COMPARISON OF NUMERICAL AND ANALYTICAL APPROACHES FOR REDUCTION OF ROTATIONAL AND VIBRATION-ROTATIONAL SPECTRA OF DIATOMIC MOLECULES TO PARAMETERS OF RADIAL FUNCTIONS

JOHN A. COXON, *Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada B3H 4J3*; and MARCIN MOLSKI, *Theoretical Chemistry Department, A. Mickiewicz University, ul. Grunwaldzka 6, PL 60-780 Poznań, Poland*..

The talk presents a numerical test[a] of the three most popular methods used for direct inversion of the highly resolved IR and MW spectra of diatomic systems: (A) the numerical techniques such as those described by Coxon[b], Bernath[c], Le Roy[d] and their co-workers, (B) the analytical approach of Ogilvie[e], implemented in the computer program Radiatom, and (C) its improved version, called deformational self-consistent procedure (DS-cP), proposed by Molski[f]. The test calculations show that the Ogilvie's Radiatom program does not produce sufficiently accurate radial parameters and energy term values for their export to other utilities employed in the spectral analysis of diatomic systems.

---

[a] J. A. Coxon and M. Molski, *Phys. Chem. Comm.* 2001, **21** 1; J. A. Coxon and M. Molski, *Spectrochim. Acta A* 2002, submitted for publication.

[b] J. A. Coxon and P. G. Hajigeorgiou, *J. Mol. Spectrosc.*, 1991, **150**, 1; J. A. Coxon, *J. Mol. Spectrosc.*, 1992, **152**, 274.

[c] J. M. Campbell, M. Dulick, D. Klapstein, J. B. White and P. F. Bernath, *J. Chem. Phys.*, 1993, **99**, 8379; H. G. Hedderich, M. Dulick and P. F. Bernath, *J. Chem. Phys.*, 1993, **99**, 8363; M. Dulick, K. Q. Zhang, B. Guo and P. F. Bernath, *J. Mol. Spectrosc.*, 1998, **188**, 14.

[d] J. Y. Seto, R. J. Le Roy, J. Verges and C. Amiot, *J. Chem. Phys.*, 2000, **113**, 3067.

[e] J. F. Ogilvie, *J. Phys. B*, 1994, **27**, 47; J. F. Ogilvie, *The Vibrational and Rotational Spectrometry of Diatomic Molecules*, Academic Press, London, 1998.

[f] M. Molski, *J. Phys. Chem.*, 1999, **103**, 5269; M. Molski, *Chem. Phys. Lett.*, 1999, **306**, 88. M. Molski, *Chem. Phys. Lett.* 2001, **342**, 293.