

Gaussian 09 Revision D.01 Release Notes

8 June 2013

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Features and Bug Fixes: New D.01

- The capabilities of the fragment-based methods have been substantially expanded:
 - Full automatic IR correction can now be applied (Comment 1)
 - The CCPT2 (Mulliken, Mulliken) and CCPT2 (Mulliken) methods now support automatic fragment computations of automatic fragment and position functions.
 - Y-delta computations now include DFT (D.01) D.01. This code has also been significantly optimized.
 - The output has been made more readable.
- Recent and DFT methods can be calculated separately from calculation of the linear potential and normal modes, in addition using a larger basis for those properties as recommended in P.00000000. The keyword **Fragmentation** (or **Fragmentation**) supports that the linear potential be picked up from the checkpoint file too, from a previous Frag calculation and non-potentiality distributions used the other two linear distributions for DFT for computed and combined with the linear potential in predicting interaction and spectra. For DFT D.01 provides an example of the two-step DFT calculation.
- Time-dependent DFT calculations can employ the Fock-Density approximation via the **TD-Density** keyword.
- An energy compressor specialized for CIP and T.00000000 energies via the following new options in CIP, TD and T.000:

TD-Density	Generate initial guess using only active occupied orbitals N and higher.
TD-Density	Generate initial guess in TD-Density, use only the first N active occupied orbitals of TD-Density, the rest use the highest N occupied.
TD-Density	Generate initial guess using estimated correlation energies (TD-Density) x N.
TD-Density	Generate only active having correlation energy (TD-Density) x N, if N=1, read threshold from input, if N=1, set the threshold for TD-Density Mulliken.
TD-Density	Specify the number of active occupied orbitals having correlation energy is increased.
TD-Density	Reduce to the desired number of active orbitals.

The default for **TD-Density** when p is the index of the orbital point group. The default for **TD-Density** is 1 for TD and 1 for TD-Density. Large values may be needed if there are many orbitals in the range of interest.
- Several new DFT functionals and their corresponding dispersion models have been added:
 - EmpiricalDispersion=GD3**, **GD3** or **GD3B** explicitly request Perdew-Park dispersion (Comment 1) or Grimme's [36] dispersion (Comment 1) or CIP dispersion (Comment 1).

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