

# Supplementary Material

## Searching for Systems with Planar Hexacoordinate Carbons

**Diego Inostroza<sup>1,2</sup>, Luis Leyva-Parra<sup>1,2</sup>, Osvaldo Yañez<sup>3,\*</sup>, José Solar-Encinas<sup>1,2</sup>, Alejandro Vásquez-Espinal<sup>4</sup>, Maria Luisa Valenzuela<sup>5</sup> and William Tiznado<sup>1,\*</sup>**

<sup>1</sup> Computational and Theoretical Chemistry Group, Departamento de Ciencias Química, Facultad de Ciencias Exactas, Universidad Andrés Bello, República 275, Santiago, Chile; wtiznado@unab.cl ; leyvaluis177@gmail.com ; dinostro92@gmail.com ; j.solarencinas@uandresbello.edu

<sup>2</sup> Programa de Doctorado en Fisicoquímica Molecular, Facultad de Ciencias Exactas, Universidad Andrés Bello, Av. República 275, Santiago 8370146; l.leyvaparra@uandresbello.edu ; dinostro92@gmail.com ; j.solarencinas@uandresbello.edu

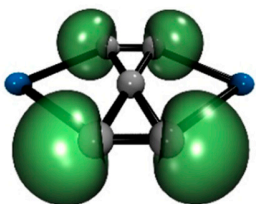
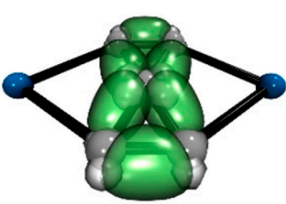
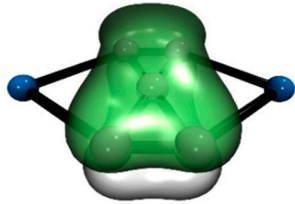
<sup>3</sup> Núcleo de Investigación en Data Science, Facultad de Ingeniería y Negocios, Universidad de las Américas, Santiago 7500000, Chile; oyanez@udla.cl

<sup>4</sup> Química y Farmacia, Facultad de Ciencias de la Salud, Universidad Arturo Prat, Casilla 121, Iquique 1100000, Chile; alvasquez@unap.cl


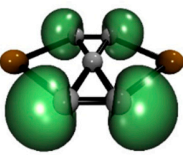
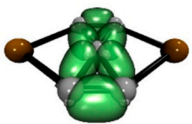

<sup>5</sup> Grupo de Investigación en Energía y Procesos Sustentables, Instituto de Ciencias Químicas Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile, Av. El Llano Subercaseaux 2801, Santiago 8900000, Chile; maria.valenzuela@uautonoma.cl

\* Correspondence: wtiznado@unab.cl ; oyanez@udla.cl; Tel.: (optional; include country code; if there are multiple corresponding authors, add author initials)

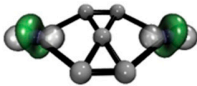
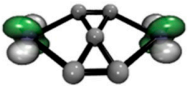
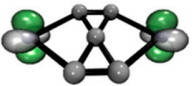
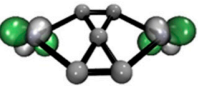
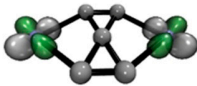
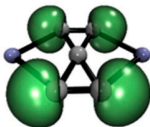
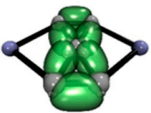
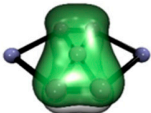
**Figure S1.** Adaptive Natural Density Partitioning bonding pattern of the  $M_2C_5^{2+}$  ( $M = \text{Be}, \text{Ca}, \text{Mg}$ ) at the  $\omega\text{b97XD/Def2-TZVP}$  level.

	E-LPs	E-E $\sigma$ -bonds	E-E $\pi$ -bond
			
	4 x 1c-2e	6 x 2c-2e	1 x 5c-2e
<b>E = C, M = Be</b>	ON = 1.80  e	ON = 1.97 – 1.78  e	ON = 1.99  e
<b>E = C, M = Mg</b>	ON = 1.85  e	ON = 1.97 – 1.78  e	ON = 1.99  e
<b>E = C, M = Ca</b>	ON = 1.88  e	ON = 1.96 – 1.77  e	ON = 1.99  e

