Supplementary material

Searching for systems with planar hexacoordinate carbons

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Figure S1. Adaptive Natural Density Partitioning bonding pattern of the $M_2C_5^{2+}$ (M = Be, Ca, Mg) at the ωb97XD/Def2-TZVP level.

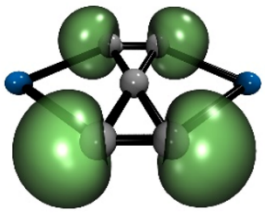
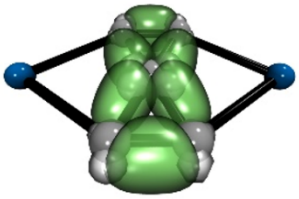
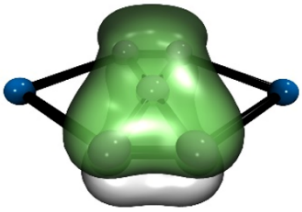
	E-LPs	E-E σ-bonds	E-E π-bond
			
	4 x 1c-2e	6 x 2c-2e	1 x 5c-2e
E = C, M = Be	ON = 1.80 |e|	ON = 1.97 – 1.78 |e|	ON = 1.99 |e|
E = C, M = Mg	ON = 1.85 |e|	ON = 1.97 – 1.78 |e|	ON = 1.99 |e|
E = C, M = Ca	ON = 1.88 |e|	ON = 1.96 – 1.77 |e|	ON = 1.99 |e|

Figure S2. Adaptive Natural Density Partitioning bonding pattern of the M_2C_5 (M = Al, Ga, In) at the ωb97XD/Def2-TZVP level.

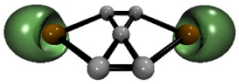
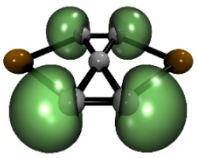
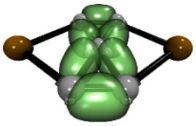
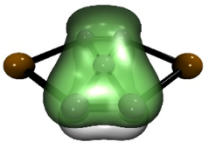
	M-LPs	E-LPs	E-E σ-bonds	E-E π-bond
				
	2 x 1c-2e	4 x 1c-2e	6 x 2c-2e	1 x 5c-2e
E = C, M = Al	ON = 1.97 |e|	ON = 1.81 |e|	ON = 1.97 – 1.78 |e|	ON = 1.99 |e|
E = C, M = Ga	ON = 1.97 |e|	ON = 1.81 |e|	ON = 1.96 – 1.78 |e|	ON = 1.99 |e|
E = C, M = In	ON = 1.98 |e|	ON = 1.82 |e|	ON = 1.96 – 1.78 |e|	ON = 1.99 |e|

Figure S3. Adaptive Natural Density Partitioning bonding pattern of the $Zn_2C_5^{2+}$ at the ωb97XD/Def2-TZVP level.

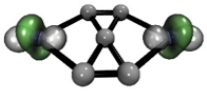
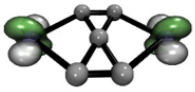
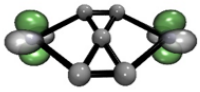
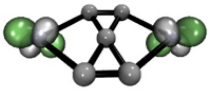
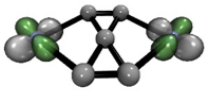
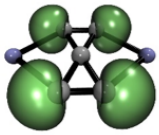
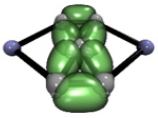
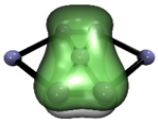
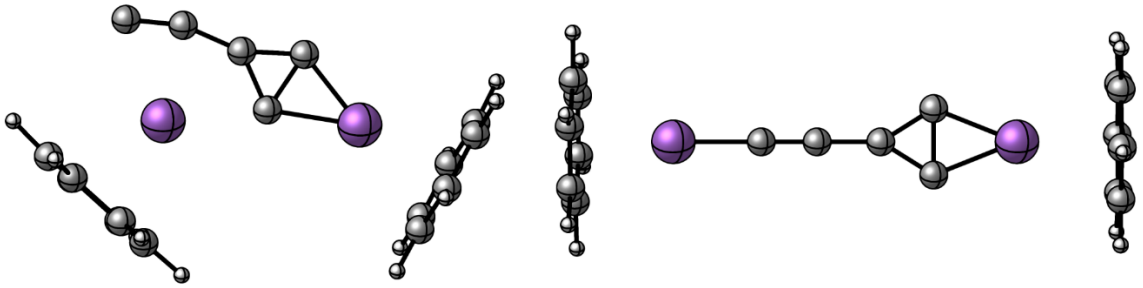
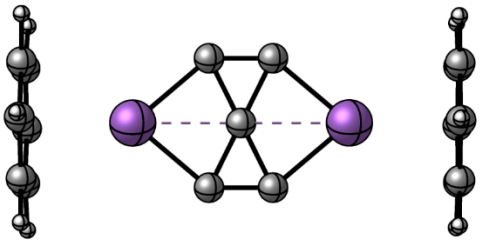
	Zn-LPs			
				
	2 x 1c-2e	2 x 1c-2e	2 x 1c-2e	2 x 1c-2e
$C_5Zn_2^{2+}$	ON = 1.99 |e|	ON = 1.99 |e|	ON = 1.99 |e|	ON = 1.99 |e|
	Zn-LPs	C-LPs	C-C σ-bonds	C-C π-bond
				
	2 x 1c-2e	4 x 1c-2e	6 x 2c-2e	1 x 5c-2e
$C_5Zn_2^{2+}$	ON = 1.99 |e|	ON = 1.74 |e|	ON = 1.97 – 1.77 |e|	ON = 1.99 |e|

Figure S4. Putative global minimum and low-lying isomers of complex $(C_6H_6)_2$-Li_2C_5. Relative energies are shown in kcal·mol^{-1} at ωb97XD/def2-TZVP level including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in cm^{-1}.



