

Collision-induced spectra of hydrogen and nitrogen from quantum calculations with an anisotropic potential

Tijs Karman, Gerrit C. Groenenboom, and Ad van der Avoird

Theoretical Chemistry, Institute for Molecules and Materials,

Radboud University Nijmegen, The Netherlands

Apolar molecules such as H₂ and N₂ absorb infrared radiation in the gas and liquid phase, because of the dipole moments induced in the molecules during collisions. The dominant contribution in H₂ and N₂ is the dipole induced by the electric field of the quadrupole moments of their collision partners, but when the molecules approach closely contributions from exchange and higher order electrostatic interactions become important as well. In almost all of the earlier theoretical calculations of collision-induced absorption (CIA) it was assumed that the molecules behave as spherical objects in collisions and the exchange of identical molecules was neglected. Recently, we derived an efficient method for the calculation of CIA spectra from quantum scattering calculations in which the anisotropic interactions and exchange between the colliding molecules are fully taken into account. This method was applied, with the use of *ab initio* calculated intermolecular potential and dipole moment surfaces, to compute the CIA spectra of H₂ and N₂ [1, 2]. Comparison with the results from calculations that include only the isotropic potential, with or without taking into account exchange, shows that the exchange effects are generally small, but that the inclusion of anisotropic interactions is very important at lower collision energies especially for N₂. They have a substantial effect on the CIA spectrum of N₂ over the whole rotation-translation far-infrared region, but yield an important contribution also in the higher-frequency wing of the H₂ spectrum. It is also demonstrated that the isotropic potential approximation works well for the CIA spectra at higher temperatures.

-
- [1] T. Karman, A. van der Avoird, and G. C. Groenenboom, *J. Chem. Phys.* **142**, 084305 (2015).
[2] T. Karman, E. Miliordos, K. L. C. Hunt, G. C. Groenenboom, and A. van der Avoird, *J. Chem. Phys.* **142**, 084306 (2015).