Cationic beryllium-group 13 heterobimetallic dimetallocenes with donor-acceptor bond

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Supplementary Information

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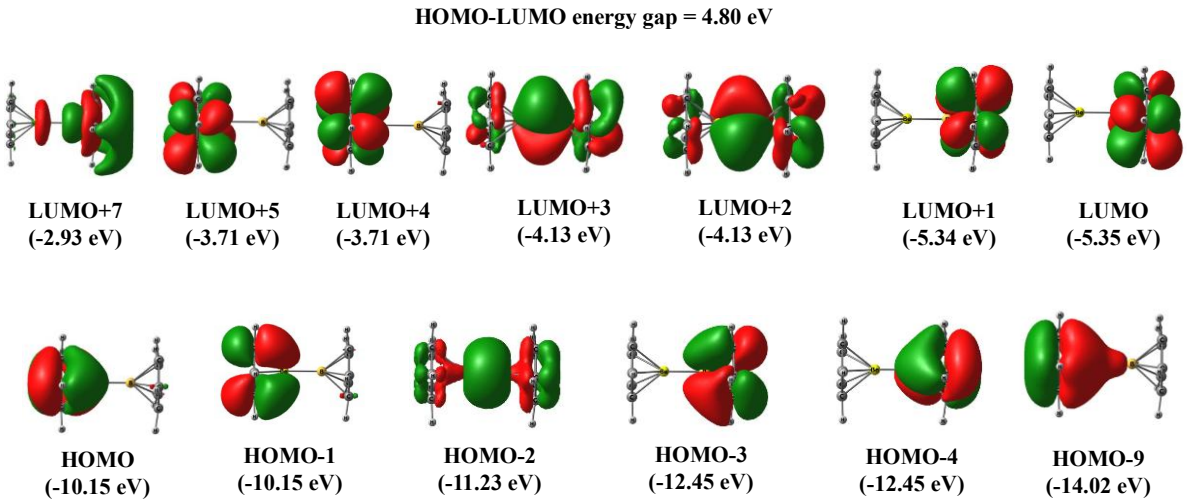

Figure S1. Molecular orbitals of [Cp-Be-B-Cp]$^+$ at BP86/def2-TZVP level of theory; eigen values are given in eV in parentheses; isosurface value = 0.03.

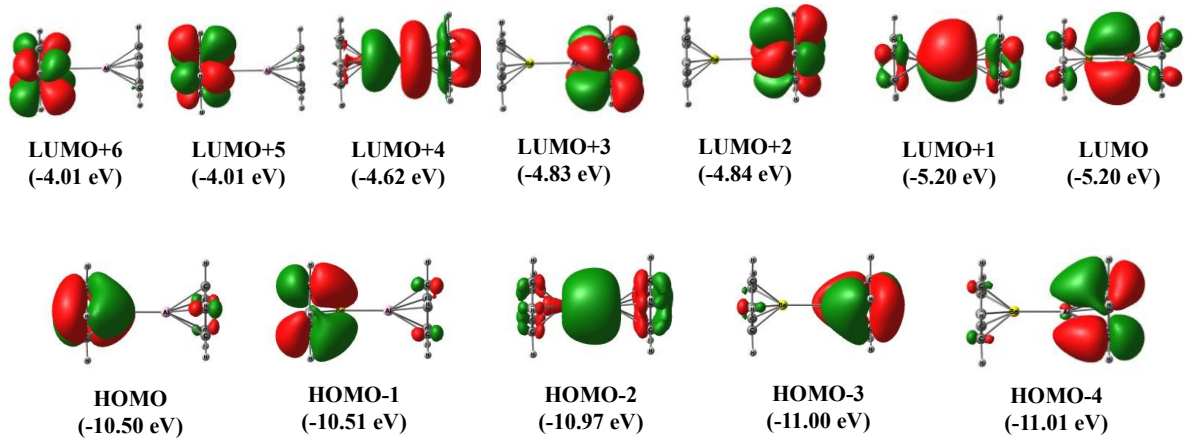

Figure S2. Molecular orbitals of [Cp-Be-Al-Cp]$^+$ at BP86/def2-TZVP level of theory; eigen values are given in eV in parentheses; isosurface value = 0.03.