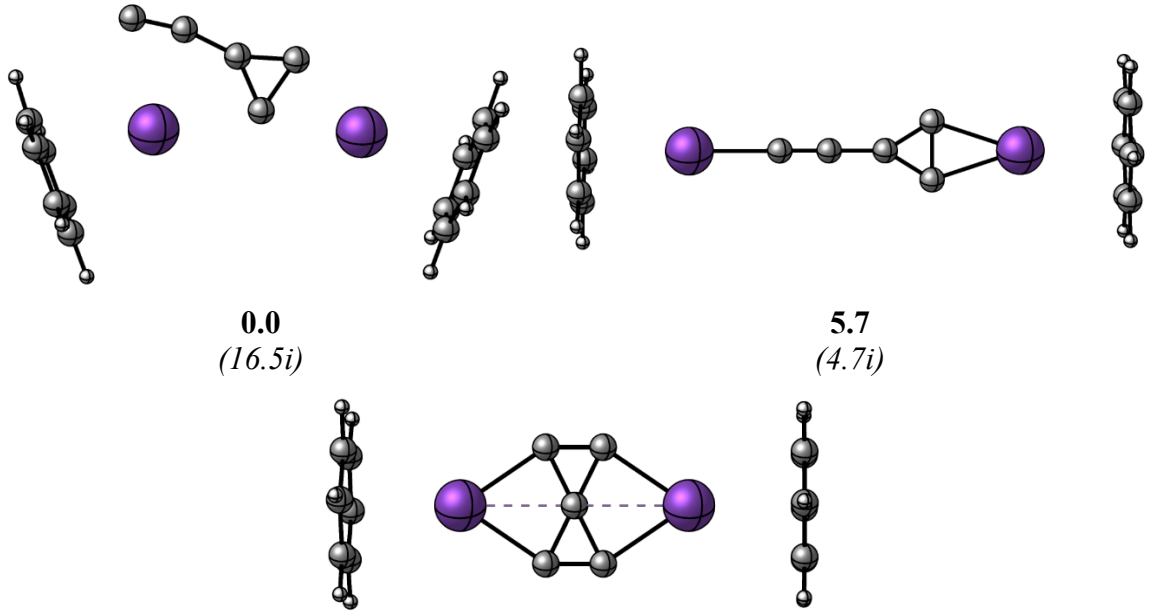
0.0
(11.9)

0.1
(2.7)



13.0
(7.7)

Figure S5. Putative global minimum and low-lying isomers of complex $(C_6H_6)_2$-Na_2C_5. Relative energies are shown in kcal·mol^{-1} at ωb97XD/def2-TZVP level including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in cm^{-1}.

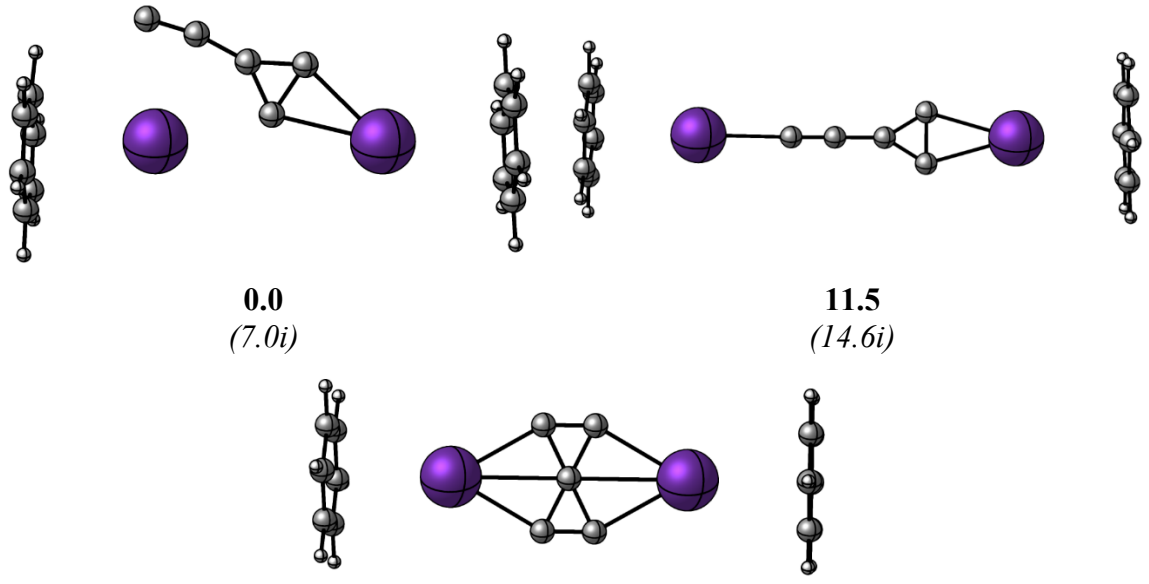


0.0
(16.5i)

5.7
(4.7i)

14.8
(10.2i)

Figure S6. Putative global minimum and low-lying isomers of complex $(C_6H_6)_2$-K_2C_5. Relative energies are shown in kcal·mol^{-1} at ωb97XD/def2-TZVP level including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in cm^{-1}.

