9143 3.1461 2.5264 1.9883 1.3406 1.2454 1.0334 1.0334 0.8761 0.7894

0.7625 0.6573 0.6169

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107343.66329204

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.85638221

PAW double counting = 52191.10855329 -52254.03771526

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.29750909

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76785121 eV

energy without entropy = -1202.76785121 energy(sigma->0) = -1202.76785121

---------- Iteration 13(15) ----------

POTLOK: cpu time 0.1669: real time 0.1689

SETDIJ: cpu time 0.0101: real time 0.0102

EDDIAG: cpu time 1.9274: real time 1.9339

RMM-DIIS: cpu time 4.7194: real time 4.7402

ORTHCH: cpu time 0.3601: real time 0.3612

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5265: real time 0.5285

MIXING: cpu time 0.0090: real time 0.0090

LOOP: cpu time 7.7198: real time 7.7521

eigenvalue-minimisations : 1281

total energy-change (2. order) :-0.2289620E-05 (-0.1467913E-08)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7408984 magnetization 0.0542681

Broyden mixing:

rms(total) = 0.87674E-05 rms(broyden)= 0.87627E-05

rms(prec) = 0.14056E-04

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.8907

7.5068 4.0069 2.5537 2.3369 1.8061 1.5317 1.0353 1.0353 1.0291 0.8757

0.8011 0.6906 0.6186 0.6425

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107343.66474909

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.85637250

PAW double counting = 52191.10895551 -52254.03811874

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.29604335

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76785350 eV

energy without entropy = -1202.76785350 energy(sigma->0) = -1202.76785350

---------- Iteration 13(16) ----------

POTLOK: cpu time 0.1643: real time 0.1791

SETDIJ: cpu time 0.0098: real time 0.0099

EDDIAG: cpu time 1.9247: real time 1.9311

RMM-DIIS: cpu time 4.8116: real time 4.8325

ORTHCH: cpu time 0.3530: real time 0.3542

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5262: real time 0.5281

MIXING: cpu time 0.0102: real time 0.0102

LOOP: cpu time 7.8002: real time 7.8454

eigenvalue-minimisations : 1312

total energy-change (2. order) :-0.1648314E-05 (-0.1303079E-08)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7408987 magnetization 0.0542681

Broyden mixing:

rms(total) = 0.41857E-05 rms(broyden)= 0.41824E-05

rms(prec) = 0.70445E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9035

7.8643 4.5611 2.6209 2.5057 1.9104 1.3857 1.0411 1.0411 1.0176 1.0176

0.8257 0.8257 0.6841 0.6167 0.6353

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107343.66560637

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.85635697

PAW double counting = 52191.10630533 -52254.03547130

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.29516945

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76785515 eV

energy without entropy = -1202.76785515 energy(sigma->0) = -1202.76785515

---------- Iteration 13(17) ----------

POTLOK: cpu time 0.1703: real time 0.1725

SETDIJ: cpu time 0.0099: real time 0.0100

EDDIAG: cpu time 1.9386: real time 1.9448

RMM-DIIS: cpu time 4.2734: real time 4.2873

ORTHCH: cpu time 0.3553: real time 0.3564

DOS: cpu time 0.0004: real time 0.0004

CHARGE: cpu time 0.5254: real time 0.5272

MIXING: cpu time 0.0096: real time 0.0096

LOOP: cpu time 7.2829: real time 7.3081

eigenvalue-minimisations : 1046

total energy-change (2. order) :-0.3504101E-06 (-0.2954215E-09)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7408986 magnetization 0.0542681

Broyden mixing:

rms(total) = 0.27162E-05 rms(broyden)= 0.27153E-05

rms(prec) = 0.47157E-05

weight for this iteration 100.00

eigenvalues of (default mixing * dielectric matrix)

average eigenvalue GAMMA= 1.9269

8.0614 4.9591 2.7569 2.5493 1.9932 1.5107 1.5107 1.0375 1.0375 1.0540

0.8807 0.8005 0.7549 0.6781 0.6148 0.6316

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107343.66583546

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.85635561

PAW double counting = 52191.10467360 -52254.03384116

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.29493776

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76785550 eV

energy without entropy = -1202.76785550 energy(sigma->0) = -1202.76785550

---------- Iteration 13(18) ----------

POTLOK: cpu time 0.1687: real time 0.1887

SETDIJ: cpu time 0.0142: real time 0.0179

```
      EDDIAG:  cpu time        1.9315: real time        1.9379
 RMM-DIIS:  cpu time        4.2957: real time        4.3226
      ORTHCH:  cpu time        0.3528: real time        0.3540
         DOS:  cpu time        0.0004: real time        0.0004
      CHARGE:  cpu time        0.5244: real time        0.5261
      MIXING:  cpu time        0.0102: real time        0.0103
      ------------------------------------------
        LOOP:  cpu time        7.2979: real time        7.3579

eigenvalue-minimisations  :  1060
total energy-change (2. order) :-0.2259840E-06  (-0.1785141E-09)
number of electron       518.9999715 magnetization             0.9999998
augmentation part          11.7408985 magnetization             0.0542682

Broyden mixing:
 rms(total) = 0.19290E-05        rms(broyden)= 0.19281E-05
 rms(prec ) = 0.29924E-05
 weight for this iteration        100.00

eigenvalues of (default mixing * dielectric matrix)
 average eigenvalue GAMMA=      1.9717
 8.2619   5.4959   3.1894   2.5684   2.2690   1.8506   1.3872   1.0391   1.0391   1.0730
```

1.0730 0.8305 0.8305 0.6972 0.6682 0.6157 0.6296

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107343.66588577

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.85635284

PAW double counting = 52191.10401072 -52254.03317867

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.29488452

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76785573 eV

energy without entropy = -1202.76785573 energy(sigma->0) = -1202.76785573

---------- Iteration 13(19) ----------

POTLOK: cpu time 0.1643: real time 0.1725

SETDIJ: cpu time 0.0101: real time 0.0101

EDDIAG: cpu time 1.9238: real time 1.9307

RMM-DIIS: cpu time 4.1888: real time 4.2060

ORTHCH: cpu time 0.3557: real time 0.3569

DOS: cpu time 0.0003: real time 0.0003

LOOP: cpu time 6.6431: real time 6.6765

eigenvalue-minimisations : 988

total energy-change (2. order) :-0.7505878E-07 (-0.9728574E-10)

number of electron 518.9999715 magnetization 0.9999998

augmentation part 11.7408985 magnetization 0.0542682

Free energy of the ion-electron system (eV)

---

alpha Z PSCENC = 233.50077011

Ewald energy TEWEN = 91336.43504288

-Hartree energ DENC = -107343.66587034

-exchange EXHF = 0.00000000

-V(xc)+E(xc) XCENC = 1743.85634892

PAW double counting = 52191.10418114 -52254.03334866

entropy T*S EENTRO = -0.00000000

eigenvalues EBANDS = -5814.29489654

atomic energy EATOM = 18704.32991668

Solvation Ediel_sol = 0.00000000

---

free energy TOTEN = -1202.76785580 eV

energy without entropy = -1202.76785580 energy(sigma->0) = -1202.76785580

---

average (electrostatic) potential at core

the test charge radii are 0.5201 0.6991 1.0621 0.7215

(the norm of the test charge is 1.0000)

1 -40.7509	2 -40.7487	3 -40.7502	4 -40.7487	5 -40.7509
6 -40.7530	7 -40.7506	8 -40.7583	9 -40.7502	10 -40.7578
11 -40.7516	12 -40.7536	13 -40.6470	14 -40.6939	15 -40.7672
16 -40.6960	17 -40.6901	18 -40.8602	19 -40.6772	20 -40.6642
21 -40.6866	22 -40.6597	23 -40.0868	24 -40.1283	25 -57.4568
26 -57.6677	27 -57.6548	28 -57.4665	29 -57.6610	30 -57.4568
31 -57.6675	32 -57.6544	33 -57.4645	34 -57.6658	35 -57.4576
36 -57.6694	37 -57.6544	38 -57.4668	39 -57.6717	40 -57.4567
41 -57.6734	42 -57.6546	43 -57.4716	44 -57.6864	45 -57.4567
46 -57.6724	47 -57.6554	48 -57.4719	49 -57.6773	50 -57.4578
51 -57.6690	52 -57.6552	53 -57.4695	54 -57.6637	55 -57.6346
56 -57.6605	57 -57.6845	58 -57.6804	59 -57.6642	60 -57.6671
61 -57.6873	62 -57.6718	63 -57.6348	64 -57.6600	65 -57.6866
66 -57.6920	67 -57.6625	68 -57.6669	69 -57.6910	70 -57.6981
71 -57.6343	72 -57.6614	73 -57.6942	74 -57.7189	75 -57.6634
76 -57.6675	77 -57.7033	78 -57.7480	79 -57.6345	80 -57.6640
81 -57.7080	82 -57.7495	83 -57.6666	84 -57.6690	85 -57.7348
86 -57.8387	87 -57.6369	88 -57.6647	89 -57.7099	90 -57.7143
91 -57.6713	92 -57.6693	93 -57.7395	94 -57.7563	95 -57.6353
96 -57.6628	97 -57.6936	98 -57.6878	99 -57.6686	100 -57.6680

101 -57.7052	102 -57.6830	103 -57.6580	104 -57.6285	105 -57.6425
106 -57.2862	107 -57.3856	108 -57.6289	109 -57.5941	110 -57.6569
111 -57.6285	112 -57.6390	113 -57.3049	114 -57.3913	115 -57.6282
116 -57.5960	117 -57.6562	118 -57.6203	119 -57.6950	120 -57.6782
121 -57.3850	122 -57.6270	123 -57.7060	124 -57.6571	125 -57.6230
126 -57.8293	127 -58.3163	128 -57.3584	129 -57.6323	130 -58.1389
131 -57.6651	132 -57.6323	133 -57.7969	134 -57.4116	135 -57.3696
136 -57.6362	137 -58.0738	138 -57.6615	139 -57.6280	140 -57.6682
141 -57.2951	142 -57.3757	143 -57.6315	144 -57.6445	145 -60.8684
146 -57.3151	147 -81.3358			

E-fermi : -2.3779 XC(G=0): -2.7342 alpha+bet : -2.2521

spin component 1

k-point 1 : 0.0000 0.0000 0.0000

band No.	band energies	occupation
1	-27.1411	1.00000
2	-21.5658	1.00000

3	-21.4693	1.00000
4	-21.0967	1.00000
5	-21.0660	1.00000
6	-21.0122	1.00000
7	-20.9765	1.00000
8	-20.9745	1.00000
9	-20.8889	1.00000
10	-20.5549	1.00000
11	-20.5007	1.00000
12	-20.4095	1.00000
13	-20.3958	1.00000
14	-20.1237	1.00000
15	-19.9737	1.00000
16	-19.7005	1.00000
17	-19.6247	1.00000
18	-19.5971	1.00000
19	-19.5814	1.00000
20	-19.5265	1.00000
21	-19.5247	1.00000
22	-19.4965	1.00000
23	-19.4789	1.00000
24	-19.1093	1.00000

25	-19.0726	1.00000
26	-18.9764	1.00000
27	-18.9627	1.00000
28	-18.8980	1.00000
29	-18.7315	1.00000
30	-18.5021	1.00000
31	-18.3566	1.00000
32	-18.2732	1.00000
33	-18.2500	1.00000
34	-18.1809	1.00000
35	-18.1788	1.00000
36	-18.0777	1.00000
37	-18.0738	1.00000
38	-17.5591	1.00000
39	-17.3112	1.00000
40	-17.2849	1.00000
41	-17.2802	1.00000
42	-17.2078	1.00000
43	-17.2014	1.00000
44	-17.1743	1.00000
45	-17.0202	1.00000
46	-16.9478	1.00000

47	-16.9302	1.00000
48	-16.8910	1.00000
49	-16.8892	1.00000
50	-16.8479	1.00000
51	-16.8395	1.00000
52	-16.8183	1.00000
53	-16.8164	1.00000
54	-16.7273	1.00000
55	-16.7240	1.00000
56	-16.1747	1.00000
57	-15.7274	1.00000
58	-15.6899	1.00000
59	-15.6580	1.00000
60	-15.6343	1.00000
61	-15.6141	1.00000
62	-15.5516	1.00000
63	-15.5478	1.00000
64	-15.1724	1.00000
65	-14.8081	1.00000
66	-14.6058	1.00000
67	-14.5761	1.00000
68	-14.5328	1.00000

69	-14.4963	1.00000
70	-14.4663	1.00000
71	-14.4397	1.00000
72	-14.3314	1.00000
73	-14.3033	1.00000
74	-14.2775	1.00000
75	-14.2697	1.00000
76	-14.1805	1.00000
77	-14.1766	1.00000
78	-13.8886	1.00000
79	-13.7571	1.00000
80	-13.5910	1.00000
81	-13.5462	1.00000
82	-13.5273	1.00000
83	-13.4950	1.00000
84	-13.4435	1.00000
85	-13.3621	1.00000
86	-13.3435	1.00000
87	-13.1859	1.00000
88	-12.7841	1.00000
89	-12.7573	1.00000
90	-12.7251	1.00000

91	-12.6940	1.00000
92	-12.6842	1.00000
93	-12.6213	1.00000
94	-12.4591	1.00000
95	-12.4444	1.00000
96	-12.3795	1.00000
97	-12.3223	1.00000
98	-12.2110	1.00000
99	-12.2014	1.00000
100	-12.1629	1.00000
101	-11.9491	1.00000
102	-11.6836	1.00000
103	-11.6281	1.00000
104	-11.6092	1.00000
105	-11.5842	1.00000
106	-11.1194	1.00000
107	-11.0868	1.00000
108	-10.8974	1.00000
109	-10.8860	1.00000
110	-10.8314	1.00000
111	-10.7087	1.00000
112	-10.6820	1.00000

113	-10.6616	1.00000
114	-10.6443	1.00000
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spin component 2

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274	-0.0544	0.00000
275	-0.0453	0.00000
276	0.0162	0.00000
277	0.0425	0.00000
278	0.0827	0.00000
279	0.2105	0.00000
280	0.2580	0.00000
281	0.2822	0.00000
282	0.4367	0.00000
283	0.4548	0.00000
284	0.4853	0.00000
285	0.6031	0.00000
286	0.7025	0.00000
287	0.8221	0.00000

288	0.8819	0.00000
289	1.0559	0.00000
290	1.1072	0.00000
291	1.1453	0.00000
292	1.1795	0.00000
293	1.2327	0.00000
294	1.2512	0.00000
295	1.3101	0.00000
296	1.3205	0.00000
297	1.3612	0.00000
298	1.4323	0.00000
299	1.4798	0.00000
300	1.5016	0.00000
301	1.5790	0.00000
302	1.6041	0.00000
303	1.6577	0.00000
304	1.6875	0.00000
305	1.7591	0.00000
306	1.7746	0.00000
307	1.8776	0.00000
308	1.9025	0.00000
309	1.9102	0.00000

310	1.9272	0.00000
311	2.1385	0.00000
312	2.1973	0.00000
313	2.2212	0.00000
314	2.2562	0.00000
315	2.2907	0.00000
316	2.2969	0.00000
317	2.3371	0.00000
318	2.3622	0.00000
319	2.3843	0.00000
320	2.4096	0.00000
321	2.4303	0.00000
322	2.4361	0.00000
323	2.4557	0.00000
324	2.4588	0.00000
325	2.4697	0.00000
326	2.5249	0.00000
327	2.5430	0.00000
328	2.7065	0.00000
329	2.7346	0.00000
330	2.7544	0.00000
331	2.7600	0.00000

332	2.7736	0.00000
333	2.8327	0.00000
334	2.8490	0.00000
335	2.8714	0.00000
336	2.9027	0.00000
337	2.9334	0.00000
338	2.9571	0.00000
339	2.9841	0.00000
340	3.0075	0.00000
341	3.0387	0.00000
342	3.0527	0.00000
343	3.0720	0.00000
344	3.0932	0.00000
345	3.1522	0.00000
346	3.1725	0.00000
347	3.1892	0.00000
348	3.1998	0.00000
349	3.3067	0.00000
350	3.3268	0.00000
351	3.3603	0.00000
352	3.3704	0.00000
353	3.3930	0.00000

354	3.4369	0.00000
355	3.4813	0.00000
356	3.4920	0.00000
357	3.4967	0.00000
358	3.5070	0.00000
359	3.6390	0.00000
360	3.6771	0.00000
361	3.6988	0.00000
362	3.7380	0.00000
363	3.7567	0.00000
364	3.7616	0.00000
365	3.7777	0.00000
366	3.7995	0.00000
367	3.8160	0.00000
368	3.8422	0.00000
369	3.8480	0.00000
370	3.8672	0.00000
371	3.8814	0.00000
372	3.8942	0.00000
373	3.9219	0.00000
374	3.9367	0.00000
375	3.9498	0.00000

376	3.9599	0.00000
377	3.9828	0.00000
378	3.9864	0.00000
379	4.0223	0.00000
380	4.0793	0.00000
381	4.1708	0.00000
382	4.2588	0.00000
383	4.2622	0.00000
384	4.2691	0.00000
385	4.2929	0.00000
386	4.3213	0.00000
387	4.3344	0.00000
388	4.3505	0.00000
389	4.3818	0.00000
390	4.3867	0.00000
391	4.4233	0.00000
392	4.4487	0.00000
393	4.4737	0.00000
394	4.4831	0.00000
395	4.4935	0.00000
396	4.4991	0.00000
397	4.5202	0.00000

398	4.5556	0.00000
399	4.5942	0.00000
400	4.6106	0.00000
401	4.6294	0.00000
402	4.6464	0.00000
403	4.6600	0.00000
404	4.6859	0.00000
405	4.7092	0.00000
406	4.7378	0.00000
407	4.7514	0.00000
408	4.7705	0.00000
409	4.7874	0.00000
410	4.7899	0.00000
411	4.8034	0.00000
412	4.8331	0.00000
413	4.8694	0.00000
414	4.8856	0.00000
415	4.9038	0.00000
416	4.9421	0.00000
417	4.9937	0.00000
418	5.0101	0.00000
419	5.0134	0.00000

