Supporting information

10-π-electron arenes *à la carte*: Structure and Bonding of the $[E\text{-}(C_nH_n)\text{-}E]^{n-6}$ (E = Ca, Sr, Ba; n = 6-8) complexes

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Table 1-SI. Structural parameters for the lowest-lying energy structures of the $E_2(C_6H_6)$, $E_2(C_7H_7)^+$, and $E_2(C_8H_8)^{2+}$ (E = Ca, Sr, Ba) combinations obtained at the PBE0-D3/def2-TZVP and PBE0-D3/def2-TZVPD level. The distances of the E atoms from the ring centers (**r**) and the C–C bond lengths ($\mathbf{r_{c\text{-}c}}$) (in Å) are given.

	PBE0-D3/def2-TZVP		PBE0-D3/def2-TZVPD	
System	r	$r_{c\text{-}c}$	r	$r_{c\text{-}c}$
$Ca_2C_6H_6$	1.889	1.469	1.889	1.469
$Sr_2C_6H_6$	2.074	1.466	2.074	1.466
$Ba_2C_6H_6$	2.275	1.458	2.275	1.458
$Ca_2C_7H_7^+$	1.839	1.435	1.839	1.435
$Sr_2C_7H_7^+$	2.031	1.441	2.030	1.435
$Ba_2C_7H_7^+$	2.233	1.433	2.233	1.433
$Ca_2C_8H_8^{2+}$	1.834	1.415	1.840	1.415
$Sr_2C_8H_8^{2+}$	2.044	1.415	2.044	1.415
$Ba_2C_8H_8^{2+}$	2.256	1.414	2.263	1.414

Table 2-SI. The results of EDA at the PBE0/TZ2P level for $[Ba\text{-}(C_7H_7)\text{-}Ba]^+$ using different schemes . Energy values are in kcal/mol.[a]

	$[C_7H_7]^+ + [Ba\cdots Ba]$	$[C_7H_7]^+ + [Ba\cdots Ba]$	$[C_7H_7]^{3-} + [Ba\cdots Ba]^{4+}$
	$(a'_1)^2(a''_2)^2(e'_1)^0$	$(a'_1)^0(a''_2)^0(e'_1)^4$	$(a'_1)^0(a''_2)^0(e'_1)^0$
ΔE_{int}	-199.9	-298.4	-1394.8
ΔE_{Pauli}	699.6	971.8	218.8
ΔE_{elstat}	-370.1	-633.0	-1372.0 (85.0)
ΔE_{orb}	-529.3	-637.2	-241.6 (15.0)
a'_1	196.7	-3.4	-19.4 (8.0)
a'_2	0.0	0.0	0.0
e'_1	-5.6	203.4	-38.7 (16.0)
e'_2	-2.4	-3.3	-28.2 (11.7)
e'_3	1.4	-0.1	-15.3 (6.3)
a''_1	0.0	0.0	0.0
a''_2	226.6	-3.8	-11.9 (4.9)
e''_1	-28.9	-29.4	-61.7 (25.5)
e''_2	-917.1	-800.7	-66.4 (27.5)
e''_3	0.0	0.0	0.0

[a]The values in parentheses are the percentage contributions to the total attractive interactions, $\Delta E_{elstat} + \Delta E_{orb}$. The values in parentheses for the irreducible representations are the percentage contributions to the total orbital interaction, ΔE_{orb}.

