Quasibound dimers formed in collisions of different molecules: classical trajectory study and spectroscopic manifestations

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Stable bimolecular complexes (tightly bound dimers) in the gas phase are usually formed in the course of third body stabilization of their unstable precursors - quasibound complexes (QC, or collision complexes). The latter can form provided at least one of colliding partners has internal degree of freedom (see, e.g. [1] and references therein). The principal difference is clearly demonstrated between commonly known "orbitings" [2] and QC in the classical non-reactive scattering picture. Hamilton equations, trajectory examples and statistical analysis of QC formation are presented for various molecular pairs (atom–diatom, diatom–diatom, atom–linear molecule, linear molecule–linear molecule, atom–spherical top). Explicit formulae are derived displaying the role of QC in collisional relaxation phenomena and broadening and shifting of spectral lines. Special consideration is given to the general problem of adequate simulation of QC formation at different gas temperatures and pressures. Possible manifestation of non-impact effects in core-region of spectral line shapes due to QC is discussed.

[1] S. V. Ivanov, *Molec. Phys.* **2004**, *102,* 1871.
[2] J. O. Hirschfelder, C. F. Curtiss, R. B. Bird. Molecular Theory of Gases and Liquids. Wiley, **1954**.