Supplementary Material for PCCP

The observation of the electronic spectrum of Fe_2Cl_6 in the gas phase

Philip J. Hodges, Ian R. Beattie and John M. Brown

Supplementary Information

Contents:
1. Details of calibration procedure for LIF spectrum, and dispersed fluorescence spectrum.
2. Table: Vacuum wavenumbers and approximate relative intensities for the vibrational features in the laser excitation spectrum of Fe_2Cl_6 between 353 and 400 nm.

1a. Details of calibration procedure for LIF spectrum.
The laser-induced fluorescence was focused onto a photomultiplier tube mounted at right angles to both the molecular beam and the laser beam. Either an Andover UG-1 filter or a bandpass filter centred at 390 nm (Andover) was located in front of the PMT, improving the signal-to-noise by blocking out the majority of the blackbody radiation from the heated nozzle whilst allowing the laser-induced fluorescence to pass. The laser power was measured with a photodiode and the laser wavelength monitored using a Burleigh uv pulsed wavemeter (model WA55-00). At the end of the experiment the fluorescence signal was normalized to laser power and the wavelength calibrated against the readings from the wavemeter. From previous work, the dye laser scanning system has been found to be highly linear in wavelength. From repeat recordings of this spectrum, the uncertainty in absolute vacuum wavenumber determination is estimated to be 0.2 cm^{-1}.

1b. Details of calibration procedure for dispersed fluorescence spectra.
The dispersed fluorescence spectra were calibrated by first recording the spectrum of a hollow cathode lamp to acquire a calibration curve for the diffraction grating. The scan was close to linear in wavelength but there was an almost constant offset of 6 cm^{-1} over the range of these experiments. The spectra were subsequently calibrated with respect to the excitation band. The typical linewidth (FWHM) is 150 cm^{-1}. We estimate that the uncertainty of measurement is 15 cm^{-1} for ground state vibrational features.

2. Vacuum wavenumbers and approximate relative intensities for the vibrational features in the laser excitation spectrum of Fe_2Cl_6 between 353 and 400 nm.

