```
[c0251:44143] [[27432,0],0] ORTE_ERROR_LOG: Data unpack would read past end of buffer in file ../../openmpi-3.1.1/orte/util/
show_help.c at line 501
 DBCSR| Multiplication driver                                              XSMM
 DBCSR| Multrec recursion limit                                            512
 DBCSR| Multiplication stack size                                         1000
 DBCSR| Maximum elements for images                                  UNLIMITED
 DBCSR| Multiplicative factor virtual images                               1
 DBCSR| Multiplication size stacks                                         3
 DBCSR| Number of 3D layers                                           SINGLE
 DBCSR| Use MPI memory allocation                                          T
 DBCSR| Use RMA algorithm                                                  F
 DBCSR| Use Communication thread                                           T
 DBCSR| Communication thread load                                         60


  **** **** ******  **  PROGRAM STARTED AT               2024-05-28 15:40:36.788
 ***** ** ***  *** **   PROGRAM STARTED ON                                 c0251
 **    ****   ******    PROGRAM STARTED BY                             benazzi.m
 ***** **    ** ** **   PROGRAM PROCESS ID                                 44142
  **** **  *******  **  PROGRAM STARTED IN /home/benazzi.m/CP2K/Al_CO2_C1/Cubic_
                                          Unit_Cell/MethanolModel

 CP2K| version string:                                         CP2K version 6.1
 CP2K| source code revision number:                                  svn:18464
 CP2K| cp2kflags: omp libint fftw3 libxc parallel mpi3 scalapack xsmm libderiv_m
 CP2K|            ax_am1=5 libint_max_am=6
 CP2K| is freely available from                            https://www.cp2k.org/
 CP2K| Program compiled at                           Thu Dec  6 14:46:17 EST 2018
 CP2K| Program compiled on                                              c0004
 CP2K| Program compiled for                                             local
 CP2K| Data directory path                  /shared/centos7/cp2k/cp2k-6.1.0/data
 CP2K| Input file name        /home/benazzi.m/CP2K/Al_CO2_C1/Cubic_Unit_Cell/Met

 GLOBAL| Force Environment number                                          1
 GLOBAL| Basis set file name            /shared/centos7/cp2k/cp2k-6.1.0-gpu/data
 GLOBAL| Potential file name            /shared/centos7/cp2k/cp2k-6.1.0-gpu/data
 GLOBAL| MM Potential file name                                  MM_POTENTIAL
 GLOBAL| Coordinate file name                                co2_c1_melt.xyz
 GLOBAL| Method name                                                    CP2K
 GLOBAL| Project name                                 co2_c1_melt_highprint
 GLOBAL| Preferred FFT library                                         FFTW3
 GLOBAL| Preferred diagonalization lib.                                  SL
 GLOBAL| Run type                                                        MD
 GLOBAL| All-to-all communication in single precision                     F
 GLOBAL| FFTs using library dependent lengths                             F
 GLOBAL| Global print level                                             HIGH
 GLOBAL| Total number of message passing processes                        1
 GLOBAL| Number of threads for this process                               8
 GLOBAL| This output is from process                                      0
 GLOBAL| CPU model name :  Intel(R) Xeon(R) CPU E5-2690 v3 @ 2.60GHz

 MEMORY| system memory details [Kb]
 MEMORY|                        rank 0           min           max       average
 MEMORY| MemTotal            131141092     131141092     131141092     131141092
 MEMORY| MemFree             100274232     100274232     100274232     100274232
 MEMORY| Buffers                 17376         17376         17376         17376
 MEMORY| Cached               19006992      19006992      19006992      19006992
 MEMORY| Slab                   523096        523096        523096        523096
 MEMORY| SReclaimable           392116        392116        392116        392116
 MEMORY| MemLikelyFree       119690716     119690716     119690716     119690716


 *** Fundamental physical constants (SI units) ***

 *** Literature: B. J. Mohr and B. N. Taylor,
 ***             CODATA recommended values of the fundamental physical
 ***             constants: 2006, Web Version 5.1
 ***             http://physics.nist.gov/constants

 Speed of light in vacuum [m/s]                                  2.99792458000000E+08
 Magnetic constant or permeability of vacuum [N/A**2]            1.25663706143592E-06
 Electric constant or permittivity of vacuum [F/m]               8.85418781762039E-12
 Planck constant (h) [J*s]                                       6.62606896000000E-34
 Planck constant (h-bar) [J*s]                                   1.05457162825177E-34
 Elementary charge [C]                                           1.60217648700000E-19
 Electron mass [kg]                                              9.10938215000000E-31
 Electron g factor [ ]                                          -2.00231930436220E+00
 Proton mass [kg]                                                1.67262163700000E-27
 Fine-structure constant                                         7.29735253760000E-03
 Rydberg constant [1/m]                                          1.09737315685270E+07
 Avogadro constant [1/mol]                                       6.02214179000000E+23
 Boltzmann constant [J/K]                                        1.38065040000000E-23
 Atomic mass unit [kg]                                           1.66053878200000E-27
 Bohr radius [m]                                                 5.29177208590000E-11

 *** Conversion factors ***

 [u] -> [a.u.]                                                   1.82288848426455E+03
 [Angstrom] -> [Bohr] = [a.u.]                                   1.88972613288564E+00
 [a.u.] = [Bohr] -> [Angstrom]                                   5.29177208590000E-01
 [a.u.] -> [s]                                                   2.41888432650478E-17
 [a.u.] -> [fs]                                                  2.41888432650478E-02
 [a.u.] -> [J]                                                   4.35974393937059E-18
 [a.u.] -> [N]                                                   8.23872205491840E-08
 [a.u.] -> [K]                                                   3.15774647902944E+05
 [a.u.] -> [kJ/mol]                                              2.62549961709828E+03
 [a.u.] -> [kcal/mol]                                            6.27509468713739E+02
 [a.u.] -> [Pa]                                                  2.94210107994716E+13
 [a.u.] -> [bar]                                                 2.94210107994716E+08
```

```
[a.u.] -> [atm]                                          2.90362800883016E+08
[a.u.] -> [eV]                                           2.72113838565563E+01
[a.u.] -> [Hz]                                           6.57968392072181E+15
[a.u.] -> [1/cm] (wave numbers)                          2.19474631370540E+05
[a.u./Bohr**2] -> [1/cm]                                 5.14048714338585E+03


CELL_TOP| Volume [angstrom^3]:                                       5832.156
CELL_TOP| Vector a [angstrom    18.000    -0.000    -0.000    |a| =     18.000
CELL_TOP| Vector b [angstrom    -0.000    18.000    -0.000    |b| =     18.000
CELL_TOP| Vector c [angstrom    -0.000    -0.000    18.000    |c| =     18.000
CELL_TOP| Angle (b,c), alpha [degree]:                                    90.001
CELL_TOP| Angle (a,c), beta  [degree]:                                    90.000
CELL_TOP| Angle (a,b), gamma [degree]:                                    90.002
CELL_TOP| Numerically orthorhombic:                                        NO


SUBCELL GRID  INFO FOR THE NONBONDED NEIGHBOR LISTS

   NUMBER OF SUBCELLS             ::                   7         7         6
   NUMBER OF PERIODIC      IMAGES ::                   1         1         1
   NUMBER OF INTERACTING SUBCELLS ::                   2         2         2

GENERATE|  Preliminary Number of Bonds generated:                          0
GENERATE|  Achieved consistency in connectivity generation.

CELL| Volume [angstrom^3]:                                          5832.156
CELL| Vector a [angstrom]:      18.000    -0.000    -0.000    |a| =     18.000
CELL| Vector b [angstrom]:      -0.000    18.000    -0.000    |b| =     18.000
CELL| Vector c [angstrom]:      -0.000    -0.000    18.000    |c| =     18.000
CELL| Angle (b,c), alpha [degree]:                                       90.001
CELL| Angle (a,c), beta  [degree]:                                       90.000
CELL| Angle (a,b), gamma [degree]:                                       90.002
CELL| Numerically orthorhombic:                                           NO

CELL_REF| Volume [angstrom^3]:                                      5832.156
CELL_REF| Vector a [angstrom    18.000    -0.000    -0.000    |a| =     18.000
CELL_REF| Vector b [angstrom    -0.000    18.000    -0.000    |b| =     18.000
CELL_REF| Vector c [angstrom    -0.000    -0.000    18.000    |c| =     18.000
CELL_REF| Angle (b,c), alpha [degree]:                                    90.001
CELL_REF| Angle (a,c), beta  [degree]:                                    90.000
CELL_REF| Angle (a,b), gamma [degree]:                                    90.002
CELL_REF| Numerically orthorhombic:                                        NO

*******************************************************************************
*******************************************************************************
**                                                                           **
**     #####                          ##             ##                     **
**    ##   ##            ##          ##             ##                     **
**   ##     ##                       ##            ######                  **
**   ##     ##  ##   ##  ##   #####  ##  ##   ####   ##    #####    #####   **
**   ##     ##  ##   ##  ##  ##      ## ##   ##      ##   ##   ##  ##   ##   **
**   ##  ## ##  ##   ##  ##  ##      ####     ###    ##   ######   ######    **
**    ##  ###   ##   ##  ##  ##      ## ##      ##   ##   ##       ##        **
**     #######   #####   ##   #####  ##  ##  ####    ##    #####   ##        **
**           ##                                                  ##        **
**                                                                           **
**                                          ... make the atoms dance         **
**                                                                           **
**            Copyright (C) by CP2K developers group (2000 - 2018)           **
**                                                                           **
*******************************************************************************

RADII: ORBITAL BASIS in angstrom            Kind   Label     Radius  OCE Radius
                                               1   Al      5.918567    5.918567
                                               2   O       5.902583    5.902583
                                               3   C       6.607519    6.607519

RADII: SHELL SETS OF ORBITAL BASIS in angstrom   Kind  Label   Set       Radius
                                                    1  Al        1     5.918567
                                                    2  O         1     5.902583
                                                    3  C         1     6.607519

RADII: PRIMITIVE GAUSSIANS OF ORBITAL BASIS in anKindomLabel   Set       Radius
                                                    1  Al        1     1.447112
                                                                       2.374969
                                                                       3.577377
                                                                       5.918567
                                                    2  O         1     0.521068
                                                                       0.818805
                                                                       1.295514
                                                                       2.003103
                                                                       2.965599
                                                                       4.380024
                                                                       5.902583
                                                    3  C         1     0.711311
                                                                       1.114719
                                                                       1.762165
                                                                       2.595017
                                                                       4.046615
                                                                       5.491987
                                                                       6.607519

RADII: AUXILLIARY BASIS in angstrom         Kind   Label     Radius  OCE Radius
                                                      1   Al        no basis
                                                      2   O         no basis
                                                      3   C         no basis

RADII: SHELL SETS OF AUXILLIARY BASIS in angstromKind  Label   Set       Radius
                                                    1   Al              no basis
```

	2	O	no basis
	3	C	no basis

RADII: PRIMITIVE GAUSSIANS OF AUXILLIARY BASIS in	Kind	Label	Set	Radius
	1	Al		no basis
	2	O		no basis
	3	C		no basis

RADII: LOCAL RI BASIS in angstrom	Kind	Label	Radius	OCE Radius
	1	Al		no basis
	2	O		no basis
	3	C		no basis

RADII: SHELL SETS OF LOCAL RI BASIS in angstrom	Kind	Label	Set	Radius
	1	Al		no basis
	2	O		no basis
	3	C		no basis

RADII: PRIMITIVE GAUSSIANS OF LOCAL RI BASIS in a	Kind	Label	Set	Radius
	1	Al		no basis
	2	O		no basis
	3	C		no basis

RADII: CORE CHARGE DISTRIBUTIONS in angstrom	Kind	Label	Radius
	1	Al	1.793683
	2	O	1.017201
	3	C	1.376023

RADII: LOCAL PART OF GTH/ELP PP in angstrom	Kind	Label	Radius
	1	Al	0.866959
	2	O	0.528197
	3	C	0.699284

RADII: NON-LOCAL PART OF GTH PP in angstrom	Kind	Label	Radius
	1	Al	1.588550
	2	O	0.622773
	3	C	0.838527

