INFRARED SPECTRA OF $^{12}C^{16}O$ IN ABSORPTION AND EVALUATION OF RADIAL FUNCTIONS FOR POTENTIAL ENERGY AND ELECTRIC DIPOLAR MOMENT

J. F. OGILVIE, *Centre for Experimental and Constructive Mathematics, Department of Mathematics, Simon Fraser University, 8888 University drive, Burnaby, British Columbia V5A 1S6 Canada*; SWEE-LAN CHEAH, YUAN-PERN LEE, *Department of Chemistry, National Tsing Hua University, Hsinchu 30013, Taiwan*; S. P. A. SAUER, *Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK 2100 Copenhagen O, Denmark.*

From quantum-chemical calculations of rotational g factor and new experimental measurements of strengths of lines in infrared spectra of vibration-rotational bands in absorption[a], with $v'' = 0$ and $1 \leq v' \leq 4$, of $^{12}C^{16}O$, and from analysis of 16947 frequencies and wave numbers assigned to pure rotational and vibration-rotational transitions within electronic ground state $X\ ^1\Sigma^+$, including new measurements of band 4 – 0 of $^{12}C^{16}O$, we evaluate radial functions[b] for potential energy and electric dipolar moment, the latter both in polynomial form and as a rational function that has qualitatively correct behaviour under limiting conditions.

---

[a]J. F. Ogilvie, S-L. Cheah, Y.-P. Lee and S. P. A. Sauer, *Theoretical Chemistry Accounts*, in press (2002)
[b]J. F. Ogilvie, *The Vibrational and Rotational Spectrometry of Diatomic Molecules*, Academic Press, London U.K. (1998)
