5.80 Small-Molecule Spectroscopy and Dynamics

Fall 2008

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Chemistry 5.76
Spring 1980

Problem Set #2

1. See Problem Set # 2, 1977, question # 1.

2. See Problem Set # 2, 1977, question # 2.

3. See Problem Set # 2, 1977, question # 3.

4. See Problem Set # 2, 1977, question # 4.

5. See Problem Set # 2, 1977, question # 5.

6. (a) See Problem Set # 2, 1977, question # 6(a).

   (b) See Problem Set # 2, 1977, question # 6(b).

   (c) Is the energy level diagram for Dk sufficiently complete that the electronic partition function

$$q_e = \sum_{\text{all states } i} g_i \exp[-E_i/kT],$$

   may be calculated at 3000K? If one or more electronic terms are missing, what would be the fractional error in q_e, assuming plausible term energies? Can you devise an experiment which samples $q_e(T)$ with accuracy sufficient to locate a missing low-lying electronic term?