Reparm: Genesis

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June 9, 2016

1 Geometry array creation

The expected kenergy of an atom is

$$\langle E_{atom} \rangle = \frac{3}{2} K_b T \tag{1}$$

where K_b is the boltzman constant $1.38064853E^{-23}m^2kgS^{-2}K^{-1}$ and T is temperature which is defaulted to $298K$ the default for Gaussian 09. Gaussian 09 sets all translational and rotational modes to zero. The total energy of the molecule is then.

$$\langle E_{molecule} \rangle = \sum_{i=atom}^{N} E_{atom} \tag{2}$$

where N is the number of atoms. Of course this is the expected value. We therefore need to use a random number from a normal distribution to modify it. The variance of molecule energy is

$$\sigma^2 = \frac{2}{3N} \langle E_{molecule} \rangle \tag{3}$$

Leading to the molecule energy

$$E_{molecule} = \langle E_{molecule} \rangle + R \tag{4}$$

where R is the random value generated from a normal distribution with aforementioned variance. We then distribute this energy among the normal

modes using a uniform random number generator, giving us a new vector E_{mode}. Now, normal modes are represented by harmonic oscillators, so

$$E_{mode} = \frac{1}{2}kx^2 \tag{5}$$

$$x = \sqrt{\frac{2E}{k}} \tag{6}$$

where k is the spring constant given and x is the maximum displacement from equilibrium. Now these maximum diplacements, $\mathbf{x}$, can be made in any direction, so we once again apply a random number generator to flip the sign of some some of these modes. We now have our maximum displacement vector $\mathbf{x}$. Our normal modes are extracted from gaussian 09 and placed into a matrix $\mathbf{M}$ with the columns representing the coordinates for each atom, X_{atom1}, Y_{atom1}, Z_{atom1}, X_{atom2}, etc., and the rows representing the normal modes. Our final diplacement vector is thus,

$$\mathbf{d} = \mathbf{x} \cdot \mathbf{M} \tag{7}$$

This vector is then added to the optimized structured $\mathbf{o}$ to get the new structure

$$\mathbf{s} = \mathbf{o} + \mathbf{d} \tag{8}$$