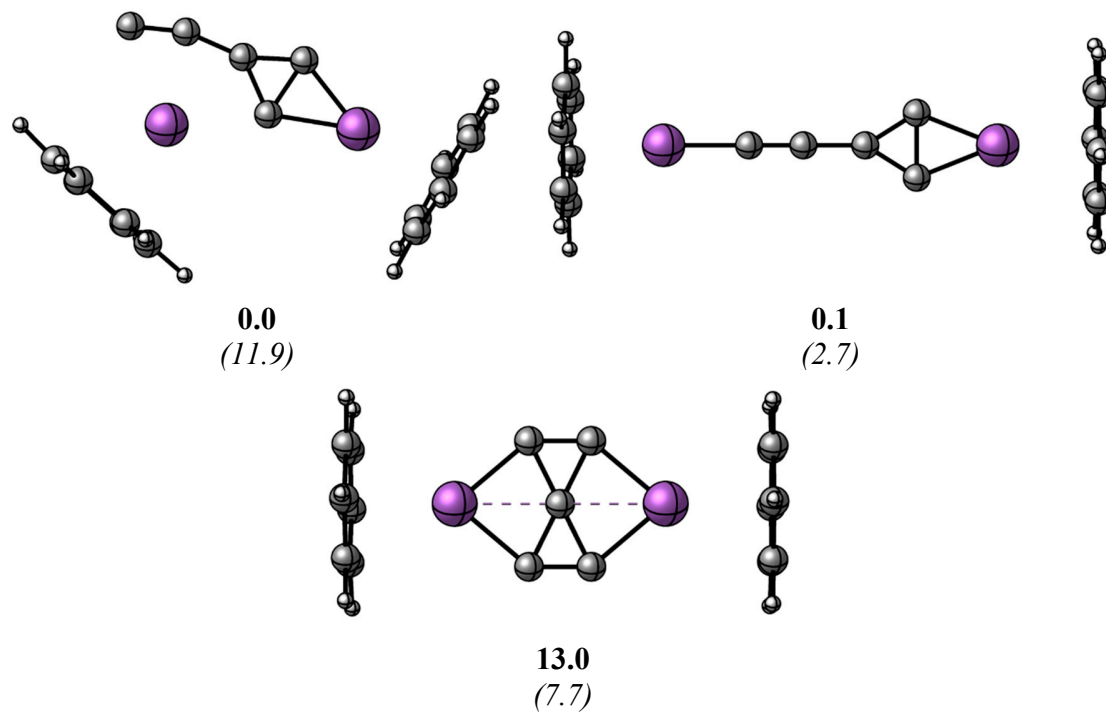
**Figure S2.** Adaptive Natural Density Partitioning bonding pattern of the  $M_2C_5$  ( $M = \text{Al}, \text{Ga}, \text{In}$ ) at the  $\omega\text{b97XD/Def2-TZVP}$  level.

	M-LPs	E-LPs	E-E $\sigma$ -bonds	E-E $\pi$ -bond
				
	2 x 1c-2e	4 x 1c-2e	6 x 2c-2e	1 x 5c-2e
<b>E = C, M = Al</b>	ON = 1.97  e	ON = 1.81  e	ON = 1.97 – 1.78  e	ON = 1.99  e
<b>E = C, M = Ga</b>	ON = 1.97  e	ON = 1.81  e	ON = 1.96 – 1.78  e	ON = 1.99  e
<b>E = C, M = In</b>	ON = 1.98  e	ON = 1.82  e	ON = 1.96 – 1.78  e	ON = 1.99  e

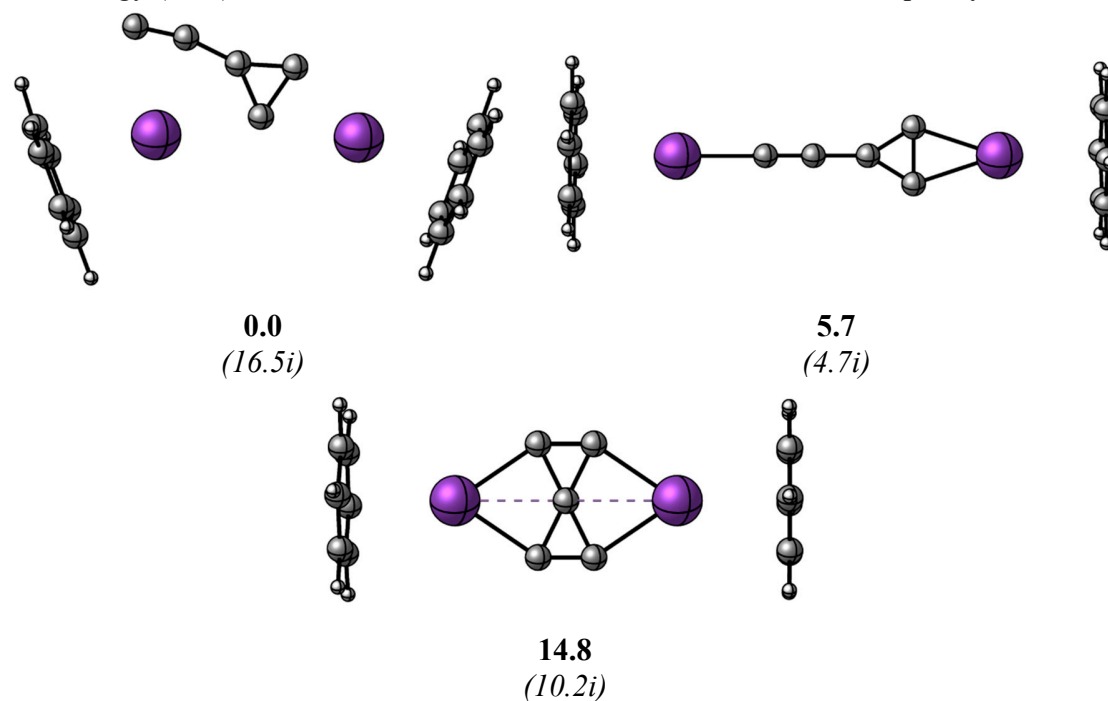
**Figure S3.** Adaptive Natural Density Partitioning bonding pattern of the  $\text{Zn}_2\text{C}_5^{2+}$  at the  $\omega\text{b97XD/Def2-TZVP}$  level.