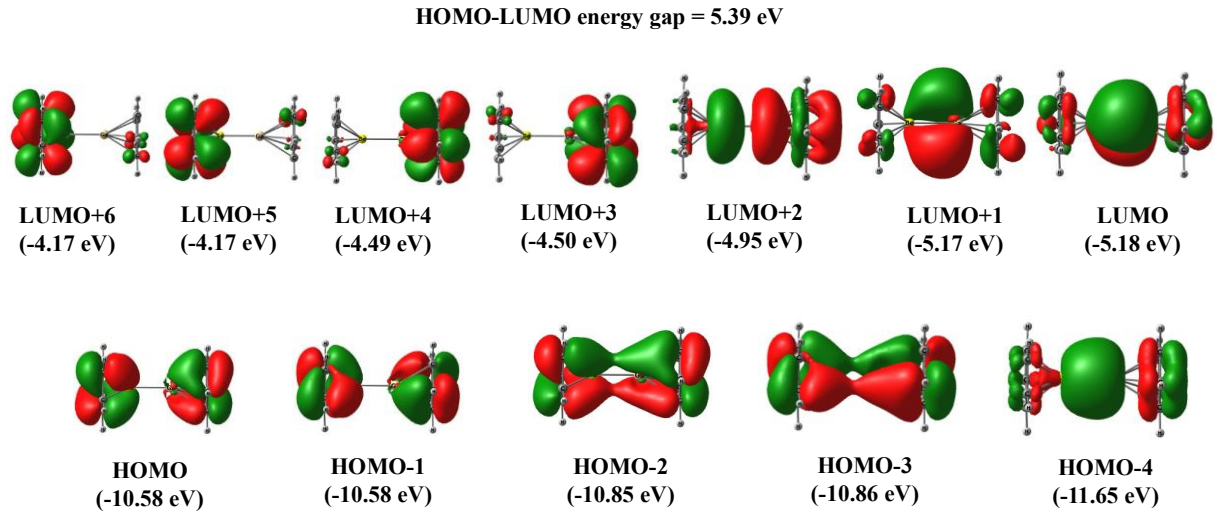

Figure S3. Molecular orbitals of [Cp-Be-Ga-Cp]$^+$ at BP86/def2-TZVP level of theory; eigen values are given in eV in parentheses; isosurface value = 0.03.

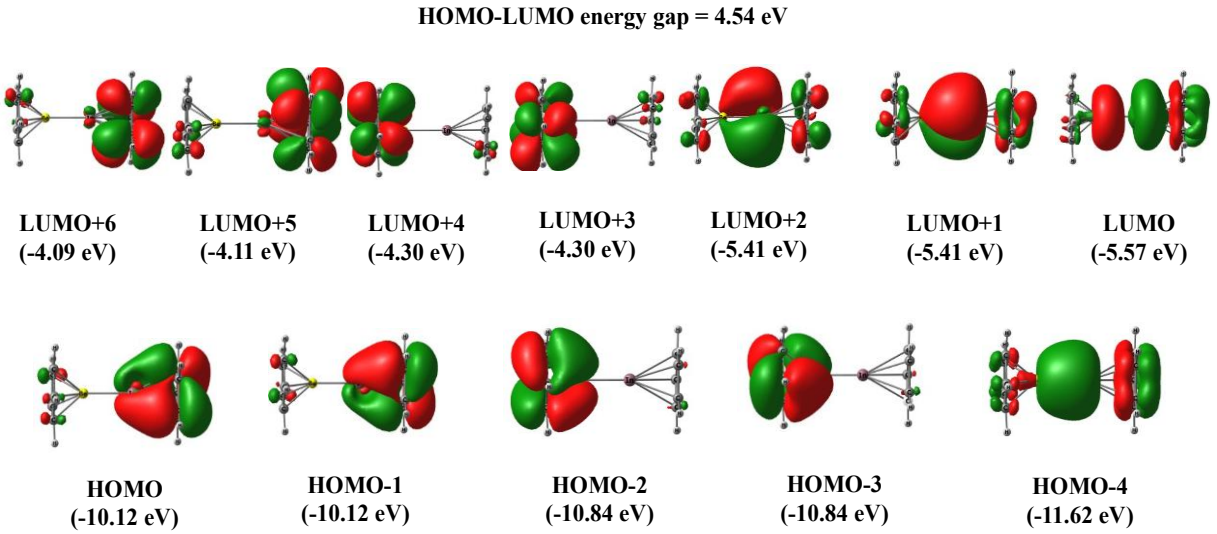

Figure S4. Molecular orbitals of [Cp-Be-In-Cp]$^+$ at BP86/def2-TZVP level of theory; eigen values are given in eV in parentheses; isosurface value = 0.03.