Table 3-SI. The results of EDA at the PBE0/TZ2P level for $[Ba\text{-}(C_8H_8)\text{-}Ba]^{2+}$ using different schemes. Energy values are in kcal/mol.[a]

	$[C_8H_8]^{2+} + [Ba\cdots Ba]$	$[C_8H_8]^{2+} + [Ba\cdots Ba]$	$[C_8H_8]^{2-} + [Ba\cdots Ba]^{4+}$
	$(a_{1g})^2(a_{2u})^2(e_{1u})^0$	$(a_{1g})^0(a_{2u})^0(e_{1u})^4$	$(a_{1g})^0(a_{2u})^0(e_{1u})^0$
ΔE_{int}	-350.4	-450.8	-935.7
ΔE_{Pauli}	613.2	919.9	136.4
ΔE_{elstat}	-289.6	-626.0	-889.3 (82.9)
ΔE_{orb}	-674.1	-744.7	-182.8 (17.1)
a_{1g}	394.2	-3.0	-14.7 (8.0)
a_{2g}	0.0	0.0	0.0
b_{1g}	0.7	0.1	-4.0 (2.2)
b_{2g}	0.2	0.1	-1.6 (0.9)
e_{1g}	-20.2	-20.6	-42.5 (23.2)
e_{2g}	-1.9	-2.7	-23.3 (12.7)
e_{3g}	0.0	0.0	0.0
a_{1u}	0.0	0.0	0.0
a_{2u}	385.5	-4.2	-8.6 (4.7)
b_{1u}	0.0	0.0	0.0
b_{2u}	0.0	0.0	0.0
e_{1u}	-4.8	613.9	-29.1 (15.9)
e_{2u}	-1428.9	-1328.0	-45.5 (24.9)
e_{3u}	1.2	-0.2	-13.6 (7.4)

[a]The values in parentheses are the percentage contributions to the total attractive interactions, $\Delta E_{elstat} + \Delta E_{orb}$. The values in parentheses for the irreducible representations are the percentage contributions to the total orbital interaction, ΔE_{orb}.

Table 4-SI. The results of EDA at the PBE0/TZ2P level. All the energies are in kcal/mol.[a]

	$[C_6H_6] + [E\cdots E]$		$[C_6H_6] + [E\cdots E]$		$[C_6H_6]^{4-} + [E\cdots E]^{4+}$	
	$(a_{1g})^2(a_{2u})^2(e_{1u})^0$		$(a_{1g})^0(a_{2u})^0(e_{1u})^4$		$(a_{1g})^0(a_{2u})^0(e_{1u})^0$	
	Ca	Sr	Ca	Sr	Ca	Sr
ΔE_{int}	-28.8	-17.4	-214.1	-202.6	-1823.3	-1724.3
ΔE_{Pauli}	791.5	720.4	988.4	871.4	245.1	257.4
ΔE_{elstat}	-471.9 (57.5)	-435.7 (59.1)	-633.6 (52.7)	-554.2 (51.6)	-1434.7 (69.4)	-1417.4 (71.5)
ΔE_{orb}	-348.4 (42.2)	-302.1 (40.9)	-569.0 (47.3)	-519.8 (48.4)	-633.6 (30.6)	-564.4 (28.5)
a_{1g}	1.3	16.6	-6.8 (1.2)	-6.1 (1.2)	-6.8 (1.1)	-5.9 (1.0)
a_{2g}	0.0	0.0	0.0	0.0	0.0	0.0
b_{1g}	0.0	0.0	0.0	0.0	0.0	0.0
b_{2g}	0.0	0.0	0.0	0.0	0.0	0.0
e_{1g}	-35.9	-34.3	-39.1 (6.9)	-40.9 (7.9)	-48.3 (7.6)	-45.5 (8.1)
e_{2g}	-4.1	-2.8	-4.9 (0.9)	-3.6 (0.7)	-1.5 (0.2)	0.2 (0.0)
a_{1u}	0.0	0.0	0.0	0.0	0.0	0.0
a_{2u}	62.9	64.1	-4.6 (0.8)	-5.8 (1.1)	-2.8 (0.4)	-4.5 (0.8)
b_{1u}	0.0	0.0	-0.1 (0.0)	0.0	0.6	0.7
b_{2u}	0.4	0.5	0.1	0.3	1.8	1.7
e_{1u}	-11.6	-8.0	-240.8 (42.3)	-175.8 (33.8)	5.7	-6.2 (1.1)
e_{2u}	-361.5	-338.7	-272.7 (47.9)	-287.9 (55.4)	-582.3 (91.9)	-504.8 (89.4)

[a] The values in parentheses are the percentage contributions to the total attractive interactions, $\Delta E_{elstat} + \Delta E_{orb}$. The values in parentheses for the irreducible representations are the percentage contributions to the total orbital interaction, ΔE_{orb}.

