Density derived electrostatic and chemical (DDEC) electron density partitioning

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Atoms-in-molecule electron density partitioning is a useful post-processing analysis tool for computing atomic charges (as well as higher order atomic multipoles) from the total electron density. ONETEP uses the DDEC3 method [1,3] for this purpose, as the computed charges are both chemically meaningful and reproduce the electrostatic potential of the underlying QM calculation. Options are also available for computing *Hirshfeld* and *iterated stockholder atoms* (ISA) charges [3,4].

A DDEC3 calculation to partition the electron density and output atomic charges, multipoles and volumes is performed by specifying:

```
ddec_calculate :  T
ddec_multipole :  T
ddec_moment :  3
```

along with the ddec_rcomp block for your system (see below). Iterated stockholder atoms (ISA) partitioning may be performed instead by additionally specifying:

```
ddec_IH_fraction :  0.00
```

Classical Hirshfeld partitioning may be performed instead by additionally specifying:

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```
ddec_classical_hirshfeld :  T
ddec_IH_fraction :  1.00
ddec_maxit :  1
```

The reference ion densities for use with DDEC3 are read in from an external library kindly provided by Thomas A. Manz and Nidia Gabaldon Limas (please cite Refs. [1,2]), and are available for download from the ONETEP website:

http://www.onetep.org/pmwiki/uploads/Main/Utilities/ddec_atomic_densities.tar.gz

The paths to the reference densities are specified in the block 'ddec_rcomp'. Specify one core and one total density file for each species in your system (except for hydrogen and helium which do not require a core density file). The example below is for methanol:

```
%block ddec_rcomp
H ALL "H_c2.refconf"
O ALL "O_c2.refconf"
O CORE "O_c2.coreconf"
C ALL "C_c2.refconf"
C CORE "C_c2.coreconf"
%endblock ddec_rcomp
```

References

For the development of the DDEC method:

[1] T.A. Manz and D.S. Sholl, "Improved Atoms-in-Molecule Charge Partitioning Functional for Simultaneously Reproducing the Electrostatic Potential and Chemical States in Periodic and Non-Periodic Materials," J. Chem. Theory Comput. 8 (2012) 2844-2867.
[2] T. A. Manz and D. S. Sholl, "Chemically Meaningful Atomic Charges that Reproduce the Electrostatic Potential in Periodic and Nonperiodic Materials", J. Chem. Theory Comput. 6 (2010) 2455-2468.

And its implementation in ONETEP:

[3] L. P. Lee, N. Gabaldon Limas, D. J. Cole, M. C. Payne, C.-K. Skylaris, T. A. Manz, "Expanding the Scope of Density Derived Electrostatic and Chemical Charge Partitioning to Thousands of Atoms", J. Chem. Theory Comput., 10 (2014) 5377.
[4] L. P. Lee, D. J. Cole, C.-K. Skylaris, W. L. Jorgensen, M. C. Payne, "Polarized Protein-Specific Charges from Atoms-in-Molecule Electron Density Partitioning", J. Chem. Theory Comput., 9 (2013), 2981.