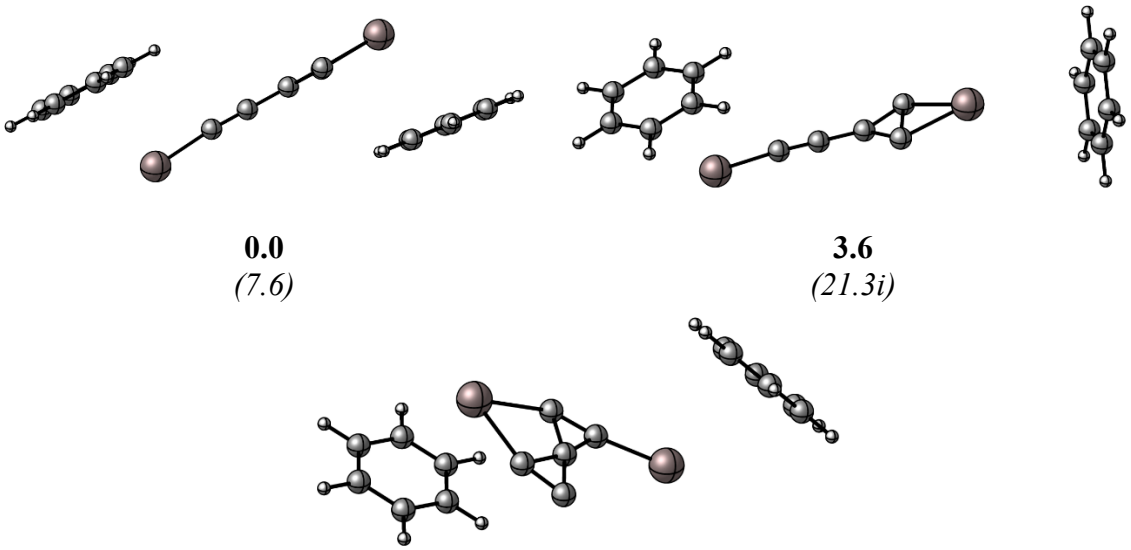


0.0
(7.0i)

11.5
(14.6i)

20.8
(6.8i)

Figure S7. Putative global minimum and low-lying isomers of complex $(C_6H_6)_2$-Al_2C_5. Relative energies are shown in kcal·mol^{-1} at ωb97XD/def2-TZVP level including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in cm^{-1}.

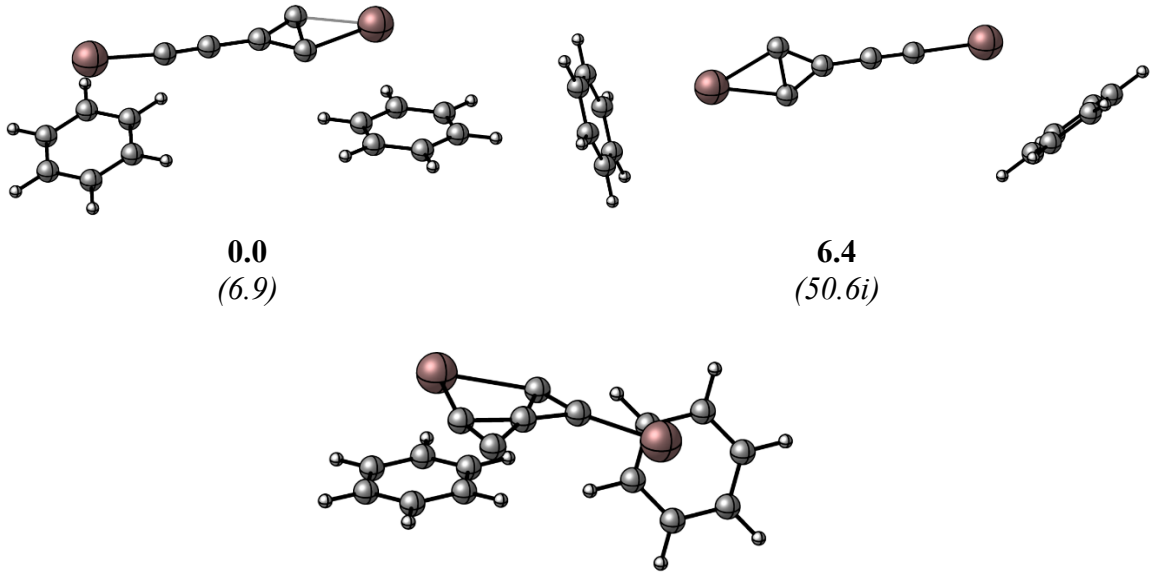


0.0
(7.6)

3.6
(21.3i)

39.1
(11.4)

Figure S8. Putative global minimum and low-lying isomers of complex $(C_6H_6)_2$- Ga_2C_5. Relative energies are shown in kcal·mol^{-1} at ωb97XD/def2-TZVP level including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in cm^{-1}.

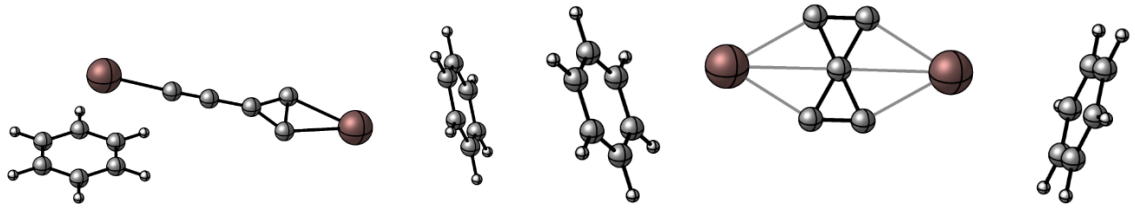


0.0
(6.9)

6.4
(50.6i)

36.8
(10.9)

