DETERMINATION OF ELECTRIC AND MAGNETIC PROPERTIES OF DIATOMIC MOLECULES FROM PURE ROTATIONAL AND VIBRATION- ROTATIONAL SPECTRA

MARCIN MOLSKI, JERZY KONARSKI, *Theoretical Chemistry Department, A. Mickiewicz University, ul. Grunwaldzka 6, PL 60-780 Poznań, Poland*.

We extended[a] Dunham's approach to analytic treatment of vibration-rotational spectra of diatomic molecules and applied the method to GaH and LiH in their ground electronic states $X^1\Sigma^+$. The vibrational displacements of nuclei are considered in the vicinity of dynamical reference conformation R_{vJ} that depends not only on the rotational quantum number J, through the action of centrifugal force, but also on the vibrational v one, through nonadiabatic vibrational effects of high order. Published wavenumbers of assigned transitions are reproduced with fewer parameters for potential energy than reported elsewhere. From parameters representing nonadiabatic rotational effects we estimate at R_0 the rotational $g-$factor and electric dipolar moment. They conform acceptably with magnitudes from published experiments on Stark and Zeeman effects and from quantum-chemical calculations of electronic structure.

[a] J. Konarski, Int. J. Quantum Chem. 51, 439 (1994); M. Molski, Phys. Rev. 50A, 4380 (1994); *Idem* J. Mol. Spectrosc. 181, 1 (1997); *Ibid* 185, 256 (1997); *Ibid* 193, 244 (1999).