Vacuum waveumber (cm^{-1})	rel intensity[a]	Vacuum waveumber (cm^{-1})	rel intensity[a]	Vacuum waveumber (cm^{-1})	rel intensity[a]	Vacuum waveumber (cm^{-1})	rel intensity[a]
25018.6	0.1	25671.1	0.15	26029.9	0.2	26350.8	0.1
25039.4	0.2	25672.3	0.3	26033.4	0.5	26351.8	0.3
25055.1	0.2	25674.6	0.2	26040.6	0.4	26353.9	0.3
25056.8	0.05	25676.6	0.3	26046.0	0.4	26359.3	0.3
25070.7	0.25	25680.8	0.2	26050.2	0.6	26366.6	0.6
25072.2	0.1	25686.0	0.3	26052.9	0.2	26376.3	0.4
25100.6	0.1	25689.4	0.2	26055.1	0.1	26382.8	0.2
25113.5	0.1	25691.1	0.2	26057.7	0.5	26391.7	0.4
25131.8	0.05	25709.6	0.3	26065.0	0.3	26405.6	0.4
25147.6	0.1	25723.1	1.5	26071.3	0.7	26408.0	0.2
25149.2	0.1	25729.8	0.1	26073.0	0.4	26431.8	0.1
25185.6	0.6	25733.4	0.1	26077.9	0.8	26464.7	0.1
25188.9	0.3	25743.3	0.1	26080.6	0.2	26550.6	0.1
25203.7	0.5	25753.0	0.1	26083.5	0.1	26551.7	0.05
25205.8	0.5	25763.6	0.3	26089.3	0.1	26561.7	0.1
25214.8	0.1	25774.2	1.5	26098.9	0.4	26570.9	0.1
25216.4	0.05	25790.8	0.3	26102.4	0.8	26587.3	0.3
25241.6	0.55	25802.1	0.1	26104.6	0.4	26596.3	0.3
25261.0	0.2	25805.5	0.1	26108.7	0.3	26652.0	0.05
25281.0	0.15	25809.5	0.1	26116.4	0.3	26671.2	0.1
25308.0	0.4	25816.2	0.1	26125.3	0.6	26681.1	0.1
25324.8	0.1	25818.5	0.1	26127.2	1	26688.1	0.1
25343.1	0.1	25820.1	0.1	26135.2	1	26690.6	0.2
25347.0	0.05	25824.1	0.5	26140.5	4.5	26750.2	0.2
25351.2	0.05	25830.5	0.3	26143.6	1.2	26776.7	0.025
25357.3	0.6	25843.8	0.6	26148.0	0.7	26853.9	0.2
25362.8	0.4	25846.5	0.2	26150.9	0.8	26873.0	0.4
25378.0	0.6	25855.9	0.6	26153.1	0.8	26961.0	0.3
25405.3	0.1	25864.2	0.2	26166.8	0.2	26977.4	0.4
25407.5	0.15	25865.2	0.2	26169.2	0.6	27019.5	0.1
25432.6	0.5	25884.6	0.3	26174.9	0.6	27033.0	0.1
25435.0	2	25898.7	6	26179.0	0.6	27095.5	0.1
25440.4	0.9	25909.1	0.2	26181.6	0.6	27107.6	0.1
25449.9	1.5	25909.5	0.2	26184.0	0.4	27110.6	0.1
25466.6	0.5	25917.5	2	26191.3	0.4	27113.0	0.1
25473.6	0.4	25922.2	4	26199.2	0.5	27121.8	0.1
25482.5	2.1	25928.3	0.2	26200.1	0.5	27131.7	0.1
25500.1	0.5	25939.4	0.2	26207.3	0.5	27133.6	0.1
25564.8	0.1	25940.7	0.2	26217.9	0.6	27135.8	0.1
25565.0	0.05	25953.9	0.2	26220.0	0.6	27143.5	0.4
25580.0	0.1	25960.3	0.4	26227.9	0.6	27166.7	3
25588.7	0.1	26966.0	0.2	26230.2	0.4	27394.2	10
25590.0	0.2	25967.2	0.1	26231.9	0.4	27584.6	0.3
25596.2	0.2	25968.2	0.2	26232.4	0.3	27490.6	0.3
25594.6	0.05	25972.9	0.3	26239.4	0.6	27528.5	0.5
25596.0	0.1	25978.3	0.2	26240.7	0.6	27571.8	0.3
25597.7	0.05	25979.8	0.5	26242.0	0.6	27591.5	0.3
25605.0	0.05	25985.7	0.2	26250.5	0.2	27625.1	0.6
25604.8	0.15	25986.7	0.1	26254.1	0.2	27676.3	0.4
25613.7	0.15	25989.1	0.5	26260.3	0.2	27720.1	0.3
25621.9	0.2	25995.2	0.5	26310.6	0.8	27721.6	0.2
25634.3	0.6	25997.1	0.5	26313.0	0.5	27882.2	0.8
25638.5	0.2	25999.9	0.5	26317.7	1.3	27917.2	1.5
25636.6	0.2	26007.2	0.5	26319.2	0.7	27933.6	0.4
25643.6	0.2	26018.2	0.6	26326.0	1	27969.5	1.1
25644.9	0.1	26019.2	0.5	26327.2	0.8	28003.2	0.9
25656.8	0.3	26019.9	0.3	26330.0	0.6	28026.0	1.5
25662.2	0.3	26025.3	0.6	26342.3	0.4	28035.4	0.8
25667.0	0.1	26027.0	0.3	26347.3	1.2	28046.4	0.2

[a] Estimate of relative intensity on a scale of 1 to 10. Due to marked fluctuations in molecular concentration, and errors introduced when scaling adjacent scans, the relative intensities are only reliable for lines that are closely separated.