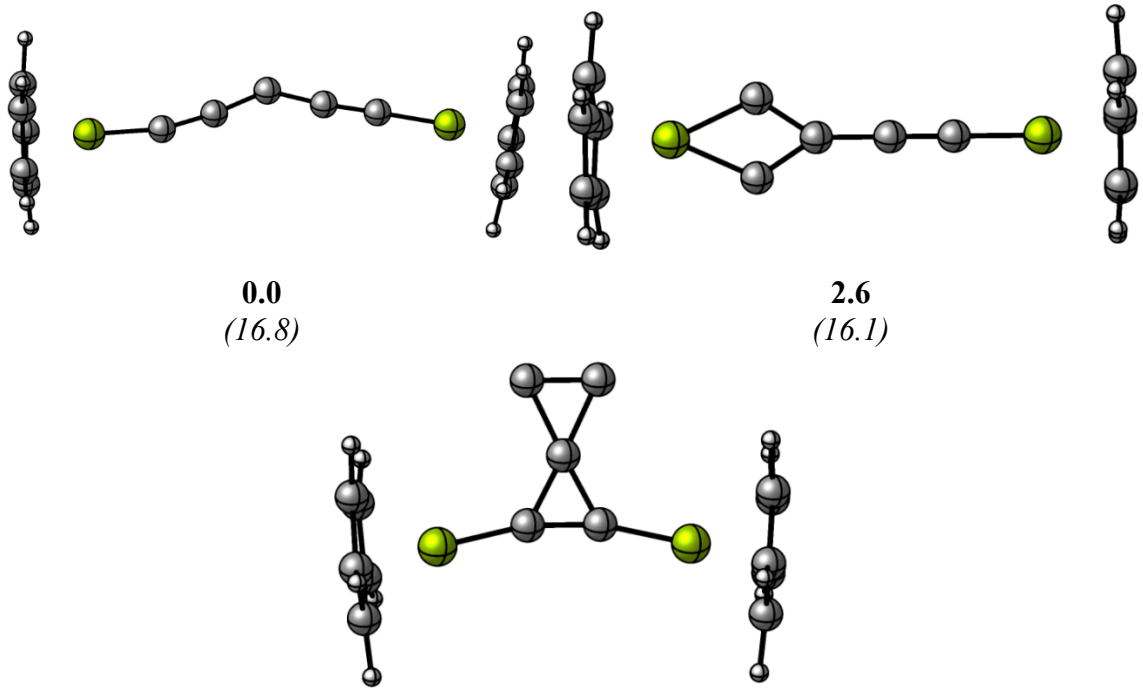
Figure S9. Putative global minimum and low-lying isomers of complex $(C_6H_6)_2$-In_2C_5. Relative energies are shown in kcal·mol^{-1} at ωb97XD/def2-TZVP level including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in cm^{-1}.



0.0
(6.8)

38.7
(18.2i)

Figure S10. Putative global minimum and low-lying isomers of $(C_5H_5^-)_2$- $Be_2C_5^{2+}$. Relative energies are shown in kcal·mol^{-1} at ωb97XD/def2-TZVP level including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in cm^{-1}.

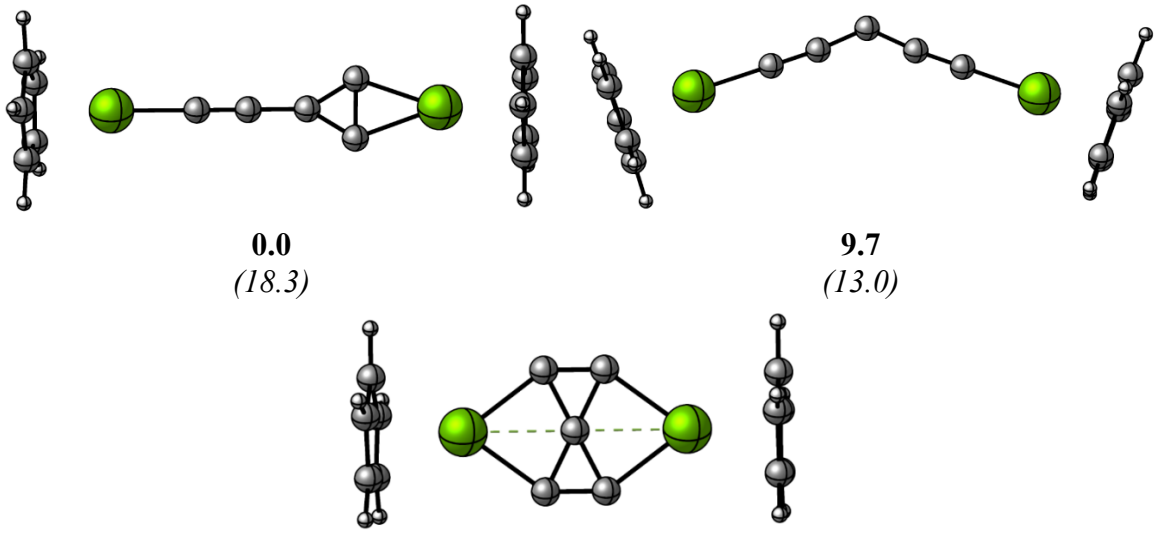


0.0
(16.8)

2.6
(16.1)

35.6
(5.2)

Figure S11. Putative global minimum and low-lying isomers of $(C_5H_5^-)_2$- $Mg_2C_5^{2+}$. Relative energies are shown in kcal·mol^{-1} at ωb97XD/def2-TZVP level including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in cm^{-1}.

