

## R(0) LINE SHAPE PARAMETERS OF CO IN ARGON

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A state of the art study of the parameters of the pure rotational R(0) line of carbon monoxide molecule ( $^{12}\text{C}^{16}\text{O}$ ) perturbed by Ar is presented.

Experimental spectra were obtained at room temperature using three microwave spectrometers<sup>1</sup> differing by the principle of absorption measurement and covering a wide pressure range from less than one mTorr to several atmospheres. The experimental spectra were obtained with a signal-to-noise ratio of several thousands. The line shape analysis was performed using sophisticated profiles including speed-dependence and line mixing effects allowing the determination of the corresponding parameters.

Quantum dynamical calculations of scattering matrix elements were performed on two different 3-dimensional potential energy surfaces (PES): the PES of Sumiyoshi et al.<sup>2</sup> and our recently calculated PES. For the R<sub>0</sub>(0) line of CO, calculations were performed for kinetic energies varying between 0.1 and 2000 cm<sup>-1</sup>. The obtained S-matrix elements (relevant to that electric dipole transition) were further used to calculate the generalized Hess spectroscopic cross sections<sup>3</sup>. The thermally averaged values of these cross sections provided us the pressure broadening and shift coefficients as well as the real and imaginary parts of the Dicke frequency of the velocity changing collisions<sup>4</sup>. In addition, our calculations allowed the speed dependence of these line shape parameters to be determined. We are thus in the position to perform an accurate line shape analysis.

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<sup>3</sup>[doi:10.1063/1.451277](https://doi.org/10.1063/1.451277), L. Monchick and L. Hunter, *J. Chem. Phys.*, **85**, 713-718, (1986).

<sup>4</sup>[doi:10.1016/j.jqsrt.2017.08.014](https://doi.org/10.1016/j.jqsrt.2017.08.014), F. Thibault, K. Patkowski, P.S. Żuchowski, H. Józwiak, R. Ciuryło, P. Wcisło, *JQSRT*, **202**, 308-320, (2017).