

Supplementary information

A New Kind of Sandwich-Electride Complexes of Cyclooctatetraene Ligand $M^1_2(\eta^8-C_8H_8)_2M^2_2$ ($M^1 = Na, K$ and $M^2 = Ca, Mg$): A Theoretical Study

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Table S1 WBI index of the reported complex

Molecule	WBI index	
	C-M ¹	C-M ²
Na ₂ (C ₈ H ₈) ₂ Mg ₂	0.01	0.03
Na ₂ (C ₈ H ₈) ₂ Ca ₂	0.01	0.03
K ₂ (C ₈ H ₈) ₂ Mg ₂	0.01	0.03
K ₂ (C ₈ H ₈) ₂ Ca ₂	0.01	0.03

Table S2 Atomic and orbital contribution towards the M²-M² bond

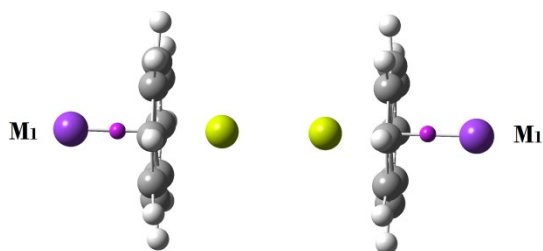
Molecule	Atomic (percentage) contribution of M ² to M ² -M ² bond	Orbital (percentage) contribution of M ² to M ² -M ² bond
Na ₂ (C ₈ H ₈) ₂ Mg ₂	Mg(50%)-Mg(50%)	Mg : s(74.26%)p 0.34(25.39%)
		Mg : s(74.34%)p 0.34(25.31%)
Na ₂ (C ₈ H ₈) ₂ Ca ₂	Ca(50%)-Ca(50%)	Ca: s(72.76%)p 0.37(26.60%)
		Ca: s(72.76%)p 0.37(26.60%)
K ₂ (C ₈ H ₈) ₂ Mg ₂	Mg(50%)-Mg(50%)	Mg: s(73.63%)p 0.35(26.05%)
		Mg: s(73.67%)p 0.35(26.00%)
K ₂ (C ₈ H ₈) ₂ Ca ₂	Ca(50%)-Ca(50%)	Ca: s(72.16%)p 0.38(27.19%)
		Ca: s(72.15%)p 0.38(27.19%)

Table S3. ELF values of population of the reported electrone systems

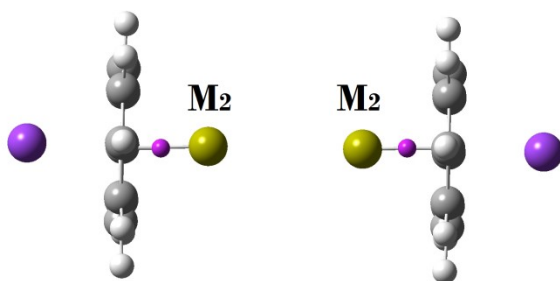
Electrone System reported	N(pop)
Be ₂ (η ⁵ -C ₅ H ₅) ₂	2.15
Mg ₂ (η ⁵ -C ₅ H ₅) ₂	1.91

Table S4 Comparison of the γ_{avg} (au) of the reported system with our studied system.

Electride System reported	γ_{avg}	Studied system	γ_{avg}
$\text{Be}_2(\eta^5\text{-C}_5\text{H}_5)_2$	6.3×10^4	$\text{Na}_2(\text{C}_8\text{H}_8)_2\text{Mg}_2$	2.56×10^5
$\text{Mg}_2(\eta^5\text{-C}_5\text{H}_5)_2$	1.1×10^5	$\text{Na}_2(\text{C}_8\text{H}_8)_2\text{Ca}_2$	1.44×10^6
		$\text{K}_2(\text{C}_8\text{H}_8)_2\text{Mg}_2$	2.61×10^5
		$\text{K}_2(\text{C}_8\text{H}_8)_2\text{Ca}_2$	1.39×10^6

