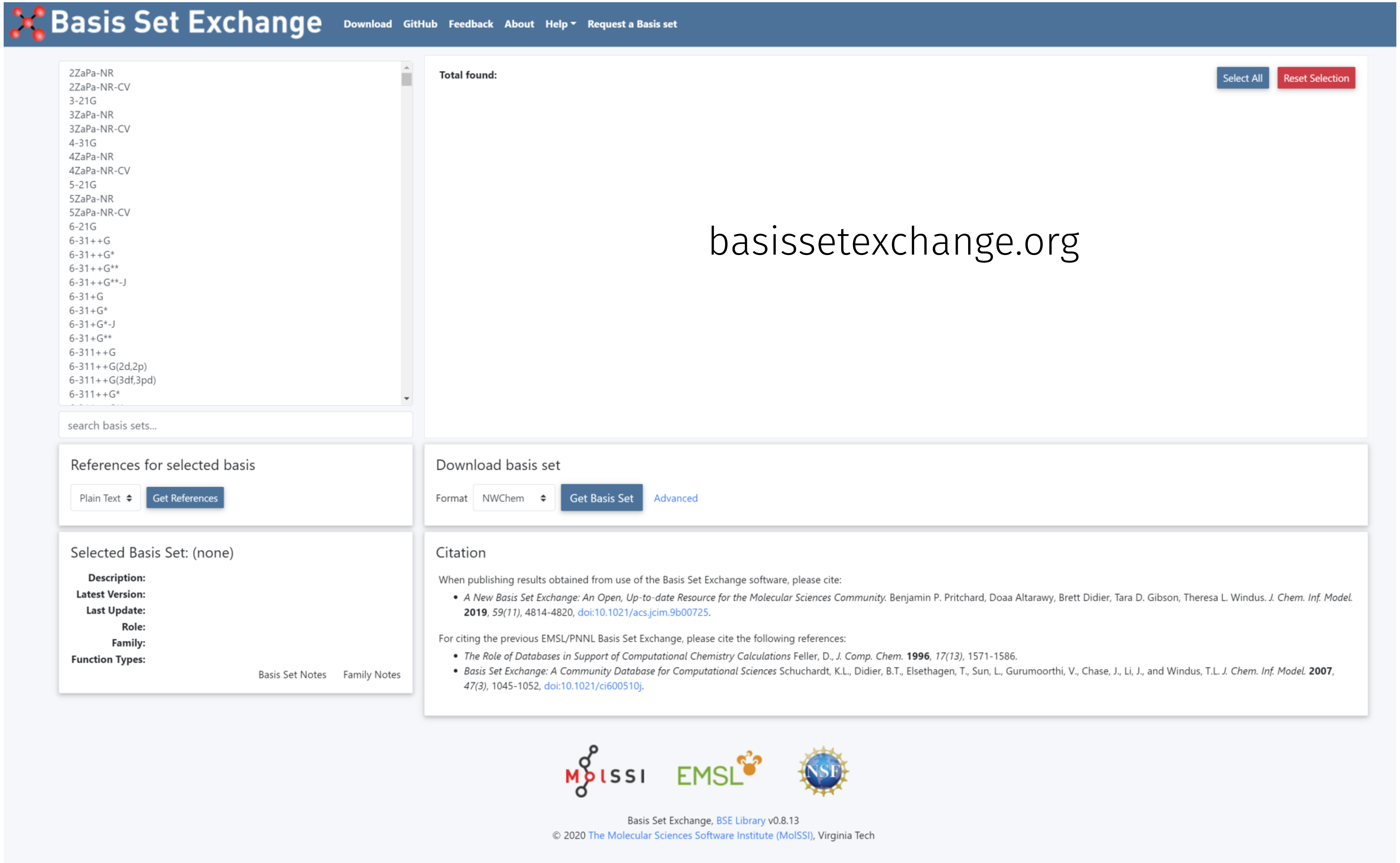
Basis Sets

Basis Sets



2ZaPa-NR
2ZaPa-NR-CV
3-21G
3ZaPa-NR
3ZaPa-NR-CV
4-31G
4ZaPa-NR
4ZaPa-NR-CV
5-21G
5ZaPa-NR
5ZaPa-NR-CV
6-21G
6-31++G
6-31++G*
6-31++G**
6-31++G**-J
6-31+G
6-31+G*
6-31+G*-J
6-31+G**
6-311++G
6-311++G(2d,2p)
6-311++G(3df,3pd)
6-311++G*

Total found:

basissetexchange.org

References for selected basis

Download basis set

Format: NWChem

Selected Basis Set: (none)

Description:
Latest Version:
Last Update:
Role:
Family:
Function Types:

Citation

When publishing results obtained from use of the Basis Set Exchange software, please cite:

- *A New Basis Set Exchange: An Open, Up-to-date Resource for the Molecular Sciences Community.* Benjamin P. Pritchard, Doaa Altarawy, Brett Didier, Tara D. Gibson, Theresa L. Windus. *J. Chem. Inf. Model.* **2019**, *59(11)*, 4814-4820, doi:10.1021/acs.jcim.9b00725.

