Mesp test on electron density isosurface of 0.001 au

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Details on computation of electron density

Molecule: Catechin
Number of atoms: 35
Type of calculation: MP2
LCAO program: NwChem
Basis set: DZP (Dunning)
Number of basis functions: 385
Results in convergence:

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SCF energy              -1025.506542418239
Correlation energy         -3.373250480378
Singlet pairs              -2.099306813488
Triplet pairs              -1.273943666890
Total MP2 energy        -1028.879792898617
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This calculation has been kindly supplied to us by Dr. Noel Ferro.

Details on DAM computation of electron density (MED) and electrostatic potential (MESP)

Length of DAM partition/exansion of MED: $l_{max} = 10$
Grid size for MED tabulation: 257x257x257 (16 974 593 points)
Grid dimensions for MED tabulation: $x, y, z \in [-17, 17]$ bohr
MED value for isosurface: 0.001
Number of triangles for MED isosurface: 179 852
Number of vertices for MED isosurface: 90 656
Wall-clock time of MED grid computation: 475 sec (in a system with an Intel(R) Core(TM) i7-2630QM CPU @ 2.00GHz and 4 cores)

Results of MESP surface extrema computed with the current algorithm

Number of local maxima (higher than mesp = 0.73E-01) found =   5

Positions and mesp values of the local maxima in the mesh
----
x = -0.10090E+02 y = 0.37188E+01 z = -0.79681E+00 mesp = 0.89468E-01
x = -0.29761E+00 y = 0.12883E+02 z = -0.39838E+00 mesp = 0.91452E-01
x = 0.51798E+01 y = -0.12575E+02 z = -0.53119E+00 mesp = 0.80414E-01
x = 0.82345E+01 y = 0.29219E+01 z = 0.13712E+01 mesp = 0.78107E-01
x = -0.46484E+01 y = -0.54453E+01 z = 0.45670E+01 mesp = 0.78653E-01

Number of local minima (lower than mesp = -0.65E-01) found =   1

Positions and mesp values of the local minima in the mesh
----
x = -0.79681E+00 y = -0.11578E+02 z = 0.37188E+01 mesp = -0.80831E-01

***************************** MESP statistics *****************************

     Total surface with positive MESP = 0.49282E+03
     Total surface with negative MESP = 0.58480E+03

     MESP average = 0.73496E-04
     Positive MESP average = 0.27731E-01
     Negative MESP average = -0.23234E-01

     MESP variance = 0.76617E-03
     Positive MESP variance = 0.49598E-03
     Negative MESP variance = 0.27020E-03

     MESP average deviation = 0.25297E-01

     MESP nu parameter = 0.22829E+00

                         TIMING (in seconds)

 Processor 0 (user, system, total):   (0.11208E+03, 0.40000E+01, 0.11608E+03)
 Processor 1 (user, system, total):   (0.11345E+03, 0.47552E+00, 0.11393E+03)
 Processor 2 (user, system, total):   (0.11490E+03, 0.18774E+00, 0.11509E+03)
 Processor 3 (user, system, total):   (0.72241E+02, 0.23997E+01, 0.74640E+02)

Results of MESP surface extrema computed with eq (36) of main text

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Number of local maxima (higher than mesp =  0.73E-01) found =   5

Positions and mesp values of the local maxima in the mesh
-----------------------------------------------------------------------
x = -0.10090E+02 y =  0.37188E+01 z = -0.79681E+00 mesp =  0.89467E-01
x = -0.29761E+00 y =  0.12883E+02 z = -0.39838E+00 mesp =  0.91451E-01
x =  0.51798E+01 y = -0.12575E+02 z = -0.53119E+00 mesp =  0.80413E-01
x =  0.82345E+01 y =  0.29219E+01 z =  0.13712E+01 mesp =  0.78107E-01
x = -0.46484E+01 y = -0.54453E+01 z =  0.45670E+01 mesp =  0.78652E-01

Number of local minima (lower than mesp = -0.65E-01) found =   1

Positions and mesp values of the local minima in the mesh
-----------------------------------------------------------------------
x = -0.79681E+00 y = -0.11578E+02 z =  0.37188E+01 mesp = -0.80831E-01



***************************** MESP statistics *****************************


     Total surface with positive MESP =  0.49282E+03
     Total surface with negative MESP =  0.58480E+03

     MESP average =  0.73524E-04
     Positive MESP average =  0.27731E-01
     Negative MESP average = -0.23234E-01

     MESP variance =  0.76617E-03
     Positive MESP variance =  0.49597E-03
     Negative MESP variance =  0.27019E-03

     MESP average deviation =  0.25297E-01

     MESP nu parameter =  0.22829E+00

                         TIMING (in seconds)

 Processor  0 (user, system, total):    ( 0.80432E+04, 0.26885E+03, 0.83121E+04)
 Processor  1 (user, system, total):    ( 0.79180E+04, 0.18680E+01, 0.79199E+04)
 Processor  2 (user, system, total):    ( 0.83063E+04, 0.19510E+01, 0.83083E+04)
 Processor  3 (user, system, total):    ( 0.75441E+02, 0.29307E+01, 0.78371E+02)
```

MESP surface extrema on density isosurface (0.001 au)