

General Comments on DeFT

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The following is a list of quick comments about the program. I will add to this list as others ask questions that I fail to address in the other documents. Of course, gradually, this information will work its way into the appropriate documentation.

- DeFT was written during my postdoctoral stay in the group of Professor Peter A. Kollman, Department of Pharmaceutical Chemistry, University of California, San Francisco, as well as at my present address, the Department of Chemistry at the University of Ottawa.
- We request that all improvements to the code be sent back to the University of Ottawa so that others can subsequently take advantage of them (contributors will be appropriately acknowledged).
- The basis set files unfortunately are restricted to first row atoms (other basis sets will be made available as they are published by their developers: N. Godbout, D. Salahub, J. Andzelm, and E. Wimmer).
- In lieu of DFT optimized basis sets, basis sets from conventional *ab initio* methods (such as Pople's 6-31G** basis sets) may be used, and appropriate auxiliary basis sets can be constructed, using the precise format appearing in the *bases* file.
- It is important to make sure that the basis sets are specified in the same order as the atoms appear in the input of the geometry.
- No makefile exists for this program.
- The executable is created by compiling all the subroutines and then linking.
- When redimensioning the code, only the information in *main.f* need be changed as all information is passed to the subroutines by argument and not through COMMON blocks (subsequently, only *main.f* need be recompiled before relinking).
- In *main.f*, "natoms" is the maximum number of atoms.
- In *main.f*, "ncontractions" is the maximum number of contractions in the orbital bases.
- In *main.f*, "nprimitives" is the maximum number of primitives in the orbital bases.

- In *main.f*, “nauxiliary” is the maximum number of fitting functions in either the charge density or exchange and correlation auxiliary fitting bases.
- In *main.f*, “nmaxpts” is the maximum number of grid points about an atom (this should remain fixed until a larger grid becomes an option to DeFT).
- In *main.f*, “nreal” and “ninteger” are the sizes of the real and integer work vectors (the program will halt and tell the user if these values need to be raised).
- In *main.f*, all other parameters should remain as they are as they are functions of the above parameters.
- Unfortunately, the LCGTO-DFT energy gradients are not exact, therefore, the energy may rise at the end of a geometry optimization.
- The *hessian* file required for transition state optimizations (optional for geometry optimizations in internal coordinates) is fixed format and must be produced by another program in fixed format. A sample file, *hessian*, is supplied in the directory containing sample inputs and outputs and is required to locate the transition state in the sample run studying the isomerization of HCN to HNC (input file *hcn-to-hnc*). Since I like to obtain my Hessians from MOPAC, the coordinates are in angstroms and the second derivative matrix is in millidynes Å⁻². The format for the file is the following for an N atom system: for each atom, the *x*, *y*, *z* coordinates are listed, followed by 9 × N × N lines listing the full second derivative matrix (i.e., one element per line).
- When performing a vibrational analysis, it is wise to make both the SCF convergence and geometry optimization convergence criteria about one order of magnitude more stringent, i.e., smaller, than the default values. This is necessary to keep the “trivial” frequencies associated with translations and rotations as small as possible.
- When performing a vibrational analysis, a restart file from a previously completed geometry optimization (remember to make that run’s convergence criterion a bit more stringent than the default value) is required. The geometry at which the vibrational analysis is performed is that in the restart file, **not** that in the input file.
- In a vibrational analysis, only the non-“trivial” frequencies are printed out. The algorithm in *irspectrum.f* ensures that these modes are orthogonal to pure translational and rotational modes.