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

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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–CF₄ adducts, but revealed that the interaction of He and Ne with CCl₄ features an appreciable contribution of chemical components, arising from the anisotropy of the electron density of CCl₄ 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 CCl₄–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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