Zn-LPs				
$\text{C}_5\text{Zn}_2^{2+}$				
	2 x 1c-2e	2 x 1c-2e	2 x 1c-2e	2 x 1c-2e
	ON = 1.99  e	ON = 1.99  e	ON = 1.99  e	ON = 1.99  e
$\text{C}_5\text{Zn}_2^{2+}$				
	2 x 1c-2e	4 x 1c-2e	6 x 2c-2e	1 x 5c-2e
	ON = 1.99  e	ON = 1.74  e	ON = 1.97 – 1.77  e	ON = 1.99  e

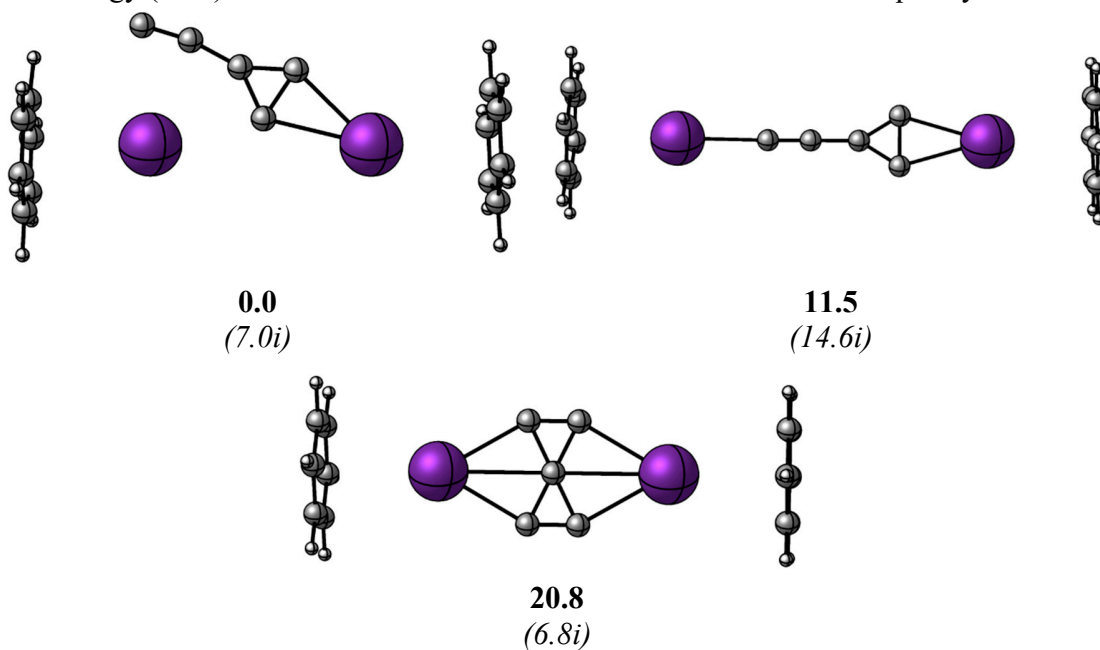
**Figure S4.** Putative global minimum and low-lying isomers of complex  $(\text{C}_6\text{H}_6)_2\text{-Li}_2\text{C}_5$ . Relative energies are shown at the  $\text{kcal}\cdot\text{mol}^{-1}$  at  $\omega\text{b97XD/def2-TZVP}$  level, including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in  $\text{cm}^{-1}$ .



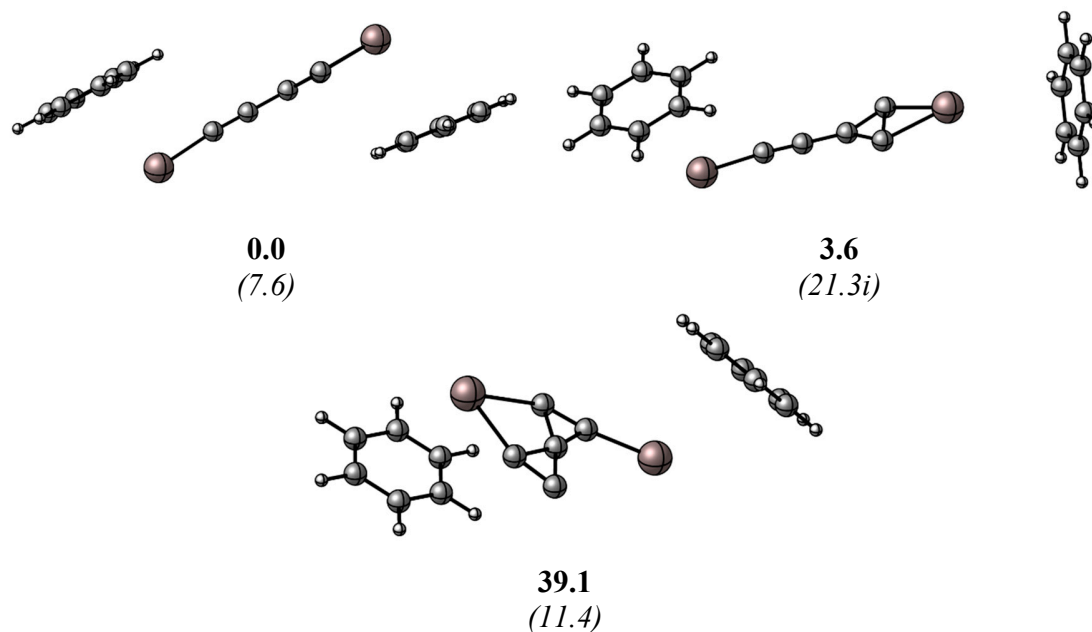
**Figure S5.** Putative global minimum and low-lying isomers of complex  $(\text{C}_6\text{H}_6)_2\text{-Na}_2\text{C}_5$ . Relative energies are shown in  $\text{kcal}\cdot\text{mol}^{-1}$  at the  $\omega\text{b97XD/def2-TZVP}$  level, including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in  $\text{cm}^{-1}$ .