RADII: ONE CENTER PROJECTORS in angstrom	Kind	Label	Radius

DISTRIBUTION OF THE MOLECULES	Process	Number of molecules
	0	68
	Sum	68

Process	Kind	Local molecules (global indices)
0	1	1
	2	2
	3	3
	4	4
	5	5
	6	6
	7	7
	8	8
	9	9
	10	10
	11	11
	12	12
	13	13
	14	14
	15	15
	16	16
	17	17
	18	18
	19	19
	20	20
	21	21
	22	22
	23	23
	24	24
	25	25
	26	26
	27	27
	28	28
	29	29
	30	30
	31	31
	32	32
	33	33
	34	34
	35	35
	36	36
	37	37
	38	38
	39	39
	40	40
	41	41
	42	42
	43	43
	44	44
	45	45
	46	46
	47	47
	48	48
	49	49
	50	50
	51	51
	52	52
	53	53
	54	54
	55	55

```
              56        56
              57        57
              58        58
              59        59
              60        60
              61        61
              62        62
              63        63
              64        64
              65        65
              66        66
              67        67
              68        68

 DISTRIBUTION OF THE PARTICLES                    Process    Number of particles
                                                        0                     68
                                                      Sum                     68

  Process   Kind   Local particles (global indices)
        0      1        1     2     3     4     5     6     7     8     9    10
                       11    12    13    15    16    17    18    19    20    21
                       22    23    24    25    26    27    28    29    30    31
                       32    33    34    35    36    37    38    39    41    42
                       44    45    46    47    48    49    50    51    52    53
                       54    55    56    57    58    59    60    61    62    63
                       64    65    66    67    68
              2        14    43
              3        40

 DFT| Spin restricted Kohn-Sham (RKS) calculation                          RKS
 DFT| Multiplicity                                                         2
 DFT| Number of spin states                                               1
 DFT| Charge                                                              0
 DFT| Self-interaction correction (SIC)                                   NO
 DFT| Cutoffs: density                                            1.000000E-10
 DFT|          gradient                                           1.000000E-10
 DFT|          tau                                                1.000000E-10
 DFT|          cutoff_smoothing_range                             0.000000E+00
 DFT| XC density smoothing                                             NONE
 DFT| XC derivatives                                                     PW
 FUNCTIONAL| ROUTINE=NEW
 FUNCTIONAL| PBE:
 FUNCTIONAL| J.P.Perdew, K.Burke, M.Ernzerhof, Phys. Rev. Letter, vol. 77, n 18,
 FUNCTIONAL|  pp. 3865-3868, (1996){spin unpolarized}

 QS| Method:                                                             GPW
 QS| Density plane wave grid type                       NON-SPHERICAL FULLSPACE
 QS| Number of grid levels:                                              5
 QS| Density cutoff [a.u.]:                                           300.0
 QS| Multi grid cutoff [a.u.]: 1) grid level                          300.0
 QS|                            2) grid level                          100.0
 QS|                            3) grid level                           33.3
 QS|                            4) grid level                           11.1
 QS|                            5) grid level                            3.7
 QS| Grid level progression factor:                                      3.0
 QS| Relative density cutoff [a.u.]:                                    20.0
 QS| Consistent realspace mapping and integration
 QS| Interaction thresholds: eps_pgf_orb:                           1.0E-05
 QS|                         eps_filter_matrix:                     0.0E+00
 QS|                         eps_core_charge:                       1.0E-12
 QS|                         eps_rho_gspace:                        1.0E-10
 QS|                         eps_rho_rspace:                        1.0E-10
 QS|                         eps_gvg_rspace:                        1.0E-05
 QS|                         eps_ppl:                               1.0E-02
 QS|                         eps_ppnl:                              1.0E-07


 ATOMIC KIND INFORMATION

 1. Atomic kind: Al                                 Number of atoms:      65

    Orbital Basis Set                                       SZV-MOLOPT-SR-GTH

      Number of orbital shell sets:                                          1
      Number of orbital shells:                                              2
      Number of primitive Cartesian functions:                               4
      Number of Cartesian basis functions:                                   4
      Number of spherical basis functions:                                   4
      Norm type:                                                             2

      Normalised Cartesian orbitals:

                        Set   Shell   Orbital          Exponent    Coefficient

                          1       1    2s             1.212902       0.147703
                                                      0.454181       0.176942
                                                      0.242419      -0.255412
                                                      0.078268      -0.047918

                          1       2    3px            1.212902       0.054477
                                                      0.454181       0.028713
                                                      0.242419      -0.164201
                                                      0.078268      -0.027375
                          1       2    3py            1.212902       0.054477
                                                      0.454181       0.028713
                                                      0.242419      -0.164201
                                                      0.078268      -0.027375
                          1       2    3pz            1.212902       0.054477
                                                      0.454181       0.028713
                                                      0.242419      -0.164201
```

```
                                                 0.078268      -0.027375

   GTH Potential information for                                GTH-PBE-q3

     Description:                       Goedecker-Teter-Hutter pseudopotential
                                         Goedecker et al., PRB 54, 1703 (1996)
                                        Hartwigsen et al., PRB 58, 3641 (1998)
                                                    Krack, TCA 114, 145 (2005)

     Gaussian exponent of the core charge distribution:              2.469136
     Electronic configuration (s p d ...):                             2   1

     Parameters of the local part of the GTH pseudopotential:

                      rloc        C1          C2          C3          C4
                    0.450000   -7.554761

     Parameters of the non-local part of the GTH pseudopotential:

                 l      r(l)      h(i,j,l)

                 0    0.487435    6.959938   -1.888836
                                 -1.888836    2.438477
                 1    0.562189    1.865299

2. Atomic kind: O                                  Number of atoms:       2

   Orbital Basis Set                                        SZV-MOLOPT-GTH

     Number of orbital shell sets:                                       1
     Number of orbital shells:                                           2
     Number of primitive Cartesian functions:                            7
     Number of Cartesian basis functions:                                4
     Number of spherical basis functions:                                4
     Norm type:                                                          2

     Normalised Cartesian orbitals:

                    Set    Shell   Orbital          Exponent    Coefficient

                      1        1    2s             12.015955      -0.284499
                                                     5.108150      -0.322498
                                                     2.048398       0.148191
                                                     0.832382       0.295475
                                                     0.352316       0.150829
                                                     0.142977       0.015788
                                                     0.046761      -0.000019

                      1        2    3px            12.015955       1.192141
                                                     5.108150       1.354170
                                                     2.048398       0.897267
                                                     0.832382       0.408839
                                                     0.352316       0.116648
                                                     0.142977       0.022184
                                                     0.046761       0.000308
                      1        2    3py            12.015955       1.192141
                                                     5.108150       1.354170
                                                     2.048398       0.897267
                                                     0.832382       0.408839
                                                     0.352316       0.116648
                                                     0.142977       0.022184
                                                     0.046761       0.000308
                      1        2    3pz            12.015955       1.192141
                                                     5.108150       1.354170
                                                     2.048398       0.897267
                                                     0.832382       0.408839
                                                     0.352316       0.116648
                                                     0.142977       0.022184
                                                     0.046761       0.000308

   GTH Potential information for                                GTH-PBE-q6

     Description:                       Goedecker-Teter-Hutter pseudopotential
                                         Goedecker et al., PRB 54, 1703 (1996)
                                        Hartwigsen et al., PRB 58, 3641 (1998)
                                                    Krack, TCA 114, 145 (2005)

     Gaussian exponent of the core charge distribution:              8.360253
     Electronic configuration (s p d ...):                             2   4

     Parameters of the local part of the GTH pseudopotential:

                      rloc        C1          C2          C3          C4
                    0.244554  -16.667215    2.487311

     Parameters of the non-local part of the GTH pseudopotential:

                 l      r(l)      h(i,j,l)

                 0    0.220956   18.337458
                 1    0.211332

3. Atomic kind: C                                  Number of atoms:       1

   Orbital Basis Set                                        SZV-MOLOPT-GTH

     Number of orbital shell sets:                                       1
     Number of orbital shells:                                           2
     Number of primitive Cartesian functions:                            7
     Number of Cartesian basis functions:                                4
```

```
 Number of spherical basis functions:                                  4
 Norm type:                                                            2

 Normalised Cartesian orbitals:

                  Set    Shell   Orbital          Exponent    Coefficient

                    1        1    2s             6.132625      -0.263661
                                                 2.625196      -0.231112
                                                 1.045457       0.042712
                                                 0.478316       0.306085
                                                 0.178617       0.065483
                                                 0.075145       0.000568
                                                 0.030287       0.000417

                    1        2    3px            6.132625       0.562677
                                                 2.625196       0.633910
                                                 1.045457       0.379157
                                                 0.478316       0.235193
                                                 0.178617       0.052379
                                                 0.075145       0.003677
                                                 0.030287       0.000105
                    1        2    3py            6.132625       0.562677
                                                 2.625196       0.633910
                                                 1.045457       0.379157
                                                 0.478316       0.235193
                                                 0.178617       0.052379
                                                 0.075145       0.003677
                                                 0.030287       0.000105
                    1        2    3pz            6.132625       0.562677
                                                 2.625196       0.633910
                                                 1.045457       0.379157
                                                 0.478316       0.235193
                                                 0.178617       0.052379
                                                 0.075145       0.003677
                                                 0.030287       0.000105

     GTH Potential information for                                GTH-PBE-q4

       Description:                    Goedecker-Teter-Hutter pseudopotential
                                        Goedecker et al., PRB 54, 1703 (1996)
                                       Hartwigsen et al., PRB 58, 3641 (1998)
                                                   Krack, TCA 114, 145 (2005)

       Gaussian exponent of the core charge distribution:          4.364419
       Electronic configuration (s p d ...):                          2   2

       Parameters of the local part of the GTH pseudopotential:

                         rloc        C1          C2          C3          C4
                      0.338471   -8.803674    1.339211

       Parameters of the non-local part of the GTH pseudopotential:

                    l      r(l)      h(i,j,l)

                    0    0.302576    9.622487
                    1    0.291507


 MOLECULE KIND INFORMATION


 All atoms are their own molecule, skipping detailed information


 TOTAL NUMBERS AND MAXIMUM NUMBERS

  Total number of            - Atomic kinds:                             3
                             - Atoms:                                   68
                             - Shell sets:                              68
                             - Shells:                                 136
                             - Primitive Cartesian functions:          281
                             - Cartesian basis functions:              272
                             - Spherical basis functions:              272

  Maximum angular momentum of- Orbital basis functions:                  1
                             - Local part of the GTH pseudopotential:    2
                             - Non-local part of the GTH pseudopotential: 2


 MODULE QUICKSTEP:  ATOMIC COORDINATES IN angstrom

  Atom  Kind  Element       X           Y           Z          Z(eff)       Mass

       1     1 Al  13    8.279093    8.323659   15.647941      3.00      26.9815
       2     1 Al  13   11.189505   10.656350   15.274053      3.00      26.9815
       3     1 Al  13   15.194412    9.903552    9.898627      3.00      26.9815
       4     1 Al  13   11.167902   14.722923   10.168862      3.00      26.9815
       5     1 Al  13   13.632521   12.843004    8.581516      3.00      26.9815
       6     1 Al  13   10.076545   13.320823    7.353197      3.00      26.9815
       7     1 Al  13   12.688350   12.699727    4.953944      3.00      26.9815
       8     1 Al  13   10.517221   16.225418    4.843259      3.00      26.9815
       9     1 Al  13   11.202464   13.865577    1.840208      3.00      26.9815
      10     1 Al  13   12.049374   10.801115    2.093025      3.00      26.9815
      11     1 Al  13   13.638367   10.887955   12.773330      3.00      26.9815
      12     1 Al  13   11.551994    7.853282   12.437442      3.00      26.9815
      13     1 Al  13   14.651940    7.800037   13.425820      3.00      26.9815
      14     2 O    8   11.148781   10.844312   10.203052      6.00      15.9994
      15     1 Al  13   14.564169    9.606387    4.101855      3.00      26.9815
```

```
    16     1 Al  13    3.618538    1.193203    8.139333      3.00      26.9815
    17     1 Al  13   12.713635    6.961509    5.529462      3.00      26.9815
    18     1 Al  13    1.533441    4.346449    6.987767      3.00      26.9815
    19     1 Al  13   12.390727    7.338794    2.313104      3.00      26.9815
    20     1 Al  13   10.138314    5.318144    3.638417      3.00      26.9815
    21     1 Al  13   13.828339    5.359548   10.713286      3.00      26.9815
    22     1 Al  13   11.076674    4.288691    9.106602      3.00      26.9815
    23     1 Al  13   14.072376    4.759893    7.522961      3.00      26.9815
    24     1 Al  13   11.703740    3.180539    5.755232      3.00      26.9815
    25     1 Al  13   10.793587    1.736271    2.911778      3.00      26.9815
    26     1 Al  13    2.537864   11.684127    1.628812      3.00      26.9815
    27     1 Al  13    4.682635   10.540255   13.066198      3.00      26.9815
    28     1 Al  13    8.214919   12.565693   10.099022      3.00      26.9815
    29     1 Al  13    5.847388   14.951629   10.040380      3.00      26.9815
    30     1 Al  13    8.487485   16.183397    8.157484      3.00      26.9815
    31     1 Al  13   16.813524    9.047519    1.761576      3.00      26.9815
    32     1 Al  13    8.523704   11.608749    3.717234      3.00      26.9815
    33     1 Al  13    7.080841   14.848127    5.651844      3.00      26.9815
    34     1 Al  13    7.328232   14.165839    2.120737      3.00      26.9815
    35     1 Al  13    5.686176   11.101047    1.674039      3.00      26.9815
    36     1 Al  13    7.310036    7.851822   13.425484      3.00      26.9815
    37     1 Al  13    3.912670    7.229264   12.847885      3.00      26.9815
    38     1 Al  13    9.000500    7.187660   10.528412      3.00      26.9815
    39     1 Al  13    6.219024    9.449381   10.230952      3.00      26.9815
    40     3 C    6    8.962107    9.741311    8.202917      4.00      12.0107
    41     1 Al  13    6.254725    6.388755    8.332291      3.00      26.9815
    42     1 Al  13    9.394256    6.523550    6.629359      3.00      26.9815
    43     2 O    8    7.637563    8.994978    5.182418      6.00      15.9994
    44     1 Al  13    8.784025    8.547866    2.700471      3.00      26.9815
    45     1 Al  13    7.147393    6.059522    4.374909      3.00      26.9815
    46     1 Al  13   10.757512    4.749429   12.425068      3.00      26.9815
    47     1 Al  13    7.801794    3.640378   11.065659      3.00      26.9815
    48     1 Al  13    7.567702    3.285833    7.662128      3.00      26.9815
    49     1 Al  13    4.905468    3.603198    5.384615      3.00      26.9815
    50     1 Al  13    8.087425    2.553754    4.406235      3.00      26.9815
    51     1 Al  13    6.786731   13.284309   12.885307      3.00      26.9815
    52     1 Al  13    4.265325   12.309836   10.494852      3.00      26.9815
    53     1 Al  13    3.887011   13.353535    7.181815      3.00      26.9815
    54     1 Al  13    3.230889    9.585342    4.174282      3.00      26.9815
    55     1 Al  13    4.627864   13.222807    3.936552      3.00      26.9815
    56     1 Al  13    1.681442    9.856737   10.851636      3.00      26.9815
    57     1 Al  13    3.230541    6.243208    9.619445      3.00      26.9815
    58     1 Al  13    3.911949    9.944457    7.755230      3.00      26.9815
    59     1 Al  13    3.488434    6.761864    6.575889      3.00      26.9815
    60     1 Al  13    5.912831    7.619135    1.450854      3.00      26.9815
    61     1 Al  13    4.427509    3.930432   11.739732      3.00      26.9815
    62     1 Al  13    4.177462    3.223895    8.566292      3.00      26.9815
    63     1 Al  13    3.753495    5.952504    3.489852      3.00      26.9815
    64     1 Al  13    7.892537   15.232825   15.546030      3.00      26.9815
    65     1 Al  13    3.337304   12.644625   15.442140      3.00      26.9815
    66     1 Al  13    3.511682   15.990806   12.624651      3.00      26.9815
    67     1 Al  13   15.833883    2.708346   13.899598      3.00      26.9815
    68     1 Al  13   13.373626    1.192041   11.921109      3.00      26.9815


 REQUESTED STRUCTURE DATA


 SCF PARAMETERS         Density guess:                            ATOMIC
                        ----------------------------------------------------
                        max_scf:                                     300
                        max_scf_history:                               0
                        max_diis:                                      4
                        ----------------------------------------------------
                        eps_scf:                                1.00E-06
                        eps_scf_history:                        0.00E+00
                        eps_diis:                               1.00E-01
                        eps_eigval:                             1.00E-05
                        ----------------------------------------------------
                        level_shift [a.u.]:                          0.00
                        added MOs                                 26    0
                        ----------------------------------------------------
                        Mixing method:                      BROYDEN_MIXING
                                              charge density mixing in g-space
                        ----------------------------------------------------
                        Smear method:                          FERMI_DIRAC
                        Electronic temperature [K]:                  300.0
                        Electronic temperature [a.u.]:           9.50E-04
                        Accuracy threshold:                      1.00E-10
                        ----------------------------------------------------
                        No outer SCF

 PW_GRID| Information for grid number                                    1
 PW_GRID| Cutoff [a.u.]                                               300.0
 PW_GRID| spherical cutoff:                                            NO
 PW_GRID|   Bounds   1          -135     134               Points:      270
 PW_GRID|   Bounds   2          -135     134               Points:      270
 PW_GRID|   Bounds   3          -135     134               Points:      270
 PW_GRID| Volume element (a.u.^3)  0.2000E-02     Volume (a.u.^3)     39357.3399
 PW_GRID| Grid span                                                 FULLSPACE

 PW_GRID| Information for grid number                                    2
 PW_GRID| Cutoff [a.u.]                                               100.0
 PW_GRID| spherical cutoff:                                            NO
 PW_GRID|   Bounds   1           -80      79               Points:      160
 PW_GRID|   Bounds   2           -80      79               Points:      160
 PW_GRID|   Bounds   3           -80      79               Points:      160
 PW_GRID| Volume element (a.u.^3)  0.9609E-02     Volume (a.u.^3)     39357.3399
 PW_GRID| Grid span                                                 FULLSPACE
```

```
 PW_GRID| Information for grid number                                    3
 PW_GRID| Cutoff [a.u.]                                                33.3
 PW_GRID| spherical cutoff:                                             NO
 PW_GRID|   Bounds   1            -45      44               Points:     90
 PW_GRID|   Bounds   2            -45      44               Points:     90
 PW_GRID|   Bounds   3            -45      44               Points:     90
 PW_GRID| Volume element (a.u.^3)  0.5399E-01     Volume (a.u.^3)     39357.3399
 PW_GRID| Grid span                                                  FULLSPACE

 PW_GRID| Information for grid number                                    4
 PW_GRID| Cutoff [a.u.]                                                11.1
 PW_GRID| spherical cutoff:                                             NO
 PW_GRID|   Bounds   1            -27      26               Points:     54
 PW_GRID|   Bounds   2            -27      26               Points:     54
 PW_GRID|   Bounds   3            -27      26               Points:     54
 PW_GRID| Volume element (a.u.^3)  0.2499         Volume (a.u.^3)     39357.3399
 PW_GRID| Grid span                                                  FULLSPACE

 PW_GRID| Information for grid number                                    5
 PW_GRID| Cutoff [a.u.]                                                 3.7
 PW_GRID| spherical cutoff:                                             NO
 PW_GRID|   Bounds   1            -15      14               Points:     30
 PW_GRID|   Bounds   2            -15      14               Points:     30
 PW_GRID|   Bounds   3            -15      14               Points:     30
 PW_GRID| Volume element (a.u.^3)   1.458         Volume (a.u.^3)     39357.3399
 PW_GRID| Grid span                                                  FULLSPACE

 POISSON| Solver                                                    PERIODIC
 POISSON| Periodicity                                                    XYZ

 RS_GRID| Information for grid number                                    1
 RS_GRID|   Bounds   1           -135     134               Points:    270
 RS_GRID|   Bounds   2           -135     134               Points:    270
 RS_GRID|   Bounds   3           -135     134               Points:    270

 RS_GRID| Information for grid number                                    2
 RS_GRID|   Bounds   1            -80      79               Points:    160
 RS_GRID|   Bounds   2            -80      79               Points:    160
 RS_GRID|   Bounds   3            -80      79               Points:    160

 RS_GRID| Information for grid number                                    3
 RS_GRID|   Bounds   1            -45      44               Points:     90
 RS_GRID|   Bounds   2            -45      44               Points:     90
 RS_GRID|   Bounds   3            -45      44               Points:     90

 RS_GRID| Information for grid number                                    4
 RS_GRID|   Bounds   1            -27      26               Points:     54
 RS_GRID|   Bounds   2            -27      26               Points:     54
 RS_GRID|   Bounds   3            -27      26               Points:     54

 RS_GRID| Information for grid number                                    5
 RS_GRID|   Bounds   1            -15      14               Points:     30
 RS_GRID|   Bounds   2            -15      14               Points:     30
 RS_GRID|   Bounds   3            -15      14               Points:     30

 DISTRIBUTION OF THE PARTICLES (ROWS)
              Process row      Number of particles         Number of matrix rows
                        0                       68                           -1
                      Sum                       68                           -1

 DISTRIBUTION OF THE PARTICLES (COLUMNS)
              Process col      Number of particles      Number of matrix columns
                        0                       68                           -1
                      Sum                       68                           -1

 <distribution_2d> {      id_nr=         1      ref_count=         1,
    n_row_distribution=             68,
      row_distribution= (     0,     0,     0,     0,     0,     0,     0,     0,
     0,     0,     0,     0,     0,     0,     0,     0,
     0,     0,     0,     0,     0,     0,     0,     0,
     0,     0,     0,     0,     0,     0,     0,     0,
     0,     0,     0,     0,     0,     0,     0,     0,
     0,     0,     0,     0,     0,     0,     0,     0,
     0,     0,     0,     0,     0,     0,     0,     0,
     0,     0,     0,     0,),
    n_col_distribution=             68,
      col_distribution= (     0,     0,     0,     0,     0,     0,     0,     0,
     0,     0,     0,     0,     0,     0,     0,     0,
     0,     0,     0,     0,     0,     0,     0,     0,
     0,     0,     0,     0,     0,     0,     0,     0,
     0,     0,     0,     0,     0,     0,     0,     0,
     0,     0,     0,     0,     0,     0,     0,     0,
     0,     0,     0,     0,     0,     0,     0,     0,
     0,     0,     0,     0,),
    n_local_rows= (    65,     2,     1,),
      local_rows=(
 (      1,     2,     3,     4,     5,
     6,     7,     8,     9,    10,
    11,    12,    13,    15,    16,
    17,    18,    19,    20,    21,
    22,    23,    24,    25,    26,
    27,    28,    29,    30,    31,
    32,    33,    34,    35,    36,
    37,    38,    39,    41,    42,
    44,    45,    46,    47,    48,
    49,    50,    51,    52,    53,
    54,    55,    56,    57,    58,
```

```
    59,    60,    61,    62,    63,
    64,    65,    66,    67,    68 )
(     14,    43 )
(     40 )
 ),
    n_local_cols= (    65,     2,     1,),
      local_cols=(
(      1,     2,     3,     4,     5,
     6,     7,     8,     9,    10,
    11,    12,    13,    15,    16,
    17,    18,    19,    20,    21,
    22,    23,    24,    25,    26,
    27,    28,    29,    30,    31,
    32,    33,    34,    35,    36,
    37,    38,    39,    41,    42,
    44,    45,    46,    47,    48,
    49,    50,    51,    52,    53,
    54,    55,    56,    57,    58,
    59,    60,    61,    62,    63,
    64,    65,    66,    67,    68 )
(     14,    43 )
(     40 )
 ),
    blacs_env=  group=         0, ref_count=         5,
  mepos=(       0,       0),
  num_pe=(       1,       1),
  blacs2mpi=      0
  para_env=<cp_para_env id=     0>,
  my_pid=         0, n_pid=         1 }
 }

 MD| Molecular Dynamics Protocol
 MD| Ensemble Type                                                  NPT_F
 MD| Number of Time Steps                                          25000
 MD| Time Step [fs]                                                 0.10
 MD| Temperature [K]                                             1200.00
 MD| Temperature tolerance [K]                                      0.00
 MD| Pressure [Bar]                                                 1.01
 MD| Barostat time constant [  fs]                               1000.00
 MD| Print MD information every                                 1 step(s)
 MD| File type     Print frequency[steps]                      File names
 MD| Coordinates            1                    co2_c1_melt_highprint-pos-1.xyz
 MD| Simulation Cel         1                       co2_c1_melt_highprint-1.cell
 MD| Velocities             1                    co2_c1_melt_highprint-vel-1.xyz
 MD| Energies               1                       co2_c1_melt_highprint-1.ener
 MD| Dump                   1                    co2_c1_melt_highprint-1.restart

 ROT| Rotational Analysis Info
 ROT| Principal axes and moments of inertia in atomic units:
 ROT|                                1                2                3
 ROT| EIGENVALUES           0.367025125E+09  0.378040229E+09  0.400683241E+09
 ROT|      X                   -0.481758691       0.032427637      -0.875703724
 ROT|      Y                    0.865915321      -0.135802316      -0.481402521
 ROT|      Z                    0.134533340       0.990205120      -0.037344359
 ROT| Numer of Rotovibrational vectors:     6

 Calculation of degrees of freedom
                                             Number of atoms:        68
                                Number of Intramolecular constraints:         0
                                Number of Intermolecular constraints:         0
                                 Invariants(translation + rotations):         3
                                             Degrees of freedom:       201


 Restraints Information
                                 Number of Intramolecular restraints:         0
                                 Number of Intermolecular restraints:         0

 THERMOSTAT| Thermostat Info for PARTICLES
 THERMOSTAT| Type of thermostat           Canonical Sampling/Velocity Rescaling
 THERMOSTAT| CSVR time constant [  fs]                                 1000.00
 THERMOSTAT| Initial Kinetic Energy                                   0.000000
 THERMOSTAT| End of Thermostat Info for PARTICLES


