Collision-induced absorption spectra: improved theory applied to H$_2$-H$_2$ and N$_2$-N$_2$

Tijs Karman, Evangelos Miliordos, Katharine L. C. Hunt, Ad van der Avoird, and Gerrit C. Groenenboom

We present a method for including anisotropic interactions in the quantum mechanical calculation of collision-induced absorption spectra.

We apply this method to the H$_2$-H$_2$ and N$_2$-N$_2$ systems,and compare with calculations in the usual isotropic interaction approximation. For H$_2$-H$_2$, the isotropic interaction approximation is generally very accurate, although significant effects of anisotropic interactions are observed in the far wing of the spectrum.

For N$_2$-N$_2$, angular localization of the scattering wave functions due to anisotropic interactions increases the line strength at low energies by two orders of magnitude.

The effect of anisotropy decreases at higher energy, hence the isotropic interaction approximation can be used as a high-temperature approximation for the calculation of collision-induced absorption spectra.