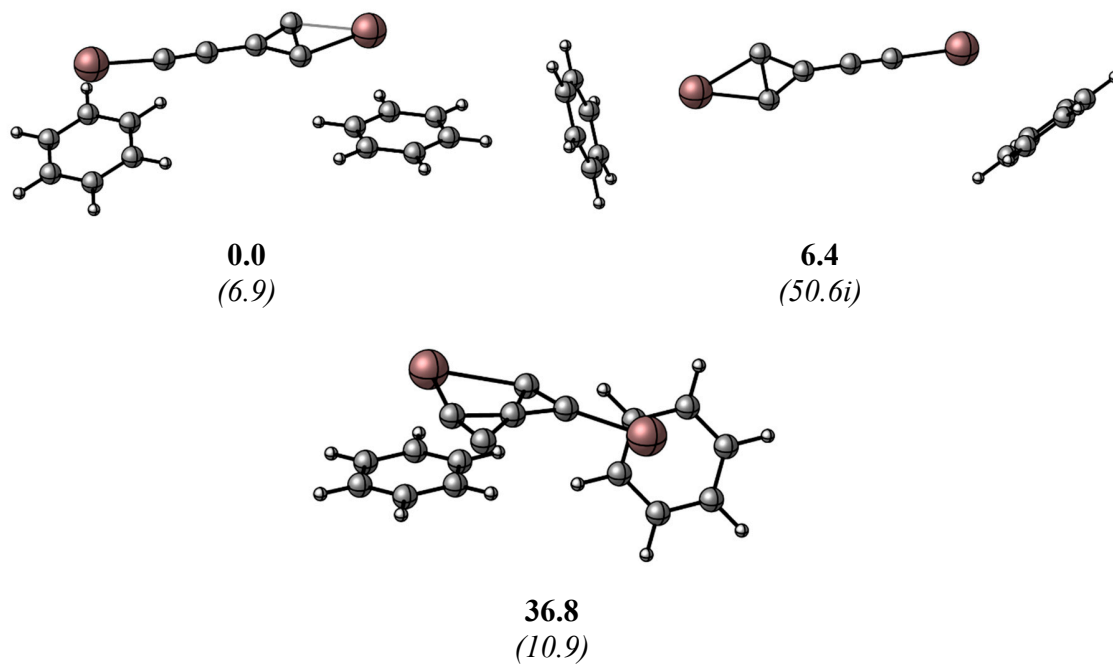
**Figure S6.** Putative global minimum and low-lying isomers of complex  $(\text{C}_6\text{H}_6)_2\text{-K}_2\text{C}_5$ . Relative energies are shown in  $\text{kcal}\cdot\text{mol}^{-1}$  at the  $\omega\text{b97XD/def2-TZVP}$  level, including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in  $\text{cm}^{-1}$ .



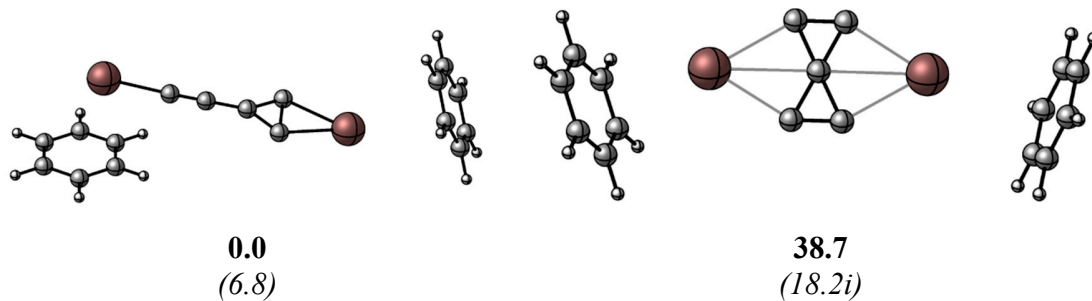
**Figure S7.** Putative global minimum and low-lying isomers of complex  $(\text{C}_6\text{H}_6)_2\text{-Al}_2\text{C}_5$ . Relative energies are shown in  $\text{kcal}\cdot\text{mol}^{-1}$  at the  $\omega\text{b97XD/def2-TZVP}$  level, including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in  $\text{cm}^{-1}$ .



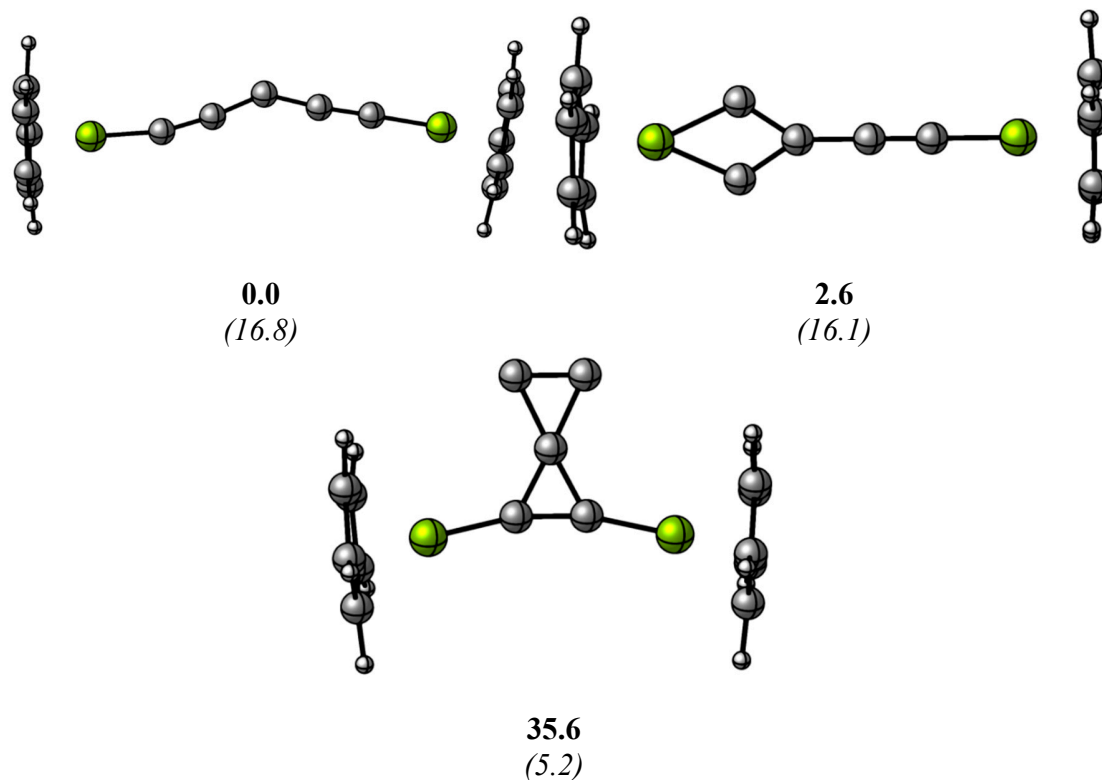
**Figure S8.** Putative global minimum and low-lying isomers of complex  $(\text{C}_6\text{H}_6)_2\text{-Ga}_2\text{C}_5$ . Relative energies are shown in  $\text{kcal}\cdot\text{mol}^{-1}$  at the  $\omega\text{b97XD/def2-TZVP}$  level, including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in  $\text{cm}^{-1}$ .



