Catching the role of chemical interactions in neutral complexes of helium and neon by molecular beam experiments and charge displacement calculations

David Cappelletti*[1], Alessio Bartocci[1], Felice Grandinetti[2], Stefano Falcinelli[3], Leonardo Belpassi[4], Francesco Tarantelli[1,4] and Fernando Pirani[1]

[1]*Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, via Elce di Sotto 8, 06123 Perugia, Italy*
[2]*Dipartimento per la Innovazione nei sistemi Biologici, Agroalimentari e Forestali (DIBAF), Università della Tuscia, 01100 Viterbo, Italy*
[3]*Dipartimento di Ingegneria Civile ed Ambientale, Università degli Studi di Perugia, 06125 Perugia, Italy*
[4]*Istituto di Tecnologie e Scienze Molecolari del CNR, via Elce di Sotto 8, 06123 Perugia Italy*

*(presenting author) david.cappelletti@unipg.it;

The complexes of helium and neon with gaseous neutral molecules are generally perceived as van der Waals adducts, held together by physical (non covalent) forces, due to the combination of size (exchange) repulsion with dispersion/induction attraction. The molecular beam experiments discussed at the workshop confirmed that this is the case for He-, Ne-CF_4 adducts, but revealed that the interaction of He and Ne with CCl_4 features an appreciable contribution of chemical components, arising from the anisotropy of the electron density of CCl_4 that enhances a charge transfer from Ng (Ng = He, Ne). These findings furnish a novel assay of the bonding capabilities of helium and neon, and invite to revisit the neutral complexes of these elements as systems of chemical relevance. The CCl_4-Ng are also peculiar examples of halogen bonds, a group of interactions of major current concern. Finally, our investigation preludes to the development of semi-empirical models for force fields aimed to the unified description of static and dynamical properties of systems of comparable or higher complexity.

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