

Reparm: Genesis

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June 8, 2016

1 Geometry array creation

The expected energy of an atom is

$$\langle E_{atom} \rangle = \frac{3}{2} K_b T \quad (1)$$

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. The total energy of the molecule is then.

$$\langle E_{molecule} \rangle = \sum_{i=atom}^N E_{atom} \quad (2)$$

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

$$\sigma^2 = \frac{2}{3N} \langle E_{molecule} \rangle \quad (3)$$

Leading to the molecule energy

$$E_{molecule} = \langle E_{molecule} \rangle + R \quad (4)$$

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

$$E_{mode} = \frac{1}{2}kx^2 \quad (5)$$

$$x = \sqrt{\frac{2E}{k}} \quad (6)$$

where k is the spring constant given and x is the displacement from equilibrium. Now these displacements, \mathbf{x} , can be made in any direction, so we once again apply a random number generator to flip the sign of some of these modes. We now have our displacement vector \mathbf{x} . For simplification of calculations, we make this a diagonal matrix \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 displacement matrix is thus,

$$\mathbf{D} = \mathbf{X}\mathbf{M} \quad (7)$$

When we sum the rows we obtain the displacement vector \mathbf{d} , which is then applied to the optimized coordinates.