5.80 Small-Molecule Spectroscopy and Dynamics
Fall 2008

Problem Set #4

1. See Problem Set # 4, 1977, question # 1.

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

3. See Problem Set # 4, 1977, question # 3.

    (a) See Problem Set # 4, 1977, question # 3a.

    (b) See Problem Set # 4, 1977, question # 3b.

    (c) The ground electronic state of C_3O_2 is nondegenerate. What is the degeneracy of ψ_{mol} when C_3O_2 is in its ground electronic state with $v_1 = v_2 = v_3 = v_4 = v_5 = v_6 = 0$, $v_7 = 1$, and the rotational quantum number $J = 5$? The normal coordinate Q_7 is antisymmetric with respect to simultaneous interchange of all pairs of equivalent nuclei. What is the degeneracy of ψ_{mol} for the above state with $J = 6$ instead of 5?

4. See Problem Set # 4, 1977, question # 6.

5. $^{16}O^{12}C^{32}S$ is a linear molecule. The bond lengths are

    $r_{CO} = 1.16\text{Å}$

    $r_{CS} = 1.56\text{Å}$

    and the observed fundamental vibrational frequencies are

    $v_1 = 858.9$ cm^{-1} stretch

    $v_2 = 520.4$ cm^{-1} bend

    $v_3 = 2062.2$ cm^{-1} stretch.

    (a) Obtain k_{CS}, k_{CO}, and $k_\theta[r_{CO}r_{CS}]^{-1}$ in dynes/cm.

    (b) What are the amplitudes for C-O and C-S stretch in v_1?

    (c) What are the vibrational frequencies for $^{18}O^{12}C^{32}S$?