CHEM 26700 (Experimental Physical Chemistry) Lab Reports

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1 UV-VIS ANALYSIS OF IODINE

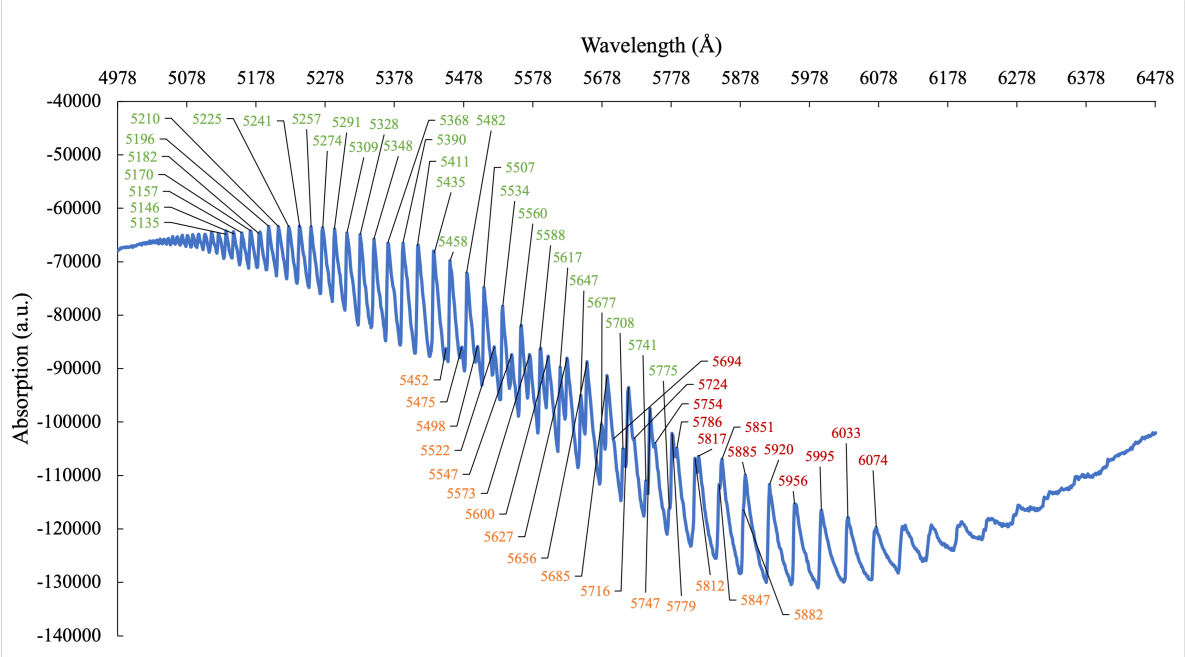

Figure 1: The absorption spectrum of gaseous I_2 between $\lambda = 5000 - 6500\,\text{Å}$.

v'	v''	ω (cm^{-1})	v'	v''	ω (cm^{-1})	v'	v''	ω (cm^{-1})
						10	2	16463
						11	2	16575
						12	2	16680
			13	1	17001	13	2	16789
14	0	17316	14	1	17102	14	2	16891
15	0	17418	15	1	17205	15	2	16992
16	0	17519	16	1	17304	16	2	17091
17	0	17614	17	1	17400	17	2	17190
18	0	17708	18	1	17494	18	2	17283
19	0	17803	19	1	17590	19	2	17379
20	0	17895	20	1	17680	20	2	17470
21	0	17985	21	1	17771	21	2	17562
22	0	18070	22	1	17857			
23	0	18158	23	1	17943			
24	0	18241	24	1	18027			
25	0	18321	25	1	18109			
26	0	18399	26	1	18188			
27	0	18480	27	1	18264			
28	0	18552	28	1	18341			
29	0	18628						
30	0	18698						
31	0	18768						
32	0	18835						
33	0	18900						
34	0	18960						
35	0	19022						
36	0	19080						
37	0	19138						
38	0	19193						
39	0	19245						
40	0	19297						
41	0	19342						
42	0	19391						
43	0	19432						
44	0	19474						

Table 1: Peaks and their corresponding transitions.