Table 5-SI. The results of EDA at the PBE0/TZ2P level. All the energies are in kcal/mol.[a]

	$[C_7H_7]^+ + [E\cdots E]$		$[C_7H_7]^+ + [E\cdots E]$		$[C_7H_7]^{3-} + [E\cdots E]^{4+}$	
	$(a'_1)^2(a''_2)^2(e'_1)^0$		$(a'_1)^0(a''_2)^0(e'_1)^4$		$(a'_1)^0(a''_2)^0(e'_1)^0$	
	Ca	Sr	Ca	Sr	Ca	Sr
ΔE_{int}	-168.9	-167.7	-349.5	-349.2	-1553.6	-1462.1
ΔE_{Pauli}	769.9	708.5	1064.1	955.4	190.8	201.6
ΔE_{elstat}	-397.9 (42.4)	-368.3 (42.0)	-681.2 (48.2)	-598.7 (45.9)	-1446.5 (82.9)	-1412.1 (84.9)
ΔE_{orb}	-541.0 (57.6)	-507.9 (58.0)	-732.3 (51.8)	-705.9 (54.1)	-298.0 (17.1)	-251.5 (15.1)
a'_1	213.0	217.2	-6.3	-5.7	-22.4 (7.5)	-20.0 (8.0)
a'_2	0.0	0.0	0.0	0.0	0.0	0.0
e'_1	-11.4	-7.6	181.8	214.7	-50.7 (17.0)	-42.7 (17.0)
e'_2	-5.1	-3.3	-5.7	-4.1	-40.6 (13.6)	-33.3 (13.2)
e'_3	1.0	1.3	0.2	0.9	-21.4 (7.2)	-18.0 (7.2)
a''_1	0.0	0.0	0.0	0.0	0.0	0.0
a''_2	241.6	236.5	-5.3	-5.4	-11.3 (3.8)	-10.8 (4.3)
e''_1	-28.9	-27.1	-31.5	-33.1	-59.9 (20.1)	-56.8 (22.6)
e''_2	-951.1	-924.9	-865.4	-873.3	-91.7 (30.8)	-70.1 (27.9)
e''_3	0.0	0.0	0.0	0.0	0.0	0.0

[a]The values in parentheses are the percentage contributions to the total attractive interactions, $\Delta E_{elstat} + \Delta E_{orb}$. The values in parentheses for the irreducible representations are the percentage contributions to the total orbital interaction, ΔE_{orb}.

Table 6-SI. The results of EDA at the PBE0/TZ2P level. All the energies are in kcal/mol unit.[a]