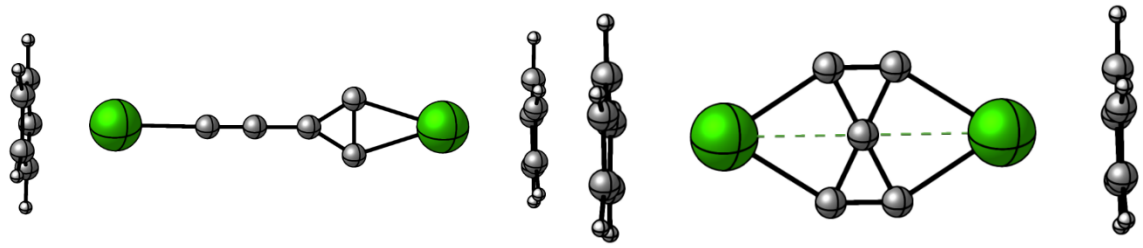


0.0
(18.3)

9.7
(13.0)

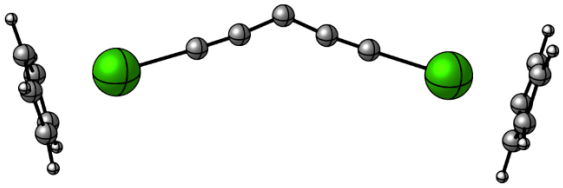
22.5
(11.8)

Figure S12. Putative global minimum and low-lying isomers of $(C_5H_5^-)_2$- $Ca_2C_5^{2+}$. Relative energies are shown in kcal·mol^{-1} at ωb97XD/def2-TZVP level including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in cm^{-1}.



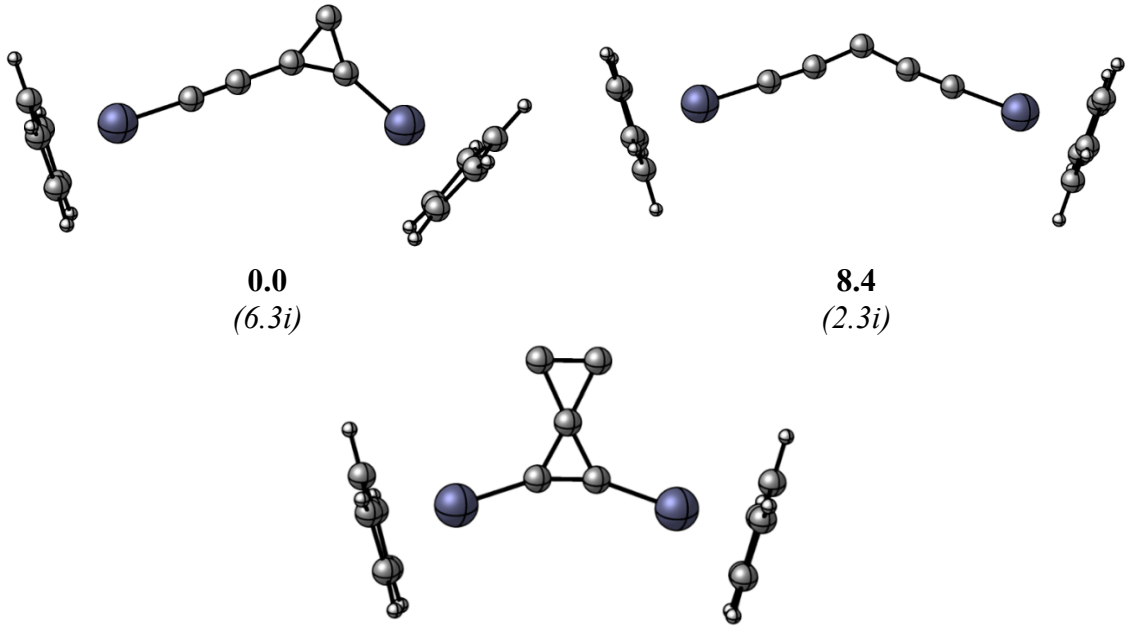
0.0
(18.9)

8.0
(8.9)



18.8
(11.5)

Figure S13. Putative global minimum and low-lying isomers of $(C_5H_5^-)_2$- $Zn_2C_5^{2+}$. Relative energies are shown in kcal·mol^{-1} at ωb97XD/def2-TZVP level including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in cm^{-1}.

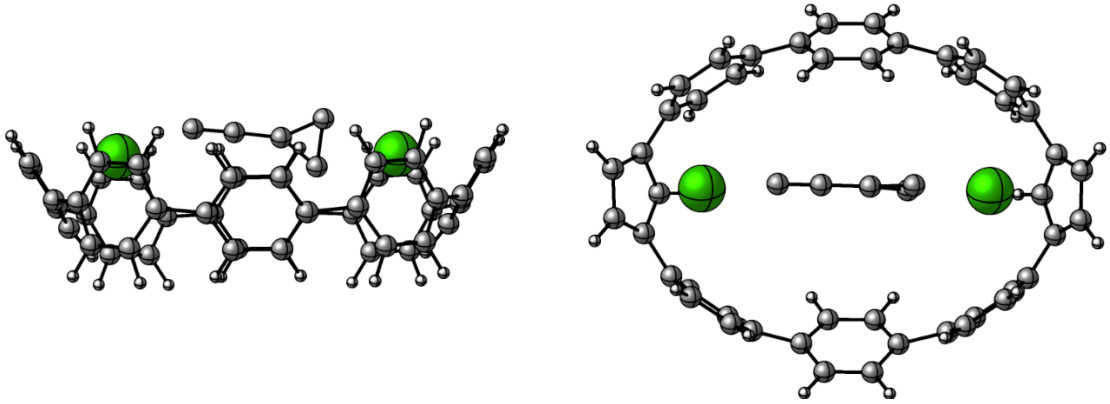


0.0
(6.3i)

8.4
(2.3i)

