EFFECTIVE DIPOLE MOMENT MODEL FOR AXIALLY SYMMETRIC C_{3v} MOLECULES: APPLICATION TO THE PRECISE STUDY OF ABSOLUTE LINE STRENGTHS OF THE ν_6 FUNDAMENTAL OF CH_3Cl

O. N. ULENIKOV, E. S. BEKHTEREVA, O. V. GROMOVA, A. L. FOMCHENKO, *National Research Tomsk Polytechnic University, 30, av. Lenina, 634050 Tomsk, Russia*; **C. SYDOW and S. BAUERECKER**, *Institut für Physikalische und Theoretische Chemie, Technische Universität Braunschweig, D - 38106, Braunschweig, Germany*

The effective dipole moment model for molecules of axial C_{3v} symmetry is derived on the basis of the symmetry properties of a molecule which, on the one hand, is of the same order of efficiency (but much simpler and clearer in applications) as the analogous models derived on the basis of the irreducible tensorial sets theory and, on the other hand, mathematically more correct in comparison with concepts like the Herman–Walles function used in the models. As an application of the general results obtained, we discuss high resolution infrared spectra of CH_3Cl, recorded with the Zürich prototype ZP2001 (Bruker IFS125 HR) Fourier transform infrared spectrometer at a resolution of 0.001 cm^{-1} and analyzed in the region of 880–1190 cm^{-1}. Absolute strengths of more than 2800 transitions (2081 lines) were obtained from the fit of their shapes both with Voigt and Hartmann–Tran profiles, and parameters of the effective dipole moment of the ν_6 band were determined by the computer code SYMTOMLIST (SYMmetric TOp Molecules: LIne STrengths), created on the basis of a derived theoretical model. As the first step of the analysis of the experimental data, assignments of the recorded lines were made. A total of about 5180 transitions with J^{max} = 68, K^{max} = 21 were assigned to the ν_6 band. The weighted fit of 2077 upper energy values obtained from the experimentally recorded transitions was made with a Hamiltonian which takes into account different types of ro–vibrational effects in doubly degenerate vibrational states of the $C_{3v}-$symmetric molecule. As the result, a set of 25 fitted parameters was obtained which reproduces the initial 2077 upper "experimental" ro–vibrational energy values with a root mean square deviation $d_{\mathrm{rms}} = 4.7 \times 10^{-5}$ cm^{-1}. At the second step of the analysis, the computer code SYMTOMLIST was used for determination of the parameters of the derived effective dipole moment model. Six effective dipole moment parameters were obtained from the weighted fit procedure which reproduces absolute experimental strengths of the 2804 initial experimental transitions with a relative $d_{\mathrm{rms}} = 3.4\%$.

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