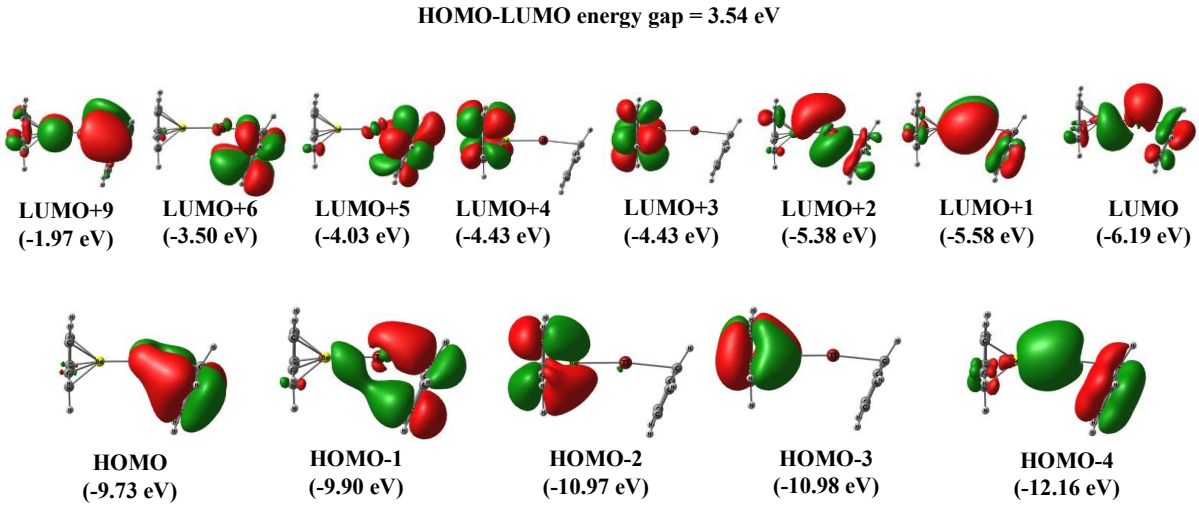

Figure S5. Molecular orbitals of [Cp-Be-Tl-Cp]$^{+}$ at BP86/def2-TZVP level of theory; eigen values are given in eV in parentheses; isosurface value = 0.03.

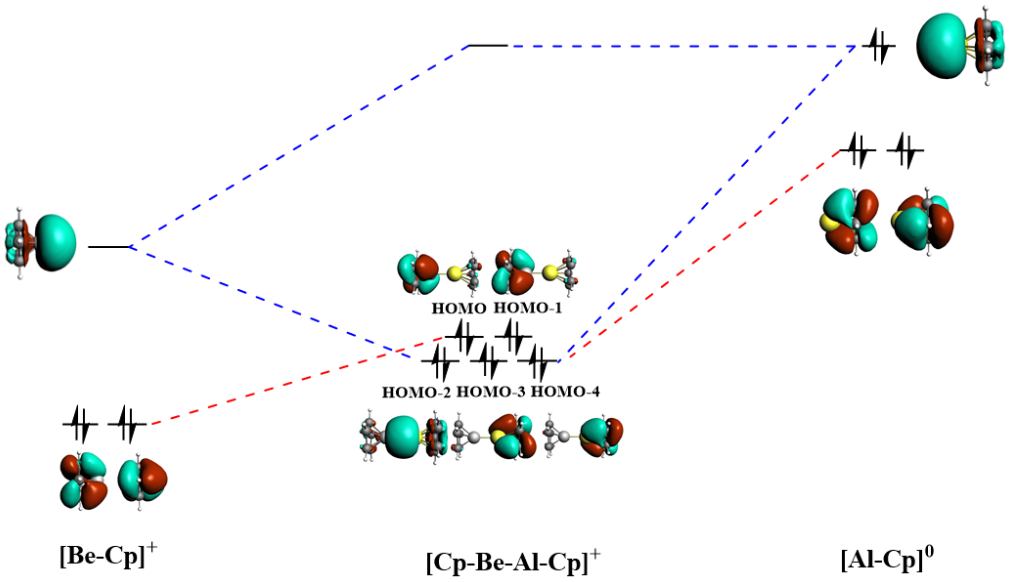

Figure S6. Orbital interaction diagrams of [Cp-Be-Al-Cp]$^{+}$ dimetallocene showing frontier valence MOs.

