

Can a base be turned into a super-acid? The magical effect of non-covalent interactions and other niceties

Prof. Otilia M^o

^aDepartamento de Química, Facultad de Ciencias, Módulo 13, and Institute of Advanced Chemical Sciences (IadChem), Universidad Autónoma de Madrid. Campus de Excelencia UAM-CSIC, Cantoblanco, 28049-Madrid. Spain.

X₂M alkaline earth derivatives (M = Be, Mg) yield very stable complexes when interacting with conventional Lewis bases [1], due to their electron-deficient nature. Nothing surprising in this statement; but what is really interesting is that these interactions trigger changes in the electronic density in the two interacting systems, which are reflected in **dramatic** variations in their intrinsic reactivity, in particular in the reactivity of the Lewis base, to the point that conventional bases become extra strong acids [2]. In a similar way they reinforce other non-covalent interactions [3,4], or favor the appearance of sigma holes [5]; but what is certainly more striking is that the interactions of bases with alkaline-earth derivatives can lead to the exergonic and barrierless formation of radicals [6] (see Figure 1).

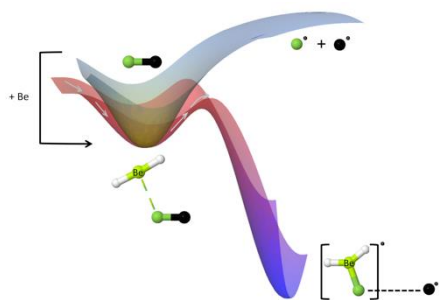


Figure 1. Potential energy curves associated with the dissociation of the FCl molecule and the dissociation of the F-Cl bond in the ClF: BeH₂ complex.

The electron-deficient nature of these derivatives is also behind the enormous electron and anionic affinity of some Be-containing derivatives, such as 1,8-diBeX-naphthalene compounds[7] through the formation of one-electro two centers and three centers bonds.

- [1] M. Yáñez, P. Sanz, O. M^o, I. Alkorta, J. Elguero, J. Chem. Theor. Comput. 2009, 5, 2763.
- [2] M. Yáñez, O. M^o, I. Alkorta, J. Elguero, Chem. Eur. J. 2013, 35, 11637.
- [3] O. M^o, M. Yáñez, I. Alkorta, J. Elguero, J. Chem. Theory Comput. 2012,8, 2293.
- [4] L. Albrecht, R.J. Boyd, O. M^o, M. Yáñez, Phys. Chem. Chem. Phys. 2012, 14, 14540.
- [5] O. Brea, O. M^o, M. Yáñez, I. Alkorta, J. Elguero, Chem. Eur. J, 21, 2015, 12676.
- [6] O. Brea, I. Alkorta, O. M^o, M. Yáñez, J. Elguero, I. Corral, Angew. Chem. Eng. Int. Ed. 2016, 55, 8736.
- [7] O. Brea, I. Corral, O. M^o, M. Yáñez, I. Alkorta, J. Elguero, Chem. Eur. J. 2016, 22, 18322.