For citing the previous EMSL/PNNL Basis Set Exchange, please cite the following references:

- *The Role of Databases in Support of Computational Chemistry Calculations* Feller, D., *J. Comp. Chem.* **1996**, *17(13)*, 1571-1586.
- *Basis Set Exchange: A Community Database for Computational Sciences* Schuchardt, K.L., Didier, B.T., Elsethagen, T., Sun, L., Gurumoorthi, V., Chase, J., Li, J., and Windus, T.L. *J. Chem. Inf. Model.* **2007**, *47(3)*, 1045-1052, doi:10.1021/ci600510j.

Basis Set Exchange, BSE Library v0.8.13
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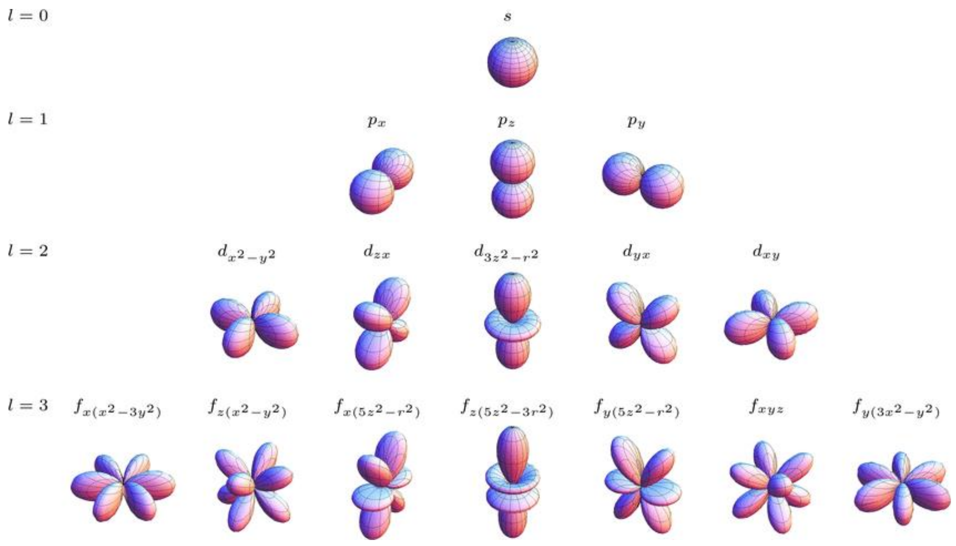
Basis Sets

- Set = multiple basis functions
  - s-orbital: 1 basis function
  - p-orbital: 3 basis functions (px, py, pz)
- Finite
- Big families
  - atom-centered
    - Slater-type orbitals (STO): expensive integrals
    - Gaussian-type orbitals (GTO)
      - Primitive gaussian functions build up orbitals
  - plane waves
  - Wavelets
    - Systematically improving, rare
- Typically defined per element: problem for quantum alchemy
- Connection locality and cost
- Minimal basis set: one basis function for each orbital
- Polarization functions: asymmetry close to the nucleus: bonds
- Diffuse functions: asymmetry away from the nuclei: hydrogen bond, dipoles



Plane waves

- Path to complete basis set (CBS limit)
- Easy and elegant implementation except HF
- Easy derivatives
- Requires “fake” boundary conditions
- Empty space is not free
- Pseudopotentials required as cutoff too high
- Commonly used for materials

Atom-centered basis functions

- Localised, so empty space is free
- Scales linearly with number of atoms
- Numerical issues if atoms close together
- Any boundary conditions possible
- No path to complete basis set limit: empirical schemes necessary
- Harder to implement
- Commonly used for molecules / mixed settings

Real-Space and Wavelets

Real-Space

- Multi-dimensional grid
- Easiest to approach CBS
- Hard to implement
- Slow in evaluation
- Mostly used for technical demonstrations / settling one-off questions