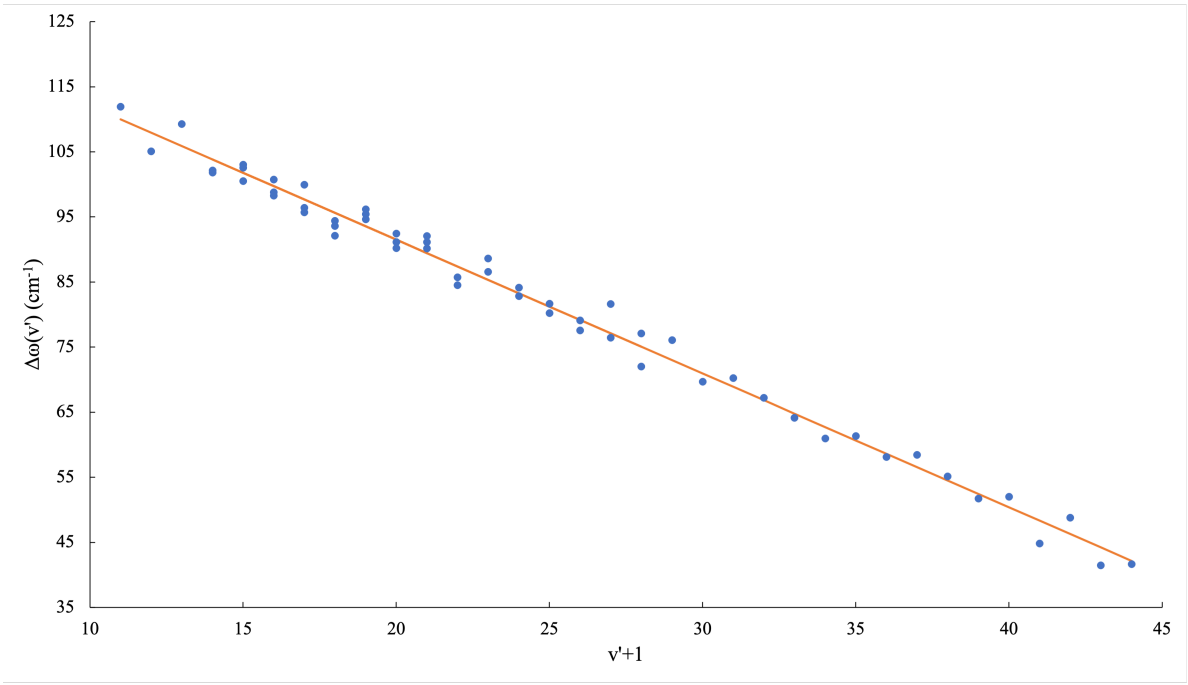

Figure 2: Birge-Sponer plot for the B state.

	$\bar{\nu}'_e$	$\bar{\nu}'_e x'_e$	D'_e	D'_0	$\bar{\nu}''_e$	$\bar{\nu}''_e x''_e$	D''_e	D''_0	T_e
Calculated values	132.62	1.0279	4277.2	4211.1	216.10	1.2583	9278.5	9170.7	12 604
Literature values[1,2]	125.69	0.764	4112	4046	214.50	0.614	12 244	12 137	15 769.01

Table 2: Calculated spectroscopic constants and their reported values.

Note that the units for all values in Table 2 is cm^{-1}.

