Chem. 542
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Normal Modes – Problem 2

Apply the normal mode transformation to a diatomic molecule AB in three dimensions, where the two atoms have masses m_1 and m_2 and are constrained to move along a fixed line. Assume the potential interaction between the two atoms is quadratic, i.e.,

$$V(\mathbf{r}) = \frac{1}{2} k \left[(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2 \right]$$

where x_i, y_i, z_i are the Cartesian displacement coordinates.

Your normal mode frequencies should be identical to those you found in the 1D case. In fact, even though you are working in 3D, this is effectively a 1D problem. The reason is that the given form of the potential is correct only if the molecule is oriented along a fixed axis. (Otherwise we should subtract the equilibrium bond length from the interatomic distance, and we wouldn't be able to get it in this form!)