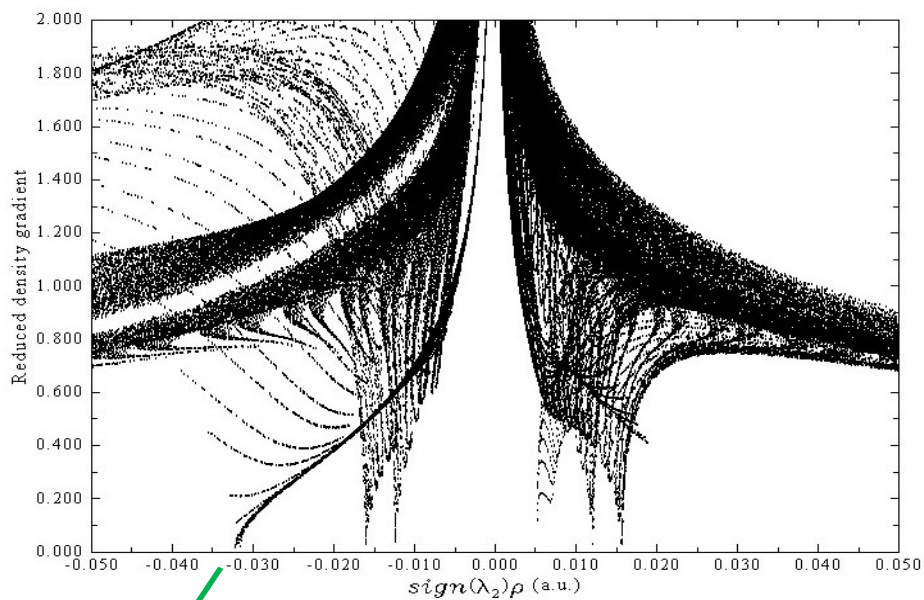


Ghost atom placed 1\AA towards M^1

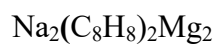


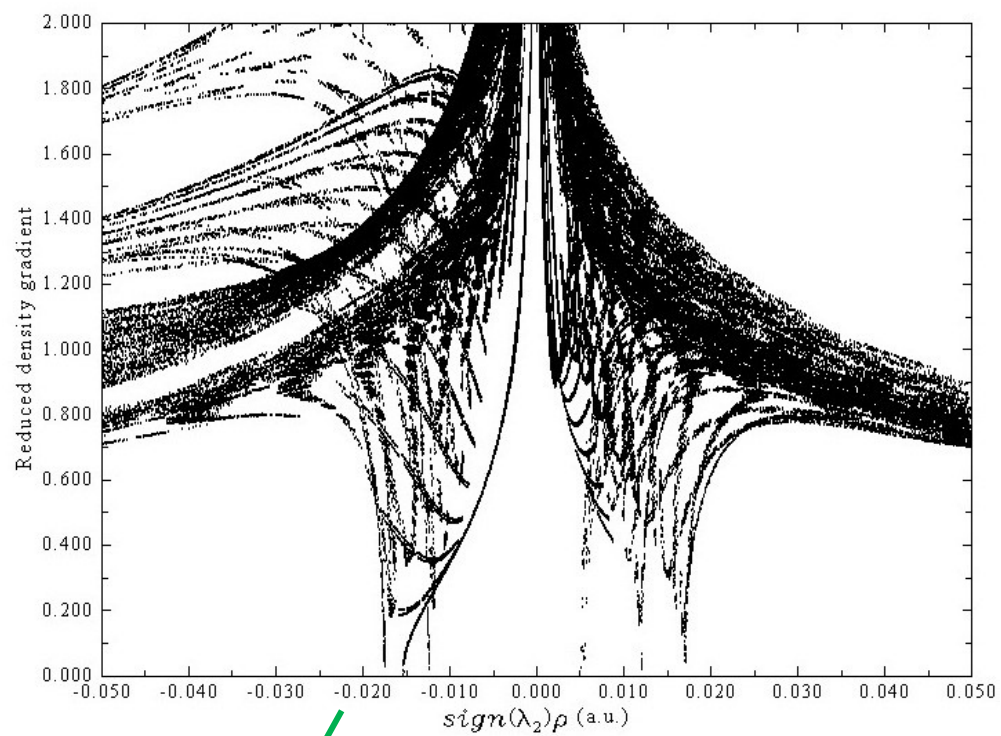
Ghost atom placed 1 Å towards M^2

Fig . S1 Placement of the ghost atom 1 Å away from the ring.