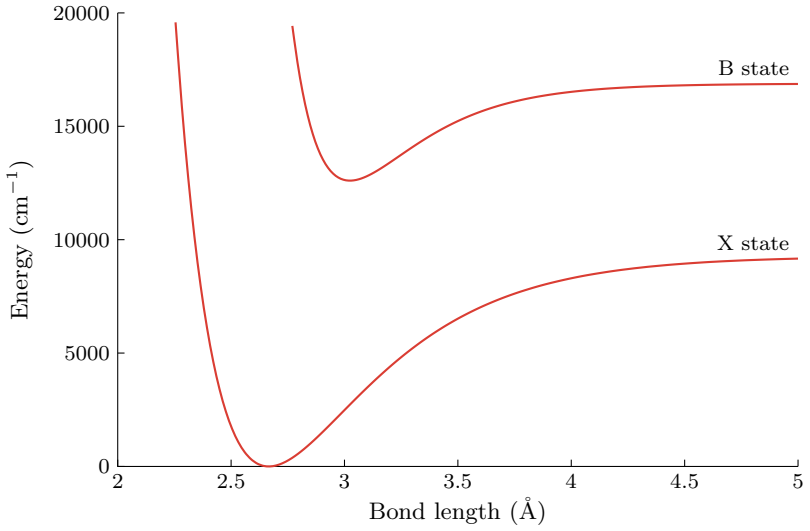

Figure 3: Morse potential curves.

References

(1) Huber, K. P.; Herzberg, G. H. In *NIST Chemistry WebBook, NIST Standard Reference Database Number 69*, Linstrom, P. J., Mallard, W. G., Eds., `https://doi.org/10.18434/T4D303`; National Institute of Standards and Technology: Gaithersburg MD, 20899; Chapter Constants of Diatomic Molecules.

(2) McNaught, I. J. The Electronic Spectrum of Iodine Revisited. *J. Chem. Educ.* **1980**, *57*, 101–105.

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2 TITLE

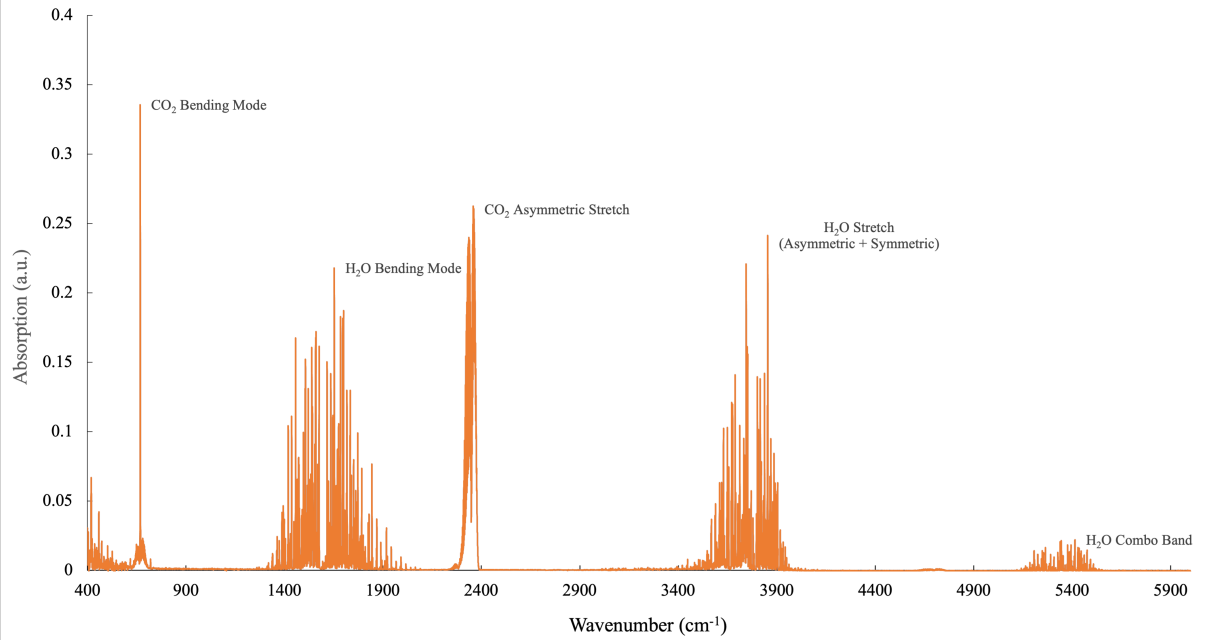
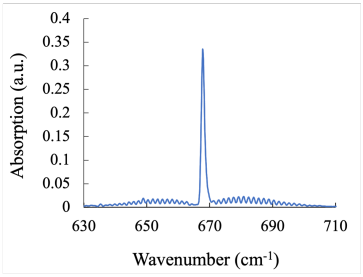
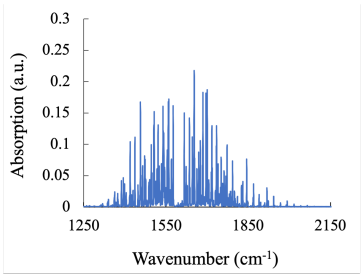