 THERMOSTAT| Thermostat Info for BAROSTAT
 THERMOSTAT| Type of thermostat           Canonical Sampling/Velocity Rescaling
 THERMOSTAT| CSVR time constant [  fs]                                 1000.00
 THERMOSTAT| Initial Kinetic Energy                                   0.000000
 THERMOSTAT| End of Thermostat Info for BAROSTAT

 ************************** Velocities initialization **************************
 Initial Temperature                                                1200.00 K
 COM velocity:           -0.000000000000     -0.000000000000      0.000000000000
 *******************************************************************************


 DISTRIBUTION OF THE NEIGHBOR LISTS
              Total number of particle pairs:                          2883
              Total number of matrix elements:                        46128
              Average number of particle pairs:                        2883
              Maximum number of particle pairs:                        2883
              Average number of matrix element:                        46128
              Maximum number of matrix elements:                       46128


 DISTRIBUTION OF THE OVERLAP MATRIX
              Number  of non-zero blocks:                              2205
              Percentage non-zero blocks:                             93.99
              Average number of blocks per CPU:                        2205
```

```
             Maximum number of blocks per CPU:                          2205
             Average number of matrix elements per CPU:                35290
             Maximum number of matrix elements per CPU:                35290

 Initializing the DDAPC Environment

 Number of electrons:                                                    211
 Number of occupied orbitals:                                            106
 Number of molecular orbitals:                                           132

 Number of orbital functions:                                            272
 Number of independent orbital functions:                                272

 Extrapolation method: initial_guess

 Atomic guess: The first density matrix is obtained in terms of atomic orbitals
               and electronic configurations assigned to each atomic kind

 Guess for atomic kind: Al

 Electronic structure
    Total number of core electrons                                     10.00
    Total number of valence electrons                                   3.00
    Total number of electrons                                          13.00
    Multiplicity                                                 not specified
    S   [  2.00  2.00] 2.00
    P   [  6.00] 1.00


 ********************************************************************************
                   Iteration          Convergence                      Energy [au]
 ********************************************************************************
                           1         0.00000                        -1.839916641139

 Energy components [Hartree]           Total Energy ::              -1.839916641139
                                        Band Energy ::              -1.480244384359
                                      Kinetic Energy ::               0.902481093321
                                    Potential Energy ::              -2.742397734460
                                       Virial (-V/T) ::               3.038731508898
                                        Core Energy ::              -2.804511037042
                                          XC Energy ::              -0.662033911062
                                     Coulomb Energy ::               1.626628306965
                         Total Pseudopotential Energy ::              -3.744899388934
                         Local Pseudopotential Energy ::              -4.214375415915
                      Nonlocal Pseudopotential Energy ::               0.469476026981
                                     Confinement ::                   0.379072585704

 Orbital energies  State     L     Occupation   Energy[a.u.]          Energy[eV]

                       1     0          2.000      -0.568042          -15.457219

                       1     1          1.000      -0.344160           -9.365060


 Total Electron Density at R=0:                                         0.000909

 Guess for atomic kind: O

 Electronic structure
    Total number of core electrons                                          2.00
    Total number of valence electrons                                       6.00
    Total number of electrons                                               8.00
    Multiplicity                                                  not specified
    S   [  2.00] 2.00
    P      4.00


 ********************************************************************************
                   Iteration          Convergence                      Energy [au]
 ********************************************************************************
                           1         0.00000                       -15.656397804158

 Energy components [Hartree]           Total Energy ::              -15.656397804158
                                        Band Energy ::               -9.711402808750
                                      Kinetic Energy ::               11.894390277343
                                    Potential Energy ::              -27.550788081501
                                       Virial (-V/T) ::                2.316284184317
                                        Core Energy ::              -26.206889069409
                                          XC Energy ::               -3.172436912785
                                     Coulomb Energy ::               13.722928178036
                         Total Pseudopotential Energy ::              -38.135868095610
                         Local Pseudopotential Energy ::              -39.418531219003
                      Nonlocal Pseudopotential Energy ::                1.282663123393
                                     Confinement ::                    0.345887488582

 Orbital energies  State     L     Occupation   Energy[a.u.]          Energy[eV]

                       1     0          2.000      -2.010675          -54.713244

                       1     1          4.000      -1.422513          -38.708556


 Total Electron Density at R=0:                                         0.000021

 Guess for atomic kind: C

 Electronic structure
    Total number of core electrons                                          2.00
    Total number of valence electrons                                       4.00
    Total number of electrons                                               6.00
```

```
   Multiplicity                                                not specified
   S   [  2.00] 2.00
   P      2.00


 ******************************************************************************
                  Iteration          Convergence                      Energy [au]
 ******************************************************************************
                          1         0.00000                      -5.193179266359

 Energy components [Hartree]           Total Energy ::           -5.193179266359
                                        Band Energy ::           -2.747025210180
                                    Kinetic Energy ::            4.338444617531
                                  Potential Energy ::           -9.531623883890
                                     Virial (-V/T) ::            2.197014073978
                                     Core Energy ::             -8.574505764553
                                       XC Energy ::             -1.533265579935
                                    Coulomb Energy ::            4.914592078128
                         Total Pseudopotential Energy ::        -12.939213155833
                         Local Pseudopotential Energy ::        -13.491979661493
                      Nonlocal Pseudopotential Energy ::          0.552766505660
                                     Confinement ::              0.262627737492

 Orbital energies  State     L     Occupation   Energy[a.u.]          Energy[eV]

                       1     0          2.000      -0.839535          -22.844921

                       1     1          2.000      -0.533977          -14.530257


 Total Electron Density at R=0:                                        0.012643
 Re-scaling the density matrix to get the right number of electrons
                  # Electrons             Trace(P)               Scaling factor
                          211              211.000                       1.000


 SCF WAVEFUNCTION OPTIMIZATION

  Step     Update method      Time    Convergence         Total energy    Change
  ---------------------------------------------------------------------------

  Trace(PS):                                 211.0000000000
  Electronic density on regular grids:      -210.9999999820        0.0000000180
  Core density on regular grids:             210.9999999523       -0.0000000477
  Total charge density on r-space grids:      -0.0000000297
  Total charge density g-space grids:         -0.0000000297


  Core Hamiltonian energy:                                        109.5898111520
  Hartree energy:                                                 245.3460575096
  Exchange-correlation energy:                                    -53.8152656492
  Coulomb (electron-electron) energy:                             166.8213593191
        Maximum deviation from MO S-orthonormality                    0.1000E+01
        Minimum/Maximum MO magnitude             0.0000E+00           0.0000E+00
     1 NoMix/Diag. 0.40E+00   29.3     0.83155048      -161.9900483780 -1.62E+02

  Trace(PS):                                 211.0000000000
  Electronic density on regular grids:      -210.9999999831        0.0000000169
  Core density on regular grids:             210.9999999523       -0.0000000477
  Total charge density on r-space grids:      -0.0000000309
  Total charge density g-space grids:         -0.0000000309


  Core Hamiltonian energy:                                        105.8343542581
  Hartree energy:                                                 244.9856141946
  Exchange-correlation energy:                                    -53.8100145989
  Coulomb (electron-electron) energy:                             169.8084135829
        Maximum deviation from MO S-orthonormality                    0.5903E-14
        Minimum/Maximum MO magnitude             0.4790E+00           0.1326E+01
     2 Broy./Diag. 0.40E+00   36.8     1.95611699      -166.1051607326 -4.12E+00

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999843        0.0000000157
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000320
 Total charge density g-space grids:         -0.0000000320


 Core Hamiltonian energy:                                         89.8161015969
 Hartree energy:                                                 246.4632245604
 Exchange-correlation energy:                                    -53.4003717482
 Coulomb (electron-electron) energy:                             167.5069693090
       Maximum deviation from MO S-orthonormality                    0.3865E-14
       Minimum/Maximum MO magnitude             0.4786E+00           0.1316E+01
    3 Broy./Diag. 0.40E+00   37.0     1.93368488      -180.2367643796 -1.41E+01

 Trace(PS):                                 211.0000000000
 Electronic density on regular grids:      -210.9999999852        0.0000000148
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000330
 Total charge density g-space grids:         -0.0000000330


 Core Hamiltonian energy:                                        104.6491288924
 Hartree energy:                                                 247.0810998970
 Exchange-correlation energy:                                    -53.2371816561
 Coulomb (electron-electron) energy:                             167.7178819207
       Maximum deviation from MO S-orthonormality                    0.4854E-14
       Minimum/Maximum MO magnitude             0.4793E+00           0.1309E+01
    4 Broy./Diag. 0.40E+00   37.2     0.43309743      -164.6233509242  1.56E+01
```

```
Trace(PS):                                 210.9999999998
Electronic density on regular grids:      -210.9999999857        0.0000000143
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000334
Total charge density g-space grids:         -0.0000000334


Core Hamiltonian energy:                                          104.6264581510
Hartree energy:                                                   247.3775325168
Exchange-correlation energy:                                      -53.1706142429
Coulomb (electron-electron) energy:                               168.2092783899
      Maximum deviation from MO S-orthonormality                      0.4566E-14
      Minimum/Maximum MO magnitude              0.4795E+00            0.1302E+01
   5 Broy./Diag. 0.40E+00   37.4     0.37198062      -164.2829314242  3.40E-01

Trace(PS):                                 210.9999999998
Electronic density on regular grids:      -210.9999999861        0.0000000139
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000339
Total charge density g-space grids:         -0.0000000339


Core Hamiltonian energy:                                          101.3992490992
Hartree energy:                                                   247.8370386682
Exchange-correlation energy:                                      -53.0664500138
Coulomb (electron-electron) energy:                               168.2451914476
      Maximum deviation from MO S-orthonormality                      0.4517E-14
      Minimum/Maximum MO magnitude              0.4794E+00            0.1306E+01
   6 Broy./Diag. 0.40E+00   37.6     0.46794601      -166.9473376724 -2.66E+00

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999862        0.0000000138
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000339
Total charge density g-space grids:         -0.0000000339


Core Hamiltonian energy:                                           98.7097254827
Hartree energy:                                                   248.0325043096
Exchange-correlation energy:                                      -53.0178962555
Coulomb (electron-electron) energy:                               168.0458061713
      Maximum deviation from MO S-orthonormality                      0.3240E-14
      Minimum/Maximum MO magnitude              0.4795E+00            0.1304E+01
   7 Broy./Diag. 0.40E+00   37.6     0.64087560      -169.3927216123 -2.45E+00

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999864        0.0000000136
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000341
Total charge density g-space grids:         -0.0000000341


Core Hamiltonian energy:                                          101.1377386177
Hartree energy:                                                   248.2686879553
Exchange-correlation energy:                                      -52.9659275460
Coulomb (electron-electron) energy:                               168.0130895638
      Maximum deviation from MO S-orthonormality                      0.3412E-14
      Minimum/Maximum MO magnitude              0.4794E+00            0.1303E+01
   8 Broy./Diag. 0.40E+00   37.7     0.37422861      -166.6765651030  2.72E+00

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999867        0.0000000133
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000345
Total charge density g-space grids:         -0.0000000345


Core Hamiltonian energy:                                          100.6481369914
Hartree energy:                                                   248.8298935210
Exchange-correlation energy:                                      -52.8428752225
Coulomb (electron-electron) energy:                               167.9811403983
      Maximum deviation from MO S-orthonormality                      0.3707E-14
      Minimum/Maximum MO magnitude              0.4794E+00            0.1304E+01
   9 Broy./Diag. 0.40E+00   37.5     0.24639549      -166.4825590992  1.94E-01

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999868        0.0000000132
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000345
Total charge density g-space grids:         -0.0000000345


Core Hamiltonian energy:                                           98.9973619054
Hartree energy:                                                   249.0102556286
Exchange-correlation energy:                                      -52.8026270426
Coulomb (electron-electron) energy:                               167.8747361990
      Maximum deviation from MO S-orthonormality                      0.3048E-14
      Minimum/Maximum MO magnitude              0.4794E+00            0.1304E+01
  10 Broy./Diag. 0.40E+00   37.6     0.23144862      -167.9121582924 -1.43E+00

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000346
Total charge density g-space grids:         -0.0000000346


Core Hamiltonian energy:                                          100.3683119588
Hartree energy:                                                   249.2019969861
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Exchange-correlation energy:                                -52.7595121899
Coulomb (electron-electron) energy:                         167.8381774730
      Maximum deviation from MO S-orthonormality                 0.3197E-14
      Minimum/Maximum MO magnitude          0.4794E+00           0.1304E+01
  11 Broy./Diag. 0.40E+00   37.8     0.11467181      -166.3067873938  1.61E+00

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.3808997898
Hartree energy:                                             249.3344489910
Exchange-correlation energy:                                -52.7329609206
Coulomb (electron-electron) energy:                         167.8282560755
      Maximum deviation from MO S-orthonormality                 0.3407E-14
      Minimum/Maximum MO magnitude          0.4794E+00           0.1304E+01
  12 Broy./Diag. 0.40E+00   37.7     0.09105076      -166.1349292286  1.72E-01

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999870        0.0000000130
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.1130654098
Hartree energy:                                             249.4009258476
Exchange-correlation energy:                                -52.7177777022
Coulomb (electron-electron) energy:                         167.8131864037
      Maximum deviation from MO S-orthonormality                 0.3260E-14
      Minimum/Maximum MO magnitude          0.4794E+00           0.1304E+01
  13 Broy./Diag. 0.40E+00   37.7     0.03651566      -166.3214698335 -1.87E-01

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.3475410735
Hartree energy:                                             249.3520319401
Exchange-correlation energy:                                -52.7290271850
Coulomb (electron-electron) energy:                         167.8473757973
      Maximum deviation from MO S-orthonormality                 0.3291E-14
      Minimum/Maximum MO magnitude          0.4794E+00           0.1303E+01
  14 Broy./Diag. 0.40E+00   37.7     0.05934560      -166.1470842406  1.74E-01

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.0907662936
Hartree energy:                                             249.3919310343
Exchange-correlation energy:                                -52.7201543397
Coulomb (electron-electron) energy:                         167.8204516099
      Maximum deviation from MO S-orthonormality                 0.3003E-14
      Minimum/Maximum MO magnitude          0.4794E+00           0.1304E+01
  15 Broy./Diag. 0.40E+00   37.7     0.08372763      -166.3550165174 -2.08E-01

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.4133739139
Hartree energy:                                             249.3827069975
Exchange-correlation energy:                                -52.7220913562
Coulomb (electron-electron) energy:                         167.8392416997
      Maximum deviation from MO S-orthonormality                 0.3338E-14
      Minimum/Maximum MO magnitude          0.4794E+00           0.1304E+01
  16 Broy./Diag. 0.40E+00   37.7     0.04700929      -166.0436968626  3.11E-01

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.1770003056
Hartree energy:                                             249.4221654560
Exchange-correlation energy:                                -52.7139951522
Coulomb (electron-electron) energy:                         167.8451393294
      Maximum deviation from MO S-orthonormality                 0.3228E-14
      Minimum/Maximum MO magnitude          0.4794E+00           0.1304E+01
  17 Broy./Diag. 0.40E+00   37.9     0.02298721      -166.2324631147 -1.89E-01

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
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 Total charge density g-space grids:          -0.0000000347


 Core Hamiltonian energy:                                      100.2767032219
 Hartree energy:                                               249.4364411318
 Exchange-correlation energy:                                  -52.7099979975
 Coulomb (electron-electron) energy:                           167.8417231332
       Maximum deviation from MO S-orthonormality                   0.3247E-14
       Minimum/Maximum MO magnitude              0.4794E+00         0.1304E+01
   18 Broy./Diag. 0.40E+00   37.8     0.05776178      -166.1145029097  1.18E-01

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                      100.5051227250
 Hartree energy:                                               249.4258257342
 Exchange-correlation energy:                                  -52.7137568157
 Coulomb (electron-electron) energy:                           167.8590655550
       Maximum deviation from MO S-orthonormality                   0.3997E-14
       Minimum/Maximum MO magnitude              0.4794E+00         0.1304E+01
   19 Broy./Diag. 0.40E+00   37.9     0.05567654      -165.9002552240  2.14E-01

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                      100.2313530787
 Hartree energy:                                               249.4442063616
 Exchange-correlation energy:                                  -52.7103609473
 Coulomb (electron-electron) energy:                           167.8687300357
       Maximum deviation from MO S-orthonormality                   0.3234E-14
       Minimum/Maximum MO magnitude              0.4794E+00         0.1304E+01
   20 Broy./Diag. 0.40E+00   37.9     0.00889137      -166.1524485575 -2.52E-01

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                      100.3007427028
 Hartree energy:                                               249.4340542294
 Exchange-correlation energy:                                  -52.7124858618
 Coulomb (electron-electron) energy:                           167.8749677206
       Maximum deviation from MO S-orthonormality                   0.3230E-14
       Minimum/Maximum MO magnitude              0.4794E+00         0.1304E+01
   21 Broy./Diag. 0.40E+00   37.8     0.03792071      -166.0953414894  5.71E-02

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                      100.2052728749
 Hartree energy:                                               249.4396870930
 Exchange-correlation energy:                                  -52.7116766668
 Coulomb (electron-electron) energy:                           167.8732293061
       Maximum deviation from MO S-orthonormality                   0.3093E-14
       Minimum/Maximum MO magnitude              0.4794E+00         0.1304E+01
   22 Broy./Diag. 0.40E+00   37.7     0.03011979      -166.1842963588 -8.90E-02

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                      100.2998325856
 Hartree energy:                                               249.4374248357
 Exchange-correlation energy:                                  -52.7121896420
 Coulomb (electron-electron) energy:                           167.8789786783
       Maximum deviation from MO S-orthonormality                   0.3289E-14
       Minimum/Maximum MO magnitude              0.4794E+00         0.1304E+01
   23 Broy./Diag. 0.40E+00   38.0     0.02064323      -166.0925725218  9.17E-02

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                      100.2137051405
 Hartree energy:                                               249.4499129740
 Exchange-correlation energy:                                  -52.7105278664
 Coulomb (electron-electron) energy:                           167.8931655438
       Maximum deviation from MO S-orthonormality                   0.3294E-14
       Minimum/Maximum MO magnitude              0.4794E+00         0.1304E+01
   24 Broy./Diag. 0.40E+00   37.8     0.02020768      -166.1645419084 -7.20E-02
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Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.3135079749
Hartree energy:                                                 249.4474966153
Exchange-correlation energy:                                    -52.7115838125
Coulomb (electron-electron) energy:                             167.8998369502
      Maximum deviation from MO S-orthonormality                    0.3218E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  25 Broy./Diag. 0.40E+00   37.9     0.00644503      -166.0682010935  9.63E-02

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2744360764
Hartree energy:                                                 249.4487636191
Exchange-correlation energy:                                    -52.7121011419
Coulomb (electron-electron) energy:                             167.9138547194
      Maximum deviation from MO S-orthonormality                    0.3208E-14
      Minimum/Maximum MO magnitude              0.4794E+00          0.1304E+01
  26 Broy./Diag. 0.40E+00   37.9     0.01035103      -166.1065406405 -3.83E-02

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2555751650
Hartree energy:                                                 249.4526390520
Exchange-correlation energy:                                    -52.7120270845
Coulomb (electron-electron) energy:                             167.9223898330
      Maximum deviation from MO S-orthonormality                    0.3181E-14
      Minimum/Maximum MO magnitude              0.4794E+00          0.1304E+01
  27 Broy./Diag. 0.40E+00   37.9     0.01150757      -166.1214329862 -1.49E-02

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2784374095
Hartree energy:                                                 249.4503869111
Exchange-correlation energy:                                    -52.7119191702
Coulomb (electron-electron) energy:                             167.9179234511
      Maximum deviation from MO S-orthonormality                    0.3225E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  28 Broy./Diag. 0.40E+00   37.9     0.02096925      -166.1007402787  2.07E-02

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2696504054
Hartree energy:                                                 249.4544869206
Exchange-correlation energy:                                    -52.7127072917
Coulomb (electron-electron) energy:                             167.9359520527
      Maximum deviation from MO S-orthonormality                    0.3216E-14
      Minimum/Maximum MO magnitude              0.4794E+00          0.1304E+01
  29 Broy./Diag. 0.40E+00   38.0     0.01447751      -166.1061596623 -5.42E-03

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.3153127215
Hartree energy:                                                 249.4517362971
Exchange-correlation energy:                                    -52.7136994971
Coulomb (electron-electron) energy:                             167.9434104206
      Maximum deviation from MO S-orthonormality                    0.3234E-14
      Minimum/Maximum MO magnitude              0.4794E+00          0.1304E+01
  30 Broy./Diag. 0.40E+00   37.9     0.00880696      -166.0642817581  4.19E-02

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2463647224
Hartree energy:                                                 249.4521747725
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Exchange-correlation energy:                                -52.7136828690
Coulomb (electron-electron) energy:                         167.9429185976
      Maximum deviation from MO S-orthonormality                 0.3553E-14
      Minimum/Maximum MO magnitude           0.4795E+00          0.1304E+01
  31 Broy./Diag. 0.40E+00   38.0     0.01008756      -166.1327828623 -6.85E-02

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2949147889
Hartree energy:                                             249.4517833282
Exchange-correlation energy:                                -52.7143017669
Coulomb (electron-electron) energy:                         167.9504847600
      Maximum deviation from MO S-orthonormality                 0.3221E-14
      Minimum/Maximum MO magnitude           0.4795E+00          0.1304E+01
  32 Broy./Diag. 0.40E+00   38.1     0.00812050      -166.0852315530  4.76E-02

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2757457482
Hartree energy:                                             249.4501374405
Exchange-correlation energy:                                -52.7146436540
Coulomb (electron-electron) energy:                         167.9509767180
      Maximum deviation from MO S-orthonormality                 0.3251E-14
      Minimum/Maximum MO magnitude           0.4795E+00          0.1304E+01
  33 Broy./Diag. 0.40E+00   38.1     0.00759041      -166.1063929242 -2.12E-02

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2651069154
Hartree energy:                                             249.4510416214
Exchange-correlation energy:                                -52.7147513568
Coulomb (electron-electron) energy:                         167.9528581072
      Maximum deviation from MO S-orthonormality                 0.3188E-14
      Minimum/Maximum MO magnitude           0.4795E+00          0.1304E+01
  34 Broy./Diag. 0.40E+00   37.9     0.00963540      -166.1162186795 -9.83E-03

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2822790503
Hartree energy:                                             249.4502376120
Exchange-correlation energy:                                -52.7151245387
Coulomb (electron-electron) energy:                         167.9556715564
      Maximum deviation from MO S-orthonormality                 0.3155E-14
      Minimum/Maximum MO magnitude           0.4795E+00          0.1304E+01
  35 Broy./Diag. 0.40E+00   37.9     0.00321172      -166.1002393575  1.60E-02

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2706226290
Hartree energy:                                             249.4506860143
Exchange-correlation energy:                                -52.7150605649
Coulomb (electron-electron) energy:                         167.9559606623
      Maximum deviation from MO S-orthonormality                 0.3213E-14
      Minimum/Maximum MO magnitude           0.4795E+00          0.1304E+01
  36 Broy./Diag. 0.40E+00   38.1     0.00248608      -166.1113873993 -1.11E-02

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2837616570
Hartree energy:                                             249.4497522522
Exchange-correlation energy:                                -52.7153490371
Coulomb (electron-electron) energy:                         167.9579384691
      Maximum deviation from MO S-orthonormality                 0.3553E-14
      Minimum/Maximum MO magnitude           0.4795E+00          0.1304E+01
  37 Broy./Diag. 0.40E+00   38.0     0.00387970      -166.0994643668  1.19E-02

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
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 Total charge density g-space grids:          -0.0000000347


 Core Hamiltonian energy:                                     100.2597675275
 Hartree energy:                                              249.4499368188
 Exchange-correlation energy:                                 -52.7156313164
 Coulomb (electron-electron) energy:                          167.9604419335
       Maximum deviation from MO S-orthonormality                 0.3199E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   38 Broy./Diag. 0.40E+00   38.0     0.00307129      -166.1235573179 -2.41E-02

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2789548433
 Hartree energy:                                              249.4494912689
 Exchange-correlation energy:                                 -52.7159853675
 Coulomb (electron-electron) energy:                          167.9639021651
       Maximum deviation from MO S-orthonormality                 0.3194E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   39 Broy./Diag. 0.40E+00   38.2     0.00170195      -166.1051731158  1.84E-02

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2756805050
