

# Alkaline-earth (Be, Mg, Ca) bonds at the origin of huge acidity enhancements

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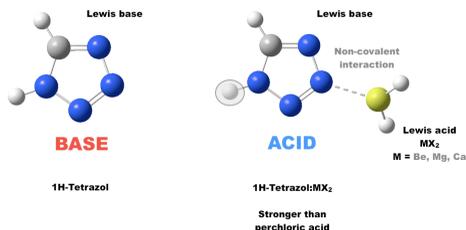
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## Abstract

The interaction between alkaline-earth derivatives of general formula  $X_2M$  ( $X = H, F, Cl$ ;  $M = Be, Mg, Ca$ ) and a set of Lewis bases including first and second-row hydrides, namely  $YH_n$  ( $Y = O, N, F, S, P, Cl$ ) hydrides, as well as other typical cyclic organic bases such as aniline, 1H-1,2,3-triazole, 1H-tetrazole and phenylphosphine, was investigated at the G4 *ab initio* composite method. Contrary to what might be expected, it was found that the interactions involving Mg and Ca derivatives are not necessarily weaker than those with beryllium bonds. The origin is two-folded, the larger deformation of the interacting systems when Be-derivatives are involved, and the appearance of secondary non-covalent interactions in the formation of some of the Mg and Ca-containing complexes. Hence, the dissociation of the latter complexes may require higher enthalpies than the Be ones.



**Figure 1.** Upon association with  $MX_2$  ( $M = Be, Mg, Ca$ ) alkaline-earth derivatives conventional bases become very strong acids.

These deformations are triggered by a significant redistribution of the electron density of the two interacting moieties, which also result in dramatic changes of the reactivity of the interacting compounds and in particular on the intrinsic basicity of the Lewis bases investigated, to the point that conventional bases such as ammonia or aniline, upon complexation with  $MCl_2$  ( $M = Be, Mg, Ca$ ), become stronger Brønsted acids than phosphoric acid, whereas other bases such as 1H-tetrazole become stronger acids than perchloric acid