Real Sociedad Española de Física

ID de la contribución : **69** Tipo : **Oral parallel contribution**

Experimental characterization of the basic intermolecular interaction components

miércoles, 19 de julio de 2017 15:15 (30)

The target of the present work is the detailed characterization of the most relevant components of the intermolecular interaction, which control the molecular dynamics under a variety of conditions. To this purpose, molecular beam experiments have been performed under conditions proper to isolate quantum effects in the single collision events, which probe in detail the projectile-target interaction. Particular attention is addressed to range, strength and anisotropy of non-covalent interaction components, due to the balance of size (or Pauli) repulsion with dispersion and induction attraction, to which must be added electrostatic contributions, and of other components of covalent (chemical) nature, mostly affected by charge (electron) transfer effects. The analysis of several experimental findings has been important to develop suitable analytical representations of the potential energy surfaces (PESs), tested and improved by exploiting also the comparison with results of ab initio calculations, useful to provide an internally consistent description of the intermolecular interaction both in the most and less stable configurations of the interacting system. The proper formulation of the PESs is crucial not only to describe the dynamics of elementary processes occurring in interstellar medium and in planetary atmospheres, but also to control equilibrium a non-equilibrium phenomena of applied interest, as those occurring in combustion, flames and plasmas.

Acknowledgment

The financial support of this research is from the “Fondazione Cassa di Risparmio di Perugia” (Contract No. 2015.0331.021) and from the “Dipartimento di Chimica, Biologia e Biotecnologie, Università di Perugia”

Primary author(s) : Prof. PIRANI, Fernando (Dipartimento di Chimica, Biologia e Biotecnologie, Università di Perugia)

Presenter(s) : Prof. PIRANI, Fernando (Dipartimento di Chimica, Biologia e Biotecnologie, Università di Perugia)

Clasificación de la sesión : Molecular Physics at the Edge II

Clasificación de temáticas : Molecular Physics at the Edge