 Hartree energy:                                              249.4492208005
 Exchange-correlation energy:                                 -52.7160525574
 Coulomb (electron-electron) energy:                          167.9645391797
       Maximum deviation from MO S-orthonormality                 0.3553E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   40 Broy./Diag. 0.40E+00   38.1     0.00444642      -166.1087824776 -3.61E-03

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2714447237
 Hartree energy:                                              249.4501265362
 Exchange-correlation energy:                                 -52.7156834192
 Coulomb (electron-electron) energy:                          167.9616520599
       Maximum deviation from MO S-orthonormality                 0.3208E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   41 Broy./Diag. 0.40E+00   38.0     0.00513776      -166.1117409906 -2.96E-03

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2829738840
 Hartree energy:                                              249.4490954299
 Exchange-correlation energy:                                 -52.7163709382
 Coulomb (electron-electron) energy:                          167.9673568072
       Maximum deviation from MO S-orthonormality                 0.3242E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   42 Broy./Diag. 0.40E+00   38.1     0.00165684      -166.1019335146  9.81E-03

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2713503152
 Hartree energy:                                              249.4493771648
 Exchange-correlation energy:                                 -52.7164630254
 Coulomb (electron-electron) energy:                          167.9688529153
       Maximum deviation from MO S-orthonormality                 0.3232E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   43 Broy./Diag. 0.40E+00   37.9     0.00252467      -166.1133705001 -1.14E-02

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2842187661
 Hartree energy:                                              249.4489140785
 Exchange-correlation energy:                                 -52.7162451162
 Coulomb (electron-electron) energy:                          167.9666955793
       Maximum deviation from MO S-orthonormality                 0.3265E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   44 Broy./Diag. 0.40E+00   38.0     0.00328355      -166.1007434422  1.26E-02
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Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2619209690
Hartree energy:                                                 249.4492383675
Exchange-correlation energy:                                    -52.7164757339
Coulomb (electron-electron) energy:                             167.9689868785
      Maximum deviation from MO S-orthonormality                    0.3775E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  45 Broy./Diag. 0.40E+00   37.9     0.00343018      -166.1229406623 -2.22E-02

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2769676926
Hartree energy:                                                 249.4487670309
Exchange-correlation energy:                                    -52.7169878708
Coulomb (electron-electron) energy:                             167.9739795734
      Maximum deviation from MO S-orthonormality                    0.3247E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  46 Broy./Diag. 0.40E+00   37.9     0.00080770      -166.1088871012  1.41E-02

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2748343740
Hartree energy:                                                 249.4484897511
Exchange-correlation energy:                                    -52.7171799902
Coulomb (electron-electron) energy:                             167.9757720607
      Maximum deviation from MO S-orthonormality                    0.3298E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  47 Broy./Diag. 0.40E+00   37.9     0.00199472      -166.1114880270 -2.60E-03

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2721786133
Hartree energy:                                                 249.4489892911
Exchange-correlation energy:                                    -52.7172280325
Coulomb (electron-electron) energy:                             167.9774417687
      Maximum deviation from MO S-orthonormality                    0.3331E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  48 Broy./Diag. 0.40E+00   37.9     0.00247498      -166.1136925009 -2.20E-03

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2848409735
Hartree energy:                                                 249.4482271219
Exchange-correlation energy:                                    -52.7175072448
Coulomb (electron-electron) energy:                             167.9792572299
      Maximum deviation from MO S-orthonormality                    0.3235E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  49 Broy./Diag. 0.40E+00   37.9     0.00311263      -166.1020681028  1.16E-02

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2666658176
Hartree energy:                                                 249.4484348780
Exchange-correlation energy:                                    -52.7178097730
Coulomb (electron-electron) energy:                             167.9826767205
      Maximum deviation from MO S-orthonormality                    0.3775E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  50 Broy./Diag. 0.40E+00   37.8     0.00263453      -166.1203429383 -1.83E-02

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2805613890
Hartree energy:                                                 249.4480001764
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Exchange-correlation energy:                                -52.7176644886
Coulomb (electron-electron) energy:                         167.9811414921
      Maximum deviation from MO S-orthonormality                 0.3240E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  51 Broy./Diag. 0.40E+00   37.9     0.00353343      -166.1067368856  1.36E-02

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2666573122
Hartree energy:                                             249.4484286365
Exchange-correlation energy:                                -52.7176137196
Coulomb (electron-electron) energy:                         167.9807277817
      Maximum deviation from MO S-orthonormality                 0.3230E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  52 Broy./Diag. 0.40E+00   37.9     0.00289632      -166.1201510595 -1.34E-02

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2743154469
Hartree energy:                                             249.4484591992
Exchange-correlation energy:                                -52.7176459962
Coulomb (electron-electron) energy:                         167.9813100804
      Maximum deviation from MO S-orthonormality                 0.3268E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  53 Broy./Diag. 0.40E+00   37.9     0.00097336      -166.1125039570  7.65E-03

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2753100895
Hartree energy:                                             249.4483087972
Exchange-correlation energy:                                -52.7177650872
Coulomb (electron-electron) energy:                         167.9824252965
      Maximum deviation from MO S-orthonormality                 0.3247E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  54 Broy./Diag. 0.40E+00   37.9     0.00076942      -166.1117778692  7.26E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2734613204
Hartree energy:                                             249.4485408989
Exchange-correlation energy:                                -52.7177379771
Coulomb (electron-electron) energy:                         167.9825444300
      Maximum deviation from MO S-orthonormality                 0.3216E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  55 Broy./Diag. 0.40E+00   38.0     0.00082485      -166.1133678139 -1.59E-03

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2792195094
Hartree energy:                                             249.4482813592
Exchange-correlation energy:                                -52.7178212696
Coulomb (electron-electron) energy:                         167.9831406551
      Maximum deviation from MO S-orthonormality                 0.3291E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  56 Broy./Diag. 0.40E+00   37.9     0.00129675      -166.1079510876  5.42E-03

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2721714810
Hartree energy:                                             249.4482906953
Exchange-correlation energy:                                -52.7180174060
Coulomb (electron-electron) energy:                         167.9853582890
      Maximum deviation from MO S-orthonormality                 0.3254E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  57 Broy./Diag. 0.40E+00   37.7     0.00054226      -166.1151868854 -7.24E-03

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
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 Total charge density g-space grids:          -0.0000000347


 Core Hamiltonian energy:                                     100.2752087807
 Hartree energy:                                              249.4481093146
 Exchange-correlation energy:                                 -52.7179334017
 Coulomb (electron-electron) energy:                          167.9844797315
       Maximum deviation from MO S-orthonormality                 0.3232E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   58 Broy./Diag. 0.40E+00   37.8     0.00195379      -166.1122481580  2.94E-03

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2715764089
 Hartree energy:                                              249.4482577841
 Exchange-correlation energy:                                 -52.7180307429
 Coulomb (electron-electron) energy:                          167.9856298552
       Maximum deviation from MO S-orthonormality                 0.3223E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   59 Broy./Diag. 0.40E+00   37.8     0.00196801      -166.1158229902 -3.57E-03

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2743823789
 Hartree energy:                                              249.4484099013
 Exchange-correlation energy:                                 -52.7180059268
 Coulomb (electron-electron) energy:                          167.9856706064
       Maximum deviation from MO S-orthonormality                 0.3164E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   60 Broy./Diag. 0.40E+00   37.8     0.00113773      -166.1128452197  2.98E-03

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2769042747
 Hartree energy:                                              249.4480443420
 Exchange-correlation energy:                                 -52.7181348251
 Coulomb (electron-electron) energy:                          167.9864611681
       Maximum deviation from MO S-orthonormality                 0.3303E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   61 Broy./Diag. 0.40E+00   37.9     0.00106866      -166.1108174982  2.03E-03

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2694759807
 Hartree energy:                                              249.4482870680
 Exchange-correlation energy:                                 -52.7180765380
 Coulomb (electron-electron) energy:                          167.9861519622
       Maximum deviation from MO S-orthonormality                 0.3157E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   62 Broy./Diag. 0.40E+00   37.9     0.00119460      -166.1179461934 -7.13E-03

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2761536902
 Hartree energy:                                              249.4482109999
 Exchange-correlation energy:                                 -52.7181036047
 Coulomb (electron-electron) energy:                          167.9864596425
       Maximum deviation from MO S-orthonormality                 0.3240E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   63 Broy./Diag. 0.40E+00   37.9     0.00039513      -166.1113707075  6.58E-03

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2737651755
 Hartree energy:                                              249.4481712493
 Exchange-correlation energy:                                 -52.7181848939
 Coulomb (electron-electron) energy:                          167.9874033410
       Maximum deviation from MO S-orthonormality                 0.3235E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   64 Broy./Diag. 0.40E+00   37.9     0.00061164      -166.1138795926 -2.51E-03
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Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2741864661
Hartree energy:                                                 249.4482095214
Exchange-correlation energy:                                    -52.7181934800
Coulomb (electron-electron) energy:                             167.9874475955
      Maximum deviation from MO S-orthonormality                    0.3188E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  65 Broy./Diag. 0.40E+00   38.1     0.00059395      -166.1134283708  4.51E-04

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2746495419
Hartree energy:                                                 249.4480915604
Exchange-correlation energy:                                    -52.7183473502
Coulomb (electron-electron) energy:                             167.9891388426
      Maximum deviation from MO S-orthonormality                    0.3253E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  66 Broy./Diag. 0.40E+00   37.9     0.00033790      -166.1132386187  1.90E-04

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2736520832
Hartree energy:                                                 249.4483243137
Exchange-correlation energy:                                    -52.7182745619
Coulomb (electron-electron) energy:                             167.9887574718
      Maximum deviation from MO S-orthonormality                    0.3286E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  67 Broy./Diag. 0.40E+00   37.9     0.00068994      -166.1139297274 -6.91E-04

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2784105560
Hartree energy:                                                 249.4480066722
Exchange-correlation energy:                                    -52.7182832264
Coulomb (electron-electron) energy:                             167.9883424895
      Maximum deviation from MO S-orthonormality                    0.3227E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  68 Broy./Diag. 0.40E+00   38.0     0.00171192      -166.1094967877  4.43E-03

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2689772113
Hartree energy:                                                 249.4481399285
Exchange-correlation energy:                                    -52.7183742973
Coulomb (electron-electron) energy:                             167.9895401454
      Maximum deviation from MO S-orthonormality                    0.3251E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  69 Broy./Diag. 0.40E+00   37.9     0.00133088      -166.1188892669 -9.39E-03

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2749761880
Hartree energy:                                                 249.4480693480
Exchange-correlation energy:                                    -52.7184863396
Coulomb (electron-electron) energy:                             167.9908405853
      Maximum deviation from MO S-orthonormality                    0.3313E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  70 Broy./Diag. 0.40E+00   38.0     0.00056453      -166.1130732529  5.82E-03

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2736075900
Hartree energy:                                                 249.4480521798
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Exchange-correlation energy:                                -52.7183807750
Coulomb (electron-electron) energy:                         167.9896793987
      Maximum deviation from MO S-orthonormality                 0.3327E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  71 Broy./Diag. 0.40E+00   38.1     0.00110199      -166.1143529676 -1.28E-03

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2733284778
Hartree energy:                                             249.4481107263
Exchange-correlation energy:                                -52.7184253961
Coulomb (electron-electron) energy:                         167.9901564299
      Maximum deviation from MO S-orthonormality                 0.3180E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  72 Broy./Diag. 0.40E+00   38.0     0.00067252      -166.1146155632 -2.63E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2744599695
Hartree energy:                                             249.4480149154
Exchange-correlation energy:                                -52.7184872518
Coulomb (electron-electron) energy:                         167.9907406784
      Maximum deviation from MO S-orthonormality                 0.4108E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  73 Broy./Diag. 0.40E+00   38.0     0.00028949      -166.1136442592  9.71E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2727884762
Hartree energy:                                             249.4481191420
Exchange-correlation energy:                                -52.7184627721
Coulomb (electron-electron) energy:                         167.9906348446
      Maximum deviation from MO S-orthonormality                 0.3320E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  74 Broy./Diag. 0.40E+00   38.0     0.00037792      -166.1151871229 -1.54E-03

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2753850508
Hartree energy:                                             249.4480686355
Exchange-correlation energy:                                -52.7184679513
Coulomb (electron-electron) energy:                         167.9906484645
      Maximum deviation from MO S-orthonormality                 0.3272E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  75 Broy./Diag. 0.40E+00   38.0     0.00037980      -166.1126458196  2.54E-03

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2736722024
Hartree energy:                                             249.4480645455
Exchange-correlation energy:                                -52.7185022939
Coulomb (electron-electron) energy:                         167.9910187864
      Maximum deviation from MO S-orthonormality                 0.3216E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  76 Broy./Diag. 0.40E+00   38.1     0.00016873      -166.1143970598 -1.75E-03

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2742386952
Hartree energy:                                             249.4480428323
Exchange-correlation energy:                                -52.7185586364
Coulomb (electron-electron) energy:                         167.9916728933
      Maximum deviation from MO S-orthonormality                 0.3195E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  77 Broy./Diag. 0.40E+00   38.1     0.00018761      -166.1139088329  4.88E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
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Total charge density g-space grids:          -0.0000000347


Core Hamiltonian energy:                                        100.2740445486
Hartree energy:                                                 249.4479849324
Exchange-correlation energy:                                    -52.7185441240
Coulomb (electron-electron) energy:                             167.9915066812
      Maximum deviation from MO S-orthonormality                    0.3223E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  78 Broy./Diag. 0.40E+00   38.0     0.00046424      -166.1141464620 -2.38E-04

Trace(PS):                                  210.9999999999
Electronic density on regular grids:       -210.9999999869        0.0000000131
Core density on regular grids:              210.9999999523       -0.0000000477
Total charge density on r-space grids:       -0.0000000347
Total charge density g-space grids:          -0.0000000347


Core Hamiltonian energy:                                        100.2730934673
Hartree energy:                                                 249.4480806984
Exchange-correlation energy:                                    -52.7185777499
Coulomb (electron-electron) energy:                             167.9920174424
      Maximum deviation from MO S-orthonormality                    0.3211E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  79 Broy./Diag. 0.40E+00   38.0     0.00062462      -166.1150335015 -8.87E-04

Trace(PS):                                  210.9999999999
Electronic density on regular grids:       -210.9999999869        0.0000000131
Core density on regular grids:              210.9999999523       -0.0000000477
Total charge density on r-space grids:       -0.0000000347
Total charge density g-space grids:          -0.0000000347


Core Hamiltonian energy:                                        100.2752473261
Hartree energy:                                                 249.4479279305
Exchange-correlation energy:                                    -52.7186085392
Coulomb (electron-electron) energy:                             167.9920891443
      Maximum deviation from MO S-orthonormality                    0.3211E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  80 Broy./Diag. 0.40E+00   38.1     0.00049216      -166.1130646009  1.97E-03

Trace(PS):                                  210.9999999999
Electronic density on regular grids:       -210.9999999869        0.0000000131
Core density on regular grids:              210.9999999523       -0.0000000477
Total charge density on r-space grids:       -0.0000000347
Total charge density g-space grids:          -0.0000000347


Core Hamiltonian energy:                                        100.2715016332
Hartree energy:                                                 249.4480303412
Exchange-correlation energy:                                    -52.7186053334
Coulomb (electron-electron) energy:                             167.9921814147
      Maximum deviation from MO S-orthonormality                    0.3997E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  81 Broy./Diag. 0.40E+00   38.1     0.00064389      -166.1167053771 -3.64E-03

Trace(PS):                                  210.9999999999
Electronic density on regular grids:       -210.9999999869        0.0000000131
Core density on regular grids:              210.9999999523       -0.0000000477
Total charge density on r-space grids:       -0.0000000347
Total charge density g-space grids:          -0.0000000347


Core Hamiltonian energy:                                        100.2747032888
Hartree energy:                                                 249.4480113220
Exchange-correlation energy:                                    -52.7185972407
Coulomb (electron-electron) energy:                             167.9921240062
      Maximum deviation from MO S-orthonormality                    0.3284E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  82 Broy./Diag. 0.40E+00   38.0     0.00033450      -166.1135145025  3.19E-03

Trace(PS):                                  210.9999999999
Electronic density on regular grids:       -210.9999999869        0.0000000131
Core density on regular grids:              210.9999999523       -0.0000000477
Total charge density on r-space grids:       -0.0000000347
Total charge density g-space grids:          -0.0000000347


Core Hamiltonian energy:                                        100.2734729397
Hartree energy:                                                 249.4480107391
Exchange-correlation energy:                                    -52.7186074183
Coulomb (electron-electron) energy:                             167.9922303657
      Maximum deviation from MO S-orthonormality                    0.3213E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  83 Broy./Diag. 0.40E+00   38.1     0.00027541      -166.1147552519 -1.24E-03

Trace(PS):                                  210.9999999999
Electronic density on regular grids:       -210.9999999869        0.0000000131
Core density on regular grids:              210.9999999523       -0.0000000477
Total charge density on r-space grids:       -0.0000000347
Total charge density g-space grids:          -0.0000000347


Core Hamiltonian energy:                                        100.2738779194
Hartree energy:                                                 249.4480029416
Exchange-correlation energy:                                    -52.7186248953
Coulomb (electron-electron) energy:                             167.9924274266
      Maximum deviation from MO S-orthonormality                    0.3254E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  84 Broy./Diag. 0.40E+00   38.2     0.00005878      -166.1143755575  3.80E-04
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Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2738180029
Hartree energy:                                                 249.4479750090
Exchange-correlation energy:                                    -52.7186813945
Coulomb (electron-electron) energy:                             167.9930745772
      Maximum deviation from MO S-orthonormality                    0.3227E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  85 Broy./Diag. 0.40E+00   38.1     0.00008918      -166.1145199837 -1.44E-04

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2737274513
Hartree energy:                                                 249.4480183399
Exchange-correlation energy:                                    -52.7186938540
Coulomb (electron-electron) energy:                             167.9932885790
      Maximum deviation from MO S-orthonormality                    0.3220E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  86 Broy./Diag. 0.40E+00   38.0     0.00022254      -166.1145794519 -5.95E-05

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2747572054
Hartree energy:                                                 249.4478992619
Exchange-correlation energy:                                    -52.7187338002
Coulomb (electron-electron) energy:                             167.9935873024
      Maximum deviation from MO S-orthonormality                    0.3247E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  87 Broy./Diag. 0.40E+00   38.0     0.00041114      -166.1137091233  8.70E-04

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2718788161
Hartree energy:                                                 249.4479631823
Exchange-correlation energy:                                    -52.7187376650
Coulomb (electron-electron) energy:                             167.9937171183
      Maximum deviation from MO S-orthonormality                    0.3256E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  88 Broy./Diag. 0.40E+00   38.0     0.00051400      -166.1165276388 -2.82E-03

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2741556008
Hartree energy:                                                 249.4479552699
Exchange-correlation energy:                                    -52.7187422270
Coulomb (electron-electron) energy:                             167.9937912402
      Maximum deviation from MO S-orthonormality                    0.3208E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  89 Broy./Diag. 0.40E+00   37.9     0.00032971      -166.1142630648  2.26E-03

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2735612122
Hartree energy:                                                 249.4479740986
Exchange-correlation energy:                                    -52.7187157776
Coulomb (electron-electron) energy:                             167.9935248323
      Maximum deviation from MO S-orthonormality                    0.3261E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
  90 Broy./Diag. 0.40E+00   38.1     0.00027635      -166.1148120362 -5.49E-04

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2739579325
Hartree energy:                                                 249.4479600460
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Exchange-correlation energy:                                -52.7187371106
Coulomb (electron-electron) energy:                         167.9937123444
      Maximum deviation from MO S-orthonormality                 0.3299E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  91 Broy./Diag. 0.40E+00   38.0     0.00022747      -166.1144502915  3.62E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2738074700
Hartree energy:                                             249.4479449760
Exchange-correlation energy:                                -52.7187420055
Coulomb (electron-electron) energy:                         167.9937594074
      Maximum deviation from MO S-orthonormality                 0.3251E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  92 Broy./Diag. 0.40E+00   37.9     0.00006717      -166.1146212755 -1.71E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2735252679
Hartree energy:                                             249.4479588852
Exchange-correlation energy:                                -52.7187404137
Coulomb (electron-electron) energy:                         167.9937642493
      Maximum deviation from MO S-orthonormality                 0.3247E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  93 Broy./Diag. 0.40E+00   38.0     0.00006095      -166.1148878019 -2.67E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2738020872
Hartree energy:                                             249.4479517958
Exchange-correlation energy:                                -52.7187471282
Coulomb (electron-electron) energy:                         167.9938306060
      Maximum deviation from MO S-orthonormality                 0.3192E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  94 Broy./Diag. 0.40E+00   38.0     0.00001672      -166.1146248674  2.63E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2736889450
Hartree energy:                                             249.4479597073
Exchange-correlation energy:                                -52.7187495306
Coulomb (electron-electron) energy:                         167.9938699033
      Maximum deviation from MO S-orthonormality                 0.3553E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  95 Broy./Diag. 0.40E+00   37.9     0.00007050      -166.1147324880 -1.08E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2740142123
Hartree energy:                                             249.4479448232
Exchange-correlation energy:                                -52.7187588599
Coulomb (electron-electron) energy:                         167.9939604429
      Maximum deviation from MO S-orthonormality                 0.3145E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  96 Broy./Diag. 0.40E+00   38.0     0.00007733      -166.1144314111  3.01E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2736324977
Hartree energy:                                             249.4479539056
Exchange-correlation energy:                                -52.7187512836
Coulomb (electron-electron) energy:                         167.9939098813
      Maximum deviation from MO S-orthonormality                 0.3305E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
  97 Broy./Diag. 0.40E+00   37.9     0.00011736      -166.1147965573 -3.65E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
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 Total charge density g-space grids:          -0.0000000347


 Core Hamiltonian energy:                                     100.2737810736
 Hartree energy:                                              249.4479548580
 Exchange-correlation energy:                                 -52.7187633631
 Coulomb (electron-electron) energy:                          167.9940336171
       Maximum deviation from MO S-orthonormality                 0.3293E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   98 Broy./Diag. 0.40E+00   37.9     0.00009473      -166.1146588026  1.38E-04

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2739138893
 Hartree energy:                                              249.4479400568
 Exchange-correlation energy:                                 -52.7187672683
 Coulomb (electron-electron) energy:                          167.9940560335
       Maximum deviation from MO S-orthonormality                 0.3234E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
   99 Broy./Diag. 0.40E+00   38.2     0.00004847      -166.1145449630  1.14E-04

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2736366838
 Hartree energy:                                              249.4479478393
 Exchange-correlation energy:                                 -52.7187648746
 Coulomb (electron-electron) energy:                          167.9940426108
