FIRST HIGH RESOLUTION ANALYSIS OF THE ν_1, ν_2, ν_3, ν_4, ν_5, AND ν_6 BANDS OF COF^{35}Cl IN THE 600-2000 cm $^{-1}$REGION

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Concern about the implication of chlorofluorocarbons (CFCs) on the amounts of ozone in the earth's atmosphere has led to the measurement of the concentration of halogen containing compounds in the stratosphere. Of the various possible oxidation products of CFC's in the stratosphere, carbonyl chlorofluoride COFCl may receive attention. COFCl is formed by the reaction of freon11 ($CFCl_3$) with O(^{1}D) oxygen atoms which are formed by photolysis of ozone [a], [b]. High resolution atmospheric infrared spectra are potential means of monitoring COFCl. However, there is only little information on the spectroscopy of this molecule in the literature. We have recorded spectra of a ^{35}Cl enriched sample of COFCl at ca. 0.002 cm^{-1} resolution with the BRUKER Fourier transform spectrometer of the University of Wuppertal. We present here the first high resolution analyses of the six fundamentals ν_1, ν_2, ν_3, ν_4, ν_5 and ν_6 bands located at 1875.8, 1095.1, 764.4, 501.6, 408.8 and 666.6 cm^{-1} respectively for the ^{35}Cl isotopic species of COFCl. According to the results of the analyses, the ν_3, ν_4, ν_5, ν_6 are unperturbed, while the analyses of the ν_2 and ν_1 bands was complicated by numerous resonances. Excellent results were obtained for the ν_3, ν_4, ν_5, ν_6 bands and for the perturbed ν_2 band. On the other hand, for the ν_1 band for which the resonance scheme is more complex, the results of the analysis are still less satisfactory.

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[b] F.Wu, and R.W.Carr, J. Phys. Chem. 96, 1743, (1992)