DETERMINATION OF THE GROUND-STATE POTENTIAL FUNCTION OF OZONE FROM INFRARED SPECTRA

VLADIMIR G. TYUTEREV, A. BARBE, T. COURS, *Groupe de Spectroscopie Moléculaire et Atmosphérique, Equipe Associeé au CNRS, UPRESA Q 6089, U. F. R. Sciences, B. P. 1039, F-51687 Reims Cedex 2, France*; SERGEI TASHKUN, *Institute of Atmospheric Optics, Russian Academy of Science, Tomsk 634055, Russia*; PER JENSEN, *FB9 - Theoretische Chemie, Bergische Universität – Gesamthochschule Wuppertal, D-42097 Wuppertal, Germany*.

The effective ground-state potential energy function of the ozone molecule near the C_{2v} equilibrium configuration has been obtained in a least-squares fit to the largest sample of experimental, high-resolution vibration-rotation data used for this purpose so far. The fitting is based on variational calculations carried out with an extended MORBID model. The RMS (root-mean-square) deviation of the fit of ro-vibrational data up to $J = 5$ is 0.02 cm^{-1}. For the set of all 60 band centres of the $^{16}O_3$ molecule included in the Atlas of Ozone Line Parameters[a] the RMS deviation is 0.025 cm^{-1}, and for all band centres determined so far from high resolution spectra, including those recently observed and assigned in Reims corresponding to highly excited stretching and bending vibrations (v_1+v_2+$v_3 < 6$) , the RMS deviation is 0.1 cm^{-1}. The "dark states" that produce resonance perturbations in the observed bands are described with experimental accuracy up to the $(v_1v_2v_3) = (080)$ state. Extrapolation tests demonstrate the predictive power of the potential function obtained: rotational extrapolation up to $J = 10$ for the eleven lowest vibrational states results in an RMS deviation of 0.06 cm^{-1}. Also, vibrational energies measured by low-resolution Raman spectroscopy (which were not included in the input data for the fit) are calculated within the experimental accuracy of the experimental values up to the dissociation limit. The long-range behaviour of the fitted potential at the dissociation limit $O_3 \rightarrow O_2$ + O shows very good agreement with experimental data.

[a] J.-M. Flaud, C. Camy-Peyret, C. P. Rinsland, M. A. H. Smith, and V. Malathy Devi, Atlas of Ozone Line Parameters from Microwave to Medium Infrared, Academic Press, New York, 1990.