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Energy transfer in gaseous mixtures for atmospheric and astrochemical modelling

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The development of realistic kinetic models of gaseous systems is a fundamental issue in the study of Earth and planetary atmospheres, plasma chemistry, gas flows and astrochemistry. Particularly, the adoption of a state-to-state level of detail in the description of the molecular energy transfer [1,2], a desirable and necessary improvement, requires much insight into the dynamics of the inelastic collisions and the prompt availability of state-specific energy transfer probabilities and rate coefficients. Existing venerable approximated theories of the energy transfer, such as the Schwartz-Slawsky-Herzfeld one, are not really state-specific and have limited validity. Therefore probabilities and cross sections have to be calculated directly by simulation of the dynamics of the molecular collisions. The reliability of the simulations is conditional to the availability of accurate descriptions of the intermolecular interactions occurring between pairs of the molecular species present in the gas mixture. Here, we present examples of calculation of rate coefficients of energy transfer in mixtures containing CO2 and N2 [3-6] obtained applying a semiempirical approach to the interaction modelling, based on (i) a physically meaningful partition of the contribution to the interaction, (ii) the use of data from molecular beam experiments and (iii) ab initio calculations. An extension of such an approach can be also applied to the modelling dynamics and kinetics of gas-surface systems.

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