420	5.0388	0.00000
421	5.0444	0.00000
422	5.0701	0.00000
423	5.0862	0.00000
424	5.1172	0.00000
425	5.1219	0.00000
426	5.1411	0.00000
427	5.1443	0.00000
428	5.1713	0.00000
429	5.1801	0.00000
430	5.1893	0.00000
431	5.1932	0.00000
432	5.2198	0.00000
433	5.2386	0.00000
434	5.2435	0.00000
435	5.2615	0.00000
436	5.2990	0.00000
437	5.3038	0.00000
438	5.3127	0.00000
439	5.3364	0.00000
440	5.3536	0.00000
441	5.3715	0.00000

442	5.3823	0.00000
443	5.3966	0.00000
444	5.4297	0.00000
445	5.4599	0.00000
446	5.4715	0.00000
447	5.4876	0.00000
448	5.4988	0.00000
449	5.5276	0.00000
450	5.5687	0.00000
451	5.5750	0.00000
452	5.5956	0.00000
453	5.6076	0.00000
454	5.6266	0.00000
455	5.6710	0.00000
456	5.6930	0.00000
457	5.7192	0.00000
458	5.7274	0.00000
459	5.7478	0.00000
460	5.7624	0.00000
461	5.7901	0.00000
462	5.7935	0.00000
463	5.7987	0.00000

464	5.8046	0.00000
465	5.8208	0.00000
466	5.8257	0.00000
467	5.8556	0.00000
468	5.8611	0.00000
469	5.8838	0.00000
470	5.8875	0.00000
471	5.8921	0.00000
472	5.9097	0.00000
473	5.9215	0.00000
474	5.9485	0.00000
475	5.9534	0.00000
476	5.9699	0.00000
477	5.9765	0.00000
478	5.9893	0.00000
479	6.0122	0.00000
480	6.0414	0.00000

---

soft charge-density along one line, spin component 1

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

soft charge-density along one line, spin component 2

0 1 2 3 4 5 6 7 8 9

total charge-density along one line

pseudopotential strength for first ion, spin component: 1

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

pseudopotential strength for first ion, spin component: 2

-2.331 -4.014 -0.002 0.000 0.000

-4.014 -6.828 -0.006 0.000 -0.000

-0.002 -0.006 -0.336 -0.000 0.000

0.000 0.000 -0.000 -0.341 -0.000

0.000 -0.000 0.000 -0.000 -0.341

total augmentation occupancy for first ion, spin component: 1

3.579	-0.646	0.444	-0.034	-0.000
-0.646	0.130	-0.082	0.006	0.000
0.444	-0.082	0.056	-0.003	-0.000
-0.034	0.006	-0.003	0.011	0.000
-0.000	0.000	-0.000	0.000	0.007

total augmentation occupancy for first ion, spin component: 2

-0.000	0.000	-0.000	0.000	0.000
0.000	-0.000	0.000	-0.000	-0.000
-0.000	0.000	-0.000	-0.000	-0.000
0.000	-0.000	-0.000	-0.000	-0.000
0.000	-0.000	-0.000	-0.000	-0.000

---------- aborting loop because EDIFF is reached ----------

total charge

# of ion	s	p	d	tot
1	0.646	0.043	0.000	0.690
2	0.646	0.043	0.000	0.690
3	0.646	0.043	0.000	0.690
4	0.646	0.043	0.000	0.690
5	0.646	0.043	0.000	0.690
6	0.646	0.043	0.000	0.690
7	0.646	0.043	0.000	0.690
8	0.646	0.043	0.000	0.690
9	0.646	0.043	0.000	0.690
10	0.646	0.043	0.000	0.690
11	0.646	0.043	0.000	0.690
12	0.646	0.043	0.000	0.690
13	0.646	0.043	0.000	0.689
14	0.646	0.043	0.000	0.689
15	0.648	0.045	0.000	0.693
16	0.646	0.043	0.000	0.689
17	0.646	0.043	0.000	0.689
18	0.646	0.043	0.000	0.689
19	0.646	0.043	0.000	0.689
20	0.646	0.043	0.000	0.689

21	0.646	0.043	0.000	0.689
22	0.646	0.044	0.000	0.690
23	0.541	0.015	0.000	0.557
24	0.541	0.015	0.000	0.556
25	0.870	1.763	0.000	2.633
26	0.867	1.785	0.000	2.653
27	0.867	1.786	0.000	2.653
28	0.870	1.762	0.000	2.632
29	0.865	1.783	0.000	2.648
30	0.870	1.763	0.000	2.633
31	0.867	1.786	0.000	2.653
32	0.867	1.786	0.000	2.653
33	0.870	1.762	0.000	2.632
34	0.865	1.783	0.000	2.648
35	0.870	1.763	0.000	2.633
36	0.868	1.787	0.000	2.654
37	0.867	1.786	0.000	2.653
38	0.870	1.763	0.000	2.633
39	0.865	1.784	0.000	2.649
40	0.870	1.763	0.000	2.633
41	0.868	1.787	0.000	2.655
42	0.867	1.786	0.000	2.653

43	0.871	1.764	0.000	2.634
44	0.865	1.783	0.000	2.648
45	0.870	1.763	0.000	2.633
46	0.867	1.786	0.000	2.653
47	0.867	1.786	0.000	2.653
48	0.871	1.763	0.000	2.634
49	0.865	1.783	0.000	2.648
50	0.870	1.763	0.000	2.633
51	0.867	1.786	0.000	2.653
52	0.867	1.786	0.000	2.653
53	0.870	1.762	0.000	2.632
54	0.865	1.784	0.000	2.648
55	0.865	1.784	0.000	2.649
56	0.865	1.786	0.000	2.651
57	0.866	1.787	0.000	2.653
58	0.866	1.790	0.000	2.656
59	0.865	1.786	0.000	2.651
60	0.866	1.786	0.000	2.651
61	0.866	1.788	0.000	2.654
62	0.867	1.791	0.000	2.658
63	0.865	1.784	0.000	2.649
64	0.865	1.786	0.000	2.651

65	0.866	1.787	0.000	2.652
66	0.865	1.788	0.000	2.653
67	0.865	1.786	0.000	2.651
68	0.866	1.785	0.000	2.651
69	0.865	1.787	0.000	2.652
70	0.866	1.787	0.000	2.653
71	0.865	1.784	0.000	2.649
72	0.865	1.786	0.000	2.651
73	0.866	1.786	0.000	2.652
74	0.864	1.785	0.000	2.649
75	0.865	1.786	0.000	2.651
76	0.866	1.786	0.000	2.651
77	0.865	1.786	0.000	2.651
78	0.865	1.784	0.000	2.649
79	0.865	1.784	0.000	2.649
80	0.865	1.786	0.000	2.651
81	0.865	1.785	0.000	2.650
82	0.863	1.782	0.000	2.645
83	0.865	1.786	0.000	2.651
84	0.866	1.786	0.000	2.651
85	0.865	1.784	0.000	2.648
86	0.862	1.774	0.000	2.636

87	0.865	1.784	0.000	2.649
88	0.865	1.787	0.000	2.652
89	0.865	1.785	0.000	2.650
90	0.865	1.788	0.000	2.653
91	0.865	1.786	0.000	2.651
92	0.866	1.786	0.000	2.651
93	0.864	1.783	0.000	2.647
94	0.866	1.785	0.000	2.651
95	0.865	1.784	0.000	2.649
96	0.865	1.786	0.000	2.651
97	0.866	1.787	0.000	2.653
98	0.866	1.789	0.000	2.655
99	0.865	1.786	0.000	2.651
100	0.866	1.786	0.000	2.651
101	0.865	1.787	0.000	2.652
102	0.867	1.790	0.000	2.657
103	0.865	1.786	0.000	2.651
104	0.867	1.785	0.000	2.653
105	0.866	1.786	0.000	2.652
106	0.870	1.778	0.000	2.648
107	0.869	1.765	0.000	2.635
108	0.865	1.783	0.000	2.648

109	0.869	1.789	0.000	2.658
110	0.865	1.786	0.000	2.651
111	0.867	1.785	0.000	2.653
112	0.867	1.789	0.000	2.655
113	0.871	1.782	0.000	2.653
114	0.869	1.765	0.000	2.634
115	0.865	1.783	0.000	2.648
116	0.870	1.791	0.000	2.661
117	0.865	1.786	0.000	2.651
118	0.867	1.786	0.000	2.653
119	0.865	1.782	0.000	2.647
120	0.857	1.707	0.000	2.564
121	0.869	1.765	0.000	2.634
122	0.865	1.783	0.000	2.648
123	0.866	1.778	0.000	2.644
124	0.866	1.786	0.000	2.652
125	0.867	1.785	0.000	2.653
126	0.862	1.776	0.000	2.638
127	0.849	1.831	0.000	2.680
128	0.870	1.767	0.000	2.637
129	0.865	1.783	0.000	2.648
130	0.860	1.757	0.000	2.617

131	0.866	1.786	0.000	2.652
132	0.867	1.784	0.000	2.652
133	0.864	1.787	0.000	2.651
134	0.869	1.790	0.000	2.659
135	0.869	1.767	0.000	2.636
136	0.865	1.783	0.000	2.648
137	0.866	1.772	0.000	2.638
138	0.866	1.786	0.000	2.652
139	0.867	1.785	0.000	2.652
140	0.866	1.788	0.000	2.654
141	0.870	1.779	0.000	2.649
142	0.869	1.766	0.000	2.635
143	0.865	1.783	0.000	2.648
144	0.869	1.790	0.000	2.659
145	0.946	1.730	0.000	2.676
146	1.240	1.546	0.074	2.860
147	1.635	3.538	0.000	5.173
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tot	123.067	221.574	0.074	344.715

magnetization (x)

# of ion	s	p	d	tot
1	0.000	-0.000	0.000	0.000
2	-0.000	0.000	0.000	-0.000
3	0.000	-0.000	0.000	0.000
4	-0.000	0.000	0.000	-0.000
5	0.000	-0.000	0.000	0.000
6	-0.000	0.000	0.000	-0.000
7	0.000	-0.000	0.000	0.000
8	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	0.000
10	-0.000	0.000	0.000	-0.000
11	0.000	-0.000	0.000	0.000
12	-0.000	0.000	0.000	-0.000
13	0.000	-0.000	0.000	0.000
14	-0.004	0.002	0.000	-0.002
15	0.000	-0.000	0.000	0.000
16	-0.004	0.002	0.000	-0.002
17	-0.004	0.002	0.000	-0.002
18	0.000	-0.000	0.000	0.000

19	-0.003	0.001	0.000	-0.002
20	0.000	-0.000	0.000	0.000
21	-0.003	0.002	0.000	-0.002
22	-0.003	0.002	0.000	-0.002
23	-0.000	0.000	0.000	-0.000
24	-0.000	0.000	0.000	-0.000
25	-0.000	-0.007	0.000	-0.008
26	-0.000	-0.002	0.000	-0.002
27	0.000	0.003	0.000	0.003
28	0.000	0.005	0.000	0.005
29	0.000	0.003	0.000	0.003
30	-0.000	-0.007	0.000	-0.008
31	-0.000	-0.002	0.000	-0.002
32	0.000	0.003	0.000	0.003
33	0.000	0.005	0.000	0.005
34	0.000	0.002	0.000	0.002
35	-0.000	-0.007	0.000	-0.008
36	-0.000	-0.002	0.000	-0.002
37	0.000	0.003	0.000	0.003
38	0.000	0.006	0.000	0.007
39	0.000	0.002	0.000	0.002
40	-0.000	-0.007	0.000	-0.008

41	-0.000	-0.002	0.000	-0.002
42	0.000	0.002	0.000	0.003
43	0.000	0.005	0.000	0.005
44	0.000	0.004	0.000	0.004
45	-0.000	-0.007	0.000	-0.008
46	-0.000	-0.002	0.000	-0.002
47	0.000	0.002	0.000	0.003
48	0.000	0.005	0.000	0.006
49	0.000	0.001	0.000	0.001
50	-0.000	-0.007	0.000	-0.008
51	-0.000	-0.002	0.000	-0.002
52	0.000	0.002	0.000	0.003
53	0.000	0.006	0.000	0.007
54	0.000	0.002	0.000	0.002
55	-0.000	-0.005	0.000	-0.006
56	-0.000	-0.007	0.000	-0.007
57	-0.000	-0.001	0.000	-0.001
58	-0.000	-0.001	0.000	-0.001
59	0.000	0.006	0.000	0.007
60	0.000	0.003	0.000	0.003
61	0.000	0.001	0.000	0.001
62	0.000	0.003	0.000	0.003

63	-0.000	-0.005	0.000	-0.006
64	-0.000	-0.007	0.000	-0.007
65	-0.000	-0.001	0.000	-0.001
66	-0.000	-0.001	0.000	-0.001
67	0.000	0.006	0.000	0.006
68	0.000	0.003	0.000	0.003
69	0.000	0.001	0.000	0.001
70	0.000	0.002	0.000	0.002
71	-0.000	-0.005	0.000	-0.006
72	-0.000	-0.007	0.000	-0.007
73	-0.000	-0.001	0.000	-0.001
74	-0.000	-0.002	0.000	-0.002
75	0.000	0.006	0.000	0.007
76	0.000	0.003	0.000	0.004
77	0.000	0.003	0.000	0.003
78	0.000	0.001	0.000	0.001
79	-0.000	-0.005	0.000	-0.006
80	-0.000	-0.007	0.000	-0.007
81	-0.000	-0.001	0.000	-0.002
82	-0.000	-0.002	0.000	-0.002
83	0.001	0.007	0.000	0.008
84	0.000	0.003	0.000	0.003

85	0.000	0.002	0.000	0.002
86	0.000	0.005	0.000	0.006
87	-0.000	-0.005	0.000	-0.005
88	-0.000	-0.007	0.000	-0.007
89	-0.000	-0.001	0.000	-0.002
90	-0.000	-0.002	0.000	-0.002
91	0.001	0.008	0.000	0.008
92	0.000	0.003	0.000	0.003
93	0.000	0.002	0.000	0.003
94	0.000	0.001	0.000	0.001
95	-0.000	-0.005	0.000	-0.006
96	-0.000	-0.007	0.000	-0.007
97	-0.000	-0.001	0.000	-0.001
98	-0.000	-0.001	0.000	-0.001
99	0.001	0.007	0.000	0.007
100	0.000	0.003	0.000	0.004
101	0.000	0.003	0.000	0.003
102	0.000	0.002	0.000	0.002
103	-0.001	-0.010	0.000	-0.011
104	-0.003	-0.028	0.000	-0.031
105	-0.000	-0.001	0.000	-0.002
106	-0.000	-0.004	0.000	-0.005

107	0.007	0.116	0.000	0.122
108	0.001	0.010	0.000	0.011
109	0.000	0.001	0.000	0.001
110	-0.001	-0.010	0.000	-0.011
111	-0.003	-0.028	0.000	-0.031
112	-0.000	-0.001	0.000	-0.002
113	-0.000	-0.003	0.000	-0.004
114	0.007	0.120	0.000	0.127
115	0.001	0.010	0.000	0.011
116	0.000	0.001	0.000	0.002
117	-0.001	-0.010	0.000	-0.011
118	-0.003	-0.026	0.000	-0.029
119	-0.000	-0.002	0.000	-0.002
120	-0.000	-0.002	0.000	-0.002
121	0.007	0.115	0.000	0.122
122	0.001	0.010	0.000	0.010
123	0.000	0.003	0.000	0.003
124	-0.001	-0.010	0.000	-0.011
125	-0.003	-0.024	0.000	-0.027
126	-0.000	-0.002	0.000	-0.002
127	-0.000	0.001	0.000	0.001
128	0.006	0.105	0.000	0.111

129	0.001	0.009	0.000	0.010
130	0.000	0.004	0.000	0.004
131	-0.001	-0.009	0.000	-0.010
132	-0.003	-0.024	0.000	-0.027
133	-0.000	-0.002	0.000	-0.002
134	-0.000	-0.002	0.000	-0.002
135	0.006	0.097	0.000	0.102
136	0.001	0.009	0.000	0.010
137	0.000	0.004	0.000	0.005
138	-0.001	-0.010	0.000	-0.011
139	-0.003	-0.026	0.000	-0.029
140	-0.000	-0.002	0.000	-0.002
141	-0.000	-0.003	0.000	-0.004
142	0.006	0.105	0.000	0.111
143	0.001	0.010	0.000	0.010
144	0.000	0.002	0.000	0.003
145	0.000	0.005	0.000	0.006
146	-0.000	0.000	-0.000	0.000
147	0.000	0.004	0.000	0.004
---	---	---	---	---
tot	0.001	0.513	-0.000	0.514

CHARGE: cpu time 0.5207: real time 0.5225

FORLOC: cpu time 0.0200: real time 0.0200

FORNL : cpu time 2.0395: real time 2.0467

STRESS: cpu time 6.0482: real time 6.1297

FORCOR: cpu time 0.1385: real time 0.1394

FORHAR: cpu time 0.0331: real time 0.0332

MIXING: cpu time 0.0108: real time 0.0108

OFIELD: cpu time 0.0001: real time 0.0001

DFTD3 V3.0 Rev 1

Edisp (eV) -6.61796

E6 (eV) : -3.9313

E8 (eV) : -2.6867

% E8 : 40.60

FORVDW: cpu time 1.7843: real time 1.8311

FORCE on cell =-STRESS in cart. coord. units (eV):