	$[C_8H_8]^{2+} + [E\cdots E]$		$[C_8H_8]^{2+} + [E\cdots E]$		$[C_8H_8]^{2-} + [E\cdots E]^{4+}$	
	$(a_{1g})^2(a_{2u})^2(e_{1u})^0$		$(a_{1g})^0(a_{2u})^0(e_{1u})^4$		$(a_{1g})^0(a_{2u})^0(e_{1u})^0$	
	Ca	Sr	Ca	Sr	Ca	Sr
ΔE_{int}	-298.5	-311.3	-478.7	-494.0	-1077.6	-997.6
ΔE_{Pauli}	670.1	618.2	1018.0	916.1	118.2	124.0
ΔE_{elstat}	-310.0 (32.0)	-286.5 (30.8)	-667.2 (44.6)	-586.6 (41.6)	-941.6 (78.7)	-917.2 (81.8)
ΔE_{orb}	-658.6 (68.0)	-643.0 (69.2)	-829.5 (55.4)	-823.5 (58.4)	-254.1 (21.3)	-204.5 (18.2)
a_{1g}	436.4	426.7	-6.0	-5.3	-20.3 (8.0)	-16.7 (8.2)
a_{2g}	0.0	0.0	0.0	0.0	0.0	0.0
b_{1g}	0.5	0.6	0.2	0.5	-5.7 (2.2)	-4.8 (2.3)
b_{2g}	0.1	0.2	0.1	0.2	-2.6 (1.0)	-2.0 (1.0)
e_{1g}	-22.5	-20.6	-25.0	-26.2	-46.2 (18.2)	-41.8 (20.4)
e_{2g}	-4.9	-3.0	-5.4	-3.7	-36.2 (14.2)	-28.5 (13.9)
e_{3g}	0.0	0.0	0.0	0.0	0.0	0.0
a_{1u}	0.0	0.0	0.0	0.0	0.0	0.0
a_{2u}	418.0	406.1	-7.2	-6.8	-12.6 (5.0)	-10.1 (4.9)
b_{1u}	0.0	0.0	0.0	0.0	0.0	0.0
b_{2u}	0.0	0.0	0.0	0.0	0.0	0.0
e_{1u}	-10.4	-6.8	612.7	616.2	-42.4 (16.7)	-33.9 (16.6)
e_{2u}	-1476.1	-1447.0	-1398.6	-1398.8	-68.1 (26.8)	-50.2 (24.5)
e_{3u}	0.3	0.8	-0.4	0.5	-20.1 (7.9)	-16.5 (8.1)

[a]The values in parentheses are the percentage contributions to the total attractive interactions, $\Delta E_{elstat} + \Delta E_{orb}$. The values in parentheses for the irreducible representations are the percentage contributions to the total orbital interaction, ΔE_{orb}.