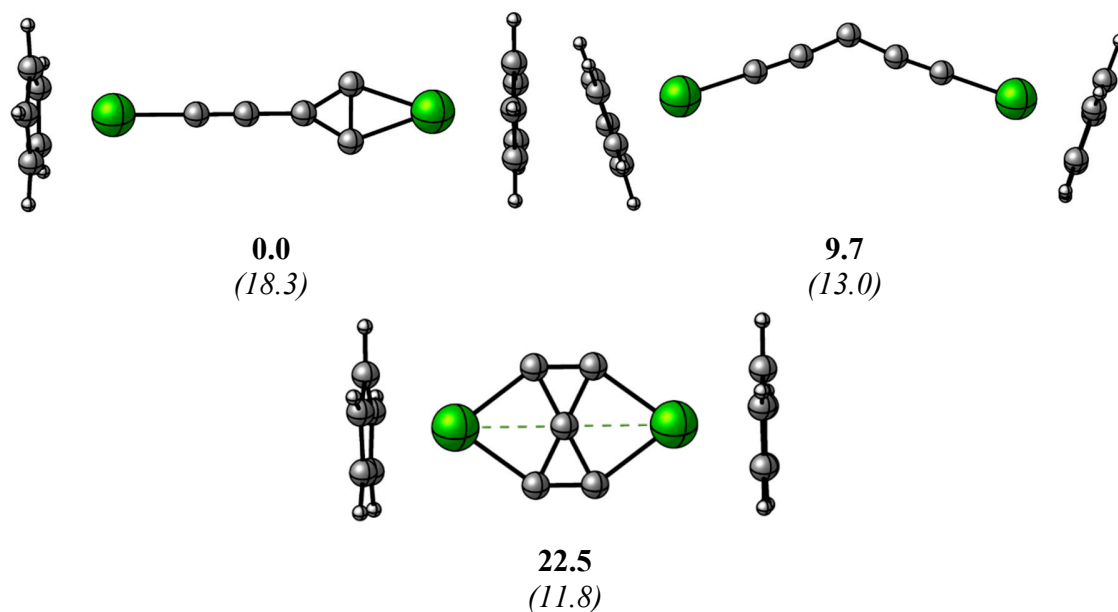
**Figure S9.** Putative global minimum and low-lying isomers of complex  $(\text{C}_6\text{H}_6)_2\text{-In}_2\text{C}_5$ . Relative energies are shown in  $\text{kcal}\cdot\text{mol}^{-1}$  at the  $\omega\text{b97XD/def2-TZVP}$  level, including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in  $\text{cm}^{-1}$ .



**Figure S10.** Putative global minimum and low-lying isomers of  $(\text{C}_5\text{H}_5^-)_2\text{-Be}_2\text{C}_5^{2+}$ . Relative energies are shown in  $\text{kcal}\cdot\text{mol}^{-1}$  at the  $\omega\text{b97XD/def2-TZVP}$  level, including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in  $\text{cm}^{-1}$ .