Direction XX YY ZZ XY YZ ZX

Alpha Z	233.50077	233.50077	233.50077			
Ewald	107585.33206	23489.11467	-39738.14176	10.22187	3453.74406	128.63845
Hartree	106105.06727	25041.40737	-23802.80868	-6.67003	2945.37234	93.20003
E(xc)	-1914.30055	-1916.63916	-1979.96915	0.13357	1.81986	0.12973
Local	**********	-53978.07964	57034.52900	-0.05361	-6356.87834	-218.39297
n-local	-472.72733	-482.63651	-439.61069	-0.69503	-0.75894	-0.32313
augment	-38.27302	-38.61717	-34.28739	0.00537	-0.98261	0.00032
Kinetic	7635.49820	7638.82569	8714.61503	-3.11030	-41.35382	-3.15643
Fock	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
vdW	-2.64123	-1.49237	-6.59252	0.00142	-0.07447	0.01226
Total	-17.71170	-14.61635	-18.76538	-0.16675	0.88807	0.10826
in kB	-4.88410	-4.03054	-5.17466	-0.04598	0.24489	0.02985

external pressure = -4.70 kB Pullay stress = 0.00 kB

VOLUME and BASIS-vectors are now :

---

energy-cutoff : 400.00

volume of cell : 5810.14

direct lattice vectors			reciprocal lattice vectors		
14.780600000	0.000000000	0.000000000	0.067656252	0.000000000	0.000000000

0.000000000 21.333900000 0.000000000 0.000000000 0.046873755 0.000000000

0.000000000 0.000000000 18.425700000 0.000000000 0.000000000 0.054272022

length of vectors

14.780600000 21.333900000 18.425700000 0.067656252 0.046873755 0.054272022

FORCES acting on ions

electron-ion (+dipol) ewald-force non-local-force convergence-correction

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0.447E-02 0.154E+03 0.361E+02 -.296E-02 -.160E+03 -.357E+02 -.180E-02 0.566E+01 -.438E+00 0.882E-07 0.729E-06 0.476E-06