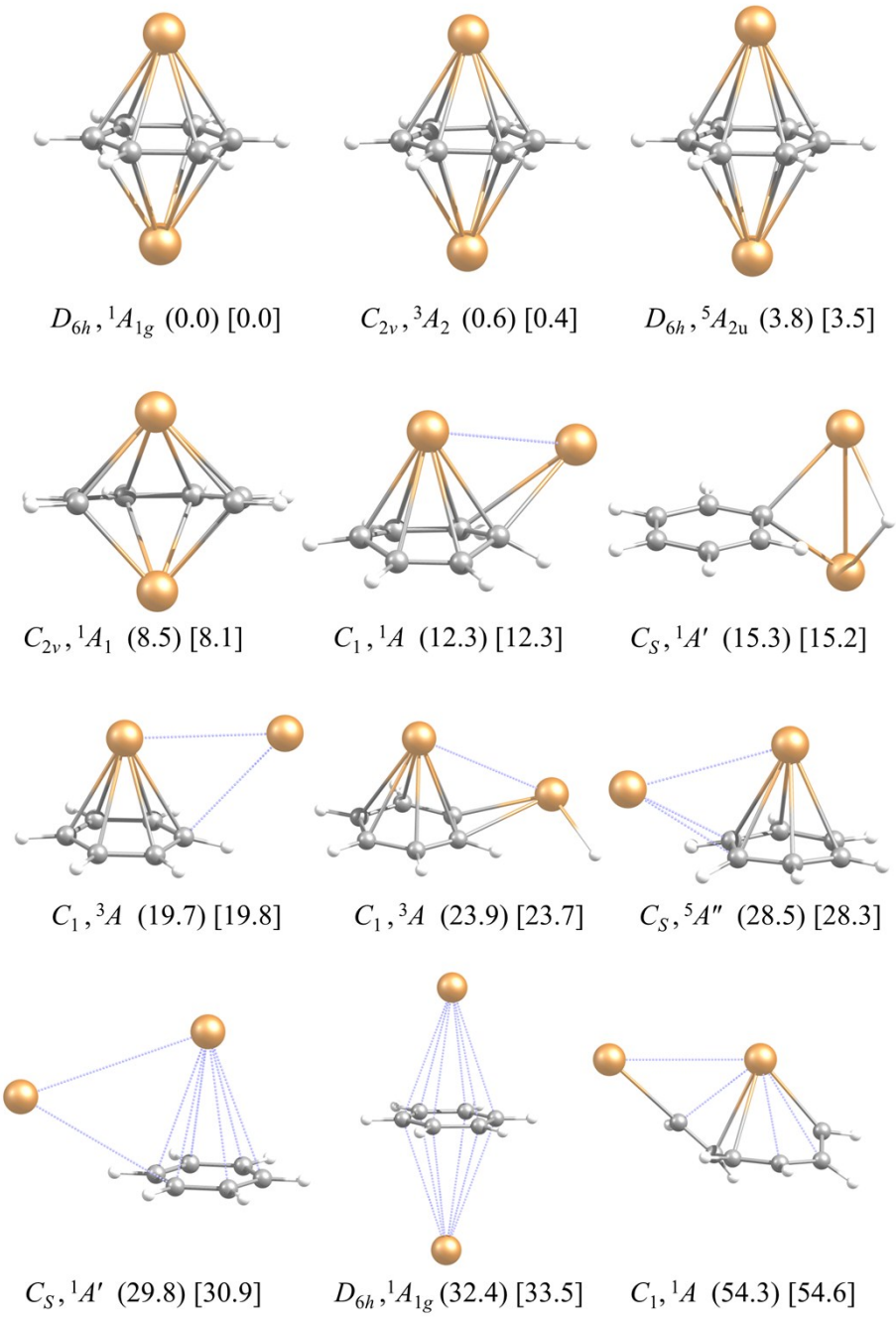

Figure 1-SI. Relative energies of the twelve low-lying energy isomers of $Ba_2(C_6H_6)$ including the ZPE correction, with respect to the lowest energy minimum (in kcal·mol^{-1}) at PBE0-D3/def2-TZVP (given in parenthesis) and PBE0-D3/def2-TZVPD levels (given in third bracket).

