BasisFit1.0 User Manual

June 30, 2013

1   Installing BasisFit

Open X11 or terminal. Navigate to the directory containing your BasisFit download *e.g.*

    cd ∼/Downloads

Create an install directory *e.g.*

    sudo mkdir /Programs

Unpack tgz file into install directory

    tar xvfz BasisFit.tgz -C /Programs

From the install directory, execute the install.osx script (for Mac OSX) or follow the instructions in the README.setup file

    cd /Programs/BasisFit

    sudo ./install.osx

Quit out of terminal or X11, and reopen. You are now ready to BasisFit!

2   Running BasisFit

BasisFit should be run from the directory containing the data files generated by GAMESS, using the command:

    process_datfile.py *dat_file_name.dat large_basis_name* (*small_basis_name*)

The name of the small basis is optional, as this will be detected from the dat file automatically, for molecules with no (C1) symmetry using a built-in basis set. If your molecule is symmetric and you have only given the symmetry unique atoms to GAMESS, you will need to give the small basis name here. If you have specified the basis set within GAMESS using an external file (EXTFIL=.TRUE.), you will also need to give the small basis name here. If your molecule is symmetric *and* you have used different basis sets for different atoms, you will need to edit the .dat file to explicitly list all atoms, change the symmetry label to C1, and specify the basis sets that describe each atom.

3 Primary Usage

BasisFit is a simple and robust method for generating physically meaningful occupied and virtual valence molecular orbitals, based upon the observation that a minimal atomic basis set generates these automatically during a Hartree-Fock calculation. These molecular orbitals are then reproduced in a larger basis by least-squares fitting the atomic minimal basis functions using a larger atomic basis, and expanding out the molecular orbitals using the minimal basis MO coefficients and the large-to-minimal basis fitting coefficients. BasisFit can be used with any type of Hartree-Fock wavefunction (RHF, UHF, ROHF). Supported basis sets are tabulated below.

basis set	atoms	basis set	atoms
STO-3G-EMSL	H – I	MINI [Huzinaga]	H – Ca
STO-3G [GAMESS version]	H – I	MINI-scaled	H – Ca
STO-6G	H – Kr		
3-21G	H – Xe	pc-0	H – Ca, Ga – Kr
6-31G	H – Zn	pc-1	H – Kr
6-31G*	H – Zn	pc-2	H – Kr
6-31G**	H – Zn	pc-3	H – Kr
6-31G(2d,2p)	H – Ar	pc-4	H – Kr
6-31G(3df,3pd)	H – Ar	aug-pc-0	H – Ca, Ga – Kr
6-31+/++G	H, Li – Ar	aug-pc-1	H – Kr
6-31+/++G*	H, Li – Ar	aug-pc-2	H – Kr
6-31+/++G**	H, Li – Ar	aug-pc-3	H – Kr
6-31+/++G(2d,2p)	H, Li – Ar	aug-pc-4	H – Kr
6-31+/++G(3df,3pd)	H, Li – Ar	cc-pVDZ	H – Ar, Sc – Kr
6-311G	H – Ca, Ga – Kr	cc-pVTZ	H – Ar, Sc – Kr
6-311G*	H – Ca, Ga – Kr	cc-pVQZ	H – Ar, Sc – Kr
6-311G**	H – Ca, Ga – Kr	cc-pV5Z	H – Ar, Sc – Kr
6-311G(2d,2p)	H – Ar	aug-cc-pVDZ	H – Ar, Sc – Kr
6-311G(3df,3pd)	H – Ar	aug-cc-pVTZ	H – Ar, Sc – Kr
6-311+/++G	H, Li – Ar	aug-cc-pVQZ	H – Ar, Sc – Kr
6-311+/++G*	H, Li – Ar	aug-cc-pV5Z	H, He, Be – Ne
6-311+/++G**	H, Li – Ar		Al – Ar, Sc – Kr
6-311+/++G(2d,2p)	H, Li – Ar		
6-311+/++G(3df,3pd)	H, Li – Ar		

When specifying the basis set to BasisFit, choose either + or ++, replace star * with s, the left bracket (with an underscore _ , and drop off the right bracket). Comments in square brackets above should also be ignored.

4 Secondary Usage

BasisFit may also be used to reproduce molecular orbitals constructed from non-minimal atomic basis sets, essentially allowing the results of any previous calculation to be used as a starting guess for a subsequent calculation with a larger atomic orbital basis set. This functionality can be used with any method that produces optimized molecular orbitals *i.e* RHF, UHF, ROHF (optimized occupied valence orbitals), CASSCF (optimized occupied and virtual orbitals, within a chosen active space. If you choose the full valence active space, this optimizes all valence orbitals). This option is designed to allow bootstrapping up from a minimal basis calculation. However, it is important to note that if your molecular orbitals are only optimized using Hartree-Fock at any point in time, your virtual orbitals will cease being physically meaningful.

5 Off-label Usage

It is also possible to construct small basis molecular orbitals from the results of a large basis calculation, although this is not generally recommended. These orbitals will be non-orthogonal, non-normalized and more cost-effectively obtained by alternative methods (bootstrapping from a smaller basis using BasisFit, or using built-in orbital guess algorithms).