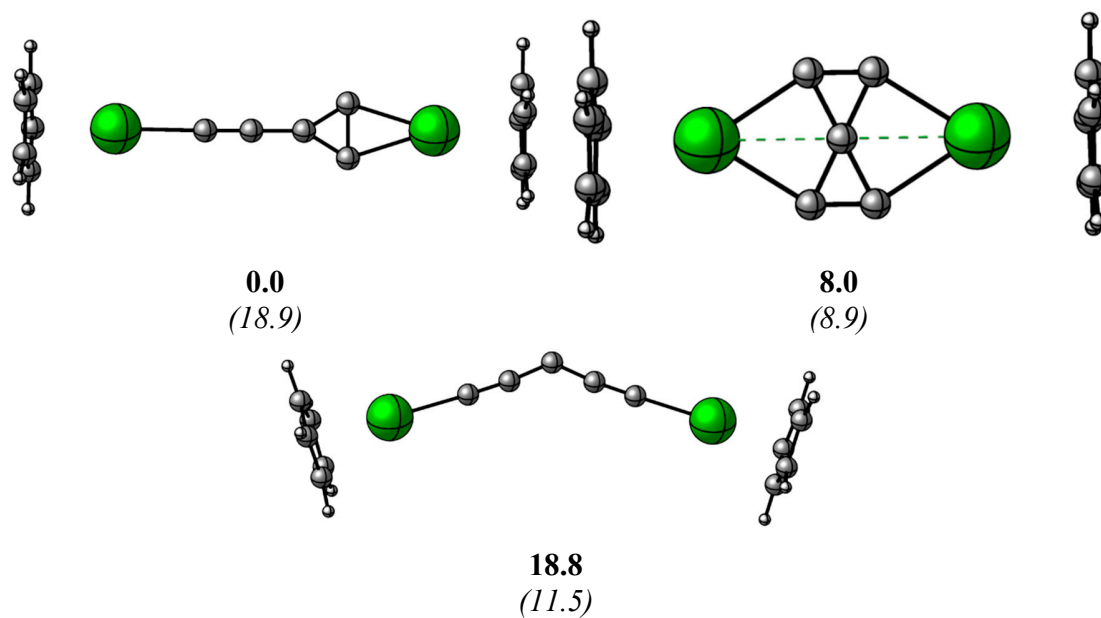


**Figure S11.** Putative global minimum and low-lying isomers of  $(\text{C}_5\text{H}_5^-)_2\text{-Mg}_2\text{C}_5^{2+}$ . Relative energies are shown in  $\text{kcal}\cdot\text{mol}^{-1}$  at the  $\omega\text{b97XD/def2-TZVP}$  level, including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in  $\text{cm}^{-1}$ .

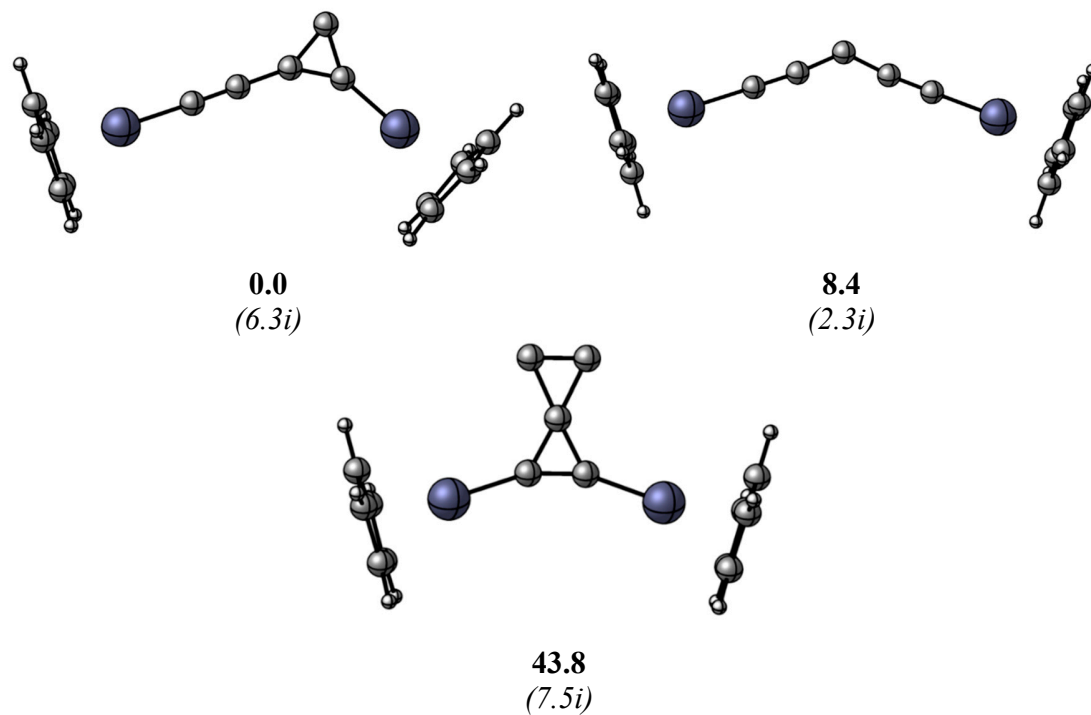




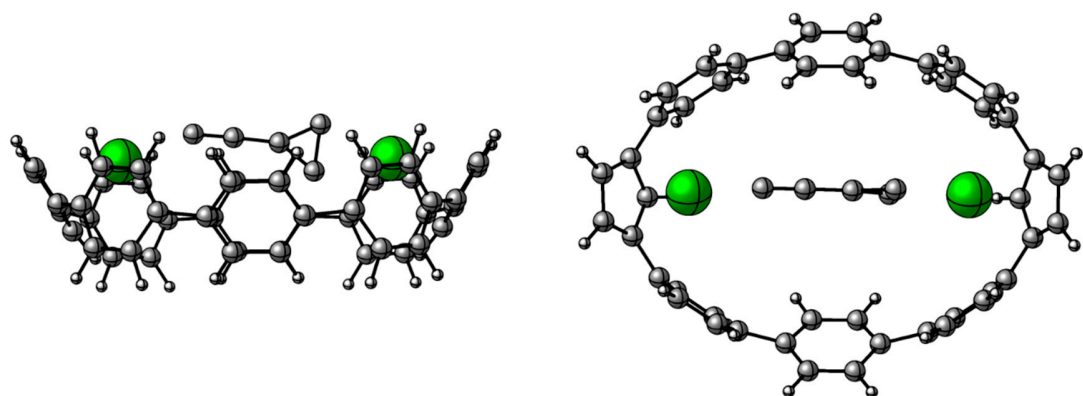
**Figure S12.** Putative global minimum and low-lying isomers of  $(\text{C}_5\text{H}_5^-)_2\text{-Ca}_2\text{C}_5^{2+}$ . Relative energies are shown in  $\text{kcal}\cdot\text{mol}^{-1}$  at the  $\omega\text{b97XD/def2-TZVP}$  level, including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in  $\text{cm}^{-1}$ .



