High Resolution IR of HCl and DCl

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1   Introduction

1.1   Purpose

Use the spectrum of HCl from vibrational-rotational spectroscopy to determine the force constant, rotational constant, and internuclear distance. Observe the differences in vibrational-rotational spectrum between HCl and DCl.

1.2   References

McQuarrie, D. A.; Simon, J. D. *Physical Chemistry: A Molecular Approach*; University Science Books: Sausalito, CA, **1997**.

Shoemaker, D. P.; Garland, C. W.; Nibler, J. W. *Experiments in Physical Chemistry, 6th edition* .p. 397-404, **1996**, The McGraw-Hill Companies.

Wiser, D.; *The Vibrational-Rotational Spectra of HCl and DCl.*; Lake Forest College: Lake Forest, IL, **2025**; pp 1-2.

1.3   Safety Information

There are no safety risk associated with this experiment.

2   Results/Data

m is related to the quantum number, J, by Shoemaker 1996 with the relationship $m = J + 1$ for the R branch on the left-hand side and $m = -J$ for the P branch on the right-hand side.
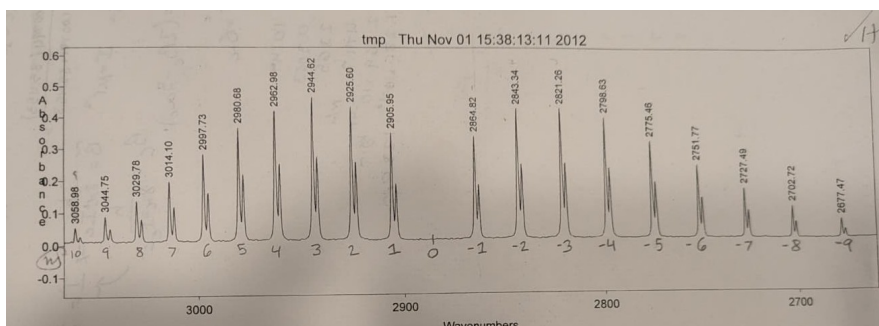

Figure 1: High resolution IR spectra of HCl label with m values.

Table 1: Comparison of experimentally calculated and literature values of properties measured by high resolution IR

	R branch				P branch		
m	$\tilde{v}$	$\Delta\tilde{v}$	$\tilde{v}_o$	m	$\tilde{v}$	$\Delta\tilde{v}$	$\tilde{v}_o$
1	2905.95	19.65	2886.20	-1	2864.82	-	2845.07
2	2925.60	19.02	2906.77	-2	2843.34	21.48	2824.51
3	2944.62	18.36	2927.32	-3	2821.26	22.08	2803.96
4	2962.98	17.70	2947.82	-4	2798.63	22.63	2783.47
5	2980.58	17.05	2968.28	-5	2775.46	23.17	2763.058
6	2997.73	16.37	2988.70	-6	2751.77	23.69	2741.74
7	3014.10	15.68	3009.05	-7	2727.49	24.28	2722.44
8	3029.78	14.97	3029.32	-8	2702.72	24.77	2702.26
9	3044.75	14.23	3049.50	-9	2677.47	25.25	2682.22
10	3058.98	-	3069.55	-	-	-	-

There was a trend of decreasing $\Delta\tilde{v}$ across the R branch and a trend of increasing $\Delta\tilde{v}$ across the P branch which lead to an over all trend for increasing $\Delta\tilde{v}$ from left to right across the spectra. A plot of Δv vs m results in a line with a slope of -2α and an intercept of $2\tilde{B} - 3\alpha$ (Fig. 2).
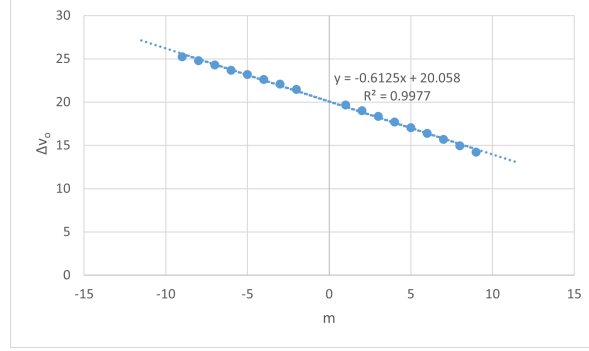

Figure 2: Graph of m vs Δv_o from HCl IR spectra.

The values of the initial frequency ($\tilde{v}_o$), force constant (k), inertia (I_e) and bond radius r were calculated following the methods outlined in Shoemaker, 1996.

Table 2: Comparison of experimentally calculated and literature values of properties measured by high resolution IR to literature values from McQuarrie, 1997

Value	Units	Experimental	Literature	% Error
B_e	cm^{-1}	10.49	-	-
α_e	cm^{-1}	0.3063	-	-
$\tilde{v}_o$	cm^{-1}	2865	2886	0.7%
k	N/m	474.2	478	0.8%
I_e	$kg \cdot m^2$	2.668 $\times 10^{-47}$	2.68×10^{-47}	0.4%
r	pm	128.0	127.5	0.4%

3 Conclusion

Changing the isotope does not change the overall force constant, but it changes the mass, so it changes the value of μ and that it changes the moment of inertia. The bond distance is also changed by changing the isotope. This has an overall effect of changing the location (frequency of the vibrations) but not the pattern. Additionally, there are 2 peaks for each of HCl because there are 2 isotopes of chlorine (^{35}Cl and ^{36}Cl) and both μ values for either isotope are very close together. D has a larger mass it helps reduce the difference between the μ values and makes the split peaks less evident.