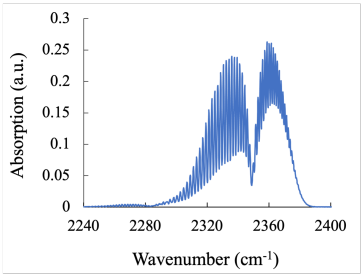
Figure 1: Infrared absorption spectrum of air (background spectrum).



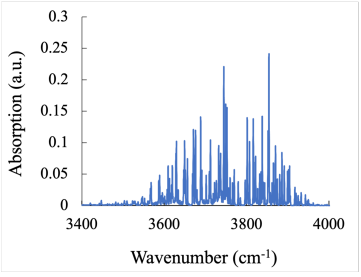
(a) CO_2 bending mode.



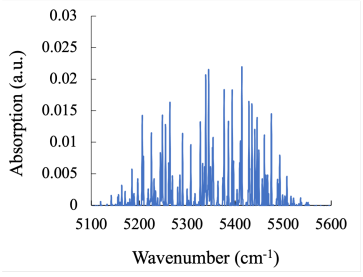
(b) H_2O bending mode.



(c) CO_2 asymmetric stretch.



(d) H_2O stretches.



(e) H_2O combo band.

Figure 2: The five primary vibrational bands in a sample of air.

Wavenumber Range (cm^{-1})	**Molecule**	**Vibrational Band**
630-710	CO_2	Bending
1250-2150	H_2O	Bending
2240-2400	CO_2	Asymmetric stretch
3400-4000	H_2O	Asymmetric & symmetric stretch
5100-5600	H_2O	Combo band

Table 1: Infrared-active vibrational modes in air molecules.