-.187E-01 0.155E+03 -.340E+02 0.163E-01 -.160E+03 0.335E+02 0.115E-02 0.565E+01 0.541E+00 -.671E-06 0.254E-06 -.265E-06

0.184E+00 0.154E+03 0.360E+02 -.184E+00 -.160E+03 -.356E+02 0.961E-05 0.565E+01 -.443E+00 -.177E-06 0.844E-06 0.246E-06

0.112E+00 0.155E+03 -.341E+02 -.989E-01 -.160E+03 0.336E+02 -.175E-01 0.565E+01 0.535E+00 0.856E-07 0.558E-06 -.504E-06

0.172E+00 0.154E+03 0.362E+02 -.173E+00 -.160E+03 -.357E+02 0.117E-02 0.566E+01 -.440E+00 -.310E-06 0.844E-06 0.705E-06

0.126E+00 0.154E+03 -.340E+02 -.108E+00 -.160E+03 0.334E+02 -.211E-01 0.565E+01

0.541E+00 0.711E-06 0.266E-06 0.254E-06

-.191E-01 0.154E+03 0.363E+02 0.179E-01 -.160E+03 -.359E+02 0.159E-02 0.566E+01 -.431E+00 -.159E-06 0.671E-06 0.139E-05

-.127E-01 0.154E+03 -.338E+02 0.196E-01 -.160E+03 0.332E+02 -.720E-02 0.565E+01 0.555E+00 0.557E-06 -.154E-06 0.119E-05

-.182E+00 0.154E+03 0.363E+02 0.182E+00 -.160E+03 -.359E+02 0.254E-03 0.566E+01 -.429E+00 0.230E-06 0.644E-06 0.158E-05

-.128E+00 0.155E+03 -.337E+02 0.115E+00 -.160E+03 0.331E+02 0.109E-01 0.565E+01 0.561E+00 -.498E-07 -.476E-06 0.140E-05

-.174E+00 0.154E+03 0.362E+02 0.176E+00 -.160E+03 -.358E+02 -.177E-02 0.566E+01 -.432E+00 0.329E-06 0.655E-06 0.115E-05

-.115E+00 0.155E+03 -.338E+02 0.961E-01 -.160E+03 0.332E+02 0.192E-01 0.565E+01 0.555E+00 -.630E-06 -.290E-06 0.689E-06

0.228E+01 -.150E+03 -.387E+02 -.227E+01 0.156E+03 0.386E+02 -.103E-01 -.566E+01 0.767E-01 0.522E-06 -.133E-07 0.192E-06

-.420E+00 -.151E+03 0.388E+02 0.421E+00 0.157E+03 -.386E+02 -.130E-02 -.567E+01 -.269E+00 -.307E-06 -.196E-06 -.254E-06

0.136E+02 -.146E+03 -.413E+02 -.138E+02 0.151E+03 0.413E+02 0.257E+00 -.567E+01 -.348E-01 0.116E-07 -.750E-07 -.880E-07

0.162E+01 -.151E+03 0.402E+02 -.162E+01 0.156E+03 -.400E+02 -.998E-03 -.567E+01 -.229E+00 0.253E-06 0.673E-07 0.570E-06

0.353E+01 -.149E+03 0.443E+02 -.353E+01 0.155E+03 -.441E+02 -.195E-02 -.567E+01 -

.180E+00 0.658E-06 0.425E-07 0.277E-06

-.149E+02 -.146E+03 -.330E+02 0.150E+02 0.151E+03 0.329E+02 -.966E-01 -.566E+01 0.498E-01 -.108E-05 0.588E-06 0.117E-05

-.297E+01 -.149E+03 0.432E+02 0.296E+01 0.155E+03 -.430E+02 0.115E-01 -.567E+01 -.241E+00 -.294E-06 -.334E-06 -.124E-05

-.380E+01 -.150E+03 -.385E+02 0.380E+01 0.156E+03 0.385E+02 -.631E-02 -.566E+01 0.241E-01 0.393E-07 -.162E-06 0.291E-06

-.208E+01 -.151E+03 0.395E+02 0.208E+01 0.156E+03 -.392E+02 0.149E-02 -.566E+01 -.282E+00 -.656E-06 -.385E-06 -.113E-05

0.775E-02 -.148E+03 0.486E+02 -.688E-04 0.154E+03 -.484E+02 -.556E-02 -.569E+01 -.158E+00 0.391E-06 -.823E-07 -.740E-06

0.196E+02 -.103E+03 0.222E+02 -.212E+02 0.103E+03 -.246E+02 0.154E+01 0.139E+00 0.238E+01 0.104E-06 -.553E-06 0.449E-06

-.191E+02 -.103E+03 0.154E+02 0.215E+02 0.103E+03 -.169E+02 -.241E+01 -.119E+00 0.152E+01 0.110E-06 -.960E-06 0.121E-05

0.709E-01 0.461E+03 0.202E+03 -.741E-01 -.462E+03 -.201E+03 0.382E-02 0.102E+01 -.219E+00 0.651E-06 0.190E-06 0.125E-05

0.212E+00 0.353E+03 -.234E+03 -.212E+00 -.353E+03 0.234E+03 0.260E-02 0.442E+00 -.370E-01 -.678E-06 0.214E-05 -.247E-05

-.255E-01 0.351E+03 0.240E+03 0.241E-01 -.351E+03 -.241E+03 0.313E-02 0.408E+00 0.563E-01 0.119E-05 -.151E-05 0.201E-05

-.173E+00 0.462E+03 -.195E+03 0.180E+00 -.463E+03 0.195E+03 -.666E-02 0.105E+01

0.233E+00 -.181E-05 0.124E-05 -.170E-05

-.623E-01 0.210E+03 -.272E+03 0.664E-01 -.210E+03 0.272E+03 -.449E-02 0.931E-01

0.560E-01 -.226E-06 0.102E-05 -.157E-05

0.562E+00 0.461E+03 0.202E+03 -.565E+00 -.462E+03 -.201E+03 0.202E-02 0.102E+01 -

.214E+00 -.626E-06 0.366E-06 0.534E-06

0.106E+01 0.352E+03 -.234E+03 -.107E+01 -.353E+03 0.234E+03 0.160E-01 0.448E+00 -

.424E-01 0.721E-06 0.181E-05 -.128E-05

0.413E+00 0.351E+03 0.240E+03 -.415E+00 -.351E+03 -.240E+03 0.302E-02 0.408E+00

0.490E-01 0.539E-08 -.137E-05 0.430E-06

0.579E+00 0.462E+03 -.195E+03 -.584E+00 -.463E+03 0.195E+03 0.481E-02 0.105E+01

0.235E+00 0.304E-06 0.222E-05 -.238E-05

0.690E+00 0.210E+03 -.272E+03 -.696E+00 -.210E+03 0.272E+03 0.602E-02 0.907E-01

0.615E-01 0.824E-07 0.397E-06 -.657E-06

0.426E+00 0.461E+03 0.202E+03 -.429E+00 -.462E+03 -.202E+03 0.387E-02 0.102E+01 -

.214E+00 -.146E-05 0.566E-06 0.227E-05

0.939E+00 0.352E+03 -.233E+03 -.956E+00 -.352E+03 0.233E+03 0.151E-01 0.440E+00 -

.377E-01 0.152E-05 -.446E-06 0.148E-05

0.479E+00 0.351E+03 0.241E+03 -.481E+00 -.351E+03 -.241E+03 0.251E-02 0.406E+00

0.511E-01 -.102E-05 -.122E-05 0.100E-05

0.705E+00 0.462E+03 -.194E+03 -.716E+00 -.463E+03 0.194E+03 0.789E-02 0.106E+01

0.242E+00 0.193E-05 0.374E-06 0.329E-06

0.725E+00 0.210E+03 -.271E+03 -.734E+00 -.210E+03 0.271E+03 0.661E-02 0.905E-01

0.593E-01 0.209E-06 -.121E-05 0.943E-06

-.181E+00 0.461E+03 0.202E+03 0.177E+00 -.462E+03 -.202E+03 0.450E-02 0.102E+01 -.218E+00 -.841E-06 0.530E-06 0.469E-05

-.294E+00 0.352E+03 -.233E+03 0.298E+00 -.352E+03 0.233E+03 -.205E-02 0.440E+00 -.299E-01 0.241E-06 -.283E-05 0.329E-05

0.410E-01 0.351E+03 0.241E+03 -.400E-01 -.351E+03 -.241E+03 0.225E-02 0.409E+00 0.556E-01 -.149E-05 -.783E-06 0.311E-05

0.505E-01 0.462E+03 -.194E+03 -.567E-01 -.463E+03 0.194E+03 0.400E-02 0.106E+01 0.232E+00 0.137E-05 -.223E-05 0.340E-05

-.477E-01 0.210E+03 -.271E+03 0.457E-01 -.210E+03 0.271E+03 -.249E-03 0.928E-01 0.325E-01 0.607E-07 -.260E-05 0.192E-05

-.552E+00 0.461E+03 0.202E+03 0.550E+00 -.462E+03 -.202E+03 0.759E-03 0.102E+01 -.220E+00 0.886E-06 0.306E-06 0.526E-05

-.119E+01 0.352E+03 -.233E+03 0.120E+01 -.353E+03 0.233E+03 -.162E-01 0.447E+00 -.330E-01 -.661E-06 -.202E-05 0.230E-05

-.352E+00 0.351E+03 0.241E+03 0.349E+00 -.351E+03 -.241E+03 0.206E-02 0.413E+00 0.622E-01 0.219E-07 -.658E-06 0.458E-05

-.412E+00 0.462E+03 -.194E+03 0.426E+00 -.463E+03 0.194E+03 -.115E-01 0.106E+01 0.230E+00 -.223E-06 -.337E-05 0.400E-05

-.561E+00 0.210E+03 -.271E+03 0.566E+00 -.210E+03 0.271E+03 -.949E-02 0.909E-01 0.525E-01 -.122E-06 -.234E-05 0.122E-05

-.476E+00 0.461E+03 0.202E+03 0.475E+00 -.462E+03 -.202E+03 0.305E-02 0.102E+01 -

.221E+00 0.142E-05 -.226E-07 0.362E-05

-.806E+00 0.353E+03 -.234E+03 0.820E+00 -.353E+03 0.234E+03 -.150E-01 0.447E+00 -.393E-01 -.105E-05 0.283E-06 -.568E-06

-.374E+00 0.351E+03 0.241E+03 0.369E+00 -.351E+03 -.241E+03 0.941E-03 0.411E+00 0.625E-01 0.126E-05 -.124E-05 0.403E-05

-.595E+00 0.462E+03 -.194E+03 0.608E+00 -.463E+03 0.194E+03 -.170E-01 0.105E+01 0.234E+00 -.166E-05 -.175E-05 0.158E-05

-.588E+00 0.210E+03 -.272E+03 0.599E+00 -.210E+03 0.272E+03 -.102E-01 0.986E-01 0.566E-01 0.145E-06 -.652E-06 -.553E-06

-.957E-02 0.206E+03 0.279E+03 0.129E-01 -.206E+03 -.279E+03 -.361E-02 0.685E-01 -.413E-01 0.102E-05 -.178E-05 0.141E-05

0.667E+00 0.303E+02 0.296E+03 -.662E+00 -.302E+02 -.296E+03 -.468E-02 -.411E-01 0.736E-02 0.722E-07 -.232E-05 0.145E-05

-.846E+00 0.144E+03 -.282E+03 0.848E+00 -.144E+03 0.282E+03 -.316E-02 0.136E+00 0.286E-01 0.151E-06 -.239E-06 -.709E-06

0.534E+00 -.215E+02 -.285E+03 -.534E+00 0.214E+02 0.285E+03 -.781E-03 0.383E-01 0.186E-01 0.371E-06 -.206E-05 0.144E-05

0.497E+00 -.294E+02 0.293E+03 -.494E+00 0.294E+02 -.293E+03 -.553E-02 0.253E-01 -.305E-01 -.395E-06 -.160E-05 0.878E-06

0.524E+00 0.139E+03 0.289E+03 -.524E+00 -.139E+03 -.289E+03 0.178E-02 0.103E+00 -.249E-01 0.555E-06 -.233E-05 0.947E-06

-.127E+01 0.364E+02 -.287E+03 0.127E+01 -.364E+02 0.287E+03 -.115E-03 -.806E-02

0.138E-01 0.984E-06 -.139E-05 0.773E-06

0.167E+01 -.130E+03 -.271E+03 -.169E+01 0.130E+03 0.271E+03 0.106E-01 -.882E-01 0.373E-01 0.489E-06 -.254E-05 0.228E-05

0.397E+00 0.207E+03 0.280E+03 -.395E+00 -.207E+03 -.280E+03 0.713E-03 0.694E-01 -.372E-01 0.471E-07 -.231E-05 0.483E-06

0.920E+00 0.312E+02 0.296E+03 -.924E+00 -.311E+02 -.296E+03 0.226E-02 -.411E-01 0.121E-01 0.503E-07 -.230E-05 0.124E-05

0.133E+01 0.144E+03 -.282E+03 -.133E+01 -.144E+03 0.282E+03 0.497E-02 0.126E+00 0.279E-01 -.206E-06 0.264E-06 -.690E-06

0.342E+01 -.199E+02 -.285E+03 -.343E+01 0.199E+02 0.285E+03 0.136E-01 0.409E-01 0.138E-01 -.172E-05 -.203E-05 0.125E-05

0.139E+01 -.287E+02 0.294E+03 -.139E+01 0.287E+02 -.294E+03 -.348E-02 0.252E-01 -.309E-01 0.250E-07 -.226E-05 0.181E-05

0.678E+00 0.139E+03 0.290E+03 -.678E+00 -.139E+03 -.290E+03 0.629E-03 0.103E+00 -.296E-01 -.368E-06 -.243E-05 0.582E-06

0.160E+01 0.367E+02 -.287E+03 -.159E+01 -.367E+02 0.287E+03 -.127E-01 -.210E-01 0.129E-01 -.601E-06 -.955E-06 0.762E-06

0.612E+01 -.125E+03 -.271E+03 -.614E+01 0.125E+03 0.271E+03 0.219E-01 -.898E-01 0.148E-01 -.162E-05 -.228E-05 0.141E-05

0.368E+00 0.207E+03 0.280E+03 -.373E+00 -.207E+03 -.280E+03 0.119E-03 0.683E-01 -.366E-01 -.782E-06 -.194E-05 0.748E-06

-.358E-01 0.319E+02 0.296E+03 0.271E-01 -.319E+02 -.296E+03 0.106E-01 -.363E-01

0.137E-01 0.184E-06 -.112E-05 0.341E-06

0.210E+01 0.144E+03 -.281E+03 -.211E+01 -.144E+03 0.281E+03 0.121E-01 0.120E+00 0.241E-01 -.887E-07 -.142E-05 0.384E-06

0.303E+01 -.171E+02 -.283E+03 -.306E+01 0.171E+02 0.283E+03 0.242E-01 0.857E-01 0.614E-01 -.943E-06 -.376E-05 0.774E-06

0.106E+01 -.272E+02 0.294E+03 -.106E+01 0.272E+02 -.294E+03 0.289E-02 0.242E-01 -.377E-01 0.597E-06 -.151E-05 0.764E-06

0.975E-01 0.140E+03 0.290E+03 -.991E-01 -.140E+03 -.290E+03 0.131E-02 0.107E+00 -.233E-01 -.661E-06 -.130E-05 0.102E-05

0.277E+01 0.387E+02 -.286E+03 -.277E+01 -.387E+02 0.286E+03 0.103E-02 -.115E-01 0.294E-01 -.828E-06 -.208E-05 0.990E-06

0.597E+01 -.115E+03 -.267E+03 -.612E+01 0.115E+03 0.267E+03 0.152E+00 -.650E-03 0.130E+00 -.259E-05 -.306E-05 0.468E-06

-.242E+00 0.207E+03 0.280E+03 0.239E+00 -.207E+03 -.280E+03 0.439E-02 0.715E-01 -.388E-01 -.996E-06 -.785E-06 0.195E-05

-.114E+01 0.314E+02 0.294E+03 0.113E+01 -.314E+02 -.294E+03 0.918E-02 -.312E-01 0.528E-02 -.727E-07 0.229E-06 -.346E-06

0.595E+00 0.144E+03 -.281E+03 -.612E+00 -.144E+03 0.281E+03 0.179E-01 0.125E+00 0.437E-01 -.891E-06 -.200E-05 0.137E-05

-.939E+00 -.159E+02 -.286E+03 0.931E+00 0.158E+02 0.286E+03 0.603E-02 0.900E-01 0.805E-01 -.152E-05 -.420E-05 0.604E-06

-.641E+00 -.265E+02 0.293E+03 0.637E+00 0.265E+02 -.293E+03 0.491E-02 0.233E-01 -

.272E-01 0.583E-06 -.850E-07 -.849E-06

-.534E+00 0.139E+03 0.289E+03 0.530E+00 -.139E+03 -.289E+03 0.655E-02 0.114E+00 -.215E-01 -.539E-06 -.937E-07 0.160E-05

0.779E+00 0.408E+02 -.287E+03 -.791E+00 -.408E+02 0.287E+03 0.525E-02 0.166E-02 -.190E-01 -.135E-05 -.353E-05 0.889E-06

-.458E+00 -.113E+03 -.276E+03 0.424E+00 0.113E+03 0.277E+03 0.349E-01 0.589E-01 -.268E+00 -.123E-05 -.378E-05 0.734E-06

-.572E+00 0.206E+03 0.279E+03 0.570E+00 -.206E+03 -.279E+03 0.115E-02 0.719E-01 -.456E-01 -.195E-06 -.241E-06 0.276E-05

-.784E+00 0.304E+02 0.294E+03 0.788E+00 -.304E+02 -.294E+03 -.756E-02 -.309E-01 -.153E-02 -.241E-06 0.180E-06 -.339E-06

-.123E+01 0.144E+03 -.281E+03 0.125E+01 -.145E+03 0.281E+03 -.159E-01 0.122E+00 0.504E-01 0.419E-06 -.331E-05 0.140E-05

-.366E+01 -.174E+02 -.283E+03 0.369E+01 0.173E+02 0.283E+03 -.307E-01 0.115E+00 0.595E-01 0.138E-05 -.472E-05 0.785E-06

-.130E+01 -.277E+02 0.291E+03 0.129E+01 0.277E+02 -.291E+03 -.133E-02 0.340E-01 -.220E-01 -.301E-06 0.572E-06 -.173E-05

-.348E+00 0.139E+03 0.289E+03 0.347E+00 -.139E+03 -.289E+03 0.121E-04 0.111E+00 -.148E-01 0.140E-06 -.119E-06 0.183E-05

-.830E+00 0.400E+02 -.287E+03 0.822E+00 -.400E+02 0.287E+03 0.125E-01 -.793E-02 -.181E-01 0.570E-06 -.423E-05 0.947E-06

-.787E+01 -.119E+03 -.267E+03 0.806E+01 0.119E+03 0.267E+03 -.189E+00 0.138E-02

0.353E-01 0.221E-05 -.399E-05 0.593E-06

-.410E+00 0.206E+03 0.279E+03 0.411E+00 -.206E+03 -.279E+03 -.281E-02 0.714E-01 -.466E-01 0.902E-06 -.902E-06 0.250E-05

-.653E-01 0.300E+02 0.294E+03 0.750E-01 -.299E+02 -.294E+03 -.949E-02 -.348E-01 0.106E-02 0.170E-07 -.104E-05 0.522E-06

-.206E+01 0.145E+03 -.282E+03 0.208E+01 -.145E+03 0.282E+03 -.189E-01 0.132E+00 0.257E-01 0.463E-06 -.239E-05 0.409E-06

-.257E+01 -.208E+02 -.285E+03 0.259E+01 0.208E+02 0.285E+03 -.292E-01 0.405E-01 0.319E-01 0.234E-05 -.281E-05 0.123E-05

-.555E+00 -.290E+02 0.291E+03 0.560E+00 0.290E+02 -.291E+03 -.286E-02 0.291E-01 -.252E-01 -.490E-06 -.950E-07 -.940E-06

0.579E-01 0.139E+03 0.289E+03 -.580E-01 -.139E+03 -.289E+03 -.354E-03 0.109E+00 -.209E-01 0.875E-06 -.121E-05 0.154E-05

-.290E+01 0.378E+02 -.286E+03 0.291E+01 -.378E+02 0.286E+03 -.147E-01 -.431E-02 0.211E-01 0.122E-05 -.280E-05 0.878E-06

-.514E+01 -.128E+03 -.271E+03 0.519E+01 0.128E+03 0.271E+03 -.463E-01 -.866E-01 0.381E-01 0.262E-05 -.315E-05 0.147E-05

0.395E+00 -.137E+03 0.280E+03 -.387E+00 0.137E+03 -.280E+03 -.971E-02 -.128E+00 -.158E-01 -.115E-05 -.898E-06 0.238E-06

0.193E+01 -.343E+03 0.233E+03 -.194E+01 0.344E+03 -.233E+03 0.910E-02 -.461E+00 -.549E-01 -.751E-06 -.318E-06 0.110E-05

-.253E+01 -.197E+03 -.259E+03 0.254E+01 0.197E+03 0.259E+03 -.941E-02 -.198E+00

0.371E-01 0.198E-05 -.360E-05 0.202E-05

0.691E+01 -.447E+03 -.198E+03 -.693E+01 0.448E+03 0.198E+03 0.966E-02 -.112E+01 0.887E-01 0.174E-05 0.941E-06 0.147E-05

-.476E+00 -.451E+03 0.204E+03 0.477E+00 0.452E+03 -.204E+03 -.213E-02 -.108E+01 -.113E+00 -.181E-05 -.447E-06 -.983E-06

0.171E+01 -.203E+03 0.269E+03 -.170E+01 0.203E+03 -.269E+03 -.481E-02 -.927E-01 -.322E-01 -.697E-06 -.127E-05 0.139E-05

-.211E+01 -.338E+03 -.222E+03 0.216E+01 0.338E+03 0.222E+03 -.441E-01 -.605E+00 0.540E-01 0.132E-05 -.558E-06 0.151E-05

0.218E+01 -.136E+03 0.282E+03 -.218E+01 0.136E+03 -.282E+03 -.634E-02 -.126E+00 -.962E-02 0.135E-06 -.153E-05 0.205E-05

0.672E+01 -.339E+03 0.238E+03 -.671E+01 0.340E+03 -.238E+03 -.126E-01 -.461E+00 -.462E-01 0.163E-05 0.271E-06 0.170E-05

0.679E+01 -.193E+03 -.259E+03 -.680E+01 0.193E+03 0.258E+03 0.111E-01 -.146E+00 0.634E-01 -.395E-06 -.287E-05 0.199E-05

0.313E+02 -.427E+03 -.198E+03 -.313E+02 0.428E+03 0.197E+03 0.727E-01 -.968E+00 0.135E+00 -.179E-05 0.281E-05 0.309E-06

0.544E+01 -.449E+03 0.209E+03 -.544E+01 0.450E+03 -.209E+03 0.654E-03 -.108E+01 -.801E-01 0.779E-06 0.268E-06 0.212E-05

0.369E+01 -.201E+03 0.272E+03 -.368E+01 0.201E+03 -.272E+03 -.701E-03 -.976E-01 -.308E-01 0.112E-05 -.870E-06 0.165E-05

0.124E+02 -.332E+03 -.223E+03 -.125E+02 0.332E+03 0.223E+03 0.120E+00 -.535E+00

0.316E-01 0.926E-06 0.481E-06 0.143E-05

0.219E+01 -.133E+03 0.283E+03 -.219E+01 0.133E+03 -.283E+03 0.578E-03 -.128E+00 -.463E-02 0.134E-05 -.530E-06 0.463E-06

0.494E+01 -.332E+03 0.245E+03 -.490E+01 0.332E+03 -.245E+03 -.319E-01 -.476E+00 -.377E-01 0.211E-05 0.102E-05 -.198E-05

0.112E+02 -.182E+03 -.258E+03 -.113E+02 0.182E+03 0.258E+03 0.469E-01 -.986E-01 -.105E+00 -.241E-05 -.302E-05 0.847E-06

0.319E+02 -.399E+03 -.175E+03 -.321E+02 0.401E+03 0.174E+03 0.292E+00 -.140E+01 0.133E+01 0.465E-05 0.588E-05 0.352E-05

0.931E+01 -.443E+03 0.219E+03 -.931E+01 0.444E+03 -.219E+03 -.546E-02 -.109E+01 -.483E-01 0.263E-05 0.914E-06 0.479E-06

0.170E+01 -.196E+03 0.273E+03 -.170E+01 0.197E+03 -.273E+03 0.551E-02 -.109E+00 -.513E-01 0.177E-05 0.499E-06 -.148E-05

0.172E+02 -.310E+03 -.216E+03 -.175E+02 0.310E+03 0.216E+03 0.324E+00 -.219E+00 0.123E+00 -.164E-05 0.165E-05 0.109E-05

-.103E+01 -.132E+03 0.281E+03 0.102E+01 0.132E+03 -.281E+03 0.103E-01 -.127E+00 -.780E-04 0.117E-05 0.700E-06 -.257E-05

-.511E+01 -.331E+03 0.239E+03 0.511E+01 0.332E+03 -.239E+03 0.877E-02 -.494E+00 -.422E-01 0.890E-06 0.157E-05 -.558E-05

0.159E+01 -.169E+03 -.261E+03 -.171E+01 0.169E+03 0.261E+03 0.116E+00 0.365E+00 -.980E-01 -.177E-05 0.115E-07 0.153E-05

-.650E+01 -.301E+03 -.189E+03 0.602E+01 0.296E+03 0.185E+03 0.469E+00 0.502E+01

0.412E+01 -.270E-05 0.840E-05 0.478E-05

-.604E+00 -.436E+03 0.227E+03 0.602E+00 0.437E+03 -.227E+03 0.157E-02 -.120E+01 -.483E-01 0.179E-05 0.134E-05 -.394E-05

-.302E+01 -.197E+03 0.268E+03 0.300E+01 0.197E+03 -.268E+03 0.146E-01 -.112E+00 -.431E-01 0.625E-06 0.116E-05 -.463E-05

0.341E+01 -.280E+03 -.215E+03 -.532E+01 0.280E+03 0.214E+03 0.191E+01 0.639E+00 0.824E+00 0.995E-06 0.914E-05 0.502E-05

-.274E+01 -.134E+03 0.277E+03 0.274E+01 0.134E+03 -.277E+03 0.246E-02 -.123E+00 -.187E-01 -.329E-06 0.115E-05 -.425E-05

-.602E+01 -.338E+03 0.230E+03 0.601E+01 0.339E+03 -.230E+03 0.112E-01 -.494E+00 -.463E-01 -.153E-05 0.105E-05 -.609E-05

-.651E+01 -.171E+03 -.257E+03 0.659E+01 0.170E+03 0.257E+03 -.760E-01 0.480E+00 0.132E-01 -.506E-06 -.115E-05 0.174E-05

-.443E+02 -.422E+03 -.184E+03 0.449E+02 0.423E+03 0.183E+03 -.563E+00 -.109E+01 0.631E+00 -.379E-05 0.633E-05 0.404E-05

-.867E+01 -.441E+03 0.211E+03 0.866E+01 0.442E+03 -.211E+03 0.143E-01 -.111E+01 -.757E-01 -.773E-06 0.107E-05 -.603E-05

-.293E+01 -.201E+03 0.265E+03 0.294E+01 0.201E+03 -.265E+03 -.918E-02 -.110E+00 -.206E-01 -.102E-05 0.103E-05 -.498E-05

-.145E+02 -.290E+03 -.209E+03 0.165E+02 0.289E+03 0.209E+03 -.197E+01 0.602E+00 0.785E+00 -.268E-05 0.851E-05 0.559E-05

-.139E+01 -.136E+03 0.277E+03 0.140E+01 0.136E+03 -.277E+03 -.102E-01 -.125E+00 -

.241E-01 -.109E-05 0.487E-06 -.298E-05

-.280E+01 -.343E+03 0.230E+03 0.278E+01 0.343E+03 -.230E+03 0.234E-01 -.473E+00 -.595E-01 -.218E-05 -.601E-07 -.307E-05

-.104E+02 -.189E+03 -.258E+03 0.105E+02 0.189E+03 0.258E+03 -.768E-01 -.139E+00 -.521E-01 0.313E-05 -.360E-05 0.843E-06

-.150E+02 -.446E+03 -.196E+03 0.150E+02 0.447E+03 0.196E+03 -.692E-01 -.112E+01 0.987E-01 0.192E-05 0.186E-05 0.783E-06

-.551E+01 -.448E+03 0.204E+03 0.552E+01 0.449E+03 -.204E+03 -.490E-02 -.108E+01 -.125E+00 -.249E-05 -.132E-06 -.507E-05

-.920E+00 -.203E+03 0.267E+03 0.929E+00 0.203E+03 -.267E+03 -.912E-02 -.102E+00 -.319E-01 -.174E-05 -.236E-06 -.203E-05

-.163E+02 -.329E+03 -.218E+03 0.167E+02 0.329E+03 0.218E+03 -.360E+00 -.480E+00 0.428E-01 0.129E-05 0.171E-05 0.133E-05

-.291E+01 -.253E+03 -.195E+03 0.184E+01 0.244E+03 0.189E+03 0.989E+00 0.789E+01 0.478E+01 0.703E-06 0.155E-04 0.138E-04

0.533E+02 -.518E+03 -.137E+03 -.544E+02 0.522E+03 0.141E+03 0.105E+01 -.395E+01 -.382E+01 0.397E-05 -.286E-05 0.313E-05

-.472E+02 -.590E+03 -.446E+03 0.532E+02 0.643E+03 0.480E+03 -.596E+01 -.518E+02 -.340E+02 -.111E-05 -.523E-05 -.165E-05

0.447E+01 0.286E+02 0.221E+02 -.291E-12 0.693E-11 0.142E-11 -.451E+01 -.286E+02 -.221E+02 0.383E-05 -.550E-04 0.102E-03

POSITION			TOTAL-FORCE (eV/Angst)		
1.24575	4.02870	5.43979	0.000048	0.000996	-0.000420
1.21024	4.07581	8.43726	-0.000975	0.002561	-0.001203
3.70862	4.02890	5.43965	0.000312	0.001868	-0.001105
3.67998	4.07733	8.43690	-0.004033	-0.000471	-0.002960
6.17157	4.02854	5.43942	-0.000005	-0.000162	-0.001765
6.14482	4.08292	8.43295	-0.002835	-0.003356	-0.003257
8.63513	4.02801	5.43869	0.000780	-0.000468	-0.002016
8.60339	4.08732	8.43089	-0.000133	-0.001225	-0.002289
11.09928	4.02784	5.43885	0.000879	0.001946	-0.002727
11.06021	4.08619	8.43099	-0.001740	0.000655	-0.000723
13.56311	4.02807	5.43972	0.000340	0.001597	-0.001634
13.52141	4.08047	8.43349	0.000413	-0.002307	0.000225
2.44241	15.48073	8.85224	-0.000619	-0.005204	0.002228
0.01714	15.44624	5.32469	0.000363	0.001540	-0.001194
4.86040	15.47728	8.86623	0.000880	0.000346	-0.000480
2.48016	15.44854	5.27562	0.000364	-0.001203	-0.000501
4.94382	15.44925	5.24869	0.001747	-0.002950	0.000241
12.31531	15.48242	9.00211	-0.002638	0.002021	0.004781

9.86772	15.44556	5.34176	0.000432	-0.001061	0.000878
14.76279	15.48245	8.89951	-0.006013	-0.000350	0.005369
12.33384	15.44510	5.36128	0.001385	-0.003197	-0.001303
7.40743	15.44616	5.26463	0.002401	0.001621	0.001339
6.44846	16.34427	7.40648	-0.001481	-0.000341	0.003869
8.60064	16.47644	7.89249	0.005279	0.001497	0.004161
1.24544	5.11881	5.35500	0.000955	0.000245	-0.002527
2.44348	5.83889	8.62292	0.002426	-0.004469	0.001184
0.01380	5.79530	5.28573	0.002078	-0.002539	0.000444
1.21063	5.16420	8.54151	0.000246	-0.000530	-0.001877
2.44351	7.27931	8.74832	-0.000082	-0.001251	-0.000152
3.70866	5.11896	5.35390	-0.000418	-0.001545	0.000263
4.90800	5.84315	8.62123	-0.001098	0.003815	-0.000812
2.47701	5.79561	5.28397	0.001451	-0.000676	-0.002634
3.67679	5.16572	8.54000	-0.000109	0.001619	-0.000026
4.90764	7.28398	8.74777	0.000742	-0.000606	0.001033
6.17184	5.11860	5.35433	0.001487	0.000480	0.000824
7.37096	5.84929	8.62094	-0.000596	0.007042	-0.002486
4.94029	5.79548	5.28340	0.000601	-0.002772	-0.001202
6.14080	5.17108	8.53715	-0.002516	0.002549	0.002485
7.37071	7.28983	8.75132	-0.001936	0.001641	0.000117
8.63543	5.11820	5.35521	0.001250	0.001453	-0.001146

