SELF- AND H_2-BROADENED LINE PARAMETERS OF CARBON MONOXIDE IN THE FIRST OVERTONE BAND

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In this study we have re-analyzed high-resolution spectra of pure CO and CO broadened by hydrogen recorded in the spectral range of the first overtone band.[a] We have used four different line shapes in the multispectrum analysis (Voigt, speed dependent Voigt, Rautian, and Rautian with speed dependence) and compared the resulting line shape parameters. The line mixing coefficients have been calculated using the Exponential Power Gap and the Energy Corrected Sudden scaling laws. A classical approach was applied to calculate CO line widths in CO-H_2 and CO-CO collisions. The formulas of classical impact theory[b] are used for calculation of dipole absorption half-widths along with exact 3D Hamilton equations for simulation of molecular motion. The calculations utilize Monte Carlo averaging over collision parameters and simple interaction potential (Tipping-Herman + electrostatic).[c,d] Molecules are treated as rigid rotors. The dependences of CO half-widths on rotational quantum number $J \leq 24$ are computed and compared with measured data at room temperature.

[a] V. Malathy Devi *et al.*, *J. Mol. Spectrosc.* **228** (2004) 580-592.

[b] R. G. Gordon, *J. Chem. Phys.* **44** (1966) 3083-3089; *ibid.*, **45** (1966) 1649-1655.

[c] J.-P. Bouanich and A. Predoi-Cross, *J. Molec. Structure* **742** (2005) 183-190.

[d] A. Predoi-Cross, J.-P. Bouanich, D. Chris Benner, A. D. May, and J. R. Drummond, *J. Chem. Phys.* **113** (2000) 158-168.