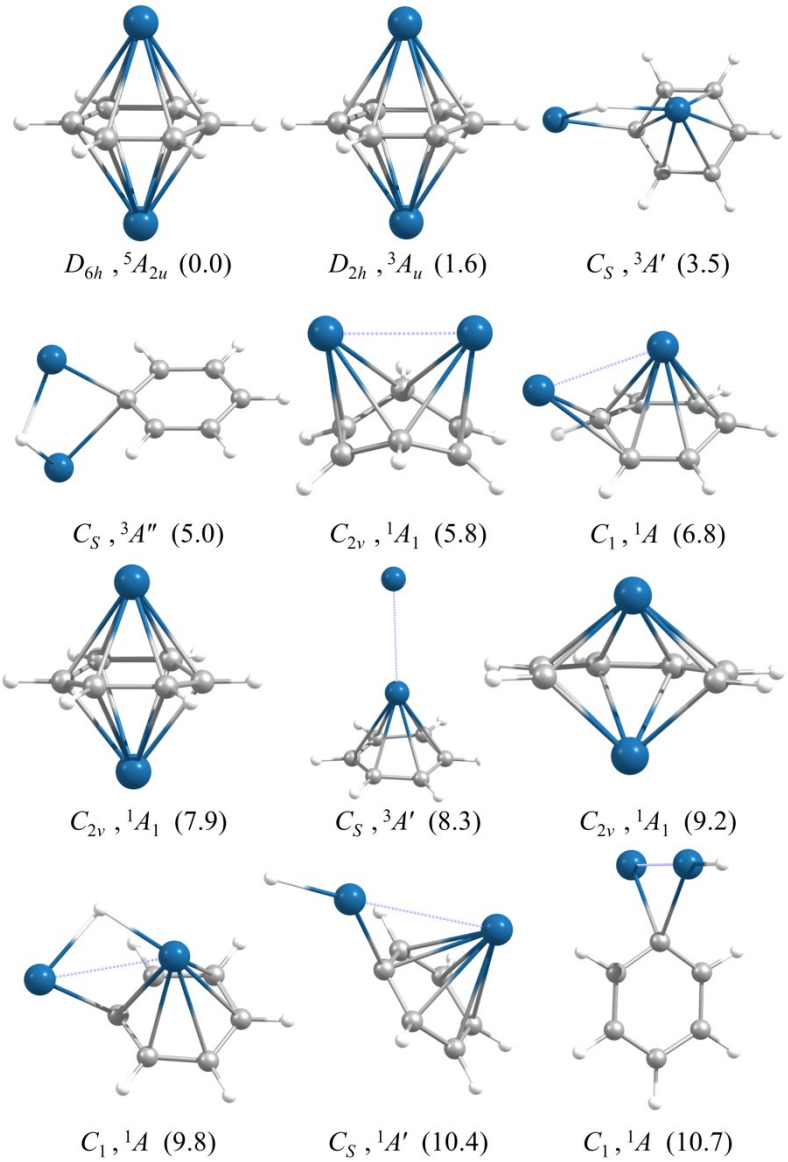

Figure 2-SI. PBE0-D3/def2-TZVP lowest energy structures of the $Ca_2(C_6H_6)$ cluster. Relative energies, including the ZPE correction, in kcal/mol with respect to the lowest energy minimum are given in parenthesis.

