ACCURATE DETERMINATION OF THE GROUND STATE CONSTANTS, INCLUDING A_0 AND D_K^0 , OF D₃Si³⁵Cl

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In a previous study^{*a*} of monoisotopic D₃Si³⁵Cl, the analysis of the fundamental bands ν_3 and ν_6 , linked by a Coriolis resonance, was reported. New Fourier transform infrared spectra of this compound were recorded in the 500 and 1000 cm⁻¹ regions. The first purpose was to obtain accurate ground state constants. The 'normal' G.S. constants B_0 , D_J^0 , and D_{JK}^0 were deduced from GSCD. As for the constants A_0 and D_K^0 , they were obtained by the now well-established method of combining data from the fundamental ν_6 , the overtone $(2\nu_6)^{\mp 2}$ and the hot band $(2\nu_6)^{\pm 2}$ - $(\nu_6)^{\pm 1}$. Special care was taken to correct calibration differences between the two spectral regions. This was done by checking closed loops such as ν_3 , $2\nu_3$, and $2\nu_3 - \nu_3$ on one hand or $\nu_6, (2\nu_6)^0$ and $(2\nu_6)^0 - \nu_6$ on the other hand. The values obtained are $A_0 = 1.427830$ cm⁻¹ and $D_K^0 = 5.36 \times 10^{-6}$ cm⁻¹ (provisional values). Some sextic H constants could also be determined. In a second stage, the upper state energies of $(2\nu_6)^{\pm 2}, (2\nu_6)^0, 2\nu_3$ and $\nu_3 + \nu_6$ were fitted together to obtain the upper state constants. Note that, due to the weakness of the $\nu_3 + \nu_6$ band, the hot bands $\nu_3 + \nu_6 - \nu_3$ and $\nu_3 + \nu_6 - \nu_6$ were used instead.

^aJ.E. Gadhi, H. Bürger, and E.B. Mkadmi, submitted to J. Mol. Spectrosc.