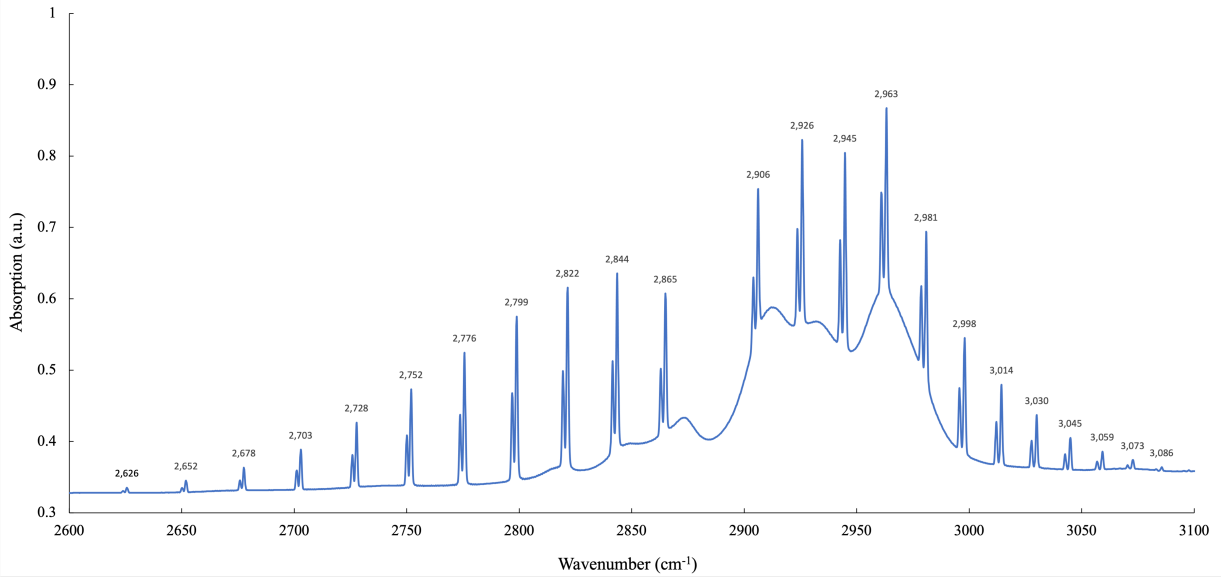


Figure 3: Rovibrational absorption spectrum of HCl.

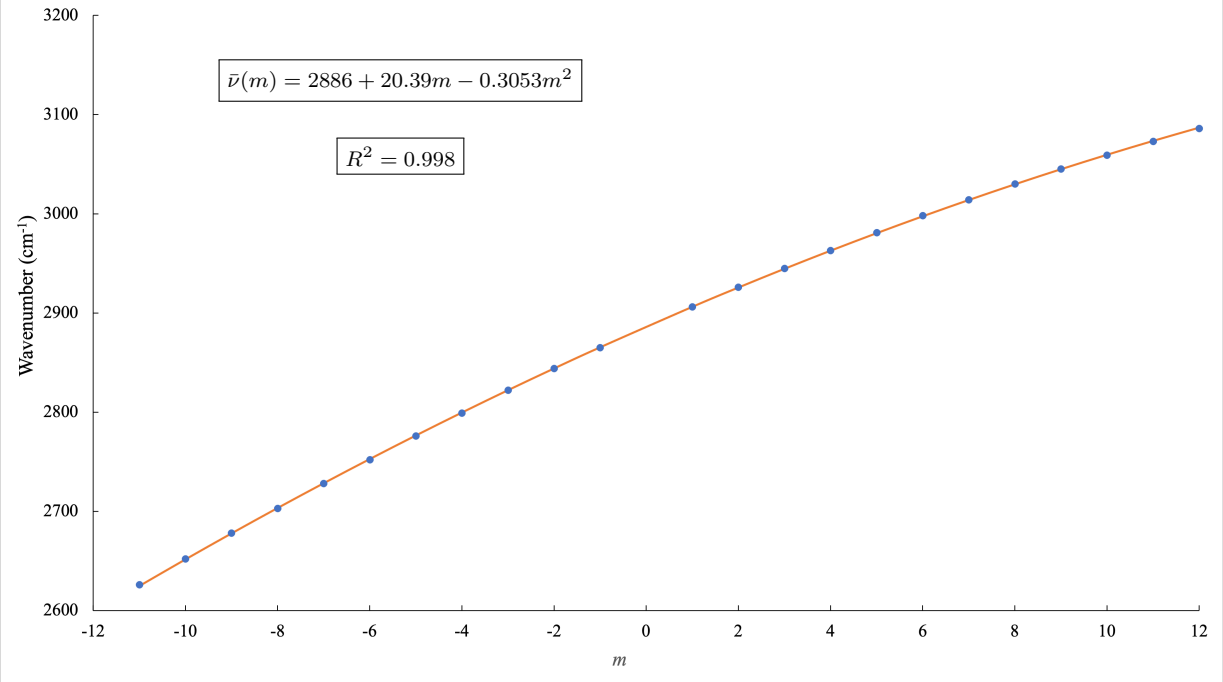


Figure 4: Fitting data on the rovibrational transition wavenumbers $\bar{\nu}$ of HCl vs. a parameter m related to the rotational energy level from which such a rovibrational transition begins.