**Figure S13.** Putative global minimum and low-lying isomers of  $(C_5H_5^-)_2-Zn_2C_5^{2+}$ . Relative energies are shown in  $\text{kcal}\cdot\text{mol}^{-1}$  at the  $\omega\text{b97XD/def2-TZVP}$  level, including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in  $\text{cm}^{-1}$ .



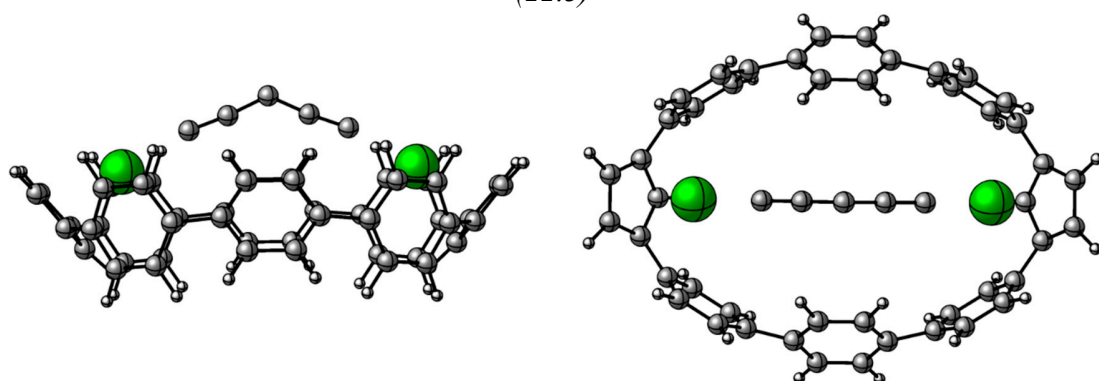
**Figure S14.** Putative global minimum and low-lying isomers of  $[8\text{-CPP}]^2\text{-}[\text{Ca}_2\text{C}_5]^{2+}$ . Relative energies are shown in  $\text{kcal}\cdot\text{mol}^{-1}$  at the  $\omega\text{b97XD/def2-TZVP}$  level, including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in  $\text{cm}^{-1}$ . A number-letter label is given to facilitate their connection with their cartesian coordinates in Table S2.



Side View

Top View

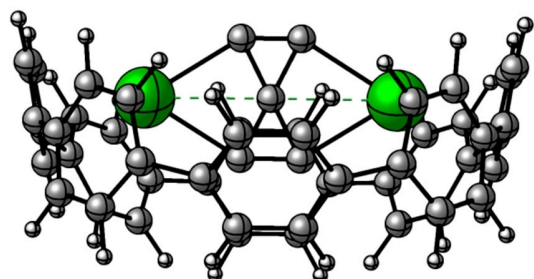
**1A. 0.0**  
(22.3)



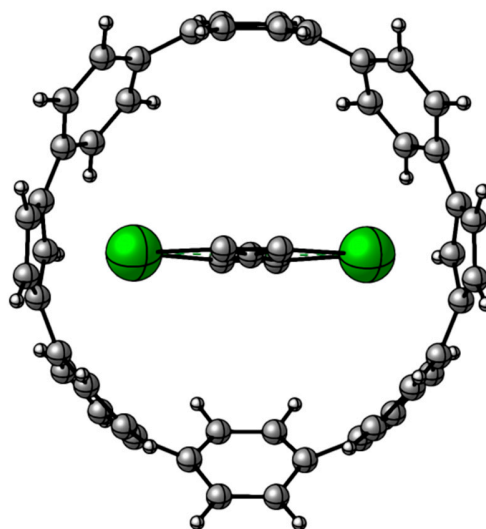
Side View

Top View

**1B.14.7**  
(19.6)



Side View



Top View

**1C. 18.5**  
(25.9)

**Table S1.** Cartesian coordinates of the  $M_2C_5^{0/2+}$  (M = Li-K, Be-Ca, Al-In, and Zn) pHc minima optimized structures at the  $\omega$ b97XD/def2-TZVP level.