9.83233	5.85166	8.62337	0.002787	0.000497	-0.001124
7.40374	5.79498	5.28512	0.003449	-0.002781	-0.001366
8.60194	5.17528	8.53759	-0.001894	-0.000385	-0.000179
9.83204	7.29110	8.75719	-0.001853	-0.002481	-0.002453
11.09930	5.11814	5.35578	-0.000861	-0.003242	-0.001441
12.29449	5.84673	8.62385	0.000033	0.005700	-0.002231
9.86750	5.79468	5.28678	-0.000748	-0.000808	0.001522
11.06261	5.17409	8.53894	0.002670	0.002734	-0.000361
12.29428	7.28729	8.75533	-0.004570	0.001231	-0.001539
13.56278	5.11829	5.35605	0.002665	0.000627	-0.002056
14.75895	5.83988	8.62434	-0.000185	-0.002683	-0.002253
12.33118	5.79480	5.28692	-0.004500	-0.001561	0.002564
13.52535	5.16844	8.54022	-0.003526	0.003816	-0.001405
14.75917	7.28012	8.75179	0.000902	0.002540	-0.000704
0.01434	7.23830	5.19017	0.000098	-0.000208	0.000041
1.24689	9.38061	5.13160	0.000545	-0.001853	-0.000038
1.21085	7.98059	8.79588	-0.000938	-0.000504	0.001498
2.44214	10.12243	8.87141	-0.000913	0.002986	-0.005031
0.01532	10.08686	5.14049	-0.002037	-0.000153	-0.002429
1.24606	7.94244	5.15775	0.002009	-0.002620	0.000802
1.21082	9.41592	8.85782	-0.000702	0.004508	0.000157
2.44072	11.55513	8.88414	-0.006183	-0.002536	0.001627

2.47747	7.23842	5.18585	0.002805	0.002878	0.001276
3.70997	9.38055	5.12566	-0.001069	-0.003000	0.000008
3.67534	7.98360	8.79349	-0.000521	0.001019	0.000907
4.90487	10.12925	8.87518	0.000285	-0.000491	-0.000038
2.47867	10.08713	5.12695	-0.002268	0.001493	0.000734
3.70939	7.94242	5.15441	0.000814	-0.004029	-0.001727
3.67589	9.41970	8.85445	-0.001499	0.002036	-0.000160
4.90263	11.56506	8.89086	-0.000578	0.001884	0.000863
4.94085	7.23830	5.18552	-0.004695	0.002252	0.000795
6.17318	9.38002	5.13173	0.002054	0.002109	0.001796
6.13864	7.99044	8.79647	0.002401	-0.000435	-0.001670
7.36780	10.13760	8.89473	-0.000924	0.002933	0.000619
4.94196	10.08682	5.12700	0.004127	0.001461	-0.001185
6.17284	7.94199	5.15766	-0.000053	0.000534	0.003002
6.13939	9.42660	8.86164	0.000765	-0.000483	-0.002120
7.36410	11.57721	8.92935	0.000172	-0.002602	0.002510
7.40426	7.23794	5.19012	0.002154	0.001767	0.001033
8.63700	9.37970	5.14543	-0.000524	0.002957	0.000909
8.60086	7.99568	8.80617	0.001076	-0.000758	-0.001180
9.83068	10.14286	8.92842	-0.002260	0.002038	-0.000445
7.40553	10.08627	5.14064	0.001187	-0.003611	0.003117
8.63637	7.94166	5.16555	0.002612	0.001759	-0.001439

8.60077	9.43254	8.88532	-0.006120	0.002633	-0.001307
9.82927	11.58244	9.00096	0.001081	0.004460	0.001417
9.86805	7.23787	5.19489	-0.000357	0.000098	-0.000254
11.10106	9.37979	5.15156	-0.003822	-0.001021	0.000620
11.06331	7.99411	8.80818	-0.000196	-0.001826	0.000008
12.29815	10.12943	8.90340	-0.000518	-0.001285	0.001463
9.86930	10.08593	5.15631	-0.005454	-0.001492	0.001378
11.10021	7.94175	5.16862	-0.000609	-0.003102	0.001361
11.06206	9.43062	8.88839	0.004659	0.002032	0.002015
12.30255	11.56557	8.94694	0.002639	-0.001068	-0.001893
12.33169	7.23799	5.19447	-0.001021	0.000242	-0.001792
13.56437	9.38021	5.14435	0.000723	0.001653	-0.000614
13.52754	7.98555	8.80171	-0.000725	-0.002685	-0.003126
14.76233	10.12320	8.88285	-0.005210	0.000687	-0.001660
12.33257	10.08637	5.15511	0.002646	0.000506	-0.001570
13.56350	7.94214	5.16485	-0.000087	-0.000909	-0.000401
13.52731	9.42040	8.86925	-0.000177	0.003093	-0.000443
14.76430	11.55727	8.90646	-0.002149	-0.000356	0.001842
0.01611	11.52516	5.16621	-0.001072	-0.002540	0.000355
1.24770	13.67535	5.22209	0.001870	-0.002135	-0.002505
1.21217	12.26335	8.89409	0.000745	-0.000466	0.001111
2.43998	14.38728	8.86748	-0.002666	-0.000044	0.000783

0.01699	14.35408	5.27295	-0.000470	-0.000924	-0.002034
1.24794	12.22963	5.17275	0.001047	0.000865	-0.001392
1.21434	13.70818	8.88771	0.001694	0.003295	0.003638
2.47958	11.52580	5.14547	-0.001613	-0.000182	-0.001523
3.71218	13.67636	5.19535	0.004555	0.000794	0.001068
3.66932	12.26248	8.88184	-0.002115	-0.000120	-0.000663
4.89370	14.38589	8.86075	0.003394	-0.002885	-0.002297
2.48000	14.35596	5.23149	0.001294	-0.001430	0.001627
3.71150	12.23022	5.15602	0.000902	-0.004508	0.000973
3.66212	13.70366	8.87117	-0.004951	0.005162	-0.000814
4.94290	11.52542	5.14351	-0.000051	-0.001747	-0.001637
6.17627	13.67505	5.20032	0.000882	0.000877	0.000057
6.13145	12.27911	8.90591	0.005218	0.006552	0.004489
7.36614	14.42967	8.88203	-0.002236	-0.002924	-0.000480
4.94347	14.35627	5.21375	0.000158	-0.002172	0.001091
6.17493	12.22917	5.16623	-0.001405	-0.001070	0.001509
6.11879	13.72336	8.87765	0.005267	0.003331	0.001166
7.40625	11.52413	5.16368	0.000929	-0.003293	0.000316
8.63876	13.67323	5.24377	0.001915	0.002421	-0.001338
8.58939	12.29067	9.00208	-0.004017	0.000009	-0.002177
9.83855	14.39048	9.30305	-0.001465	-0.028817	-0.007376
7.40672	14.35386	5.23530	-0.001128	-0.000802	-0.000780

8.63820	12.22778	5.19800	0.000303	-0.001241	0.001011
8.55571	13.73596	9.04598	0.009008	-0.004878	0.012772
9.86985	11.52338	5.18893	0.001772	-0.001919	-0.000146
11.10099	13.67352	5.27669	0.003129	-0.000571	-0.001012
11.07378	12.27333	9.00891	-0.000615	0.003336	-0.004110
12.30694	14.38896	9.00333	-0.000002	-0.003883	0.001007
9.86934	14.35300	5.29564	0.002958	-0.000358	-0.000199
11.10161	12.22804	5.21650	-0.001120	-0.002737	0.001026
11.11464	13.70636	9.07877	-0.004949	0.001616	0.007275
12.33326	11.52411	5.18815	-0.000923	0.000322	0.000502
13.56430	13.67399	5.25995	0.001604	0.000212	0.000064
13.53626	12.26601	8.93587	-0.002239	0.004156	0.001899
14.76266	14.38906	8.90426	-0.002785	0.000011	0.003752
12.33397	14.35288	5.30710	0.002752	-0.002234	-0.001828
13.56505	12.22870	5.20105	0.000085	0.000097	-0.001167
13.54921	13.70690	8.94399	-0.001244	-0.001554	0.000850
9.91126	15.53185	9.99472	-0.067463	-0.612990	-0.450926
7.28864	16.40884	8.69813	-0.003844	-0.006340	-0.007187
10.02526	16.50365	10.62998	0.079652	0.646707	0.461999

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total drift:	-0.045009	0.026010	-0.018126

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

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free energy TOTEN = -1209.38581936 eV

energy without entropy= -1209.38581936 energy(sigma->0) = -1209.38581936

d Force =-0.1156613E-03[-0.139E-01, 0.136E-01] d Energy =-0.2619393E-04-0.895E-04

d Force =-0.1441507E+02[-0.144E+02,-0.144E+02] d Ewald =-0.1441624E+02 0.117E-02

POTLOK: cpu time 0.1734: real time 0.1747

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stress matrix after NEB project (eV)

-17.71170 -0.16675 0.10826

-0.16675 -14.61635 0.88807

0.10826 0.88807 -18.76538

FORCES: max atom, RMS 0.798760 0.091163

FORCE total and by dimension 1.105288 0.646707

Stress total and by dimension 29.683967 18.765379

Finite differences progress:

Degree of freedom: 6/ 6

Displacement: 2/ 2

Total: 12/ 12

SECOND DERIVATIVES (NOT SYMMETRIZED)

	145X	145Y	145Z	147X	147Y	147Z
145X	-14.344316	-8.619292	-5.642213	5.387912	6.720885	4.507638
145Y	-8.667646	-98.734334	-59.519549	7.136466	62.909021	40.038571
145Z	-5.655137	-59.500180	-45.396676	4.651738	39.828980	30.215045
147X	5.390744	7.120607	4.646428	-3.238222	-7.284748	-4.986668
147Y	6.739275	62.913522	39.876533	-7.314380	-64.999566	-42.058262

147Z 4.513933 39.988644 30.217639 -4.997413 -42.002149 -30.542910

Eigenvectors and eigenvalues of the dynamical matrix

---

1 f = 62.138107 THz 390.425242 2PiTHz 2072.704086 cm-1 256.982647 meV

X	Y	Z	dx	dy	dz
1.245750	4.028696	5.439790	0	0	0
1.210240	4.075813	8.437264	0	0	0
3.708620	4.028896	5.439647	0	0	0
3.679981	4.077333	8.436900	0	0	0
6.171574	4.028537	5.439423	0	0	0
6.144822	4.082922	8.432952	0	0	0
8.635129	4.028007	5.438685	0	0	0
8.603386	4.087320	8.430892	0	0	0
11.099276	4.027838	5.438849	0	0	0
11.060208	4.086191	8.430988	0	0	0
13.563114	4.028068	5.439721	0	0	0
13.521407	4.080469	8.433485	0	0	0
2.442410	15.480732	8.852243	0	0	0

0.017143	15.446242	5.324686	0	0	0
4.860405	15.477285	8.866232	0	0	0
2.480161	15.448544	5.275619	0	0	0
4.943820	15.449251	5.248689	0	0	0
12.315308	15.482418	9.002109	0	0	0
9.867716	15.445563	5.341755	0	0	0
14.762794	15.482453	8.899515	0	0	0
12.333845	15.445098	5.361284	0	0	0
7.407428	15.446161	5.264635	0	0	0
6.448461	16.344273	7.406481	0	0	0
8.600641	16.476444	7.892492	0	0	0
1.245442	5.118809	5.355005	0	0	0
2.443484	5.838886	8.622924	0	0	0
0.013795	5.795296	5.285730	0	0	0
1.210631	5.164204	8.541507	0	0	0
2.443506	7.279307	8.748318	0	0	0
3.708657	5.118963	5.353897	0	0	0
4.907998	5.843148	8.621230	0	0	0
2.477011	5.795606	5.283967	0	0	0
3.676791	5.165724	8.540005	0	0	0
4.907637	7.283976	8.747768	0	0	0
6.171844	5.118599	5.354330	0	0	0

7.370958	5.849291	8.620941	0	0	0
4.940290	5.795478	5.283402	0	0	0
6.140801	5.171085	8.537152	0	0	0
7.370710	7.289828	8.751319	0	0	0
8.635429	5.118198	5.355206	0	0	0
9.832333	5.851658	8.623372	0	0	0
7.403740	5.794978	5.285116	0	0	0
8.601944	5.175280	8.537586	0	0	0
9.832040	7.291102	8.757194	0	0	0
11.099301	5.118139	5.355778	0	0	0
12.294487	5.846734	8.623846	0	0	0
9.867501	5.794678	5.286784	0	0	0
11.062615	5.174090	8.538935	0	0	0
12.294275	7.287294	8.755327	0	0	0
13.562782	5.118287	5.356054	0	0	0
14.758955	5.839879	8.624340	0	0	0
12.331181	5.794804	5.286924	0	0	0
13.525352	5.168439	8.540216	0	0	0
14.759167	7.280119	8.751789	0	0	0
0.014336	7.238301	5.190167	0	0	0
1.246890	9.380615	5.131604	0	0	0
1.210852	7.980592	8.795883	0	0	0

2.442140	10.122434	8.871408	0	0	0
0.015317	10.086865	5.140485	0	0	0
1.246057	7.942443	5.157748	0	0	0
1.210824	9.415918	8.857817	0	0	0
2.440724	11.555126	8.884137	0	0	0
2.477470	7.238419	5.185851	0	0	0
3.709968	9.380553	5.125659	0	0	0
3.675342	7.983601	8.793493	0	0	0
4.904874	10.129253	8.875180	0	0	0
2.478671	10.087127	5.126952	0	0	0
3.709392	7.942417	5.154413	0	0	0
3.675893	9.419704	8.854452	0	0	0
4.902634	11.565058	8.890860	0	0	0
4.940845	7.238299	5.185525	0	0	0
6.173182	9.380022	5.131732	0	0	0
6.138637	7.990443	8.796473	0	0	0
7.367803	10.137604	8.894732	0	0	0
4.941960	10.086817	5.126998	0	0	0
6.172836	7.941986	5.157656	0	0	0
6.139386	9.426599	8.861638	0	0	0
7.364099	11.577214	8.929347	0	0	0
7.404261	7.237943	5.190115	0	0	0

8.637001	9.379701	5.145427	0	0	0
8.600855	7.995677	8.806165	0	0	0
9.830681	10.142862	8.928417	0	0	0
7.405532	10.086269	5.140638	0	0	0
8.636371	7.941660	5.165549	0	0	0
8.600773	9.432544	8.885323	0	0	0
9.829269	11.582438	9.000960	0	0	0
9.868054	7.237874	5.194891	0	0	0
11.101065	9.379793	5.151558	0	0	0
11.063307	7.994108	8.808185	0	0	0
12.298149	10.129431	8.903401	0	0	0
9.869303	10.085933	5.156309	0	0	0
11.100208	7.941749	5.168618	0	0	0
11.062057	9.430623	8.888392	0	0	0
12.302548	11.565567	8.946939	0	0	0
12.331694	7.237995	5.194469	0	0	0
13.564367	9.380209	5.144347	0	0	0
13.527537	7.985546	8.801711	0	0	0
14.762327	10.123195	8.882854	0	0	0
12.332567	10.086366	5.155112	0	0	0
13.563503	7.942142	5.164851	0	0	0
13.527308	9.420405	8.869248	0	0	0

14.764303	11.557270	8.906463	0	0	0
0.016106	11.525163	5.166210	0	0	0
1.247700	13.675348	5.222087	0	0	0
1.212166	12.263355	8.894092	0	0	0
2.439982	14.387277	8.867485	0	0	0
0.016989	14.354079	5.272951	0	0	0
1.247937	12.229631	5.172747	0	0	0
1.214345	13.708176	8.887715	0	0	0
2.479583	11.525801	5.145468	0	0	0
3.712181	13.676356	5.195353	0	0	0
3.669320	12.262483	8.881842	0	0	0
4.893701	14.385890	8.860749	0	0	0
2.480004	14.355964	5.231485	0	0	0
3.711497	12.230218	5.156022	0	0	0
3.662122	13.703663	8.871173	0	0	0
4.942897	11.525420	5.143507	0	0	0
6.176274	13.675051	5.200324	0	0	0
6.131455	12.279109	8.905909	0	0	0
7.366144	14.429670	8.882028	0	0	0
4.943471	14.356269	5.213748	0	0	0
6.174933	12.229172	5.166227	0	0	0
6.118786	13.723364	8.877654	0	0	0

7.406253	11.524130	5.163677	0	0	0
8.638758	13.673235	5.243767	0	0	0
8.589395	12.290668	9.002075	0	0	0
9.838554	14.390477	9.303050	0	0	0
7.406718	14.353861	5.235297	0	0	0
8.638200	12.227779	5.198004	0	0	0
8.555707	13.735963	9.045978	0	0	0
9.869847	11.523381	5.188925	0	0	0
11.100990	13.673517	5.276688	0	0	0
11.073784	12.273332	9.008906	0	0	0
12.306938	14.388964	9.003328	0	0	0
9.869336	14.352999	5.295636	0	0	0
11.101606	12.228036	5.216496	0	0	0
11.114641	13.706356	9.078765	0	0	0
12.333258	11.524106	5.188149	0	0	0
13.564299	13.673994	5.259947	0	0	0
13.536260	12.266008	8.935868	0	0	0
14.762665	14.389058	8.904260	0	0	0
12.333972	14.352875	5.307100	0	0	0
13.565052	12.228698	5.201052	0	0	0
13.549212	13.706896	8.943993	0	0	0
9.911257	15.531849	9.994722	0.072317	0.696480	0.455417

7.288643	16.408837	8.698126	0	0	0
10.025257	16.503653	10.644976	-0.053949	-0.454239	-0.305020

2 f = 19.764670 THz 124.185082 2PiTHz 659.278395 cm-1 81.740133 meV

X	Y	Z	dx	dy	dz
1.245750	4.028696	5.439790	0	0	0
1.210240	4.075813	8.437264	0	0	0
3.708620	4.028896	5.439647	0	0	0
3.679981	4.077333	8.436900	0	0	0
6.171574	4.028537	5.439423	0	0	0
6.144822	4.082922	8.432952	0	0	0
8.635129	4.028007	5.438685	0	0	0
8.603386	4.087320	8.430892	0	0	0
11.099276	4.027838	5.438849	0	0	0
11.060208	4.086191	8.430988	0	0	0
13.563114	4.028068	5.439721	0	0	0
13.521407	4.080469	8.433485	0	0	0
2.442410	15.480732	8.852243	0	0	0
0.017143	15.446242	5.324686	0	0	0
4.860405	15.477285	8.866232	0	0	0
2.480161	15.448544	5.275619	0	0	0
4.943820	15.449251	5.248689	0	0	0