Wavelets

- Finite Support: easy to subdivide
- Niche implementations
- Unclear whether “best of both worlds” or “worst of both worlds”

Nomenclature

- Gaussian-type orbitals
  - Sum of Gaussians form one orbital: contraction
- Minimal basis set: “single zeta” (Zeta commonly used for the exponent in STO-nG)
- Twice/three times the basis functions for valence atomic orbitals: double-zeta, triple-zeta, …
- Split valence (single zeta for core, multiple for valence)

6-31++G**

6	One core basis function with 6 contracted Gaussians
31	Two valence basis functions with 3 and 1 contracted Gaussian respectively
*	Polarization on heavy atoms
**	Polarization also on hydrogen atoms
+	Diffuse functions on heavy atoms
++	Diffuse function also on hydrogen atoms

Nomenclature

aug-cc-cpCVDZ

aug	Diffuse functions
p	Polarization functions
DZ	Double zeta
C	core basis functions

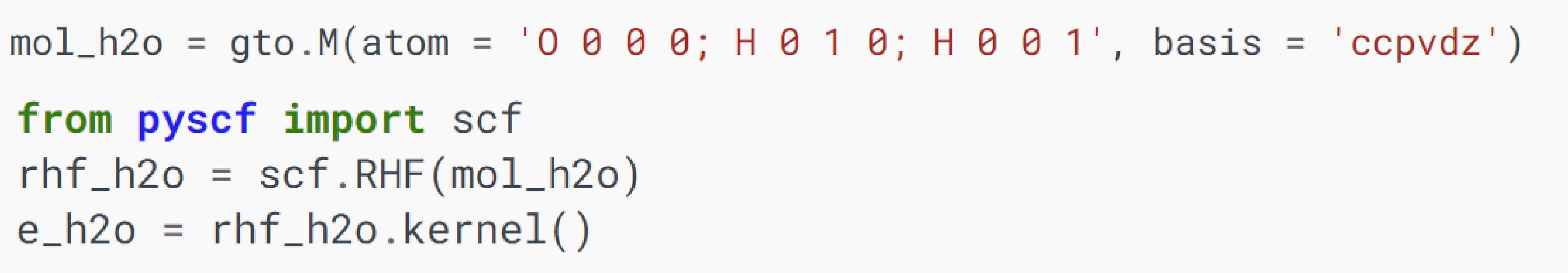
(6s,3p) → [2s,1p]

Contraction: (primitives) -> [basis functions]

Question: [3s2p1d] is how many basis functions?
Question: Ar with electron configuration [$1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$] in cc-pVTZ has how many basis functions?

PySCF example

Molecule setup



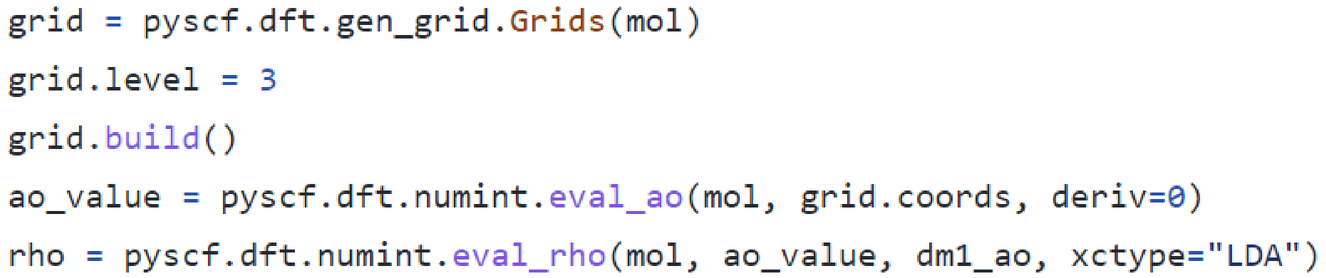
```
mol_h2o = gto.M(atom = 'O 0 0 0; H 0 1 0; H 0 0 1', basis = 'ccpvdz')

from pyscf import scf
rhf_h2o = scf.RHF(mol_h2o)
e_h2o = rhf_h2o.kernel()
```

Electron density in ao basis

```
dm1_ao = calc.make_rdm1()
```

Electron density on a grid



```
grid = pyscf.dft.gen_grid.Grids(mol)
grid.level = 3
grid.build()
ao_value = pyscf.dft.numint.eval_ao(mol, grid.coords, deriv=0)
rho = pyscf.dft.numint.eval_rho(mol, ao_value, dm1_ao, xctype="LDA")
```