       Maximum deviation from MO S-orthonormality                 0.3136E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
  100 Broy./Diag. 0.40E+00   37.8     0.00005254      -166.1148119209 -2.67E-04

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2737935202
 Hartree energy:                                              249.4479404717
 Exchange-correlation energy:                                 -52.7187673633
 Coulomb (electron-electron) energy:                          167.9940637644
       Maximum deviation from MO S-orthonormality                 0.3190E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
  101 Broy./Diag. 0.40E+00   37.9     0.00004287      -166.1146649855  1.47E-04

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2735628997
 Hartree energy:                                              249.4479481544
 Exchange-correlation energy:                                 -52.7187667306
 Coulomb (electron-electron) energy:                          167.9940671930
       Maximum deviation from MO S-orthonormality                 0.3256E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
  102 Broy./Diag. 0.40E+00   38.1     0.00005865      -166.1148872962 -2.22E-04

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2738236214
 Hartree energy:                                              249.4479461460
 Exchange-correlation energy:                                 -52.7187696078
 Coulomb (electron-electron) energy:                          167.9941051191
       Maximum deviation from MO S-orthonormality                 0.3183E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
  103 Broy./Diag. 0.40E+00   37.9     0.00004592      -166.1146314174  2.56E-04

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2737706754
 Hartree energy:                                              249.4479401724
 Exchange-correlation energy:                                 -52.7187720408
 Coulomb (electron-electron) energy:                          167.9941176769
       Maximum deviation from MO S-orthonormality                 0.3306E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
  104 Broy./Diag. 0.40E+00   37.9     0.00004916      -166.1146926958 -6.13E-05
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Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2736673990
Hartree energy:                                                 249.4479462836
Exchange-correlation energy:                                    -52.7187731329
Coulomb (electron-electron) energy:                             167.9941400309
      Maximum deviation from MO S-orthonormality                    0.3331E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
 105 Broy./Diag. 0.40E+00   38.0     0.00002556      -166.1147910498 -9.84E-05

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2738054451
Hartree energy:                                                 249.4479406096
Exchange-correlation energy:                                    -52.7187757006
Coulomb (electron-electron) energy:                             167.9941653487
      Maximum deviation from MO S-orthonormality                    0.3164E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
 106 Broy./Diag. 0.40E+00   37.8     0.00003341      -166.1146612790  1.30E-04

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2736964995
Hartree energy:                                                 249.4479452297
Exchange-correlation energy:                                    -52.7187752535
Coulomb (electron-electron) energy:                             167.9941654264
      Maximum deviation from MO S-orthonormality                    0.3240E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
 107 Broy./Diag. 0.40E+00   37.7     0.00002824      -166.1147650972 -1.04E-04

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2738498627
Hartree energy:                                                 249.4479388803
Exchange-correlation energy:                                    -52.7187759233
Coulomb (electron-electron) energy:                             167.9941641662
      Maximum deviation from MO S-orthonormality                    0.3147E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
 108 Broy./Diag. 0.40E+00   37.7     0.00004811      -166.1146187555  1.46E-04

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2736366646
Hartree energy:                                                 249.4479390000
Exchange-correlation energy:                                    -52.7187814813
Coulomb (electron-electron) energy:                             167.9942294551
      Maximum deviation from MO S-orthonormality                    0.3293E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
 109 Broy./Diag. 0.40E+00   38.0     0.00002257      -166.1148374283 -2.19E-04

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2737203546
Hartree energy:                                                 249.4479454714
Exchange-correlation energy:                                    -52.7187778881
Coulomb (electron-electron) energy:                             167.9942045807
      Maximum deviation from MO S-orthonormality                    0.3232E-14
      Minimum/Maximum MO magnitude              0.4795E+00          0.1304E+01
 110 Broy./Diag. 0.40E+00   38.1     0.00004069      -166.1147436791  9.37E-05

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2738216111
Hartree energy:                                                 249.4479314165
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Exchange-correlation energy:                                -52.7187838538
Coulomb (electron-electron) energy:                         167.9942528844
      Maximum deviation from MO S-orthonormality                 0.3202E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
 111 Broy./Diag. 0.40E+00   38.0     0.00004655      -166.1146623636  8.13E-05

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2735780944
Hartree energy:                                             249.4479395966
Exchange-correlation energy:                                -52.7187846587
Coulomb (electron-electron) energy:                         167.9942699001
      Maximum deviation from MO S-orthonormality                 0.3240E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
 112 Broy./Diag. 0.40E+00   38.0     0.00004328      -166.1148984717 -2.36E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2737634558
Hartree energy:                                             249.4479348668
Exchange-correlation energy:                                -52.7187850705
Coulomb (electron-electron) energy:                         167.9942688751
      Maximum deviation from MO S-orthonormality                 0.3175E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
 113 Broy./Diag. 0.40E+00   37.9     0.00003158      -166.1147183673  1.80E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2736092655
Hartree energy:                                             249.4479420794
Exchange-correlation energy:                                -52.7187839974
Coulomb (electron-electron) energy:                         167.9942663919
      Maximum deviation from MO S-orthonormality                 0.3258E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
 114 Broy./Diag. 0.40E+00   37.8     0.00005133      -166.1148642687 -1.46E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2738467559
Hartree energy:                                             249.4479378798
Exchange-correlation energy:                                -52.7187857344
Coulomb (electron-electron) energy:                         167.9942829002
      Maximum deviation from MO S-orthonormality                 0.3178E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
 115 Broy./Diag. 0.40E+00   38.0     0.00003187      -166.1146326767  2.32E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2737229115
Hartree energy:                                             249.4479355706
Exchange-correlation energy:                                -52.7187880621
Coulomb (electron-electron) energy:                         167.9943040666
      Maximum deviation from MO S-orthonormality                 0.3280E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
 116 Broy./Diag. 0.40E+00   37.8     0.00001657      -166.1147611635 -1.28E-04

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2737002818
Hartree energy:                                             249.4479364842
Exchange-correlation energy:                                -52.7187891877
Coulomb (electron-electron) energy:                         167.9943219259
      Maximum deviation from MO S-orthonormality                 0.3263E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
 117 Broy./Diag. 0.40E+00   37.8     0.00001288      -166.1147840353 -2.29E-05

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
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Total charge density g-space grids:          -0.0000000347


Core Hamiltonian energy:                                      100.2737287622
Hartree energy:                                               249.4479348884
Exchange-correlation energy:                                  -52.7187986692
Coulomb (electron-electron) energy:                           167.9944319235
      Maximum deviation from MO S-orthonormality                   0.3227E-14
      Minimum/Maximum MO magnitude              0.4795E+00         0.1304E+01
 118 Broy./Diag. 0.40E+00   37.9     0.00001401      -166.1147666045  1.74E-05

Trace(PS):                                  210.9999999999
Electronic density on regular grids:       -210.9999999869        0.0000000131
Core density on regular grids:              210.9999999523       -0.0000000477
Total charge density on r-space grids:       -0.0000000347
Total charge density g-space grids:          -0.0000000347


Core Hamiltonian energy:                                      100.2737701858
Hartree energy:                                               249.4479298363
Exchange-correlation energy:                                  -52.7188045121
Coulomb (electron-electron) energy:                           167.9944970617
      Maximum deviation from MO S-orthonormality                   0.3322E-14
      Minimum/Maximum MO magnitude              0.4795E+00         0.1304E+01
 119 Broy./Diag. 0.40E+00   37.9     0.00003448      -166.1147361198  3.05E-05

Trace(PS):                                  210.9999999999
Electronic density on regular grids:       -210.9999999869        0.0000000131
Core density on regular grids:              210.9999999523       -0.0000000477
Total charge density on r-space grids:       -0.0000000347
Total charge density g-space grids:          -0.0000000347


Core Hamiltonian energy:                                      100.2737432561
Hartree energy:                                               249.4479236621
Exchange-correlation energy:                                  -52.7187977301
Coulomb (electron-electron) energy:                           167.9944065895
      Maximum deviation from MO S-orthonormality                   0.3169E-14
      Minimum/Maximum MO magnitude              0.4795E+00         0.1304E+01
 120 Broy./Diag. 0.40E+00   37.7     0.00005627      -166.1147623763 -2.63E-05

Trace(PS):                                  210.9999999999
Electronic density on regular grids:       -210.9999999869        0.0000000131
Core density on regular grids:              210.9999999523       -0.0000000477
Total charge density on r-space grids:       -0.0000000347
Total charge density g-space grids:          -0.0000000347


Core Hamiltonian energy:                                      100.2734380009
Hartree energy:                                               249.4479331717
Exchange-correlation energy:                                  -52.7187989905
Coulomb (electron-electron) energy:                           167.9944340251
      Maximum deviation from MO S-orthonormality                   0.3221E-14
      Minimum/Maximum MO magnitude              0.4795E+00         0.1304E+01
 121 Broy./Diag. 0.40E+00   38.1     0.00006220      -166.1150594193 -2.97E-04

Trace(PS):                                  210.9999999999
Electronic density on regular grids:       -210.9999999869        0.0000000131
Core density on regular grids:              210.9999999523       -0.0000000477
Total charge density on r-space grids:       -0.0000000347
Total charge density g-space grids:          -0.0000000347


Core Hamiltonian energy:                                      100.2737551907
Hartree energy:                                               249.4479325401
Exchange-correlation energy:                                  -52.7188058142
Coulomb (electron-electron) energy:                           167.9945238940
      Maximum deviation from MO S-orthonormality                   0.3286E-14
      Minimum/Maximum MO magnitude              0.4795E+00         0.1304E+01
 122 Broy./Diag. 0.40E+00   37.9     0.00004358      -166.1147496733  3.10E-04

Trace(PS):                                  210.9999999999
Electronic density on regular grids:       -210.9999999869        0.0000000131
Core density on regular grids:              210.9999999523       -0.0000000477
Total charge density on r-space grids:       -0.0000000347
Total charge density g-space grids:          -0.0000000347


Core Hamiltonian energy:                                      100.2737659247
Hartree energy:                                               249.4479301969
Exchange-correlation energy:                                  -52.7188024506
Coulomb (electron-electron) energy:                           167.9944703500
      Maximum deviation from MO S-orthonormality                   0.3214E-14
      Minimum/Maximum MO magnitude              0.4795E+00         0.1304E+01
 123 Broy./Diag. 0.40E+00   38.0     0.00004230      -166.1147378617  1.18E-05

Trace(PS):                                  210.9999999999
Electronic density on regular grids:       -210.9999999869        0.0000000131
Core density on regular grids:              210.9999999523       -0.0000000477
Total charge density on r-space grids:       -0.0000000347
Total charge density g-space grids:          -0.0000000347


Core Hamiltonian energy:                                      100.2736956991
Hartree energy:                                               249.4479289576
Exchange-correlation energy:                                  -52.7188037160
Coulomb (electron-electron) energy:                           167.9944858274
      Maximum deviation from MO S-orthonormality                   0.3263E-14
      Minimum/Maximum MO magnitude              0.4795E+00         0.1304E+01
 124 Broy./Diag. 0.40E+00   37.9     0.00001004      -166.1148106833 -7.28E-05
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Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2736826542
Hartree energy:                                                 249.4479296737
Exchange-correlation energy:                                    -52.7188047240
Coulomb (electron-electron) energy:                             167.9944987477
      Maximum deviation from MO S-orthonormality                    0.3306E-14
      Minimum/Maximum MO magnitude             0.4795E+00           0.1304E+01
 125 Broy./Diag. 0.40E+00   37.9     0.00000618      -166.1148239841 -1.33E-05

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2737017694
Hartree energy:                                                 249.4479314526
Exchange-correlation energy:                                    -52.7188042901
Coulomb (electron-electron) energy:                             167.9944962439
      Maximum deviation from MO S-orthonormality                    0.3230E-14
      Minimum/Maximum MO magnitude             0.4795E+00           0.1304E+01
 126 Broy./Diag. 0.40E+00   37.9     0.00001178      -166.1148026714  2.13E-05

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2737607681
Hartree energy:                                                 249.4479288907
Exchange-correlation energy:                                    -52.7188048069
Coulomb (electron-electron) energy:                             167.9944989508
      Maximum deviation from MO S-orthonormality                    0.3216E-14
      Minimum/Maximum MO magnitude             0.4795E+00           0.1304E+01
 127 Broy./Diag. 0.40E+00   37.9     0.00001398      -166.1147467399  5.59E-05

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2736853171
Hartree energy:                                                 249.4479287513
Exchange-correlation energy:                                    -52.7188063815
Coulomb (electron-electron) energy:                             167.9945173464
      Maximum deviation from MO S-orthonormality                    0.3270E-14
      Minimum/Maximum MO magnitude             0.4795E+00           0.1304E+01
 128 Broy./Diag. 0.40E+00   37.9     0.00000422      -166.1148239096 -7.72E-05

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2737007835
Hartree energy:                                                 249.4479305744
Exchange-correlation energy:                                    -52.7188055237
Coulomb (electron-electron) energy:                             167.9945139618
      Maximum deviation from MO S-orthonormality                    0.3268E-14
      Minimum/Maximum MO magnitude             0.4795E+00           0.1304E+01
 129 Broy./Diag. 0.40E+00   37.9     0.00001900      -166.1148057651  1.81E-05

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2737290098
Hartree energy:                                                 249.4479296515
Exchange-correlation energy:                                    -52.7188064698
Coulomb (electron-electron) energy:                             167.9945201849
      Maximum deviation from MO S-orthonormality                    0.3228E-14
      Minimum/Maximum MO magnitude             0.4795E+00           0.1304E+01
 130 Broy./Diag. 0.40E+00   37.8     0.00001685      -166.1147793646  2.64E-05

Trace(PS):                                 210.9999999999
Electronic density on regular grids:      -210.9999999869        0.0000000131
Core density on regular grids:             210.9999999523       -0.0000000477
Total charge density on r-space grids:      -0.0000000347
Total charge density g-space grids:         -0.0000000347


Core Hamiltonian energy:                                        100.2737174884
Hartree energy:                                                 249.4479284245
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Exchange-correlation energy:                                -52.7188067262
Coulomb (electron-electron) energy:                         167.9945218133
      Maximum deviation from MO S-orthonormality                 0.3188E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
 131 Broy./Diag. 0.40E+00   37.9     0.00000625      -166.1147924167 -1.31E-05

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2736986031
Hartree energy:                                             249.4479273076
Exchange-correlation energy:                                -52.7188072854
Coulomb (electron-electron) energy:                         167.9945267432
      Maximum deviation from MO S-orthonormality                 0.3253E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
 132 Broy./Diag. 0.40E+00   37.9     0.00000849      -166.1148129622 -2.05E-05

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2736611156
Hartree energy:                                             249.4479293868
Exchange-correlation energy:                                -52.7188067888
Coulomb (electron-electron) energy:                         167.9945236840
      Maximum deviation from MO S-orthonormality                 0.3294E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
 133 Broy./Diag. 0.40E+00   37.9     0.00001048      -166.1148478854 -3.49E-05

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2737206526
Hartree energy:                                             249.4479287869
Exchange-correlation energy:                                -52.7188070842
Coulomb (electron-electron) energy:                         167.9945266868
      Maximum deviation from MO S-orthonormality                 0.3213E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
 134 Broy./Diag. 0.40E+00   38.0     0.00000378      -166.1147892398  5.86E-05

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2737051843
Hartree energy:                                             249.4479287065
Exchange-correlation energy:                                -52.7188075476
Coulomb (electron-electron) energy:                         167.9945321874
      Maximum deviation from MO S-orthonormality                 0.3190E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
 135 Broy./Diag. 0.40E+00   37.9     0.00000144      -166.1148052508 -1.60E-05

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2737081773
Hartree energy:                                             249.4479280232
Exchange-correlation energy:                                -52.7188084148
Coulomb (electron-electron) energy:                         167.9945408277
      Maximum deviation from MO S-orthonormality                 0.3235E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
 136 Broy./Diag. 0.40E+00   37.8     0.00000354      -166.1148038073  1.44E-06

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
Total charge density g-space grids:      -0.0000000347


Core Hamiltonian energy:                                    100.2737009596
Hartree energy:                                             249.4479278409
Exchange-correlation energy:                                -52.7188099938
Coulomb (electron-electron) energy:                         167.9945605065
      Maximum deviation from MO S-orthonormality                 0.3279E-14
      Minimum/Maximum MO magnitude          0.4795E+00           0.1304E+01
 137 Broy./Diag. 0.40E+00   38.0     0.00000396      -166.1148127956 -8.99E-06

Trace(PS):                             210.9999999999
Electronic density on regular grids:  -210.9999999869        0.0000000131
Core density on regular grids:         210.9999999523       -0.0000000477
Total charge density on r-space grids:   -0.0000000347
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 Total charge density g-space grids:          -0.0000000347


 Core Hamiltonian energy:                                     100.2737080451
 Hartree energy:                                              249.4479276702
 Exchange-correlation energy:                                 -52.7188099031
 Coulomb (electron-electron) energy:                          167.9945594716
       Maximum deviation from MO S-orthonormality                 0.3192E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
  138 Broy./Diag. 0.40E+00   37.8     0.00000804      -166.1148057839  7.01E-06

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2737170292
 Hartree energy:                                              249.4479249043
 Exchange-correlation energy:                                 -52.7188115707
 Coulomb (electron-electron) energy:                          167.9945754262
       Maximum deviation from MO S-orthonormality                 0.4219E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
  139 Broy./Diag. 0.40E+00   37.8     0.00001329      -166.1148012165  4.57E-06

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2736455932
 Hartree energy:                                              249.4479275903
 Exchange-correlation energy:                                 -52.7188107321
 Coulomb (electron-electron) energy:                          167.9945687090
       Maximum deviation from MO S-orthonormality                 0.3240E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
  140 Broy./Diag. 0.40E+00   37.9     0.00000901      -166.1148691384 -6.79E-05

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2737123853
 Hartree energy:                                              249.4479273246
 Exchange-correlation energy:                                 -52.7188106048
 Coulomb (electron-electron) energy:                          167.9945668687
       Maximum deviation from MO S-orthonormality                 0.3237E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
  141 Broy./Diag. 0.40E+00   37.8     0.00000473      -166.1148024910  6.66E-05

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2737022393
 Hartree energy:                                              249.4479276200
 Exchange-correlation energy:                                 -52.7188106069
 Coulomb (electron-electron) energy:                          167.9945682780
       Maximum deviation from MO S-orthonormality                 0.3237E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
  142 Broy./Diag. 0.40E+00   38.0     0.00000377      -166.1148123461 -9.86E-06

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2737084555
 Hartree energy:                                              249.4479271590
 Exchange-correlation energy:                                 -52.7188108285
 Coulomb (electron-electron) energy:                          167.9945694520
       Maximum deviation from MO S-orthonormality                 0.3214E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
  143 Broy./Diag. 0.40E+00   38.0     0.00000359      -166.1148068011  5.54E-06

 Trace(PS):                                 210.9999999999
 Electronic density on regular grids:      -210.9999999869        0.0000000131
 Core density on regular grids:             210.9999999523       -0.0000000477
 Total charge density on r-space grids:      -0.0000000347
 Total charge density g-space grids:         -0.0000000347


 Core Hamiltonian energy:                                     100.2737015108
 Hartree energy:                                              249.4479272083
 Exchange-correlation energy:                                 -52.7188108653
 Coulomb (electron-electron) energy:                          167.9945699940
       Maximum deviation from MO S-orthonormality                 0.3225E-14
       Minimum/Maximum MO magnitude              0.4795E+00       0.1304E+01
  144 Broy./Diag. 0.40E+00   37.8     0.00000088      -166.1148137406 -6.94E-06
```

```
 *** SCF run converged in   144 steps ***


 Electronic density on regular grids:       -210.9999999869        0.0000000131
 Core density on regular grids:              210.9999999523       -0.0000000477
 Total charge density on r-space grids:       -0.0000000347
 Total charge density g-space grids:          -0.0000000347

 Overlap energy of the core charge distribution:              0.00000000038927
 Self energy of the core charge distribution:              -463.11065139080455
 Core Hamiltonian energy:                                   100.27370151079995
 Hartree energy:                                            249.44792720834181
 Exchange-correlation energy:                               -52.71881086528722
 Coulomb Electron-Electron Interaction Energy
 - Already included in the total Hartree term               167.99456999396358
 Electronic entropic energy:                                 -0.00698020516779
 Fermi energy:                                               -0.01974482003442

 Total energy:                                             -166.11481374061290

The electron density is written in cube file format to the file:

co2_c1_melt_highprint-ELECTRON_DENSITY-1_0.cube

    Lanczos converged:  T threshold:   0.100E-02
    Est. extremal eigenvalues:    0.227E+01   0.153E+00
    Est. condition number :    0.148E+02
    NS sqrt iter    1 1.00000000   0.459E+00       0.046     1607.233
    NS sqrt iter    2 1.00000000   0.983E-01       0.066     2426.128
    NS sqrt iter    3 1.00000000   0.137E-01       0.066     2433.463
    NS sqrt iter    4 1.00000000   0.410E-03       0.063     2224.016
    NS sqrt iter    5 1.00000000   0.118E-07       0.047     1550.473
    Final NS sqrt iter    5 1.00000000   0.213E-14

 Creating energy windows. Fermi level:   -1.9777385656214161E-002
 Printing Energy Levels from  -0.58335477900447230       to   0.38988106107217751
Energy Level:    -0.5784885998 Number of states:     1 Occupation:     2.00000000327879
Energy Level:    -0.5687562414 Number of states:     1 Occupation:     2.00000008911857
Energy Level:    -0.5590238830 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.5492915246 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.5395591662 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.5298268078 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.5200944494 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.5103620910 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.5006297326 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.4908973742 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.4811650158 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.4714326574 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.4617002990 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.4519679406 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.4422355822 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.4325032238 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.4227708654 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.4130385070 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.4033061486 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.3935737902 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.3838414318 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.3741090734 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.3643767150 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.3546443566 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.3449119982 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.3351796398 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.3254472814 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.3157149230 Number of states:     1 Occupation:     1.99998141135432
Energy Level:    -0.3059825646 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.2962502062 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.2865178478 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.2767854894 Number of states:     1 Occupation:     2.00012435251769
Energy Level:    -0.2670531310 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.2573207726 Number of states:     1 Occupation:     1.99993727918226
Energy Level:    -0.2475884142 Number of states:     2 Occupation:     3.99606455559567
Energy Level:    -0.2378560558 Number of states:     3 Occupation:     6.00181502359044
Energy Level:    -0.2281236974 Number of states:     3 Occupation:     6.00699093051416
Energy Level:    -0.2183913390 Number of states:     2 Occupation:     4.00258357013222
Energy Level:    -0.2086589806 Number of states:     5 Occupation:    10.00118339449964
Energy Level:    -0.1989266222 Number of states:     5 Occupation:     9.99979278596147
Energy Level:    -0.1891942638 Number of states:     4 Occupation:     7.99512522027135
Energy Level:    -0.1794619054 Number of states:     4 Occupation:     7.99801251236016
Energy Level:    -0.1697295470 Number of states:     5 Occupation:     9.98116630542506
Energy Level:    -0.1599971886 Number of states:     6 Occupation:    11.98415606311093
Energy Level:    -0.1502648302 Number of states:     4 Occupation:     7.99874845649443
Energy Level:    -0.1405324718 Number of states:     4 Occupation:     7.99762037220080
Energy Level:    -0.1308001134 Number of states:     5 Occupation:    10.01267518633432
Energy Level:    -0.1210677550 Number of states:     5 Occupation:    10.04085927739105
Energy Level:    -0.1113353966 Number of states:     4 Occupation:     8.02576593439672
Energy Level:    -0.1016030382 Number of states:     1 Occupation:     2.00585664009739
Energy Level:    -0.0918706798 Number of states:     1 Occupation:     2.00292646103325
Energy Level:    -0.0821383214 Number of states:     0 Occupation:     0.00000000000000
Energy Level:    -0.0724059630 Number of states:     1 Occupation:     2.00800711469577
Energy Level:    -0.0626736046 Number of states:     4 Occupation:     8.03189116429309
Energy Level:    -0.0529412462 Number of states:     7 Occupation:    14.00939912483037
Energy Level:    -0.0432088878 Number of states:     9 Occupation:    17.89406557416033
Energy Level:    -0.0334765294 Number of states:     8 Occupation:    15.81562762238325
Energy Level:    -0.0237441710 Number of states:    10 Occupation:    16.20559533095322
Energy Level:    -0.0140118126 Number of states:     8 Occupation:     0.83588020838307
Energy Level:    -0.0042794542 Number of states:     9 Occupation:     0.15840773502571
Energy Level:     0.0054529042 Number of states:     9 Occupation:     0.10576477613142
Energy Level:     0.0151852626 Number of states:    10 Occupation:     0.00613720815318
Energy Level:     0.0249176210 Number of states:     8 Occupation:    -0.02977681350075
```