12.315308	15.482418	9.002109	0	0	0
9.867716	15.445563	5.341755	0	0	0
14.762794	15.482453	8.899515	0	0	0
12.333845	15.445098	5.361284	0	0	0
7.407428	15.446161	5.264635	0	0	0
6.448461	16.344273	7.406481	0	0	0
8.600641	16.476444	7.892492	0	0	0
1.245442	5.118809	5.355005	0	0	0
2.443484	5.838886	8.622924	0	0	0
0.013795	5.795296	5.285730	0	0	0
1.210631	5.164204	8.541507	0	0	0
2.443506	7.279307	8.748318	0	0	0
3.708657	5.118963	5.353897	0	0	0
4.907998	5.843148	8.621230	0	0	0
2.477011	5.795606	5.283967	0	0	0
3.676791	5.165724	8.540005	0	0	0
4.907637	7.283976	8.747768	0	0	0
6.171844	5.118599	5.354330	0	0	0
7.370958	5.849291	8.620941	0	0	0
4.940290	5.795478	5.283402	0	0	0
6.140801	5.171085	8.537152	0	0	0
7.370710	7.289828	8.751319	0	0	0

8.635429	5.118198	5.355206	0	0	0
9.832333	5.851658	8.623372	0	0	0
7.403740	5.794978	5.285116	0	0	0
8.601944	5.175280	8.537586	0	0	0
9.832040	7.291102	8.757194	0	0	0
11.099301	5.118139	5.355778	0	0	0
12.294487	5.846734	8.623846	0	0	0
9.867501	5.794678	5.286784	0	0	0
11.062615	5.174090	8.538935	0	0	0
12.294275	7.287294	8.755327	0	0	0
13.562782	5.118287	5.356054	0	0	0
14.758955	5.839879	8.624340	0	0	0
12.331181	5.794804	5.286924	0	0	0
13.525352	5.168439	8.540216	0	0	0
14.759167	7.280119	8.751789	0	0	0
0.014336	7.238301	5.190167	0	0	0
1.246890	9.380615	5.131604	0	0	0
1.210852	7.980592	8.795883	0	0	0
2.442140	10.122434	8.871408	0	0	0
0.015317	10.086865	5.140485	0	0	0
1.246057	7.942443	5.157748	0	0	0
1.210824	9.415918	8.857817	0	0	0

2.440724	11.555126	8.884137	0	0	0
2.477470	7.238419	5.185851	0	0	0
3.709968	9.380553	5.125659	0	0	0
3.675342	7.983601	8.793493	0	0	0
4.904874	10.129253	8.875180	0	0	0
2.478671	10.087127	5.126952	0	0	0
3.709392	7.942417	5.154413	0	0	0
3.675893	9.419704	8.854452	0	0	0
4.902634	11.565058	8.890860	0	0	0
4.940845	7.238299	5.185525	0	0	0
6.173182	9.380022	5.131732	0	0	0
6.138637	7.990443	8.796473	0	0	0
7.367803	10.137604	8.894732	0	0	0
4.941960	10.086817	5.126998	0	0	0
6.172836	7.941986	5.157656	0	0	0
6.139386	9.426599	8.861638	0	0	0
7.364099	11.577214	8.929347	0	0	0
7.404261	7.237943	5.190115	0	0	0
8.637001	9.379701	5.145427	0	0	0
8.600855	7.995677	8.806165	0	0	0
9.830681	10.142862	8.928417	0	0	0
7.405532	10.086269	5.140638	0	0	0

8.636371	7.941660	5.165549	0	0	0
8.600773	9.432544	8.885323	0	0	0
9.829269	11.582438	9.000960	0	0	0
9.868054	7.237874	5.194891	0	0	0
11.101065	9.379793	5.151558	0	0	0
11.063307	7.994108	8.808185	0	0	0
12.298149	10.129431	8.903401	0	0	0
9.869303	10.085933	5.156309	0	0	0
11.100208	7.941749	5.168618	0	0	0
11.062057	9.430623	8.888392	0	0	0
12.302548	11.565567	8.946939	0	0	0
12.331694	7.237995	5.194469	0	0	0
13.564367	9.380209	5.144347	0	0	0
13.527537	7.985546	8.801711	0	0	0
14.762327	10.123195	8.882854	0	0	0
12.332567	10.086366	5.155112	0	0	0
13.563503	7.942142	5.164851	0	0	0
13.527308	9.420405	8.869248	0	0	0
14.764303	11.557270	8.906463	0	0	0
0.016106	11.525163	5.166210	0	0	0
1.247700	13.675348	5.222087	0	0	0
1.212166	12.263355	8.894092	0	0	0

2.439982	14.387277	8.867485	0	0	0
0.016989	14.354079	5.272951	0	0	0
1.247937	12.229631	5.172747	0	0	0
1.214345	13.708176	8.887715	0	0	0
2.479583	11.525801	5.145468	0	0	0
3.712181	13.676356	5.195353	0	0	0
3.669320	12.262483	8.881842	0	0	0
4.893701	14.385890	8.860749	0	0	0
2.480004	14.355964	5.231485	0	0	0
3.711497	12.230218	5.156022	0	0	0
3.662122	13.703663	8.871173	0	0	0
4.942897	11.525420	5.143507	0	0	0
6.176274	13.675051	5.200324	0	0	0
6.131455	12.279109	8.905909	0	0	0
7.366144	14.429670	8.882028	0	0	0
4.943471	14.356269	5.213748	0	0	0
6.174933	12.229172	5.166227	0	0	0
6.118786	13.723364	8.877654	0	0	0
7.406253	11.524130	5.163677	0	0	0
8.638758	13.673235	5.243767	0	0	0
8.589395	12.290668	9.002075	0	0	0
9.838554	14.390477	9.303050	0	0	0

7.406718	14.353861	5.235297	0	0	0
8.638200	12.227779	5.198004	0	0	0
8.555707	13.735963	9.045978	0	0	0
9.869847	11.523381	5.188925	0	0	0
11.100990	13.673517	5.276688	0	0	0
11.073784	12.273332	9.008906	0	0	0
12.306938	14.388964	9.003328	0	0	0
9.869336	14.352999	5.295636	0	0	0
11.101606	12.228036	5.216496	0	0	0
11.114641	13.706356	9.078765	0	0	0
12.333258	11.524106	5.188149	0	0	0
13.564299	13.673994	5.259947	0	0	0
13.536260	12.266008	8.935868	0	0	0
14.762665	14.389058	8.904260	0	0	0
12.333972	14.352875	5.307100	0	0	0
13.565052	12.228698	5.201052	0	0	0
13.549212	13.706896	8.943993	0	0	0
9.911257	15.531849	9.994722	-0.109154	0.508971	0.230654
7.288643	16.408837	8.698126	0	0	0
10.025257	16.503653	10.644976	0.110052	0.669101	0.464786

3 f = 17.229065 THz 108.253405 2PiTHz 574.699715 cm-1 71.253709 meV

X	Y	Z	dx	dy	dz
1.245750	4.028696	5.439790	0	0	0
1.210240	4.075813	8.437264	0	0	0
3.708620	4.028896	5.439647	0	0	0
3.679981	4.077333	8.436900	0	0	0
6.171574	4.028537	5.439423	0	0	0
6.144822	4.082922	8.432952	0	0	0
8.635129	4.028007	5.438685	0	0	0
8.603386	4.087320	8.430892	0	0	0
11.099276	4.027838	5.438849	0	0	0
11.060208	4.086191	8.430988	0	0	0
13.563114	4.028068	5.439721	0	0	0
13.521407	4.080469	8.433485	0	0	0
2.442410	15.480732	8.852243	0	0	0
0.017143	15.446242	5.324686	0	0	0
4.860405	15.477285	8.866232	0	0	0
2.480161	15.448544	5.275619	0	0	0
4.943820	15.449251	5.248689	0	0	0
12.315308	15.482418	9.002109	0	0	0
9.867716	15.445563	5.341755	0	0	0
14.762794	15.482453	8.899515	0	0	0
12.333845	15.445098	5.361284	0	0	0

7.407428	15.446161	5.264635	0	0	0
6.448461	16.344273	7.406481	0	0	0
8.600641	16.476444	7.892492	0	0	0
1.245442	5.118809	5.355005	0	0	0
2.443484	5.838886	8.622924	0	0	0
0.013795	5.795296	5.285730	0	0	0
1.210631	5.164204	8.541507	0	0	0
2.443506	7.279307	8.748318	0	0	0
3.708657	5.118963	5.353897	0	0	0
4.907998	5.843148	8.621230	0	0	0
2.477011	5.795606	5.283967	0	0	0
3.676791	5.165724	8.540005	0	0	0
4.907637	7.283976	8.747768	0	0	0
6.171844	5.118599	5.354330	0	0	0
7.370958	5.849291	8.620941	0	0	0
4.940290	5.795478	5.283402	0	0	0
6.140801	5.171085	8.537152	0	0	0
7.370710	7.289828	8.751319	0	0	0
8.635429	5.118198	5.355206	0	0	0
9.832333	5.851658	8.623372	0	0	0
7.403740	5.794978	5.285116	0	0	0
8.601944	5.175280	8.537586	0	0	0

9.832040	7.291102	8.757194	0	0	0
11.099301	5.118139	5.355778	0	0	0
12.294487	5.846734	8.623846	0	0	0
9.867501	5.794678	5.286784	0	0	0
11.062615	5.174090	8.538935	0	0	0
12.294275	7.287294	8.755327	0	0	0
13.562782	5.118287	5.356054	0	0	0
14.758955	5.839879	8.624340	0	0	0
12.331181	5.794804	5.286924	0	0	0
13.525352	5.168439	8.540216	0	0	0
14.759167	7.280119	8.751789	0	0	0
0.014336	7.238301	5.190167	0	0	0
1.246890	9.380615	5.131604	0	0	0
1.210852	7.980592	8.795883	0	0	0
2.442140	10.122434	8.871408	0	0	0
0.015317	10.086865	5.140485	0	0	0
1.246057	7.942443	5.157748	0	0	0
1.210824	9.415918	8.857817	0	0	0
2.440724	11.555126	8.884137	0	0	0
2.477470	7.238419	5.185851	0	0	0
3.709968	9.380553	5.125659	0	0	0
3.675342	7.983601	8.793493	0	0	0

4.904874	10.129253	8.875180	0	0	0
2.478671	10.087127	5.126952	0	0	0
3.709392	7.942417	5.154413	0	0	0
3.675893	9.419704	8.854452	0	0	0
4.902634	11.565058	8.890860	0	0	0
4.940845	7.238299	5.185525	0	0	0
6.173182	9.380022	5.131732	0	0	0
6.138637	7.990443	8.796473	0	0	0
7.367803	10.137604	8.894732	0	0	0
4.941960	10.086817	5.126998	0	0	0
6.172836	7.941986	5.157656	0	0	0
6.139386	9.426599	8.861638	0	0	0
7.364099	11.577214	8.929347	0	0	0
7.404261	7.237943	5.190115	0	0	0
8.637001	9.379701	5.145427	0	0	0
8.600855	7.995677	8.806165	0	0	0
9.830681	10.142862	8.928417	0	0	0
7.405532	10.086269	5.140638	0	0	0
8.636371	7.941660	5.165549	0	0	0
8.600773	9.432544	8.885323	0	0	0
9.829269	11.582438	9.000960	0	0	0
9.868054	7.237874	5.194891	0	0	0

11.101065	9.379793	5.151558	0	0	0
11.063307	7.994108	8.808185	0	0	0
12.298149	10.129431	8.903401	0	0	0
9.869303	10.085933	5.156309	0	0	0
11.100208	7.941749	5.168618	0	0	0
11.062057	9.430623	8.888392	0	0	0
12.302548	11.565567	8.946939	0	0	0
12.331694	7.237995	5.194469	0	0	0
13.564367	9.380209	5.144347	0	0	0
13.527537	7.985546	8.801711	0	0	0
14.762327	10.123195	8.882854	0	0	0
12.332567	10.086366	5.155112	0	0	0
13.563503	7.942142	5.164851	0	0	0
13.527308	9.420405	8.869248	0	0	0
14.764303	11.557270	8.906463	0	0	0
0.016106	11.525163	5.166210	0	0	0
1.247700	13.675348	5.222087	0	0	0
1.212166	12.263355	8.894092	0	0	0
2.439982	14.387277	8.867485	0	0	0
0.016989	14.354079	5.272951	0	0	0
1.247937	12.229631	5.172747	0	0	0
1.214345	13.708176	8.887715	0	0	0

2.479583	11.525801	5.145468	0	0	0
3.712181	13.676356	5.195353	0	0	0
3.669320	12.262483	8.881842	0	0	0
4.893701	14.385890	8.860749	0	0	0
2.480004	14.355964	5.231485	0	0	0
3.711497	12.230218	5.156022	0	0	0
3.662122	13.703663	8.871173	0	0	0
4.942897	11.525420	5.143507	0	0	0
6.176274	13.675051	5.200324	0	0	0
6.131455	12.279109	8.905909	0	0	0
7.366144	14.429670	8.882028	0	0	0
4.943471	14.356269	5.213748	0	0	0
6.174933	12.229172	5.166227	0	0	0
6.118786	13.723364	8.877654	0	0	0
7.406253	11.524130	5.163677	0	0	0
8.638758	13.673235	5.243767	0	0	0
8.589395	12.290668	9.002075	0	0	0
9.838554	14.390477	9.303050	0	0	0
7.406718	14.353861	5.235297	0	0	0
8.638200	12.227779	5.198004	0	0	0
8.555707	13.735963	9.045978	0	0	0
9.869847	11.523381	5.188925	0	0	0

11.100990	13.673517	5.276688	0	0	0
11.073784	12.273332	9.008906	0	0	0
12.306938	14.388964	9.003328	0	0	0
9.869336	14.352999	5.295636	0	0	0
11.101606	12.228036	5.216496	0	0	0
11.114641	13.706356	9.078765	0	0	0
12.333258	11.524106	5.188149	0	0	0
13.564299	13.673994	5.259947	0	0	0
13.536260	12.266008	8.935868	0	0	0
14.762665	14.389058	8.904260	0	0	0
12.333972	14.352875	5.307100	0	0	0
13.565052	12.228698	5.201052	0	0	0
13.549212	13.706896	8.943993	0	0	0
9.911257	15.531849	9.994722	-0.946664	-0.014731	0.014422
7.288643	16.408837	8.698126	0	0	0
10.025257	16.503653	10.644976	0.279249	-0.130396	-0.091751

4 f = 12.865144 THz 80.834085 2PiTHz 429.135008 cm-1 53.205979 meV

X	Y	Z	dx	dy	dz
1.245750	4.028696	5.439790	0	0	0
1.210240	4.075813	8.437264	0	0	0
3.708620	4.028896	5.439647	0	0	0

3.679981	4.077333	8.436900	0	0	0
6.171574	4.028537	5.439423	0	0	0
6.144822	4.082922	8.432952	0	0	0
8.635129	4.028007	5.438685	0	0	0
8.603386	4.087320	8.430892	0	0	0
11.099276	4.027838	5.438849	0	0	0
11.060208	4.086191	8.430988	0	0	0
13.563114	4.028068	5.439721	0	0	0
13.521407	4.080469	8.433485	0	0	0
2.442410	15.480732	8.852243	0	0	0
0.017143	15.446242	5.324686	0	0	0
4.860405	15.477285	8.866232	0	0	0
2.480161	15.448544	5.275619	0	0	0
4.943820	15.449251	5.248689	0	0	0
12.315308	15.482418	9.002109	0	0	0
9.867716	15.445563	5.341755	0	0	0
14.762794	15.482453	8.899515	0	0	0
12.333845	15.445098	5.361284	0	0	0
7.407428	15.446161	5.264635	0	0	0
6.448461	16.344273	7.406481	0	0	0
8.600641	16.476444	7.892492	0	0	0
1.245442	5.118809	5.355005	0	0	0

2.443484	5.838886	8.622924	0	0	0
0.013795	5.795296	5.285730	0	0	0
1.210631	5.164204	8.541507	0	0	0
2.443506	7.279307	8.748318	0	0	0
3.708657	5.118963	5.353897	0	0	0
4.907998	5.843148	8.621230	0	0	0
2.477011	5.795606	5.283967	0	0	0
3.676791	5.165724	8.540005	0	0	0
4.907637	7.283976	8.747768	0	0	0
6.171844	5.118599	5.354330	0	0	0
7.370958	5.849291	8.620941	0	0	0
4.940290	5.795478	5.283402	0	0	0
6.140801	5.171085	8.537152	0	0	0
7.370710	7.289828	8.751319	0	0	0
8.635429	5.118198	5.355206	0	0	0
9.832333	5.851658	8.623372	0	0	0
7.403740	5.794978	5.285116	0	0	0
8.601944	5.175280	8.537586	0	0	0
9.832040	7.291102	8.757194	0	0	0
11.099301	5.118139	5.355778	0	0	0
12.294487	5.846734	8.623846	0	0	0
9.867501	5.794678	5.286784	0	0	0

11.062615	5.174090	8.538935	0	0	0
12.294275	7.287294	8.755327	0	0	0
13.562782	5.118287	5.356054	0	0	0
14.758955	5.839879	8.624340	0	0	0
12.331181	5.794804	5.286924	0	0	0
13.525352	5.168439	8.540216	0	0	0
14.759167	7.280119	8.751789	0	0	0
0.014336	7.238301	5.190167	0	0	0
1.246890	9.380615	5.131604	0	0	0
1.210852	7.980592	8.795883	0	0	0
2.442140	10.122434	8.871408	0	0	0
0.015317	10.086865	5.140485	0	0	0
1.246057	7.942443	5.157748	0	0	0
1.210824	9.415918	8.857817	0	0	0
2.440724	11.555126	8.884137	0	0	0
2.477470	7.238419	5.185851	0	0	0
3.709968	9.380553	5.125659	0	0	0
3.675342	7.983601	8.793493	0	0	0
4.904874	10.129253	8.875180	0	0	0
2.478671	10.087127	5.126952	0	0	0
3.709392	7.942417	5.154413	0	0	0
3.675893	9.419704	8.854452	0	0	0

