Minnesota density functionals available in NWChem

The following functionals developed at Minnesota are available in NWChem:

Functional	Availability
MPW3LYP	Version 4.7 and later
BB1K	Version 5.0 and later
MPW1B95	Version 5.0 and later
MPWB1K	Version 5.0 and later
PW6B95	Version 5.0 and later
PWB6K	Version 5.0 and later
M05	Version 5.0 and later
M05-2X	Version 5.0 and later
M06-L	Version 5.1 and later
M06	Version 5.1 and later
M06-2X	Version 5.1 and later
M06-HF	Version 5.1 and later

Energies and analytic gradients are available for all above functionals in NWChem.

Note: There was a bug in the DFT grid subroutine in the NWChem Version 5.0. See here for the details. This bug has been fixed in Version 5.1.

Frequently Asked Questions:

Q1. How to reproduce a Gaussian calculation using NWChem?

A1: In order to match an NWChem calculation to a G09 one, one needs to do the following:

In the Gaussian route section, specify the keywords: scf=(tight) nosym integral(grid=ultrafine)

In the NWChem "dft" section, specify: grid lebedev 90 14 ssf euler

where ssf specifies the default Stratmann-Scuseria weighting scheme in G09, and euler specifies the defaut Euler-McLaurin radial quadrature wih the transformation devised by C.W. Murray, N.C. Handy, and G.L. Laming, Mol. Phys.78, 997 (1993).

One must also be careful about using Cartesian or spherical harmonic d and f functions. Some basis sets like 6-31G(d) are defined to use Cartesian subshells for d functions, whereas others like 6-311G(2df,2p) and cc-pVTZ are defined to use spherical harmonic d and f subshells. Gaussian03 or Gaussian09 will correctly make these choices by default. But the default in NWChem is always to use Cartesian d and f functions. Thus, unless one is using a basis set like 6-31G(d), one should do the following:

In the NWChem "basis" section, specify: basis "ao basis" spherical

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This document last modified