	B_e ($\mathbf{cm^{-1}}$)	α_e ($\mathbf{cm^{-1}}$)	$\bar{\nu}_0$ ($\mathbf{cm^{-1}}$)
Calculated values	10.50	0.3053	2886
Literature values	10.59[1]	0.3072[1]	2991[1]

Table 2: Calculated spectroscopic constants and their reported values.

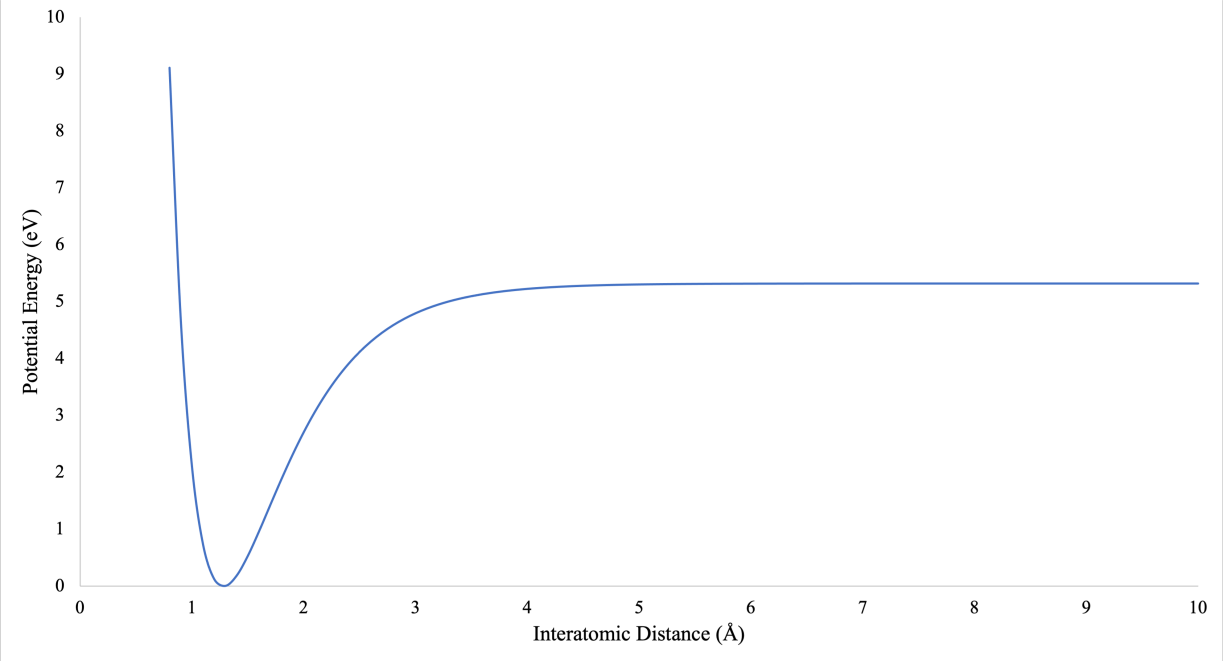


Figure 5: Morse potential curve.

	$\bar{\nu}_e$ (cm^{-1})	x_e	D_e (eV)	r_e (Å)
Calculated values	2990	0.017 41	5.320	1.281
Literature values	2991[1]	0.017 66[1]	5.319[1]	1.275[1]

Table 3: Calculated energy constants and their reported values.

References

(1) Huber, K. P.; Herzberg, G. H. In *NIST Chemistry WebBook, NIST Standard Reference Database Number 69*, Linstrom, P. J., Mallard, W. G., Eds., `https://doi.org/10.18434/T4D303`; National Institute of Standards and Technology: Gaithersburg MD, 20899; Chapter Constants of Diatomic Molecules.

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