4.902634	11.565058	8.890860	0	0	0
4.940845	7.238299	5.185525	0	0	0
6.173182	9.380022	5.131732	0	0	0
6.138637	7.990443	8.796473	0	0	0
7.367803	10.137604	8.894732	0	0	0
4.941960	10.086817	5.126998	0	0	0
6.172836	7.941986	5.157656	0	0	0
6.139386	9.426599	8.861638	0	0	0
7.364099	11.577214	8.929347	0	0	0
7.404261	7.237943	5.190115	0	0	0
8.637001	9.379701	5.145427	0	0	0
8.600855	7.995677	8.806165	0	0	0
9.830681	10.142862	8.928417	0	0	0
7.405532	10.086269	5.140638	0	0	0
8.636371	7.941660	5.165549	0	0	0
8.600773	9.432544	8.885323	0	0	0
9.829269	11.582438	9.000960	0	0	0
9.868054	7.237874	5.194891	0	0	0
11.101065	9.379793	5.151558	0	0	0
11.063307	7.994108	8.808185	0	0	0
12.298149	10.129431	8.903401	0	0	0
9.869303	10.085933	5.156309	0	0	0

11.100208	7.941749	5.168618	0	0	0
11.062057	9.430623	8.888392	0	0	0
12.302548	11.565567	8.946939	0	0	0
12.331694	7.237995	5.194469	0	0	0
13.564367	9.380209	5.144347	0	0	0
13.527537	7.985546	8.801711	0	0	0
14.762327	10.123195	8.882854	0	0	0
12.332567	10.086366	5.155112	0	0	0
13.563503	7.942142	5.164851	0	0	0
13.527308	9.420405	8.869248	0	0	0
14.764303	11.557270	8.906463	0	0	0
0.016106	11.525163	5.166210	0	0	0
1.247700	13.675348	5.222087	0	0	0
1.212166	12.263355	8.894092	0	0	0
2.439982	14.387277	8.867485	0	0	0
0.016989	14.354079	5.272951	0	0	0
1.247937	12.229631	5.172747	0	0	0
1.214345	13.708176	8.887715	0	0	0
2.479583	11.525801	5.145468	0	0	0
3.712181	13.676356	5.195353	0	0	0
3.669320	12.262483	8.881842	0	0	0
4.893701	14.385890	8.860749	0	0	0

2.480004	14.355964	5.231485	0	0	0
3.711497	12.230218	5.156022	0	0	0
3.662122	13.703663	8.871173	0	0	0
4.942897	11.525420	5.143507	0	0	0
6.176274	13.675051	5.200324	0	0	0
6.131455	12.279109	8.905909	0	0	0
7.366144	14.429670	8.882028	0	0	0
4.943471	14.356269	5.213748	0	0	0
6.174933	12.229172	5.166227	0	0	0
6.118786	13.723364	8.877654	0	0	0
7.406253	11.524130	5.163677	0	0	0
8.638758	13.673235	5.243767	0	0	0
8.589395	12.290668	9.002075	0	0	0
9.838554	14.390477	9.303050	0	0	0
7.406718	14.353861	5.235297	0	0	0
8.638200	12.227779	5.198004	0	0	0
8.555707	13.735963	9.045978	0	0	0
9.869847	11.523381	5.188925	0	0	0
11.100990	13.673517	5.276688	0	0	0
11.073784	12.273332	9.008906	0	0	0
12.306938	14.388964	9.003328	0	0	0
9.869336	14.352999	5.295636	0	0	0

11.101606	12.228036	5.216496	0	0	0
11.114641	13.706356	9.078765	0	0	0
12.333258	11.524106	5.188149	0	0	0
13.564299	13.673994	5.259947	0	0	0
13.536260	12.266008	8.935868	0	0	0
14.762665	14.389058	8.904260	0	0	0
12.333972	14.352875	5.307100	0	0	0
13.565052	12.228698	5.201052	0	0	0
13.549212	13.706896	8.943993	0	0	0
9.911257	15.531849	9.994722	0.011699	-0.455998	0.781392
7.288643	16.408837	8.698126	0	0	0
10.025257	16.503653	10.644976	0.010244	0.292567	-0.309280

5 f = 3.487700 THz 21.913864 2PiTHz 116.337141 cm-1 14.423972 meV

X	Y	Z	dx	dy	dz
1.245750	4.028696	5.439790	0	0	0
1.210240	4.075813	8.437264	0	0	0
3.708620	4.028896	5.439647	0	0	0
3.679981	4.077333	8.436900	0	0	0
6.171574	4.028537	5.439423	0	0	0
6.144822	4.082922	8.432952	0	0	0
8.635129	4.028007	5.438685	0	0	0

8.603386	4.087320	8.430892	0	0	0
11.099276	4.027838	5.438849	0	0	0
11.060208	4.086191	8.430988	0	0	0
13.563114	4.028068	5.439721	0	0	0
13.521407	4.080469	8.433485	0	0	0
2.442410	15.480732	8.852243	0	0	0
0.017143	15.446242	5.324686	0	0	0
4.860405	15.477285	8.866232	0	0	0
2.480161	15.448544	5.275619	0	0	0
4.943820	15.449251	5.248689	0	0	0
12.315308	15.482418	9.002109	0	0	0
9.867716	15.445563	5.341755	0	0	0
14.762794	15.482453	8.899515	0	0	0
12.333845	15.445098	5.361284	0	0	0
7.407428	15.446161	5.264635	0	0	0
6.448461	16.344273	7.406481	0	0	0
8.600641	16.476444	7.892492	0	0	0
1.245442	5.118809	5.355005	0	0	0
2.443484	5.838886	8.622924	0	0	0
0.013795	5.795296	5.285730	0	0	0
1.210631	5.164204	8.541507	0	0	0
2.443506	7.279307	8.748318	0	0	0

3.708657	5.118963	5.353897	0	0	0
4.907998	5.843148	8.621230	0	0	0
2.477011	5.795606	5.283967	0	0	0
3.676791	5.165724	8.540005	0	0	0
4.907637	7.283976	8.747768	0	0	0
6.171844	5.118599	5.354330	0	0	0
7.370958	5.849291	8.620941	0	0	0
4.940290	5.795478	5.283402	0	0	0
6.140801	5.171085	8.537152	0	0	0
7.370710	7.289828	8.751319	0	0	0
8.635429	5.118198	5.355206	0	0	0
9.832333	5.851658	8.623372	0	0	0
7.403740	5.794978	5.285116	0	0	0
8.601944	5.175280	8.537586	0	0	0
9.832040	7.291102	8.757194	0	0	0
11.099301	5.118139	5.355778	0	0	0
12.294487	5.846734	8.623846	0	0	0
9.867501	5.794678	5.286784	0	0	0
11.062615	5.174090	8.538935	0	0	0
12.294275	7.287294	8.755327	0	0	0
13.562782	5.118287	5.356054	0	0	0
14.758955	5.839879	8.624340	0	0	0

12.331181	5.794804	5.286924	0	0	0
13.525352	5.168439	8.540216	0	0	0
14.759167	7.280119	8.751789	0	0	0
0.014336	7.238301	5.190167	0	0	0
1.246890	9.380615	5.131604	0	0	0
1.210852	7.980592	8.795883	0	0	0
2.442140	10.122434	8.871408	0	0	0
0.015317	10.086865	5.140485	0	0	0
1.246057	7.942443	5.157748	0	0	0
1.210824	9.415918	8.857817	0	0	0
2.440724	11.555126	8.884137	0	0	0
2.477470	7.238419	5.185851	0	0	0
3.709968	9.380553	5.125659	0	0	0
3.675342	7.983601	8.793493	0	0	0
4.904874	10.129253	8.875180	0	0	0
2.478671	10.087127	5.126952	0	0	0
3.709392	7.942417	5.154413	0	0	0
3.675893	9.419704	8.854452	0	0	0
4.902634	11.565058	8.890860	0	0	0
4.940845	7.238299	5.185525	0	0	0
6.173182	9.380022	5.131732	0	0	0
6.138637	7.990443	8.796473	0	0	0

7.367803	10.137604	8.894732	0	0	0
4.941960	10.086817	5.126998	0	0	0
6.172836	7.941986	5.157656	0	0	0
6.139386	9.426599	8.861638	0	0	0
7.364099	11.577214	8.929347	0	0	0
7.404261	7.237943	5.190115	0	0	0
8.637001	9.379701	5.145427	0	0	0
8.600855	7.995677	8.806165	0	0	0
9.830681	10.142862	8.928417	0	0	0
7.405532	10.086269	5.140638	0	0	0
8.636371	7.941660	5.165549	0	0	0
8.600773	9.432544	8.885323	0	0	0
9.829269	11.582438	9.000960	0	0	0
9.868054	7.237874	5.194891	0	0	0
11.101065	9.379793	5.151558	0	0	0
11.063307	7.994108	8.808185	0	0	0
12.298149	10.129431	8.903401	0	0	0
9.869303	10.085933	5.156309	0	0	0
11.100208	7.941749	5.168618	0	0	0
11.062057	9.430623	8.888392	0	0	0
12.302548	11.565567	8.946939	0	0	0
12.331694	7.237995	5.194469	0	0	0

13.564367	9.380209	5.144347	0	0	0
13.527537	7.985546	8.801711	0	0	0
14.762327	10.123195	8.882854	0	0	0
12.332567	10.086366	5.155112	0	0	0
13.563503	7.942142	5.164851	0	0	0
13.527308	9.420405	8.869248	0	0	0
14.764303	11.557270	8.906463	0	0	0
0.016106	11.525163	5.166210	0	0	0
1.247700	13.675348	5.222087	0	0	0
1.212166	12.263355	8.894092	0	0	0
2.439982	14.387277	8.867485	0	0	0
0.016989	14.354079	5.272951	0	0	0
1.247937	12.229631	5.172747	0	0	0
1.214345	13.708176	8.887715	0	0	0
2.479583	11.525801	5.145468	0	0	0
3.712181	13.676356	5.195353	0	0	0
3.669320	12.262483	8.881842	0	0	0
4.893701	14.385890	8.860749	0	0	0
2.480004	14.355964	5.231485	0	0	0
3.711497	12.230218	5.156022	0	0	0
3.662122	13.703663	8.871173	0	0	0
4.942897	11.525420	5.143507	0	0	0

6.176274	13.675051	5.200324	0	0	0
6.131455	12.279109	8.905909	0	0	0
7.366144	14.429670	8.882028	0	0	0
4.943471	14.356269	5.213748	0	0	0
6.174933	12.229172	5.166227	0	0	0
6.118786	13.723364	8.877654	0	0	0
7.406253	11.524130	5.163677	0	0	0
8.638758	13.673235	5.243767	0	0	0
8.589395	12.290668	9.002075	0	0	0
9.838554	14.390477	9.303050	0	0	0
7.406718	14.353861	5.235297	0	0	0
8.638200	12.227779	5.198004	0	0	0
8.555707	13.735963	9.045978	0	0	0
9.869847	11.523381	5.188925	0	0	0
11.100990	13.673517	5.276688	0	0	0
11.073784	12.273332	9.008906	0	0	0
12.306938	14.388964	9.003328	0	0	0
9.869336	14.352999	5.295636	0	0	0
11.101606	12.228036	5.216496	0	0	0
11.114641	13.706356	9.078765	0	0	0
12.333258	11.524106	5.188149	0	0	0
13.564299	13.673994	5.259947	0	0	0

13.536260	12.266008	8.935868	0	0	0
14.762665	14.389058	8.904260	0	0	0
12.333972	14.352875	5.307100	0	0	0
13.565052	12.228698	5.201052	0	0	0
13.549212	13.706896	8.943993	0	0	0
9.911257	15.531849	9.994722	0.270913	-0.095741	0.129572
7.288643	16.408837	8.698126	0	0	0
10.025257	16.503653	10.644976	0.874409	-0.255961	0.265601

6 f = 2.689367 THz 16.897791 2PiTHz 89.707622 cm-1 11.122332 meV

X	Y	Z	dx	dy	dz
1.245750	4.028696	5.439790	0	0	0
1.210240	4.075813	8.437264	0	0	0
3.708620	4.028896	5.439647	0	0	0
3.679981	4.077333	8.436900	0	0	0
6.171574	4.028537	5.439423	0	0	0
6.144822	4.082922	8.432952	0	0	0
8.635129	4.028007	5.438685	0	0	0
8.603386	4.087320	8.430892	0	0	0
11.099276	4.027838	5.438849	0	0	0
11.060208	4.086191	8.430988	0	0	0
13.563114	4.028068	5.439721	0	0	0

13.521407	4.080469	8.433485	0	0	0
2.442410	15.480732	8.852243	0	0	0
0.017143	15.446242	5.324686	0	0	0
4.860405	15.477285	8.866232	0	0	0
2.480161	15.448544	5.275619	0	0	0
4.943820	15.449251	5.248689	0	0	0
12.315308	15.482418	9.002109	0	0	0
9.867716	15.445563	5.341755	0	0	0
14.762794	15.482453	8.899515	0	0	0
12.333845	15.445098	5.361284	0	0	0
7.407428	15.446161	5.264635	0	0	0
6.448461	16.344273	7.406481	0	0	0
8.600641	16.476444	7.892492	0	0	0
1.245442	5.118809	5.355005	0	0	0
2.443484	5.838886	8.622924	0	0	0
0.013795	5.795296	5.285730	0	0	0
1.210631	5.164204	8.541507	0	0	0
2.443506	7.279307	8.748318	0	0	0
3.708657	5.118963	5.353897	0	0	0
4.907998	5.843148	8.621230	0	0	0
2.477011	5.795606	5.283967	0	0	0
3.676791	5.165724	8.540005	0	0	0

4.907637	7.283976	8.747768	0	0	0
6.171844	5.118599	5.354330	0	0	0
7.370958	5.849291	8.620941	0	0	0
4.940290	5.795478	5.283402	0	0	0
6.140801	5.171085	8.537152	0	0	0
7.370710	7.289828	8.751319	0	0	0
8.635429	5.118198	5.355206	0	0	0
9.832333	5.851658	8.623372	0	0	0
7.403740	5.794978	5.285116	0	0	0
8.601944	5.175280	8.537586	0	0	0
9.832040	7.291102	8.757194	0	0	0
11.099301	5.118139	5.355778	0	0	0
12.294487	5.846734	8.623846	0	0	0
9.867501	5.794678	5.286784	0	0	0
11.062615	5.174090	8.538935	0	0	0
12.294275	7.287294	8.755327	0	0	0
13.562782	5.118287	5.356054	0	0	0
14.758955	5.839879	8.624340	0	0	0
12.331181	5.794804	5.286924	0	0	0
13.525352	5.168439	8.540216	0	0	0
14.759167	7.280119	8.751789	0	0	0
0.014336	7.238301	5.190167	0	0	0

1.246890	9.380615	5.131604	0	0	0
1.210852	7.980592	8.795883	0	0	0
2.442140	10.122434	8.871408	0	0	0
0.015317	10.086865	5.140485	0	0	0
1.246057	7.942443	5.157748	0	0	0
1.210824	9.415918	8.857817	0	0	0
2.440724	11.555126	8.884137	0	0	0
2.477470	7.238419	5.185851	0	0	0
3.709968	9.380553	5.125659	0	0	0
3.675342	7.983601	8.793493	0	0	0
4.904874	10.129253	8.875180	0	0	0
2.478671	10.087127	5.126952	0	0	0
3.709392	7.942417	5.154413	0	0	0
3.675893	9.419704	8.854452	0	0	0
4.902634	11.565058	8.890860	0	0	0
4.940845	7.238299	5.185525	0	0	0
6.173182	9.380022	5.131732	0	0	0
6.138637	7.990443	8.796473	0	0	0
7.367803	10.137604	8.894732	0	0	0
4.941960	10.086817	5.126998	0	0	0
6.172836	7.941986	5.157656	0	0	0
6.139386	9.426599	8.861638	0	0	0

7.364099	11.577214	8.929347	0	0	0
7.404261	7.237943	5.190115	0	0	0
8.637001	9.379701	5.145427	0	0	0
8.600855	7.995677	8.806165	0	0	0
9.830681	10.142862	8.928417	0	0	0
7.405532	10.086269	5.140638	0	0	0
8.636371	7.941660	5.165549	0	0	0
8.600773	9.432544	8.885323	0	0	0
9.829269	11.582438	9.000960	0	0	0
9.868054	7.237874	5.194891	0	0	0
11.101065	9.379793	5.151558	0	0	0
11.063307	7.994108	8.808185	0	0	0
12.298149	10.129431	8.903401	0	0	0
9.869303	10.085933	5.156309	0	0	0
11.100208	7.941749	5.168618	0	0	0
11.062057	9.430623	8.888392	0	0	0
12.302548	11.565567	8.946939	0	0	0
12.331694	7.237995	5.194469	0	0	0
13.564367	9.380209	5.144347	0	0	0
13.527537	7.985546	8.801711	0	0	0
14.762327	10.123195	8.882854	0	0	0
12.332567	10.086366	5.155112	0	0	0

13.563503	7.942142	5.164851	0	0	0
13.527308	9.420405	8.869248	0	0	0
14.764303	11.557270	8.906463	0	0	0
0.016106	11.525163	5.166210	0	0	0
1.247700	13.675348	5.222087	0	0	0
1.212166	12.263355	8.894092	0	0	0
2.439982	14.387277	8.867485	0	0	0
0.016989	14.354079	5.272951	0	0	0
1.247937	12.229631	5.172747	0	0	0
1.214345	13.708176	8.887715	0	0	0
2.479583	11.525801	5.145468	0	0	0
3.712181	13.676356	5.195353	0	0	0
3.669320	12.262483	8.881842	0	0	0
4.893701	14.385890	8.860749	0	0	0
2.480004	14.355964	5.231485	0	0	0
3.711497	12.230218	5.156022	0	0	0
3.662122	13.703663	8.871173	0	0	0
4.942897	11.525420	5.143507	0	0	0
6.176274	13.675051	5.200324	0	0	0
6.131455	12.279109	8.905909	0	0	0
7.366144	14.429670	8.882028	0	0	0
4.943471	14.356269	5.213748	0	0	0

6.174933	12.229172	5.166227	0	0	0
6.118786	13.723364	8.877654	0	0	0
7.406253	11.524130	5.163677	0	0	0
8.638758	13.673235	5.243767	0	0	0
8.589395	12.290668	9.002075	0	0	0
9.838554	14.390477	9.303050	0	0	0
7.406718	14.353861	5.235297	0	0	0
8.638200	12.227779	5.198004	0	0	0
8.555707	13.735963	9.045978	0	0	0
9.869847	11.523381	5.188925	0	0	0
11.100990	13.673517	5.276688	0	0	0
11.073784	12.273332	9.008906	0	0	0
12.306938	14.388964	9.003328	0	0	0
9.869336	14.352999	5.295636	0	0	0
11.101606	12.228036	5.216496	0	0	0
11.114641	13.706356	9.078765	0	0	0
12.333258	11.524106	5.188149	0	0	0
13.564299	13.673994	5.259947	0	0	0
13.536260	12.266008	8.935868	0	0	0
14.762665	14.389058	8.904260	0	0	0
12.333972	14.352875	5.307100	0	0	0
13.565052	12.228698	5.201052	0	0	0

13.549212	13.706896	8.943993	0	0	0
9.911257	15.531849	9.994722	-0.114679	-0.196333	0.334400
7.288643	16.408837	8.698126	0	0	0
10.025257	16.503653	10.644976	-0.377230	-0.421730	0.718554

Finite differences POTIM= 1.500000000000000E-002

LATTYP: Found a simple orthorhombic cell.

