Enhanced Acidity of cyclopenta-2,4-dienylborane and its Al and Ga analogues. The role of aromatization

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Supplementary Information

(total 2 pages)

Table S1. Total energies (in hartrees) and relative stability in terms of Gibbs free energies (ΔG in kJ mol^{-1}) of the anionic species produced by the C1 and Hcis deprotonation of cyclopenta-2,4-dienylgallium dihydride

method	C1	Hcis	ΔG
B3LYP/6-311+G(d,p)	-2119.05716	-2119.05804	3.5
B3LYP/6-311++G(3df,2p)//B3LYP/6-311+G(d,p)	-2119.07255	-2119.07344	3.7
B3LYP/6-311++G(3df,2p)	-2119.07262	-2119.07344	3.9
B3LYP/6-311++G(3df,2p)//CCSD/6-311+G(d,p)	-2119.07179	-2119.07094	8.0
CCSD/6-311+G(d,p)	-2116.86270	-2116.86370	3,1
CCSD(T)/6-311+G(d,p)// CCSD/6-311+G(d,p)	-2116.90384	-2116.90465	3.6

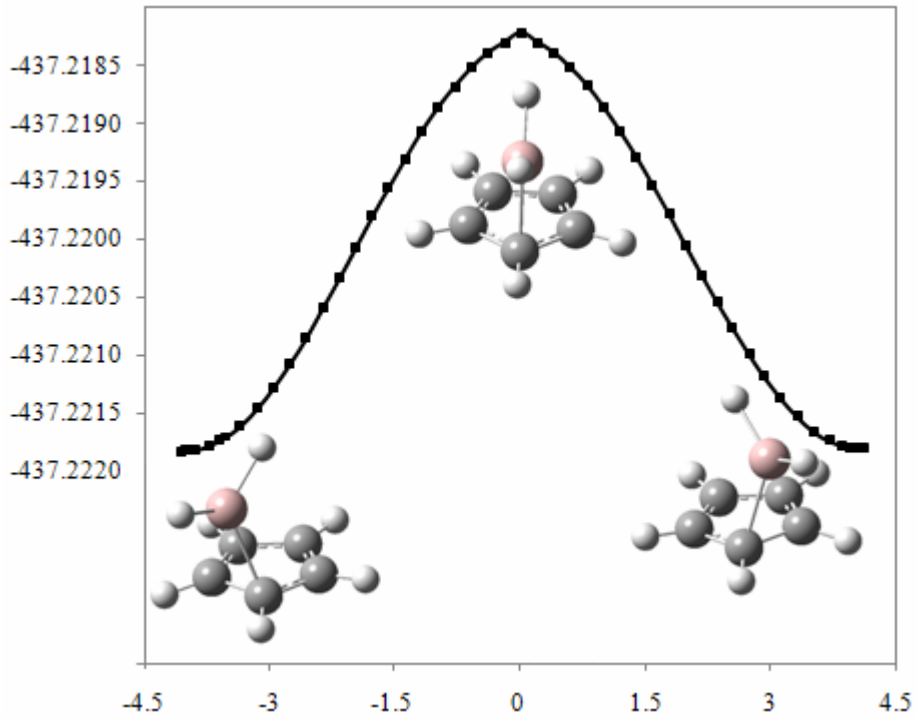

Figure S1. Potential energy curve of the sigmatropic rearrangement of AlH_2-cyclopentane derivative associated with the migration of the AlH_2 around the ciclopentadienyl ring.