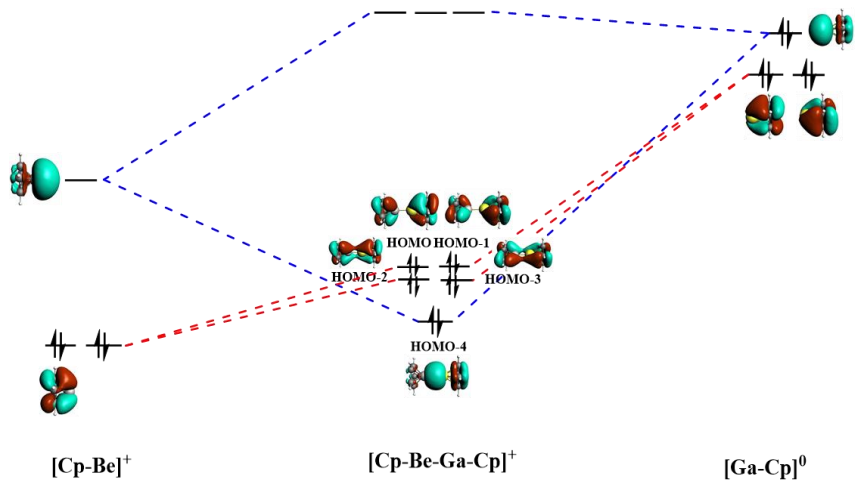

Figure S7. Orbital interaction diagrams of $[Cp\text{-}Be\text{-}Ga\text{-}Cp]^+$ dimetallocene showing frontier valence MOs.

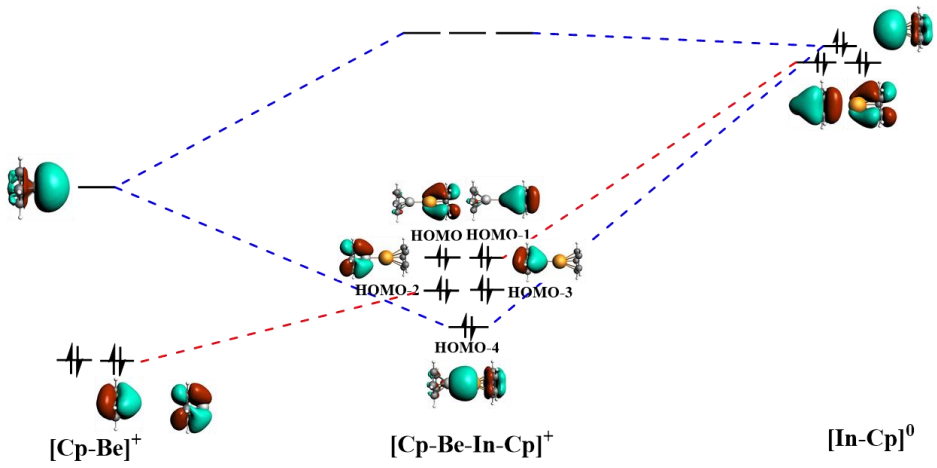

Figure S8. Orbital interaction diagrams of $[Cp\text{-}Be\text{-}In\text{-}Cp]^+$ dimetallocene showing frontier valence MOs.

