

```
import sys, math
```

```
## Covalent radii
```

$$E(\vec{\mathcal{F}}) = E(0) + \left( \frac{dE}{d\vec{\mathcal{F}}} \right)_{\vec{\mathcal{F}}=0} \vec{\mathcal{F}} + \frac{1}{2!} \left( \frac{d^2E}{d\vec{\mathcal{F}}^2} \right)_{\vec{\mathcal{F}}=0} \vec{\mathcal{F}}^2 + \frac{1}{3!} \left( \frac{d^3E}{d\vec{\mathcal{F}}^3} \right)_{\vec{\mathcal{F}}=0} \vec{\mathcal{F}}^3 + \dots$$

```
# threshold beyond average covalent radii to define bond  
bond_thresh = 1.2
```

```
# covalent (or ionic) radii by atomic element (Angstroms) from
```

```
# "Inorganic Chemistry" 3rd ed, Housecroft, Appendix 6, pgs 1013-1014
```

```
cov_radii = { 'H' : 0.37, 'C' : 0.77, 'O' : 0.73, 'N' : 0.75, 'F' : 0.71,  
'P' : 1.10, 'S' : 1.03, 'Cl' : 0.99, 'Br' : 1.14, 'I' : 1.33, 'He': 0.30,  
'Ne': 0.84, 'Ar': 1.00, 'Li': 1.02, 'Be': 0.27, 'B' : 0.88, 'Na': 1.02,  
'Mg': 0.72, 'Al': 1.30, 'Si': 1.18, 'Ga': 1.35, 'Ca': 1.00, 'Sc': 0.75,  
'Ti': 0.86, 'V' : 0.79, 'Cr': 0.73, 'Mn': 0.67, 'Fe': 0.61, 'Co': 0.64,  
'Ni': 0.55, 'Cu': 0.46, 'Zn': 0.60, 'Ga': 1.22, 'Ge': 1.22, 'As': 1.22,  
'Se': 1.17, 'Kr': 1.03, 'X' : 0.00 }
```

$$1 + 1 = 2,$$