Inter-ionic hydrogen bonds and challenging dimers

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ABSTRACT

In this contribution, we describe metastable multiply charged dimers bound by hydrogen bonds containing substituted metallocenes (metals Ru, Co, Rh, Mn) and deepen in the physical grounds that allow the existence of these species [1]. The analysis includes the structures, binding energies, and dissociation profiles, together with the study of the symmetric proton transfer that can occur in the metastable phase. The choice of DFT methodology was benchmarked against high-level ab initio methods. This work is also useful to think about the true nature of the inter-ionic hydrogen bonds (IAHBs) like the ones present in the abovementioned charged dimers. IAHBs are, as any other hydrogen bond between neutral species, mostly due to electrostatic and polarization forces [2]. These complexes are a new proof of this latter statement and the starting point of a small and recent review explaining why the use of misleading nomenclatures such as “anti-electrostatic” hydrogen bonds should be avoided to describe this kind of interactions. Naming this kind of HBs might seem only a semantic question, but it is indisputable that scientific concepts can be misinterpreted if the vocabulary does not rigorously adjust to the essence of what they are intended to describe.

References

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[2] Martín-Fernández, C.; Montero-Campillo, M. M.; Alkorta, I. Hydrogen bonds are never of “anti-electrostatic” nature: a brief tour by a misleading nomenclature. *The Journal of Physical Chemistry Letters* **2024,** *15 (15),* 4105–4110.