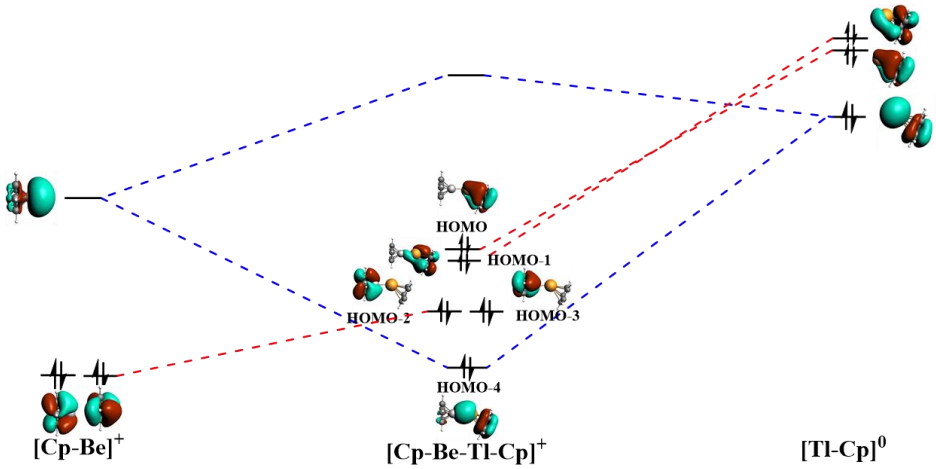

Figure S9. Orbital interaction diagrams of [Cp-Be-Tl-Cp]$^+$ dimetallocene showing frontier valence MOs.

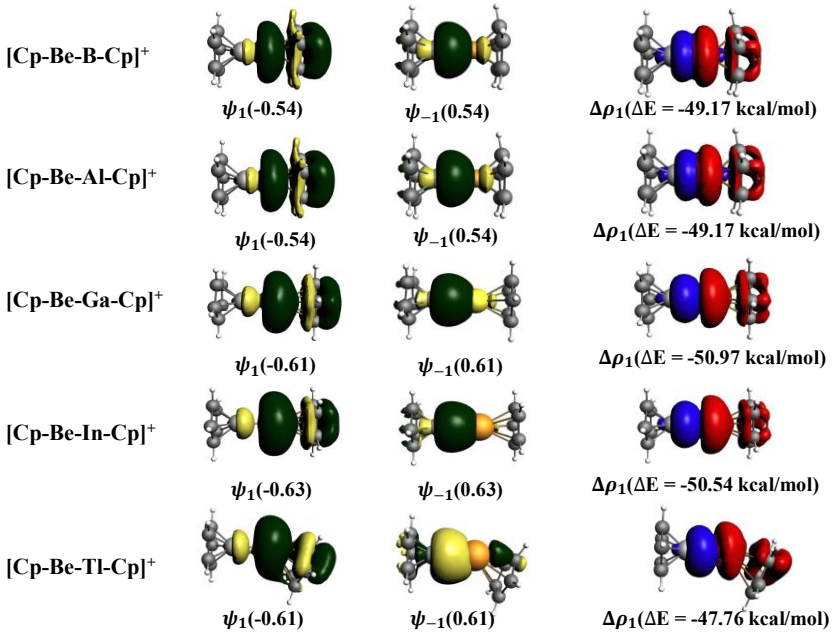

Figure S10. Plots of important NOCV pair of orbitals ψ_n/ψ_{-n} of bonding possibility A in [Cp-Be-M-Cp]$^+$ (M- B, Al, Ga, In and Tl) with their eigen values in parenthesis, the associated deformation densities $\Delta\rho_n$, and the corresponding orbital stabilization energies ΔE(kcal mol^{-1}) at the BP86/TZ2P level of theory. The direction of the charge flow in the deformation density plot is from red → blue. The isosurface values for NOCV orbitals and deformation densities are 0.03 and 0.001, respectively.

Be-M	Occupancy	Contribution from Be		Contribution from M	
		s- orbital contribution	p- orbital contribution	s- orbital contribution	p- orbital contribution
Be-B	1.99	94.20%	5.79%	5.79%	44.07%
Be-Al	1.99	91.64%	8.14%	8.14%	24.45%
Be-Ga	2.00	90.37%	9.54%	9.54%	16.25%
Be-In	2.00	90.51%	9.21%	9.21%	15.12%
Be-Tl **(LP)**	1.72	94.24%	5.63%	5.63%	-

Table S1.Bond orbital occupancy (BO) from the NBO analysis of $[Cp\text{-}Be\text{-}M\text{-}Cp]^+$ at M06/def2-TZVPP//BP86/def2-TZVP level of theory.

Be-M	Occupancy	Contribution from Be		Contribution from M		Relative Contribution (Be:M)
		s- orbital contribution	p- orbital contribution	s- orbital contribution	p- orbital contribution	
Be-B	1.99	94.20%	5.79%	5.79%	44.07%	15.3 : 84.6
Be-Al	1.99	91.64%	8.14%	8.14%	24.45%	25.8 : 74.1
Be-Ga	2.00	90.37%	9.54%	9.54%	16.25%	20.8 : 79.1
Be-In	2.00	90.51%	9.21%	9.21%	15.12%	19.9 : 80.0
Be-Tl		-	-	-	-	-