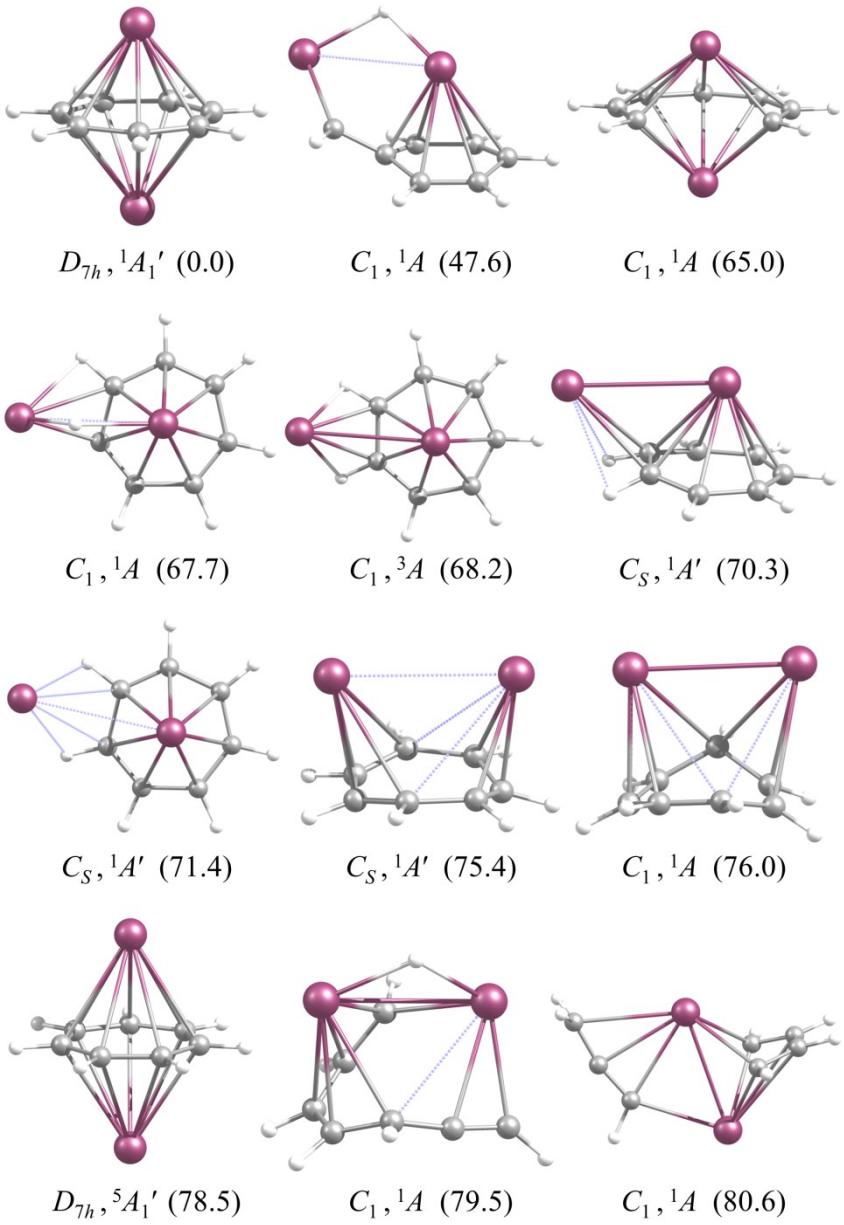

Figure 3-SI. PBE0-D3/def2-TZVP lowest energy structures of the $Sr_2(C_7H_7)^+$ cluster. Relative energies, including the ZPE correction, in kcal/mol with respect to the lowest energy minimum are given in parenthesis.

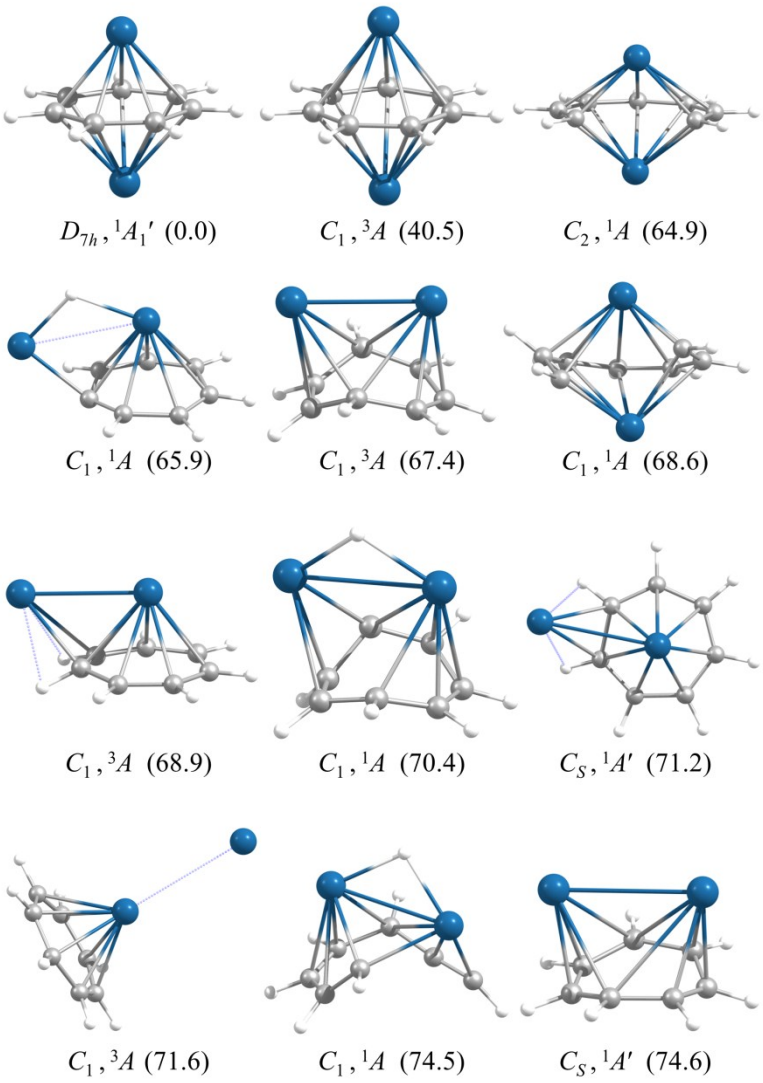

Figure 4-SI. PBE0-D3/def2-TZVP lowest energy structures of the $Ca_2(C_7H_7)^+$ cluster. Relative energies, including the ZPE correction, in kcal/mol with respect to the lowest energy minimum are given in parenthesis.

