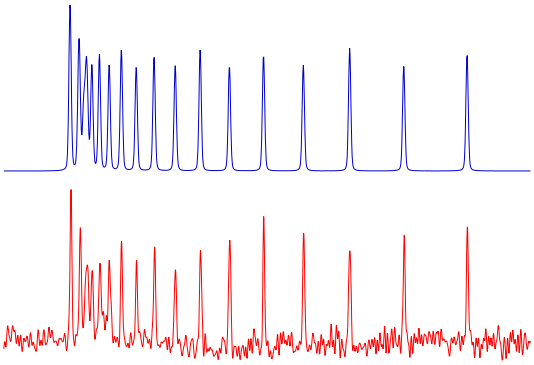
The Twenty-fourth Colloquium on High Resolution Molecular Spectroscopy



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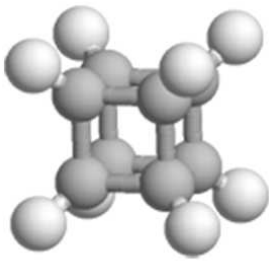

AB INITIO STUDY OF THE CH_4–Ar POTENTIAL AND INDUCED DIPOLE SURFACES: TRUE BOUND DIMER CONTENT AND COLLISION-INDUCED ABSORPTION

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The role played by methane in various industrial, environmental, atmospheric and astrophysical processes is hard to overestimate. Rigorous characterization of pair intermolecular interaction among CH_4 and other species is thus highly demanded from either the theoretical or applicative perspective. Our paper focuses on updating the *ab initio* simulation for the argon–methane potential energy surface (PES), as well as on the first construction of induced dipole surface (IDS) for this system that extends beyond multipolar approximation. Accurate knowledge of both the PES and IDS is required e.g. in order to develop a reliable model for collision-induced absorption (CIA).

First, the PES was generated assuming rigid methane and using CCSD(T) coupled cluster method with aug-cc-pVXZ (X = D, T, Q) basis sets with subsequent extrapolation to the CBS limit. Next, the IDS was calculated with aug-cc-pVTZ basis set augmented with mid-bond wave functions. Both surfaces were then subject to analytical fit in the form of an expansion over spherical harmonics. The quality of the PES was tested through calculation of the mixed second virial coefficient. Classical approach was then used to evaluate equilibrium constant for the formation of true bound CH_4–Ar dimers. Finally, our generated PES and IDS were used to trace temperature variations of the CIA rototranslational band spectral moment. The correspondence of the calculated and measured data is discussed. Estimates relevant to the Titan's atmosphere conditions are given.

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