INSTRUCTIONS

TIME LIMIT & DUE DATE. As announced in class, you may work on this as long as you like up until the due date. The exam, along with any extra pages securely stapled (see below), is due in my mailbox on Nov 11, Sat, 5 pm.

RESOURCES. All work must be done independently. You may not ask for or receive intellectual help from other students, faculty, family, clergy, or higher powers. You may not consult any print or online resources with the following exceptions: your textbook, your lecture notes, and the homework solutions posted on the web.

SHOW YOUR WORK. You may use Mathematica and the mathematical formulas in your textbook (DO YOU KNOW THE DOOR CODE FOR THE COMPUTER LAB?) However, you should try to write your answers in a way that shows in as much detail as possible, the mathematical ideas you began with and how you worked with them, and not just the final answers you obtained (if you use Mathematica, break your work down into steps that I can follow and attach a printout of your notebook). Also, include units in your answers, where appropriate.

EXTRA PAGES. Your work might very well run on to extra pages. If it does, please write your name and the problem number on each page, and indicate the sequence that the pages should be read for each problem.

Rule of the Grader – Given any answer (right or wrong), the more I understand about the thought that produced the answer, the more generous I can be towards the answer. I am grading process, not just a result.
1. The angular momentum operators, $\hat{I}_y$ and $\hat{I}_z$, for a 3D rigid rotor are shown in Engel eq. 7.29 (p. 115). Calculate $[\hat{I}_z, \hat{I}_y]$ using Cartesian coordinates.
The $\hat{I}^2$ operator for the 3D rigid rotor is a multiple of the $\hat{H}$ operator. $\hat{H}$ in spherical polar coordinates can be obtained from the Schrödinger wave equation for the rigid rotor shown in Engel eq. 7.17 (p. 112). The $\hat{I}_z$ operator in spherical polar coordinates is shown in Engel eq. 7.30 (p. 115).

2. Write $\hat{I}^2$ for the 3D rigid rotor in spherical polar coordinates.

3. Determine whether $\sin^2 \theta e^{2i\phi} + 2 \sin \phi \cos \phi e^{i\phi}$ is an eigenfunction of $\hat{I}^2$. If it is, give its eigenvalue.
4. Determine whether $\sin^2 \theta \ e^{2i\phi} + 2 \sin \theta \cos \theta \ e^{i\phi}$ is an eigenfunction of $\hat{l}_z$. If it is, give its eigenvalue.

(Extra credit: the same function appears in problems 3 & 4; if this function turns out to be an eigenfunction of one operator, $\hat{l}^2$ or $\hat{l}_z$, but not the other, explain how this is possible.)
5. The $n = 0 \rightarrow n = 3$ transition for the harmonic oscillator is not IR active. Demonstrate this by showing that the transition dipole moment, $\mu_x^{30}$, vanishes. **Note:** You need to set up and evaluate two integrals to solve this problem (see Engel eq. 8.8, p. 137), and you need use explicit formulas for two harmonic oscillator wave functions (see Engel eq. 7.5, p. 105).
6. The following rotational transitions (in MHz) have been observed for the $^{12}$C$^{32}$S molecule (ground vibration state). (Note: exact masses for these isotopes can be found in Engel, inside back cover.)

a. Calculate B, the rotational constant, in cm$^{-1}$

b. Calculate the equilibrium bond distance in pm

<table>
<thead>
<tr>
<th>Transition</th>
<th>Frequency (MHz)</th>
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<tbody>
<tr>
<td>J = 1 — 0</td>
<td>48 990.978</td>
</tr>
<tr>
<td>J = 2 — 1</td>
<td>97 980.950</td>
</tr>
<tr>
<td>J = 3 — 2</td>
<td>146 969.033</td>
</tr>
<tr>
<td>J = 4 — 3</td>
<td>195 954.226</td>
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