Basis Sets

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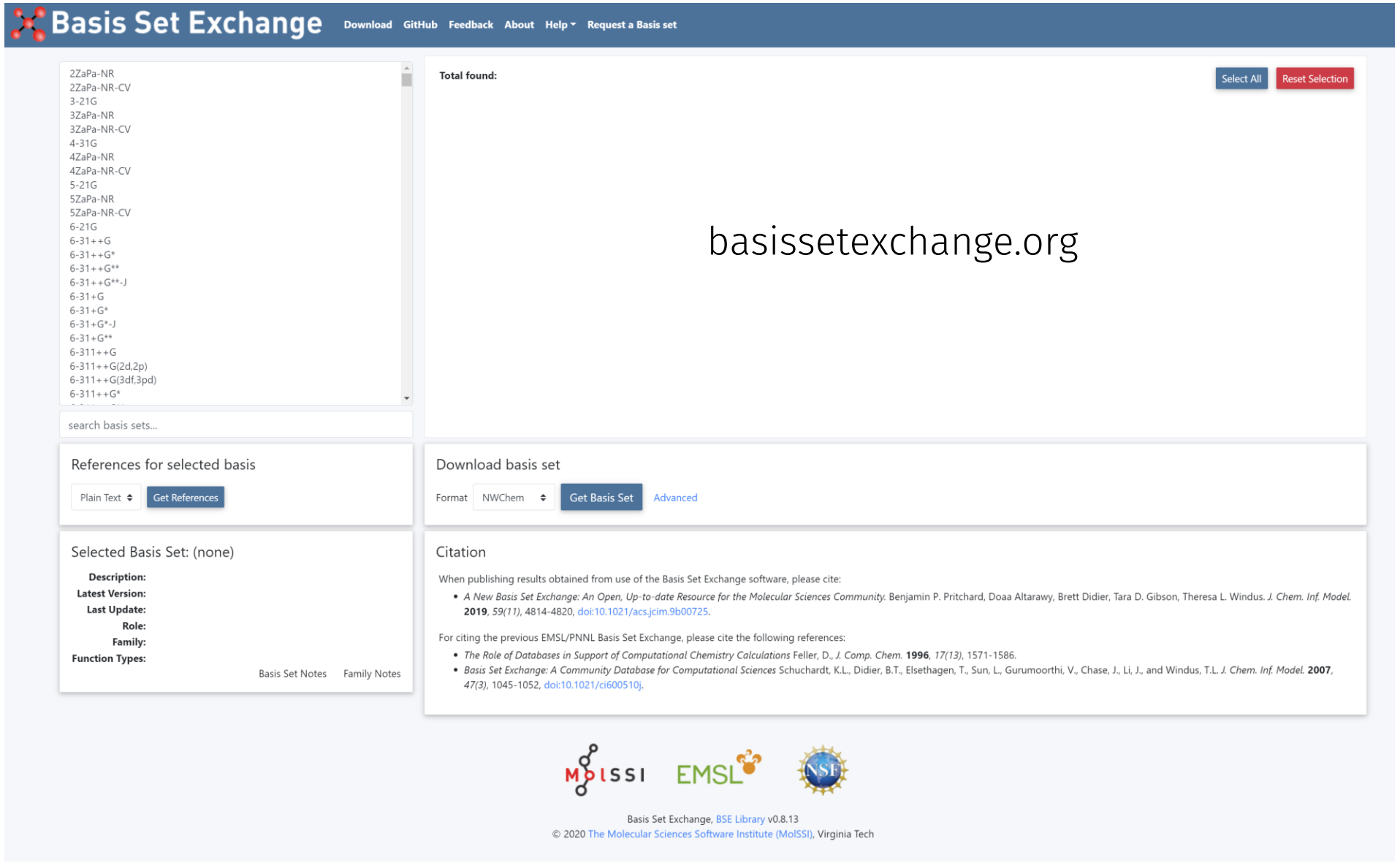
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5-21G
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5ZaPa-NR-CV
6-21G
6-31++G
6-31++G*
6-31++G**
6-31++G**-J
6-31+G
6-31+G*
6-31+G*-J
6-31+G**
6-311++G
6-311++G(2d,2p)
6-311++G(3df,3pd)
6-311++G*
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Family Notes
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.
MolSSI
EMSL
NSF
Basis Set Exchange, BSE Library v0.8.13
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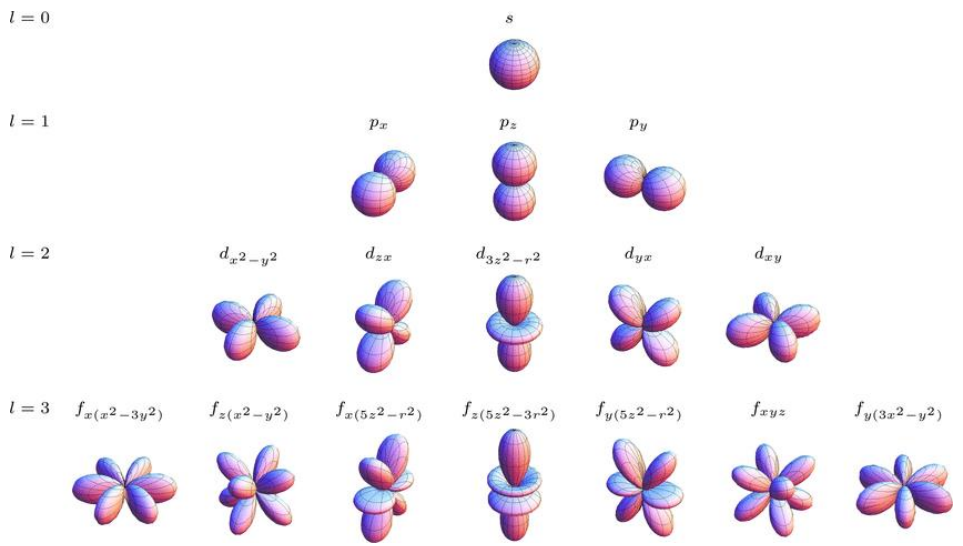
Basis Sets

