MODIFIED COMPLEX ROBERT-BONAMY LINE SHAPE CALCULATIONS FOR THE CO_2-H_2O COLLISION SYSTEM

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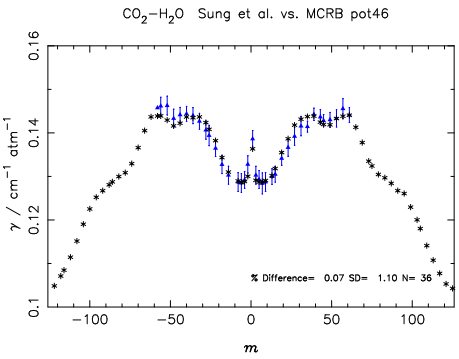
Modified Complex Robert-Bonamy (MCRB) calculations were made for the CO_2-H_2O collision system using an intermolecular potential comprised of quadrupole-dipole, quadrupole-quadrupole, atom-atom component expanded to 20^{th} order and rank 4, induction and London dispersion terms. The intermolecular potential was refined using the measurements of Sung *et al.*[1] for 46 ν_3 transitions up to *J"*=60. The final potential gives results that compare very well with the measurements of Sung *et al.*; average percent difference of 0.07 and a standard deviation of 1.10 percent. See the figure below.

This intermolecular potential was used to make calculations for all transitions in the (00001)-(00011), (00001)-(00001), and (01101)-(00001) bands for *J* up to 120 and a temperature range of 200-3000 K. The temperature dependence of the half-widths and line shifts were determined via the Gamache-Vispoel model[2]. Calculations are being made for other bands with large numbers of ν_1, ν_2, and ν_3 quanta exchanged in order to study the vibrational dependence of the half-widths and line shifts and to develop a prediction routine.[3].



[1] doi:10.1139/P08-130, K. Sung, L.R. Brown, R.A. Toth, T.J. Crawford, *Can. J. Phys.* **87**, 469-484, (2009).

[2] doi:10.1016/j.jqsrt.2018.05.019, R.R. Gamache and B. Vispoel, *J. Quant. Spectrosc. Radiat. Transfer* **217**, 440-452, (2018).

[3] doi:10.1016/j.jqsrt.2013.05.021, R.R. Gamache and J. Lamouroux, *J. Quant. Spectrosc. Radiat. Transfer* **117**, 93-103, (2013).

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