ALAT = 14.7806000000

B/A-ratio = 1.2466138046

C/A-ratio = 1.4433717170

Lattice vectors:

A1 = (-14.7806000000, 0.0000000000, 0.0000000000)

A2 = (0.0000000000, 0.0000000000, -18.4257000000)

A3 = (0.0000000000, -21.3339000000, 0.0000000000)

Analysis of symmetry for initial positions (statically):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The static configuration has the point symmetry C_1 .

Analysis of symmetry for dynamics (positions and initial velocities):

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The dynamic configuration has the point symmetry C_1 .

Analysis of constrained symmetry for selective dynamics:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The constrained configuration has the point symmetry C_1 .

Analysis of structural, dynamic, and magnetic symmetry:

==========

Subroutine PRICEL returns:

Original cell was already a primitive cell.

Routine SETGRP: Setting up the symmetry group for a

simple orthorhombic supercell.

Subroutine GETGRP returns: Found 1 space group operations

(whereof 1 operations were pure point group operations)

out of a pool of 8 trial point group operations.

The magnetic configuration has the point symmetry C_1 .

Subroutine INISYM returns: Found 1 space group operations

(whereof 1 operations are pure point group operations),

and found 1 'primitive' translations

KPOINTS: KPT-Resolved Value to Generate K-Mesh: 0

Automatic generation of k-mesh.

Space group operators:

irot	det(A)	alpha	n_x	n_y	n_z	tau_x	tau_y	tau_z
1	1.000000	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Subroutine IBZKPT returns following result:

==========

Found 1 irreducible k-points:

Following reciprocal coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

Following cartesian coordinates:

Coordinates			Weight
0.000000	0.000000	0.000000	1.000000

LOOP+: cpu time 178.2267: real time 179.2464

4ORBIT: cpu time 0.0000: real time 0.0000

total charge

# of ion	s	p	d	tot
1	0.646	0.043	0.000	0.690
2	0.646	0.043	0.000	0.690
3	0.646	0.043	0.000	0.690
4	0.646	0.043	0.000	0.690
5	0.646	0.043	0.000	0.690
6	0.646	0.043	0.000	0.690

7	0.646	0.043	0.000	0.690
8	0.646	0.043	0.000	0.690
9	0.646	0.043	0.000	0.690
10	0.646	0.043	0.000	0.690
11	0.646	0.043	0.000	0.690
12	0.646	0.043	0.000	0.690
13	0.646	0.043	0.000	0.689
14	0.646	0.043	0.000	0.689
15	0.648	0.045	0.000	0.693
16	0.646	0.043	0.000	0.689
17	0.646	0.043	0.000	0.689
18	0.646	0.043	0.000	0.689
19	0.646	0.043	0.000	0.689
20	0.646	0.043	0.000	0.689
21	0.646	0.043	0.000	0.689
22	0.646	0.044	0.000	0.690
23	0.541	0.015	0.000	0.557
24	0.541	0.015	0.000	0.556
25	0.870	1.763	0.000	2.633
26	0.867	1.785	0.000	2.653
27	0.867	1.786	0.000	2.653
28	0.870	1.762	0.000	2.632

29	0.865	1.783	0.000	2.648
30	0.870	1.763	0.000	2.633
31	0.867	1.786	0.000	2.653
32	0.867	1.786	0.000	2.653
33	0.870	1.762	0.000	2.632
34	0.865	1.783	0.000	2.648
35	0.870	1.763	0.000	2.633
36	0.868	1.787	0.000	2.654
37	0.867	1.786	0.000	2.653
38	0.870	1.763	0.000	2.633
39	0.865	1.784	0.000	2.649
40	0.870	1.763	0.000	2.633
41	0.868	1.787	0.000	2.655
42	0.867	1.786	0.000	2.653
43	0.871	1.764	0.000	2.634
44	0.865	1.783	0.000	2.648
45	0.870	1.763	0.000	2.633
46	0.867	1.786	0.000	2.653
47	0.867	1.786	0.000	2.653
48	0.871	1.763	0.000	2.634
49	0.865	1.783	0.000	2.648
50	0.870	1.763	0.000	2.633

51	0.867	1.786	0.000	2.653
52	0.867	1.786	0.000	2.653
53	0.870	1.762	0.000	2.632
54	0.865	1.784	0.000	2.648
55	0.865	1.784	0.000	2.649
56	0.865	1.786	0.000	2.651
57	0.866	1.787	0.000	2.653
58	0.866	1.790	0.000	2.656
59	0.865	1.786	0.000	2.651
60	0.866	1.786	0.000	2.651
61	0.866	1.788	0.000	2.654
62	0.867	1.791	0.000	2.658
63	0.865	1.784	0.000	2.649
64	0.865	1.786	0.000	2.651
65	0.866	1.787	0.000	2.652
66	0.865	1.788	0.000	2.653
67	0.865	1.786	0.000	2.651
68	0.866	1.785	0.000	2.651
69	0.865	1.787	0.000	2.652
70	0.866	1.787	0.000	2.653
71	0.865	1.784	0.000	2.649
72	0.865	1.786	0.000	2.651

73	0.866	1.786	0.000	2.652
74	0.864	1.785	0.000	2.649
75	0.865	1.786	0.000	2.651
76	0.866	1.786	0.000	2.651
77	0.865	1.786	0.000	2.651
78	0.865	1.784	0.000	2.649
79	0.865	1.784	0.000	2.649
80	0.865	1.786	0.000	2.651
81	0.865	1.785	0.000	2.650
82	0.863	1.782	0.000	2.645
83	0.865	1.786	0.000	2.651
84	0.866	1.786	0.000	2.651
85	0.865	1.784	0.000	2.648
86	0.862	1.774	0.000	2.636
87	0.865	1.784	0.000	2.649
88	0.865	1.787	0.000	2.652
89	0.865	1.785	0.000	2.650
90	0.865	1.788	0.000	2.653
91	0.865	1.786	0.000	2.651
92	0.866	1.786	0.000	2.651
93	0.864	1.783	0.000	2.647
94	0.866	1.785	0.000	2.651

95	0.865	1.784	0.000	2.649
96	0.865	1.786	0.000	2.651
97	0.866	1.787	0.000	2.653
98	0.866	1.789	0.000	2.655
99	0.865	1.786	0.000	2.651
100	0.866	1.786	0.000	2.651
101	0.865	1.787	0.000	2.652
102	0.867	1.790	0.000	2.657
103	0.865	1.786	0.000	2.651
104	0.867	1.785	0.000	2.653
105	0.866	1.786	0.000	2.652
106	0.870	1.778	0.000	2.648
107	0.869	1.765	0.000	2.635
108	0.865	1.783	0.000	2.648
109	0.869	1.789	0.000	2.658
110	0.865	1.786	0.000	2.651
111	0.867	1.785	0.000	2.653
112	0.867	1.789	0.000	2.655
113	0.871	1.782	0.000	2.653
114	0.869	1.765	0.000	2.634
115	0.865	1.783	0.000	2.648
116	0.870	1.791	0.000	2.661

117	0.865	1.786	0.000	2.651
118	0.867	1.786	0.000	2.653
119	0.865	1.782	0.000	2.647
120	0.857	1.707	0.000	2.564
121	0.869	1.765	0.000	2.634
122	0.865	1.783	0.000	2.648
123	0.866	1.778	0.000	2.644
124	0.866	1.786	0.000	2.652
125	0.867	1.785	0.000	2.653
126	0.862	1.776	0.000	2.638
127	0.849	1.831	0.000	2.680
128	0.870	1.767	0.000	2.637
129	0.865	1.783	0.000	2.648
130	0.860	1.757	0.000	2.617
131	0.866	1.786	0.000	2.652
132	0.867	1.784	0.000	2.652
133	0.864	1.787	0.000	2.651
134	0.869	1.790	0.000	2.659
135	0.869	1.767	0.000	2.636
136	0.865	1.783	0.000	2.648
137	0.866	1.772	0.000	2.638
138	0.866	1.786	0.000	2.652

139	0.867	1.785	0.000	2.652
140	0.866	1.788	0.000	2.654
141	0.870	1.779	0.000	2.649
142	0.869	1.766	0.000	2.635
143	0.865	1.783	0.000	2.648
144	0.869	1.790	0.000	2.659
145	0.946	1.730	0.000	2.676
146	1.240	1.546	0.074	2.860
147	1.635	3.538	0.000	5.173
tot	123.067	221.574	0.074	344.715

magnetization (x)

# of ion	s	p	d	tot
1	0.000	-0.000	0.000	0.000
2	-0.000	0.000	0.000	-0.000
3	0.000	-0.000	0.000	0.000
4	-0.000	0.000	0.000	-0.000

5	0.000	-0.000	0.000	0.000
6	-0.000	0.000	0.000	-0.000
7	0.000	-0.000	0.000	0.000
8	-0.000	0.000	0.000	-0.000
9	0.000	-0.000	0.000	0.000
10	-0.000	0.000	0.000	-0.000
11	0.000	-0.000	0.000	0.000
12	-0.000	0.000	0.000	-0.000
13	0.000	-0.000	0.000	0.000
14	-0.004	0.002	0.000	-0.002
15	0.000	-0.000	0.000	0.000
16	-0.004	0.002	0.000	-0.002
17	-0.004	0.002	0.000	-0.002
18	0.000	-0.000	0.000	0.000
19	-0.003	0.001	0.000	-0.002
20	0.000	-0.000	0.000	0.000
21	-0.003	0.002	0.000	-0.002
22	-0.003	0.002	0.000	-0.002
23	-0.000	0.000	0.000	-0.000
24	-0.000	0.000	0.000	-0.000
25	-0.000	-0.007	0.000	-0.008
26	-0.000	-0.002	0.000	-0.002

27	0.000	0.003	0.000	0.003
28	0.000	0.005	0.000	0.005
29	0.000	0.003	0.000	0.003
30	-0.000	-0.007	0.000	-0.008
31	-0.000	-0.002	0.000	-0.002
32	0.000	0.003	0.000	0.003
33	0.000	0.005	0.000	0.005
34	0.000	0.002	0.000	0.002
35	-0.000	-0.007	0.000	-0.008
36	-0.000	-0.002	0.000	-0.002
37	0.000	0.003	0.000	0.003
38	0.000	0.006	0.000	0.007
39	0.000	0.002	0.000	0.002
40	-0.000	-0.007	0.000	-0.008
41	-0.000	-0.002	0.000	-0.002
42	0.000	0.002	0.000	0.003
43	0.000	0.005	0.000	0.005
44	0.000	0.004	0.000	0.004
45	-0.000	-0.007	0.000	-0.008
46	-0.000	-0.002	0.000	-0.002
47	0.000	0.002	0.000	0.003
48	0.000	0.005	0.000	0.006

49	0.000	0.001	0.000	0.001
50	-0.000	-0.007	0.000	-0.008
51	-0.000	-0.002	0.000	-0.002
52	0.000	0.002	0.000	0.003
53	0.000	0.006	0.000	0.007
54	0.000	0.002	0.000	0.002
55	-0.000	-0.005	0.000	-0.006
56	-0.000	-0.007	0.000	-0.007
57	-0.000	-0.001	0.000	-0.001
58	-0.000	-0.001	0.000	-0.001
59	0.000	0.006	0.000	0.007
60	0.000	0.003	0.000	0.003
61	0.000	0.001	0.000	0.001
62	0.000	0.003	0.000	0.003
63	-0.000	-0.005	0.000	-0.006
64	-0.000	-0.007	0.000	-0.007
65	-0.000	-0.001	0.000	-0.001
66	-0.000	-0.001	0.000	-0.001
67	0.000	0.006	0.000	0.006
68	0.000	0.003	0.000	0.003
69	0.000	0.001	0.000	0.001
70	0.000	0.002	0.000	0.002

71	-0.000	-0.005	0.000	-0.006
72	-0.000	-0.007	0.000	-0.007
73	-0.000	-0.001	0.000	-0.001
74	-0.000	-0.002	0.000	-0.002
75	0.000	0.006	0.000	0.007
76	0.000	0.003	0.000	0.004
77	0.000	0.003	0.000	0.003
78	0.000	0.001	0.000	0.001
79	-0.000	-0.005	0.000	-0.006
80	-0.000	-0.007	0.000	-0.007
81	-0.000	-0.001	0.000	-0.002
82	-0.000	-0.002	0.000	-0.002
83	0.001	0.007	0.000	0.008
84	0.000	0.003	0.000	0.003
85	0.000	0.002	0.000	0.002
86	0.000	0.005	0.000	0.006
87	-0.000	-0.005	0.000	-0.005
88	-0.000	-0.007	0.000	-0.007
89	-0.000	-0.001	0.000	-0.002
90	-0.000	-0.002	0.000	-0.002
91	0.001	0.008	0.000	0.008
92	0.000	0.003	0.000	0.003

93	0.000	0.002	0.000	0.003
94	0.000	0.001	0.000	0.001
95	-0.000	-0.005	0.000	-0.006
96	-0.000	-0.007	0.000	-0.007
97	-0.000	-0.001	0.000	-0.001
98	-0.000	-0.001	0.000	-0.001
99	0.001	0.007	0.000	0.007
100	0.000	0.003	0.000	0.004
101	0.000	0.003	0.000	0.003
102	0.000	0.002	0.000	0.002
103	-0.001	-0.010	0.000	-0.011
104	-0.003	-0.028	0.000	-0.031
105	-0.000	-0.001	0.000	-0.002
106	-0.000	-0.004	0.000	-0.005
107	0.007	0.116	0.000	0.122
108	0.001	0.010	0.000	0.011
109	0.000	0.001	0.000	0.001
110	-0.001	-0.010	0.000	-0.011
111	-0.003	-0.028	0.000	-0.031
112	-0.000	-0.001	0.000	-0.002
113	-0.000	-0.003	0.000	-0.004
114	0.007	0.120	0.000	0.127

115	0.001	0.010	0.000	0.011
116	0.000	0.001	0.000	0.002
117	-0.001	-0.010	0.000	-0.011
118	-0.003	-0.026	0.000	-0.029
119	-0.000	-0.002	0.000	-0.002
120	-0.000	-0.002	0.000	-0.002
121	0.007	0.115	0.000	0.122
122	0.001	0.010	0.000	0.010
123	0.000	0.003	0.000	0.003
124	-0.001	-0.010	0.000	-0.011
125	-0.003	-0.024	0.000	-0.027
126	-0.000	-0.002	0.000	-0.002
127	-0.000	0.001	0.000	0.001
128	0.006	0.105	0.000	0.111
129	0.001	0.009	0.000	0.010
130	0.000	0.004	0.000	0.004
131	-0.001	-0.009	0.000	-0.010
132	-0.003	-0.024	0.000	-0.027
133	-0.000	-0.002	0.000	-0.002
134	-0.000	-0.002	0.000	-0.002
135	0.006	0.097	0.000	0.102
136	0.001	0.009	0.000	0.010

137	0.000	0.004	0.000	0.005
138	-0.001	-0.010	0.000	-0.011
139	-0.003	-0.026	0.000	-0.029
140	-0.000	-0.002	0.000	-0.002
141	-0.000	-0.003	0.000	-0.004
142	0.006	0.105	0.000	0.111
143	0.001	0.010	0.000	0.010
144	0.000	0.002	0.000	0.003
145	0.000	0.005	0.000	0.006
146	-0.000	0.000	-0.000	0.000
147	0.000	0.004	0.000	0.004
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tot	0.001	0.513	-0.000	0.514

total amount of memory used by VASP MPI-rank0 132380. kBytes

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base : 30000. kBytes

nonlr-proj: 13792. kBytes

fftplans : 5354. kBytes

grid : 63770. kBytes

one-center: 2384. kBytes

wavefun : 17080. kBytes

General timing and accounting informations for this job:

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Total CPU time used (sec):	2537.479
User time (sec):	2482.034
System time (sec):	55.445
Elapsed time (sec):	2554.695
Maximum memory used (kb):	1120776.
Average memory used (kb):	0.
Minor page faults:	2568508
Major page faults:	0
Voluntary context switches:	7791