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 Energy Level:     0.0346499794 Number of states:     8 Occupation:    -0.01807463061033
 Energy Level:     0.0443823378 Number of states:     7 Occupation:    -0.02184000101391
 Energy Level:     0.0541146962 Number of states:     8 Occupation:    -0.01737265390559
 Energy Level:     0.0638470546 Number of states:     7 Occupation:    -0.01569170277751
 Energy Level:     0.0735794130 Number of states:     7 Occupation:    -0.02360985586034
 Energy Level:     0.0833117714 Number of states:     7 Occupation:    -0.01108167717214
 Energy Level:     0.0930441298 Number of states:     7 Occupation:    -0.01141123026535
 Energy Level:     0.1027764882 Number of states:     8 Occupation:    -0.01145079795324
 Energy Level:     0.1125088467 Number of states:     6 Occupation:     0.01289473827830
 Energy Level:     0.1222412051 Number of states:     7 Occupation:     0.01048080040885
 Energy Level:     0.1319735635 Number of states:     6 Occupation:     0.00376231582597
 Energy Level:     0.1417059219 Number of states:     8 Occupation:     0.00664081539618
 Energy Level:     0.1514382803 Number of states:     7 Occupation:     0.00620939842425
 Energy Level:     0.1611706387 Number of states:     4 Occupation:     0.00187679256136
 Energy Level:     0.1709029971 Number of states:     4 Occupation:     0.00002353551114
 Energy Level:     0.1806353555 Number of states:     5 Occupation:     0.00168933238493
 Energy Level:     0.1903677139 Number of states:     5 Occupation:    -0.00291253281276
 Energy Level:     0.2001000723 Number of states:     4 Occupation:    -0.00082233940578
 Energy Level:     0.2098324307 Number of states:     2 Occupation:    -0.00199678497471
 Energy Level:     0.2195647891 Number of states:     1 Occupation:     0.00058393223865
 Energy Level:     0.2292971475 Number of states:     1 Occupation:    -0.00028071801476
 Energy Level:     0.2390295059 Number of states:     0 Occupation:     0.00000000000000
 Energy Level:     0.2487618643 Number of states:     0 Occupation:     0.00000000000000
 Energy Level:     0.2584942227 Number of states:     0 Occupation:     0.00000000000000
 Energy Level:     0.2682265811 Number of states:     0 Occupation:     0.00000000000000
 Energy Level:     0.2779589395 Number of states:     0 Occupation:     0.00000000000000
 Energy Level:     0.2876912979 Number of states:     1 Occupation:    -0.00000366761078
 Energy Level:     0.2974236563 Number of states:     0 Occupation:     0.00000000000000
 Energy Level:     0.3071560147 Number of states:     0 Occupation:     0.00000000000000
 Energy Level:     0.3168883731 Number of states:     0 Occupation:     0.00000000000000
 Energy Level:     0.3266207315 Number of states:     0 Occupation:     0.00000000000000
 Energy Level:     0.3363530899 Number of states:     0 Occupation:     0.00000000000000
 Energy Level:     0.3460854483 Number of states:     0 Occupation:     0.00000000000000
 Energy Level:     0.3558178067 Number of states:     0 Occupation:     0.00000000000000
 Energy Level:     0.3655501651 Number of states:     0 Occupation:     0.00000000000000
 Energy Level:     0.3752825235 Number of states:     0 Occupation:     0.00000000000000
 Energy Level:     0.3850148819 Number of states:     0 Occupation:     0.00000000000000