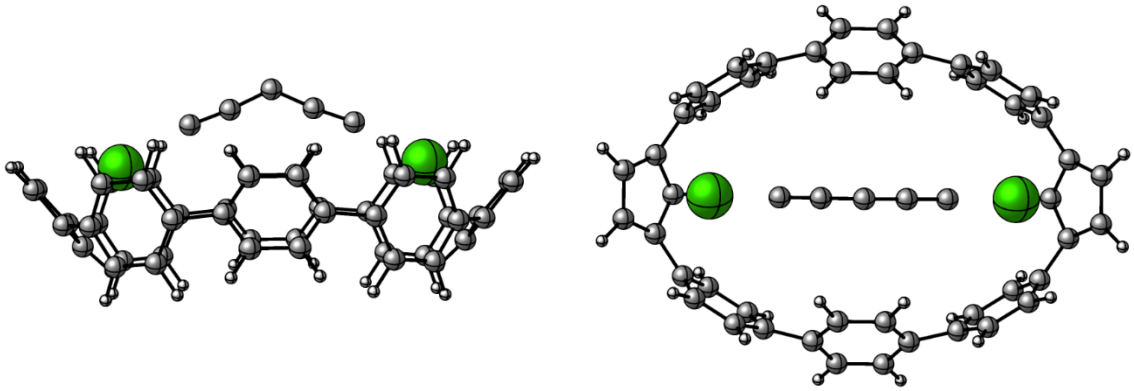
43.8
(7.5i)

Figure S14. Putative global minimum and low-lying isomers of $[8\text{-CPP}]^{2-}[Ca_2C_5]^{2+}$. Relative energies are shown in kcal·mol^{-1} at ωb97XD/def2-TZVP level including zero-point energy (ZPE) corrections and their lowest harmonic vibrational frequency in cm^{-1}. A number-letter label is given to facilitate their connection with their cartesian coordinates in Table S2.



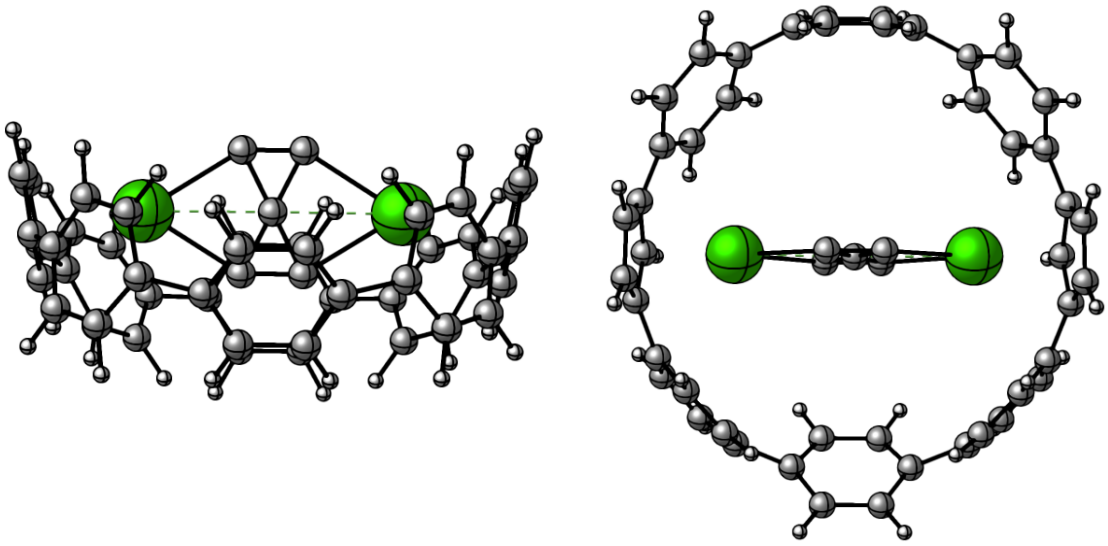
Side View **Top View**

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 ωb97XD/def2-TZVP level.

C_5Li_2				C_5Na_2			
3	-0.002663000	-2.199611000	0.021810000	11	-0.003182000	-2.605458000	0.000331000
6	-1.341344000	0.662519000	-0.016844000	6	-1.339963000	0.665290000	-0.000280000
6	1.341453000	-0.662454000	-0.016991000	6	1.340114000	-0.665186000	-0.000406000
3	0.002669000	2.199920000	0.021645000	11	0.003216000	2.605742000	0.000153000
6	1.342932000	0.659031000	-0.016882000	6	1.341629000	0.661854000	-0.000149000
6	-0.000002000	-0.000128000	0.024595000	6	-0.000033000	-0.000140000	0.000932000
6	-1.343027000	-0.658955000	-0.017029000	6	-1.341764000	-0.661778000	-0.000275000
C_5K_2				$C_5Be_2^{2+}$			
19	2.983380000	0.000000000	-0.000280000	4	0.000000000	0.000000000	1.984180000
6	-0.661900000	1.346049000	0.000316000	6	0.000000000	1.245480000	-0.663083000
6	0.661896000	-1.346036000	0.000307000	6	0.000000000	-1.245480000	0.663083000
19	-2.983371000	-0.000001000	-0.000096000	4	0.000000000	0.000000000	-1.984180000
6	-0.661895000	-1.346053000	0.000315000	6	0.000000000	-1.245480000	-0.663083000
6	-0.000018000	0.000000000	-0.000054000	6	0.000000000	0.000000000	0.000000000
6	0.661890000	1.346041000	0.000307000	6	0.000000000	1.245480000	0.663083000
$C_5Mg_2^{2+}$				$C_5Ca_2^{2+}$			
12	0.000000000	0.000000000	2.370215000	20	0.000000000	0.000000000	2.642126000
6	0.000000000	1.309623000	-0.661723000	6	0.000000000	1.338681000	-0.660199000
6	0.000000000	-1.309623000	0.661723000	6	0.000000000	-1.338681000	0.660199000
12	0.000000000	0.000000000	-2.370215000	20	0.000000000	0.000000000	-2.642126000
6	0.000000000	-1.309623000	-0.661723000	6	0.000000000	-1.338681000	-0.660199000
6	0.000000000	0.000000000	0.000000000	6	0.000000000	0.000000000	0.000000000
6	0.000000000	1.309623000	0.661723000	6	0.000000000	1.338681000	0.660199000
C_5Al_2				C_5Ga_2			
13	-2.529488000	-0.000011000	-0.000825000	31	-2.502484000	-0.009685000	-0.013081000
6	0.665615000	-1.324264000	-0.000444000	6	0.743497000	-1.288048000	0.025402000
6	-0.665644000	1.324589000	0.000885000	6	-0.746752000	1.297285000	0.033954000
13	2.529613000	0.000015000	0.000106000	31	2.505659000	0.010549000	-0.012167000
6	0.665573000	1.324285000	-0.000488000	6	0.600695000	1.375909000	0.017603000
6	-0.000293000	-0.000005000	0.000427000	6	-0.009548000	-0.002718000	0.027919000
6	-0.665604000	-1.324618000	0.000841000	6	-0.604294000	-1.386896000	0.025571000
C_5In_2				$C_5Zn_2^{2+}$			
49	2.822487000	0.000002000	-0.000621000	30	0.000000000	0.000000000	2.350986000
6	-0.665492000	1.324331000	0.001335000	6	0.000000000	1.278458000	-0.660958000
6	0.665508000	-1.324535000	0.001522000	6	0.000000000	-1.278458000	0.660958000
49	-2.822514000	-0.000004000	-0.000373000	30	0.000000000	0.000000000	-2.350986000
6	-0.665406000	-1.324386000	0.001281000	6	0.000000000	-1.278458000	-0.660958000
6	0.000185000	0.000010000	0.002510000	6	0.000000000	0.000000000	0.000000000
6	0.665427000	1.324598000	0.001468000	6	0.000000000	1.278458000	0.660958000

