# COLLISIONAL LINE MIXING IN PARALLEL AND PERPENDICULAR BANDS OF LINEAR MOLECULES BY A NON-MARKOVIAN APPROACH

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Reliable modeling of radiative transfer in planetary atmospheres requires accounting for the collisional line mixing effects in the regions of closely spaced vibrotational lines as well as in the spectral wings. Because of too high CPU cost of calculations from ab initio potential energy surfaces (if available), the relaxation matrix describing the influence of collisions is usually built by dynamical scaling laws, such as Energy-Corrected Sudden law. Theoretical approaches currently used for calculation of absorption near the band center are based on the impact approximation (Markovian collisions without memory effects) and wings are modeled via introducing some empirical parameters [1,2]. Operating with the traditional non-symmetric metric in the Liouville space, these approaches need corrections of the ECS-modeled relaxation matrix elements (”relaxation times” and ”renormalization procedure”) in order to ensure the fundamental relations of detailed balance and sum rules.We present an extension to the infrared absorption case of the previously developed [3] for rototranslational Raman scattering spectra of linear molecules non-Markovian approach of ECS-type. Owing to the specific choice of symmetrized metric in the Liouville space, the relaxation matrix is corrected for initial bath-molecule correlations and satisfies non-Markovian sum rules and detailed balance. A few standard ECS parameters determined by fitting to experimental linewidths of the isotropic $Q$-branch enable i) retrieval of these isolated-line parameters for other spectroscopies (IR absorption and anisotropic Raman scattering); ii) reproducing of experimental intensities of these spectra. Besides including vibrational angular momenta in the IR bending shapes, Coriolis effects are also accounted for. The efficiency of the method is demonstrated on OCS-He and $CO_2$-$CO_2$ spectra up to 300 and 60 atm, respectively.

[1] F. Niro, C. Boulet, and J.-M. Hartmann, J. Quant. Spectrosc. Radiat. Transf. 88, 483 (2004).
[2] H. Tran, C. Boulet, S. Stefani, M. Snels, and G. Piccioni, J. Quant. Spectrosc. Radiat. Transf. 112, 925 (2011).
[3] J. Buldyreva and L. Bonamy, Phys. Rev. A 60, 370-376 (1999).