ACCURATE DETERMINATION OF THE GROUND STATE CONSTANTS, INCLUDING A_0 AND D_K^0, OF $D_3Si^{35}Cl$

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In a previous study[a] of monoisotopic $D_3Si^{35}Cl$, 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 $2\nu_3$ - ν_3 on one hand or ν_6,$(2\nu_6)^0$ and $(2\nu_6)^0$ - ν_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 $\nu_3 + \nu_6$ - ν_3 and $\nu_3 + \nu_6$ - ν_6 were used instead.

[a] J.E. Gadhi, H. Bürger, and E.B. Mkadmi, submitted to *J. Mol. Spectrosc.*