Spectroscopy

Exercises Chapter 3B

1. For the $^{12}C^{32}S$ molecule the following millimeter wave pure rotational transitions have been observed (in MHz):

Transition	v=0	v=1
J=1←0	48'990.978	48'635.977
J=2←1	97'980.950	97'270.980
J=3←2	146'969.033	145'904.167
J=4←3	195'954.226	194'534.321

a. For each vibrational level, determine the corresponding rotational constant, B.

b. From your answers in (a), determine the vibrational-rotation interaction constant, α and determine B_e.

c. From B_e calculate r_e.

2. The S_2O molecule is a bent triatomic molecule. The S-S bond is 1.884 Å long, the S-O bond is 1.465 Å long, and the SSO angle is 118.0°.

a. Locate the center of mass and set up the moment of inertia tensor. Pick the *z*-axis out of the plane and the *x*-axis parallel to the S-S bond.

b. Diagonalize the moment of inertia tensor to find I_A, I_B, and I_C.

c. Determine the value of the asymmetry parameter κ.