Quantum Molecular Dynamics Homework 5 Spring, 2000

1. The G matrix for a non-linear triatomic molecule is a 3x3 matrix whose rows and columns refer to the three internal coordinates R_1, R_2 and the included angle ϕ. Specifically, the elements of the G-matrix are

$$G_{11} = m_1^{-1} + m_3^{-1} \qquad G_{22} = m_2^{-1} + m_3^{-1} \tag{1.1}$$

$$G_{33} = \frac{m_1^{-1}}{r_{31}^2} + \frac{m_2^{-1}}{r_{32}^2} + m_3^{-1}\left(\frac{1}{r_{31}^2} + \frac{1}{r_{32}^2} - \frac{2\cos\phi}{r_{31}r_{32}}\right) \tag{1.2}$$

$$G_{12} = m_3^{-1}\cos\phi \qquad G_{13} = \frac{-m_3^{-1}\sin\phi}{r_{32}} \qquad G_{23} = \frac{-m_3^{-1}\sin\phi}{r_{31}} \tag{1.3}$$

Write the explicit form for the G matrix for a *linear* triatomic molecule by neglecting the third row and column of the G-matrix and setting $\phi = 180^o$. Show that the kinetic energy

$$T = \frac{1}{2}\mathbf{pGp} \tag{1.4}$$

agrees with eq. 12.21.

2. Find the number of normal modes of vibration of each symmetry species for the benzene molecule.