C <sub>5</sub> Li <sub>2</sub>				C <sub>5</sub> Na <sub>2</sub>			
3	0.000000000	2.194866000		11	-2.608381000	0.000000000	
6	1.338129000	-0.662427000		6	0.662133000	1.340036000	
6	-1.338129000	0.662427000		6	-0.662133000	-1.340036000	
3	0.000000000	-2.194866000		11	2.608381000	0.000000000	
6	-1.338129000	-0.662427000		6	0.662133000	-1.340036000	
6	0.000000000	0.000000000		6	0.000000000	0.000000000	
6	1.338129000	0.662427000		6	-0.662133000	1.340036000	
C <sub>5</sub> K <sub>2</sub>				C <sub>5</sub> Be <sub>2</sub> <sup>2+</sup>			
19	0.000000000	2.985238000		4	0.000000000	1.984180000	
6	1.345568000	-0.662091000		6	1.245480000	-0.663083000	
6	-1.345568000	0.662091000		6	-1.245480000	0.663083000	
19	0.000000000	-2.985238000		4	0.000000000	-1.984180000	
6	-1.345568000	-0.662091000		6	-1.245480000	-0.663083000	
6	0.000000000	0.000000000		6	0.000000000	0.000000000	
6	1.345568000	0.662091000		6	1.245480000	0.663083000	
C <sub>5</sub> Mg <sub>2</sub> <sup>2+</sup>				C <sub>5</sub> Ca <sub>2</sub> <sup>2+</sup>			
12	0.000000000	2.370215000		20	0.000000000	2.642126000	
6	1.309623000	-0.661723000		6	1.338681000	-0.660199000	
6	-1.309623000	0.661723000		6	-1.338681000	0.660199000	
12	0.000000000	-2.370215000		20	0.000000000	-2.642126000	
6	-1.309623000	-0.661723000		6	-1.338681000	-0.660199000	
6	0.000000000	0.000000000		6	0.000000000	0.000000000	
6	1.309623000	0.661723000		6	1.338681000	0.660199000	
C <sub>5</sub> Al <sub>2</sub>				C <sub>5</sub> Ga <sub>2</sub>			
13	0.000000000	2.529551000		31	0.740798000	2.509593000	
6	1.324439000	-0.665609000		6	-1.434740000	-0.326185000	
6	-1.324439000	0.665609000		6	1.441678000	0.325119000	
13	0.000000000	-2.529551000		31	-0.740496000	-2.511480000	
6	-1.324439000	-0.665609000		6	1.135297000	-0.968509000	
6	0.000000000	0.000000000		6	0.000000000	0.007244000	
6	1.324439000	0.665609000		6	-1.143792000	0.972080000	
C <sub>5</sub> In <sub>2</sub>				C <sub>5</sub> Zn <sub>2</sub> <sup>2+</sup>			
49	0.000000000	2.822501000		30	0.000000000	2.350986000	
6	1.324463000	-0.665458000		6	1.278458000	-0.660958000	
6	-1.324463000	0.665458000		6	-1.278458000	0.660958000	
49	0.000000000	-2.822501000		30	0.000000000	-2.350986000	
6	-1.324463000	-0.665458000		6	-1.278458000	-0.660958000	
6	0.000000000	0.000000000		6	0.000000000	0.000000000	
6	1.324463000	0.665458000		6	1.278458000	0.660958000	

**Table S2.** Cartesian coordinates of the  $[8\text{-CPP}]^2\text{-}[\text{Ca}_2\text{C}_5]^{2+}$  optimized structures at the  $\omega$ b97XD/def2-TZVP level.

1A				1B			
6	1.419117000	4.409695000	0.608930000	6	1.407663000	-4.220079000	-0.277239000
6	0.689252000	3.819070000	1.638746000	6	0.690489000	-3.594915000	0.741671000
6	0.706164000	5.123292000	-0.355063000	6	0.692796000	-4.938698000	-1.234925000
6	-0.689496000	3.826506000	1.633835000	6	-0.690410000	-3.594933000	0.741603000
6	-0.679664000	5.127593000	-0.362260000	6	-0.692486000	-4.938715000	-1.234995000
6	-1.405587000	4.422166000	0.597446000	6	-1.407465000	-4.220113000	-0.277380000
1	1.238535000	5.642555000	-1.142882000	1	1.224329000	-5.471639000	-2.014472000

1	-1.212563000	3.253160000	2.387909000	1	-1.208340000	-2.996584000	1.481234000
1	-1.201101000	5.649333000	-1.155889000	1	-1.223929000	-5.471672000	-2.014593000
6	2.845439000	4.034230000	0.469092000	6	2.843959000	-3.885809000	-0.414022000
6	3.365560000	3.716181000	-0.782976000	6	3.663329000	-3.709855000	0.698226000
6	3.625377000	3.713675000	1.582903000	6	3.347186000	-3.477205000	-1.650379000
6	4.506170000	2.937083000	-0.902122000	6	4.836517000	-2.976395000	0.606201000
6	4.750845000	2.921704000	1.468219000	6	4.517216000	-2.747121000	-1.746389000
6	5.151529000	2.419827000	0.227724000	6	5.229962000	-2.381028000	-0.601643000
1	2.811422000	3.970875000	-1.677805000	1	3.342666000	-4.075402000	1.665853000
1	3.301149000	4.024011000	2.568707000	1	2.752948000	-3.635103000	-2.542324000
1	4.838031000	2.638327000	-1.893128000	1	5.417277000	-2.795268000	1.506699000
1	5.279886000	2.608578000	2.359689000	1	4.826214000	-2.357988000	-2.708539000
6	5.918320000	1.164189000	0.122820000	6	6.052289000	-1.154193000	-0.576056000
6	6.631393000	0.647145000	-0.988034000	6	6.921463000	-0.703440000	0.449461000
6	5.543544000	0.061326000	0.917454000	6	5.566109000	0.000190000	-1.228342000
6	6.654242000	-0.754051000	-0.887020000	6	6.921394000	0.703588000	0.449615000
6	5.945067000	-1.136476000	0.281817000	6	6.052279000	1.154488000	-0.575889000
1	7.105067000	1.231905000	-1.763966000	1	7.500387000	-1.331865000	1.111442000
1	4.857795000	0.120581000	1.751748000	1	4.772165000	0.000239000	-1.963634000
1	7.139891000	-1.423737000	-1.582701000	1	7.500271000	1.331923000	1.111723000
6	-2.832684000	4.053713000	0.444923000	6	-2.843759000	-3.885888000	-0.414297000
6	-3.631682000	3.758597000	1.552668000	6	-3.346887000	-3.477314000	-1.650704000
6	-3.338710000	3.722152000	-0.809605000	6	-3.663223000	-3.709934000	0.697879000
6	-4.765513000	2.977934000	1.434250000	6	-4.516937000	-2.747276000	-1.746827000
6	-4.487761000	2.955577000	-0.932868000	6	-4.836423000	-2.976507000	0.605744000
6	-5.158847000	2.468177000	0.195006000	6	-5.229797000	-2.381198000	-0.602148000
1	-3.316520000	4.080406000	2.537676000	1	-2.752563000	-3.635201000	-2.542594000
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