- 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

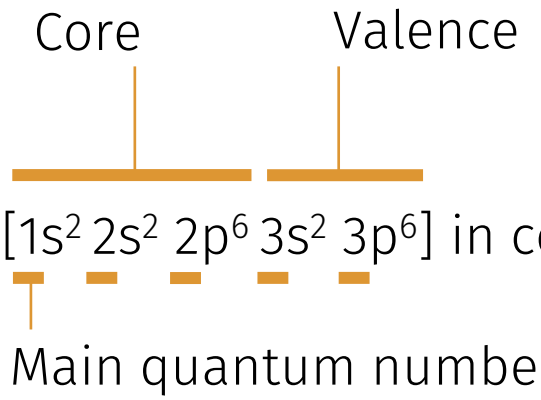
aug	Diffuse functions
p	Polarization functions
DZ	Double zeta
C	core basis functions

(6s,3p) → [2s,1p]

Contraction: (primitives) -> [basis functions]

Question: [3s2p1d] is how many basis functions? (not main quantum numbers)

Example



Ar with electron configuration [$1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^6$] in cc-pVnZ?

	[all of core]	[valence repeated n times]	[polarization of next higher angular momentum]	
DZ	1s, 2s, 2p	3s, 3s, 3p, 3p	3d	[4s, 3p, 1d] = 18
TZ	1s, 2s, 2p	3s, 3s, 3s, 3p, 3p, 3p	3d, 4d, 4f,	[5s, 4p, 2d, 1f] = 34
QZ	1s, 2s, 2p	3s, 3s, 3s, 3s, 3p, 3p, 3p, 3p	3d, 4d, 5d, 4f, 5f, 5g	[6s, 5p, 3d, 2f, 1g] = 59

…

Minimal basis set (e.g. STO-3g): 1s, 2s, 2p, 3s, 3p [3s, 2p] = 9

```
import pyscf.gto as gto
gto.M(atom='Ne 0 0 0', basis='STO-3G').ao_labels()
```

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")
```