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import sys, math

## Covarage code
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 bond length 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_rads = { 'H' : 0.37, 'C' : 0.77, 'O' : 0.73, 'N' : 0.75, 'F' : 0.71,
    'P' : 1.10, 'S' : 1.03, 'Cl' : 1.02, 'Br' : 1.14, 'I' : 1.33, 'He' : 0.30,
    'Ne' : 0.84, 'Ar' : 1.00, 'Li' : 1.02, 'Be' : 0.77, 'B' : 0.88, 'Na' : 1.02,
    'Mg' : 0.72, 'Al' : 1.30, 'Si' : 1.18, 'P' : 1.18, 'S' : 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}

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$$1 + 1 = 2,$$

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