

Physical Chemistry II
Problem Set 5
Due Thursday, April 17, 2008 (at 4:00 p.m.)
Total Number of Points = 59

- You should use very precise values for the masses of isotopes. If they are not provided in the problem, consult the table on p. 991 of Atkins and de Paula or the CRC Handbook.
1. (4 points) The molecule IF has a bond length of 1.908 Å. Calculate the location of the molecule's center of mass relative to both nuclei. (You may use, without re-derivation, results from class.)
 2. (8 points) Atkins and de Paula Exercise 9.7b. (This is not a typo.) Note:
 - Assume 300 K is known to three significant figures.
 - Do not calculate the de Broglie wavelength.
 - As we discussed in class (on March 28), the extremely small ΔE is evidence that it is "appropriate to describe this particle as behaving classically." (So I've answered the last part of the question for you.)
 3. (5 points) Atkins and de Paula Exercise 13.5b. Report the final answer in GHz.
 4. (6 points) Atkins and de Paula Exercise 13.7b. Report the moment of inertia in kg m^2 and the bond length in Å.
 5. (6 points) Atkins and de Paula Exercise 13.19b. The algebraically astute will note that only two transitions are needed to determine the constants $\tilde{\nu}$ and x_e . Therefore, use only two transitions (any two are fine).
 6. (8 points) Atkins and de Paula Problem 13.11.
 - The data given are actually ν values in units of MHz (see the original article on the back)
 - Turn in a copy of your spreadsheet and plot, with trendline and R^2 value displayed to seven significant figures. Briefly justify how you analyzed the data.
 - Report the rotational constant in cm^{-1} .
 - Skip the estimation of maximum J values—you do this in #7.
 7. (12 points) Atkins and de Paula Problem 13.12.
 - Fit the vibrational energy levels to a polynomial in $(\nu + 1/2)$.
 - Turn in a copy of your spreadsheet and plot with the appropriate trendline and R^2 value displayed. Parameters should be displayed to five significant figures.
 - Assume the data are for the "isotopomer" $^{23}\text{Na}^{127}\text{I}$
 - Report the force constant in units of kg s^{-2} and the zero-point energy in cm^{-1} .
 - Report both D_e and D_0 for NaI (in eV), assuming a Morse potential model.
 - Answers: $k = 93.802 \text{ kg s}^{-2}$; $D_0 = 3.3628 \text{ eV}$
 8. (10 points) Atkins and de Paula Problem 13.24. Answer only for the case of a diatomic rotor, and do the calculation for ICl. (Answer: $J_{\text{max}} = 30$)

Millimeter-wave spectroscopy of the iron carbonyl radical (FeCO)

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TABLE I. Rotational transitions of the FeCO radical in the ground state.

Transitions ^a $J' \leftarrow J''$	$\Omega = 0$		$\Omega = 1^f$		$\Omega = 1^e$	
	Observed ^b	O-C ^c	Observed ^b	O-C ^c	Observed ^b	O-C ^c
1 ← 0 ⁻	8 585.503 3 ^d	0.1				
2 ← 1 ⁻	17 171.067 9 ^d	-0.4				
3 ← 2 ⁻	25 756.756 0 ^d	-1.0				
4 ← 3 ⁻	34 342.631 5 ^d	1.0				
15 ← 14 ⁻	128 815.447 ⁻	-79 ^e	130 894.888 ⁻	-4 ⁻	132 989.314 ⁻	10
16 ← 15 ⁻	137 407.791 ⁻	-26 ⁻	139 618.852 ⁻	52 ^e	141 845.839 ⁻	7
17 ← 16 ⁻	146 000.952 ⁻	32 ^e	148 342.217 ⁻	-23		
24 ← 23 ⁻			209 390.752 ⁻	18 ⁻	212 628.172 ⁻	-4
25 ← 24 ⁻	214 777.719 ⁻	12 ⁻	218 109.382 ⁻	13 ⁻	221 466.094 ⁻	-12
26 ← 25 ⁻	223 378.998 ⁻	6 ⁻	226 827.246 ⁻	-24 ⁻	230 301.620 ⁻	-5
27 ← 26 ⁻	231 981.227 ⁻	7 ⁻	235 544.415 ⁻	7 ⁻	239 134.667 ⁻	-10
28 ← 27 ⁻	240 584.386 ⁻	4 ⁻	244 260.751 ⁻	-4 ⁻	247 965.206 ⁻	-4
29 ← 28 ⁻	249 188.458 ⁻	-12 ⁻	252 976.280 ⁻	1 ⁻	256 793.197 ⁻	23
30 ← 29 ⁻	257 793.462 ⁻	-8				

^a $\Omega = 0, 1^f,$ and 1^e denote the fine structure components.

^bIn MHz.

^cObserved minus calculated frequency in kHz.

^dRotational transition frequencies measured by FTMW spectroscopy (Ref. 19).

^eLess weighted in the analysis.

The footnote to Table 1 clearly indicates that the transitions are reported in MHz.