Table S2. Cartesian coordinates of the $[8\text{-CPP}]^{2-}[Ca_2C_5]^{2+}$ optimized structures at the ωb97XD/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
1	-2.768262000	3.956334000	-1.699553000	1	-3.342622000	-4.075441000	1.665542000
1	-5.311136000	2.685368000	2.322829000	1	-4.825864000	-2.358163000	-2.709007000
1	-4.812632000	2.651497000	-1.924887000	1	-5.417253000	-2.795362000	1.506194000
6	5.144904000	-2.363598000	0.468202000	6	5.229897000	2.381284000	-0.601298000
6	4.465163000	-2.612472000	1.664933000	6	4.517135000	2.747497000	-1.745997000
6	4.737139000	-3.106787000	-0.650218000	6	4.836392000	2.976436000	0.606631000
6	3.306912000	-3.366595000	1.682812000	6	3.347063000	3.477500000	-1.649893000
6	3.583328000	-3.873967000	-0.624314000	6	3.663160000	3.709818000	0.698749000
6	2.786924000	-3.931362000	0.517171000	6	2.843800000	3.885899000	-0.413483000
1	4.782887000	-2.109044000	2.569199000	1	4.826164000	2.358518000	-2.708199000
1	5.284876000	-3.013507000	-1.582649000	1	5.417150000	2.795203000	1.507111000
1	2.733467000	-3.418543000	2.600184000	1	2.752825000	3.635494000	-2.541822000
1	3.257987000	-4.363799000	-1.533750000	1	3.342460000	4.075198000	1.666428000
6	-5.947704000	1.223831000	0.094888000	6	-6.052166000	-1.154396000	-0.576655000
6	-5.589729000	0.118246000	0.893983000	6	-5.565979000	-0.000026000	-1.228957000
6	-6.680721000	0.713786000	-1.004472000	6	-6.921386000	-0.703622000	0.448816000
6	-6.733828000	-0.688479000	-0.891211000	6	-6.921548000	0.703406000	0.448758000
6	-6.024851000	-1.077012000	0.274229000	6	-6.052273000	1.154285000	-0.576617000
1	-4.909977000	0.170816000	1.734267000	1	-4.771964000	0.000020000	-1.964173000
1	-7.147916000	1.302500000	-1.781237000	1	-7.500306000	-1.332039000	1.110808000
1	-7.239014000	-1.352772000	-1.578092000	1	-7.500560000	1.331750000	1.110740000
6	-5.241861000	-2.316498000	0.466240000	6	-5.229940000	2.381123000	-0.601960000
6	-4.562969000	-2.566178000	1.663573000	6	-4.517043000	2.747344000	-1.746574000
6	-4.840707000	-3.066456000	-0.649837000	6	-4.836637000	2.976347000	0.606002000
6	-3.412309000	-3.332648000	1.683619000	6	-3.347012000	3.477395000	-1.650328000
6	-3.694796000	-3.846620000	-0.621063000	6	-3.663440000	3.709769000	0.698263000
6	-2.896590000	-3.905256000	0.519111000	6	-2.843928000	3.885838000	-0.413858000
1	-4.878043000	-2.059957000	2.567408000	1	-4.825927000	2.358330000	-2.708808000
1	-5.391321000	-2.975360000	-1.581303000	1	-5.417525000	2.795140000	1.506404000
1	-2.841121000	-3.392046000	2.602015000	1	-2.752659000	3.635388000	-2.542180000
1	-3.374139000	-4.343758000	-1.527930000	1	-3.342894000	4.075197000	1.665975000
6	1.353455000	-4.295514000	0.442280000	6	1.407488000	4.220091000	-0.276675000
6	0.633466000	-3.872762000	-0.673520000	6	0.690313000	3.594746000	0.742122000
6	0.633956000	-4.828027000	1.512586000	6	0.692621000	4.938844000	-1.234260000
6	-0.746097000	-3.864878000	-0.672946000	6	-0.690587000	3.594735000	0.742032000