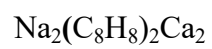


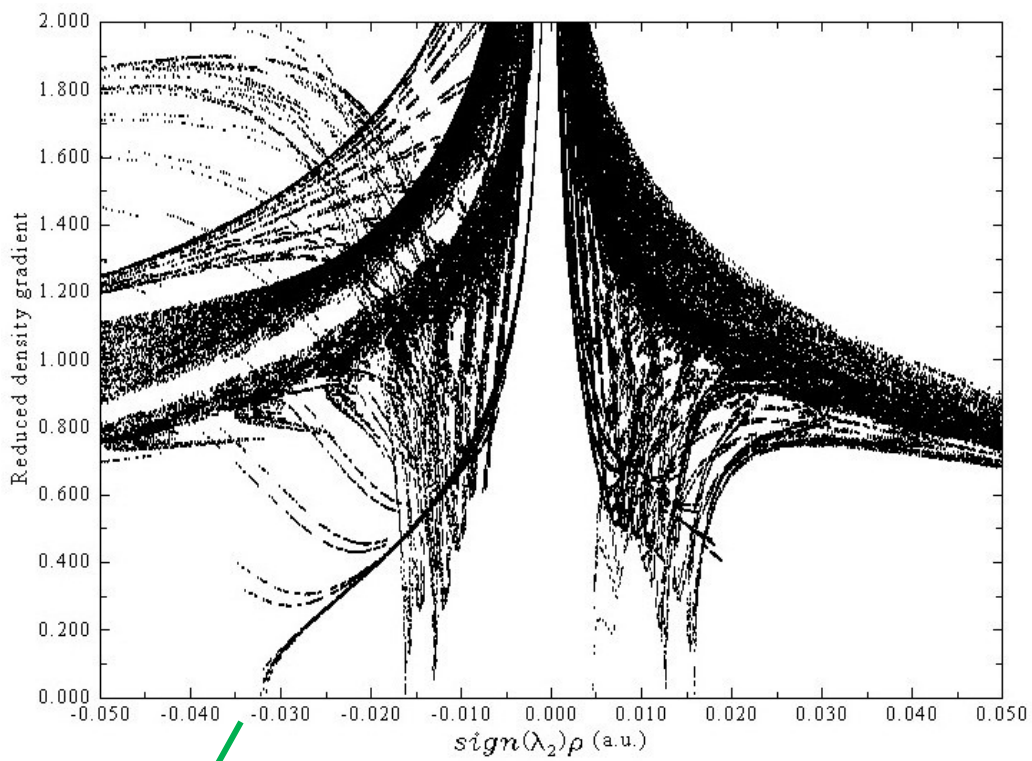
Bonding interaction



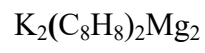


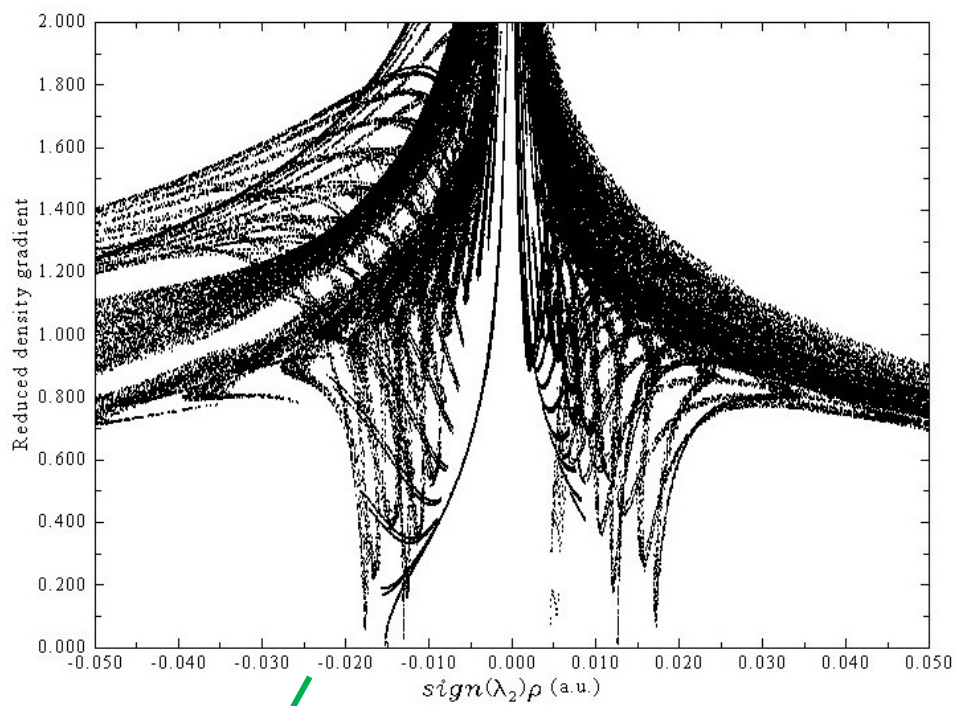
Bonding interaction





Bonding interaction





Bonding interaction

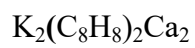


Fig .S2 .NCI plot (Reduced density gradient) versus second eigen value of the electron-density Hessian (λ_2) ρ)