 !-----------------------------------------------------------------------------!
                     Mulliken Population Analysis

 #  Atom  Element  Kind  Atomic population                         Net charge
       1     Al       1          2.991420                           0.008580
       2     Al       1          2.882478                           0.117522
       3     Al       1          2.889912                           0.110088
       4     Al       1          2.930720                           0.069280
       5     Al       1          2.938092                           0.061908
       6     Al       1          3.029900                          -0.029900
       7     Al       1          3.000823                          -0.000823
       8     Al       1          2.901707                           0.098293
       9     Al       1          2.986605                           0.013395
      10     Al       1          3.044973                          -0.044973
      11     Al       1          2.986578                           0.013422
      12     Al       1          3.007730                          -0.007730
      13     Al       1          2.977441                           0.022559
      14     O        2          6.464342                          -0.464342
      15     Al       1          3.046366                          -0.046366
      16     Al       1          2.986002                           0.013998
      17     Al       1          3.011413                          -0.011413
      18     Al       1          2.915879                           0.084121
      19     Al       1          3.000903                          -0.000903
      20     Al       1          3.068731                          -0.068731
      21     Al       1          3.057596                          -0.057596
      22     Al       1          3.033197                          -0.033197
      23     Al       1          3.010201                          -0.010201
      24     Al       1          2.995615                           0.004385
      25     Al       1          2.962979                           0.037021
      26     Al       1          2.989666                           0.010334
      27     Al       1          3.109027                          -0.109027
      28     Al       1          2.962096                           0.037904
      29     Al       1          3.068824                          -0.068824
      30     Al       1          3.020202                          -0.020202
      31     Al       1          2.833584                           0.166416
      32     Al       1          2.947782                           0.052218
      33     Al       1          3.013234                          -0.013234
      34     Al       1          3.027599                          -0.027599
      35     Al       1          3.041692                          -0.041692
      36     Al       1          3.061062                          -0.061062
      37     Al       1          2.982031                           0.017969
      38     Al       1          3.013195                          -0.013195
      39     Al       1          3.018518                          -0.018518
      40     C        3          3.901820                           0.098180
      41     Al       1          3.005632                          -0.005632
      42     Al       1          2.956243                           0.043757
      43     O        2          6.495024                          -0.495024
      44     Al       1          2.928578                           0.071422
      45     Al       1          2.988911                           0.011089
      46     Al       1          3.034310                          -0.034310
      47     Al       1          2.966360                           0.033640
      48     Al       1          2.991029                           0.008971
      49     Al       1          2.998999                           0.001001
      50     Al       1          2.988922                           0.011078
      51     Al       1          3.079907                          -0.079907
      52     Al       1          3.063300                          -0.063300
      53     Al       1          2.949055                           0.050945
      54     Al       1          2.935648                           0.064352
      55     Al       1          3.031593                          -0.031593
      56     Al       1          2.916404                           0.083596
      57     Al       1          3.060160                          -0.060160
      58     Al       1          2.988712                           0.011288
```

59	Al	1	3.056831	-0.056831
60	Al	1	2.944786	0.055214
61	Al	1	2.935174	0.064826
62	Al	1	3.223375	-0.223375
63	Al	1	3.010422	-0.010422
64	Al	1	2.812591	0.187409
65	Al	1	2.878513	0.121487
66	Al	1	2.864275	0.135725
67	Al	1	2.873447	0.126553
68	Al	1	2.909870	0.090130
# Total charge			211.000000	0.000000

!---!

!---!

Hirshfeld Charges

#Atom	Element	Kind	Ref Charge	Population	Net charge
1	Al	1	3.000	2.992	0.008
2	Al	1	3.000	2.889	0.111
3	Al	1	3.000	2.895	0.105
4	Al	1	3.000	2.934	0.066
5	Al	1	3.000	2.952	0.048
6	Al	1	3.000	3.029	-0.029
7	Al	1	3.000	3.000	-0.000
8	Al	1	3.000	2.911	0.089
9	Al	1	3.000	2.988	0.012
10	Al	1	3.000	3.039	-0.039
11	Al	1	3.000	2.994	0.006
12	Al	1	3.000	3.004	-0.004
13	Al	1	3.000	2.976	0.024
14	O	2	6.000	6.431	-0.431
15	Al	1	3.000	3.055	-0.055
16	Al	1	3.000	3.012	-0.012
17	Al	1	3.000	3.012	-0.012
18	Al	1	3.000	2.947	0.053
19	Al	1	3.000	3.004	-0.004
20	Al	1	3.000	3.048	-0.048
21	Al	1	3.000	3.057	-0.057
22	Al	1	3.000	3.031	-0.031
23	Al	1	3.000	3.009	-0.009
24	Al	1	3.000	2.999	0.001
25	Al	1	3.000	2.966	0.034
26	Al	1	3.000	2.991	0.009
27	Al	1	3.000	3.100	-0.100
28	Al	1	3.000	2.987	0.013
29	Al	1	3.000	3.058	-0.058
30	Al	1	3.000	3.024	-0.024
31	Al	1	3.000	2.830	0.170
32	Al	1	3.000	2.965	0.035
33	Al	1	3.000	3.010	-0.010
34	Al	1	3.000	3.024	-0.024
35	Al	1	3.000	3.031	-0.031
36	Al	1	3.000	3.048	-0.048
37	Al	1	3.000	2.987	0.013
38	Al	1	3.000	3.026	-0.026
39	Al	1	3.000	3.031	-0.031
40	C	3	4.000	3.849	0.151
41	Al	1	3.000	3.011	-0.011
42	Al	1	3.000	2.978	0.022
43	O	2	6.000	6.430	-0.430
44	Al	1	3.000	2.968	0.032
45	Al	1	3.000	3.000	-0.000
46	Al	1	3.000	3.037	-0.037
47	Al	1	3.000	2.973	0.027
48	Al	1	3.000	3.001	-0.001
49	Al	1	3.000	3.009	-0.009
50	Al	1	3.000	2.990	0.010
51	Al	1	3.000	3.088	-0.088
52	Al	1	3.000	3.052	-0.052
53	Al	1	3.000	2.957	0.043
54	Al	1	3.000	2.945	0.055
55	Al	1	3.000	3.027	-0.027
56	Al	1	3.000	2.930	0.070
57	Al	1	3.000	3.058	-0.058
58	Al	1	3.000	2.987	0.013
59	Al	1	3.000	3.035	-0.035
60	Al	1	3.000	2.941	0.059
61	Al	1	3.000	2.951	0.049
62	Al	1	3.000	3.140	-0.140
63	Al	1	3.000	3.009	-0.009
64	Al	1	3.000	2.807	0.193
65	Al	1	3.000	2.881	0.119
66	Al	1	3.000	2.867	0.133
67	Al	1	3.000	2.873	0.127
68	Al	1	3.000	2.914	0.086
Total Charge				0.003

!---!

Electronic kinetic energy: 79.86450419392985

LOWDIN POPULATION ANALYSIS

# Atom	Element	Kind	Atomic population	Net charge
1	Al	1	2.997713	0.002287
2	Al	1	2.883486	0.116514
3	Al	1	2.893043	0.106957
4	Al	1	2.935177	0.064823
5	Al	1	2.944952	0.055048

