AB INITIO ANHARMONIC FORCE FIELS AND EQUILIBRIUM STRUCTURE OF CARBONYL CHLOROFLUORIDE

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In this work, we report the calculation of a new anharmonic force field up to semi-diagonal quartic terms using a basis set of triple zeta quality. The accuracy of the force field is checked by comparing experimental and ab initio spectroscopic constants. To complete the infrared analysis reported previously [a], the present work involves also the identification of numerous overtone or combination bands of $COF^{35}Cl$, and for this task new low resolution Fourier transform spectra were recorded at Wuppertal. Finally, two independent equilibrium structures are determined: a purely ab initio one and a semi-experimental one.

[a] A.Perrin, J.-M.Flaud, H.Burger, G. Pawelke, S.Sander and H. Willner, J. Mol. Spectrosc. 209, 122 (2001)