6	-0.751648000	-4.821968000	1.513665000	6	-0.692661000	4.938830000	-1.234353000
6	-1.466943000	-4.284243000	0.443549000	6	-1.407641000	4.220065000	-0.276860000
1	1.151636000	-3.425099000	-1.511439000	1	1.208154000	2.996270000	1.481714000
1	1.161976000	-5.211885000	2.377356000	1	1.224155000	5.471924000	-2.013711000
1	-1.258401000	-3.401169000	-1.505829000	1	-1.208513000	2.996251000	1.481557000
1	-1.281492000	-5.202058000	2.379216000	1	-1.224103000	5.471899000	-2.013874000
1	1.201114000	3.237045000	2.393310000	1	1.208327000	-2.996549000	1.481353000
20	4.054296000	-0.170594000	-1.166685000	20	-4.414885000	0.000092000	1.053459000
20	-4.152866000	-0.169211000	-1.199598000	20	4.414782000	0.000011000	1.053971000
6	1.921760000	-0.381899000	-2.235168000	6	-2.389543000	-0.000088000	2.252068000
6	0.666452000	-0.302823000	-1.694841000	6	2.389333000	-0.000211000	2.252409000
6	-1.933833000	-0.368632000	-1.990961000	6	-1.216347000	-0.000259000	2.677323000
6	-0.715283000	-0.345137000	-1.867640000	6	1.216116000	-0.000309000	2.677607000
6	1.705887000	-0.147766000	-0.817668000	6	-0.000185000	-0.000416000	3.247580000
		1C					
6	0.919823000	-5.104230000	1.404348000				
6	1.942098000	-4.482721000	0.690332000				
6	0.054472000	-5.937044000	0.691668000				
6	1.942098000	-4.482721000	-0.690332000				
6	0.054472000	-5.937044000	-0.691668000				
6	0.919823000	-5.104230000	-1.404348000				
1	-0.696043000	-6.512790000	1.220013000				
1	2.644741000	-3.841297000	-1.206036000				
1	-0.696043000	-6.512790000	-1.220013000				
6	0.580799000	-4.543972000	2.732879000				
6	-0.752757000	-4.222722000	2.979947000				
6	1.538517000	-3.985238000	3.581688000				
6	-1.092121000	-3.230515000	3.881894000				
6	1.202850000	-2.990659000	4.481007000				
6	-0.107916000	-2.510728000	4.567594000				
1	-1.531113000	-4.652121000	2.362079000				
1	2.578711000	-4.268794000	3.475365000				
1	-2.132344000	-2.936304000	3.969812000				
1	1.981517000	-2.516410000	5.065384000				
6	-0.417423000	-1.164760000	5.074998000				
6	-1.707376000	-0.628532000	5.307310000				
6	0.462370000	-0.070629000	4.917840000				
6	-1.617614000	0.769857000	5.270531000				
6	-0.272440000	1.133574000	5.007892000				
1	-2.607478000	-1.194269000	5.499713000				
1	1.505858000	-0.160473000	4.652820000				
1	-2.444478000	1.449033000	5.416735000				
6	0.580799000	-4.543972000	-2.732879000				
6	1.538517000	-3.985238000	-3.581688000				
6	-0.752757000	-4.222722000	-2.979947000				
6	1.202850000	-2.990659000	-4.481007000				
6	-1.092121000	-3.230515000	-3.881894000				
6	-0.107916000	-2.510728000	-4.567594000				
1	2.578711000	-4.268794000	-3.475365000				
1	-1.531113000	-4.652121000	-2.362079000				
1	1.981517000	-2.516410000	-5.065384000				
1	-2.132344000	-2.936304000	-3.969812000				
6	0.171022000	2.443238000	4.498897000				
6	1.389492000	2.565411000	3.826694000				
6	-0.695266000	3.541273000	4.433593000				
6	1.620654000	3.609910000	2.952759000				
6	-0.458599000	4.590304000	3.564172000				
6	0.654359000	4.588365000	2.721643000				
1	2.124037000	1.773384000	3.889052000				
1	-1.612534000	3.535454000	5.008823000				
1	2.510985000	3.580942000	2.338013000				
1	-1.198415000	5.377024000	3.477012000				

6	-0.417423000	-1.164760000	-5.074998000	
6	0.462370000	-0.070629000	-4.917840000	
6	-1.707376000	-0.628532000	-5.307310000	
6	-1.617614000	0.769857000	-5.270531000	
6	-0.272440000	1.133574000	-5.007892000	
1	1.505858000	-0.160473000	-4.652820000	
1	-2.607478000	-1.194269000	-5.499713000	
1	-2.444478000	1.449033000	-5.416735000	
6	0.171022000	2.443238000	-4.498897000	
6	1.389492000	2.565411000	-3.826694000	
6	-0.695266000	3.541273000	-4.433593000	
6	1.620654000	3.609910000	-2.952759000	
6	-0.458599000	4.590304000	-3.564172000	
6	0.654359000	4.588365000	-2.721643000	
1	2.124037000	1.773384000	-3.889052000	
1	-1.612534000	3.535454000	-5.008823000	
1	2.510985000	3.580942000	-2.338013000	
1	-1.198415000	5.377024000	-3.477012000	
6	0.664940000	5.267718000	1.405180000	
6	-0.531197000	5.307523000	0.690565000	
6	1.840969000	5.509972000	0.691575000	
6	-0.531197000	5.307523000	-0.690565000	
6	1.840969000	5.509972000	-0.691575000	
6	0.664940000	5.267718000	-1.405180000	
1	-1.470849000	5.157279000	1.206434000	
1	2.784176000	5.588730000	1.218653000	
1	-1.470849000	5.157279000	-1.206434000	
1	2.784176000	5.588730000	-1.218653000	
20	-0.988834000	-0.076901000	2.776290000	
6	-2.328108000	0.051840000	-0.662477000	
6	0.328735000	-0.261353000	0.661720000	
20	-0.988834000	-0.076901000	-2.776290000	
6	0.328735000	-0.261353000	-0.661720000	
6	-1.000594000	-0.105548000	0.000000000	
6	-2.328108000	0.051840000	0.662477000	
1	2.644741000	-3.841297000	1.206036000	