```
     6     Al       1          3.025811                      -0.025811
     7     Al       1          2.996899                       0.003101
     8     Al       1          2.899875                       0.100125
     9     Al       1          2.996159                       0.003841
    10     Al       1          3.041071                      -0.041071
    11     Al       1          2.992642                       0.007358
    12     Al       1          2.996504                       0.003496
    13     Al       1          2.984457                       0.015543
    14     O        2          6.447404                      -0.447404
    15     Al       1          3.054224                      -0.054224
    16     Al       1          2.988637                       0.011363
    17     Al       1          3.003677                      -0.003677
    18     Al       1          2.926313                       0.073687
    19     Al       1          3.009891                      -0.009891
    20     Al       1          3.057602                      -0.057602
    21     Al       1          3.058833                      -0.058833
    22     Al       1          3.019034                      -0.019034
    23     Al       1          3.021609                      -0.021609
    24     Al       1          2.988877                       0.011123
    25     Al       1          2.982798                       0.017202
    26     Al       1          3.002467                      -0.002467
    27     Al       1          3.115266                      -0.115266
    28     Al       1          2.961695                       0.038305
    29     Al       1          3.072089                      -0.072089
    30     Al       1          3.035106                      -0.035106
    31     Al       1          2.832066                       0.167934
    32     Al       1          2.943127                       0.056873
    33     Al       1          3.001332                      -0.001332
    34     Al       1          3.038239                      -0.038239
    35     Al       1          3.033310                      -0.033310
    36     Al       1          3.051716                      -0.051716
    37     Al       1          2.989083                       0.010917
    38     Al       1          3.015683                      -0.015683
    39     Al       1          3.015527                      -0.015527
    40     C        3          3.889236                       0.110764
    41     Al       1          2.996421                       0.003579
    42     Al       1          2.958408                       0.041592
    43     O        2          6.459777                      -0.459777
    44     Al       1          2.943915                       0.056085
    45     Al       1          2.982771                       0.017229
    46     Al       1          3.044461                      -0.044461
    47     Al       1          2.971229                       0.028771
    48     Al       1          2.987846                       0.012154
    49     Al       1          2.994681                       0.005319
    50     Al       1          2.987867                       0.012133
    51     Al       1          3.083358                      -0.083358
    52     Al       1          3.051810                      -0.051810
    53     Al       1          2.954859                       0.045141
    54     Al       1          2.929814                       0.070186
    55     Al       1          3.027519                      -0.027519
    56     Al       1          2.920671                       0.079329
    57     Al       1          3.056844                      -0.056844
    58     Al       1          2.984421                       0.015579
    59     Al       1          3.046964                      -0.046964
    60     Al       1          2.951553                       0.048447
    61     Al       1          2.943754                       0.056246
    62     Al       1          3.213007                      -0.213007
    63     Al       1          3.028600                      -0.028600
    64     Al       1          2.811971                       0.188029
    65     Al       1          2.878311                       0.121689
    66     Al       1          2.863600                       0.136400
    67     Al       1          2.872187                       0.127813
    68     Al       1          2.910750                       0.089250
# Total charge                          211.000000                0.000000

 DDAP FULL DENSITY charges:
 Atom     |    Charge

     1  Al   -0.041882
     2  Al    0.034313
     3  Al    0.079489
     4  Al    0.064394
     5  Al    0.064518
     6  Al    0.090409
     7  Al   -0.010012
     8  Al    0.030308
     9  Al   -0.035131
    10  Al   -0.006885
    11  Al    0.074574
    12  Al    0.107366
    13  Al   -0.028120
    14  O    -0.571951
    15  Al   -0.041160
    16  Al   -0.087164
    17  Al    0.034983
    18  Al   -0.023475
    19  Al   -0.036901
    20  Al    0.013213
    21  Al   -0.033550
    22  Al    0.005993
    23  Al   -0.017255
    24  Al   -0.003357
    25  Al   -0.026461
    26  Al   -0.046158
    27  Al   -0.043813
    28  Al    0.170536
    29  Al   -0.042174
    30  Al   -0.064478
    31  Al    0.098639
    32  Al    0.124560
```

```
    33  Al    0.011585
    34  Al   -0.062976
    35  Al    0.036769
    36  Al    0.025959
    37  Al   -0.025340
    38  Al    0.058992
    39  Al    0.042859
    40  C    -0.087847
    41  Al    0.024935
    42  Al    0.115471
    43  O    -0.494217
    44  Al    0.082173
    45  Al    0.123056
    46  Al   -0.043672
    47  Al   -0.022514
    48  Al   -0.036673
    49  Al    0.000196
    50  Al   -0.004521
    51  Al   -0.083366
    52  Al    0.034278
    53  Al   -0.010626
    54  Al    0.049016
    55  Al    0.037023
    56  Al   -0.015848
    57  Al   -0.024000
    58  Al    0.022907
    59  Al    0.051061
    60  Al    0.002103
    61  Al   -0.012789
    62  Al    0.080579
    63  Al   -0.059414
    64  Al    0.128524
    65  Al    0.046789
    66  Al    0.066990
    67  Al    0.076950
    68  Al    0.032222
  Total      -0.000000


 ELECTRIC/MAGNETIC MOMENTS

 ********************************************************************************
 *                                                                              *
 *   ___                                                                        *
 *  /   \                                                                       *
 * [ABORT]                                                                      *
 *  \___/     Berry phase moments for non uniform MOs' occupation numbers not  *
 *    |                                  implemented                           *
 *  O/|                                                                         *
 * /| |                                                                        *
 * / \                                                    qs_moments.F:1068 *
 ********************************************************************************


 ===== Routine Calling Stack =====

            7 qs_moment_berry_phase
            6 qs_scf_post_moments
            5 scf_post_calculation_gpw
            4 qs_energies
            3 qs_forces
            2 qs_mol_dyn_low
            1 CP2K
--------------------------------------------------------------------------
MPI_ABORT was invoked on rank 0 in communicator MPI_COMM_WORLD
with errorcode 1.

NOTE: invoking MPI_ABORT causes Open MPI to kill all MPI processes.
You may or may not see output from other processes, depending on
exactly when Open MPI kills them.
--------------------------------------------------------------------------
```