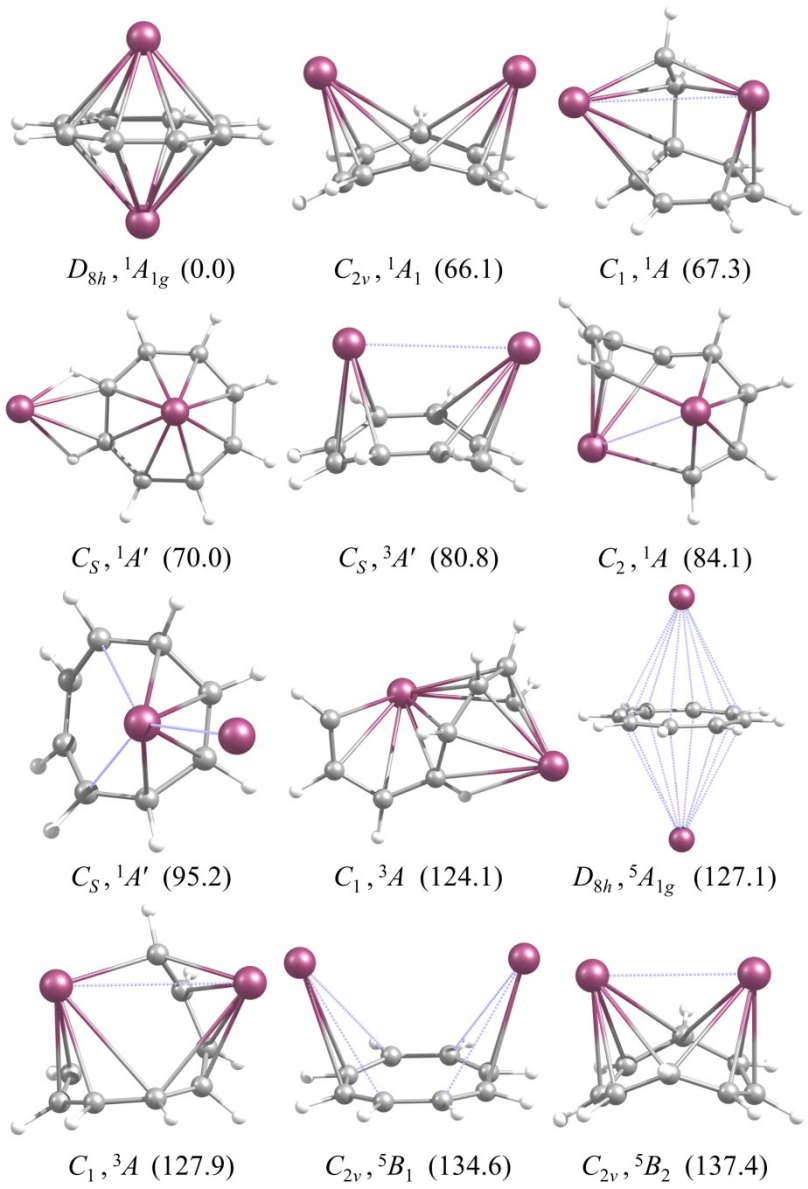

Figure 5-SI. PBE0-D3/def2-TZVP lowest energy structures of the $Sr_2(C_8H_8)^{2+}$ cluster. Relative energies, including the ZPE correction, in kcal/mol with respect to the lowest energy minimum are given in parenthesis

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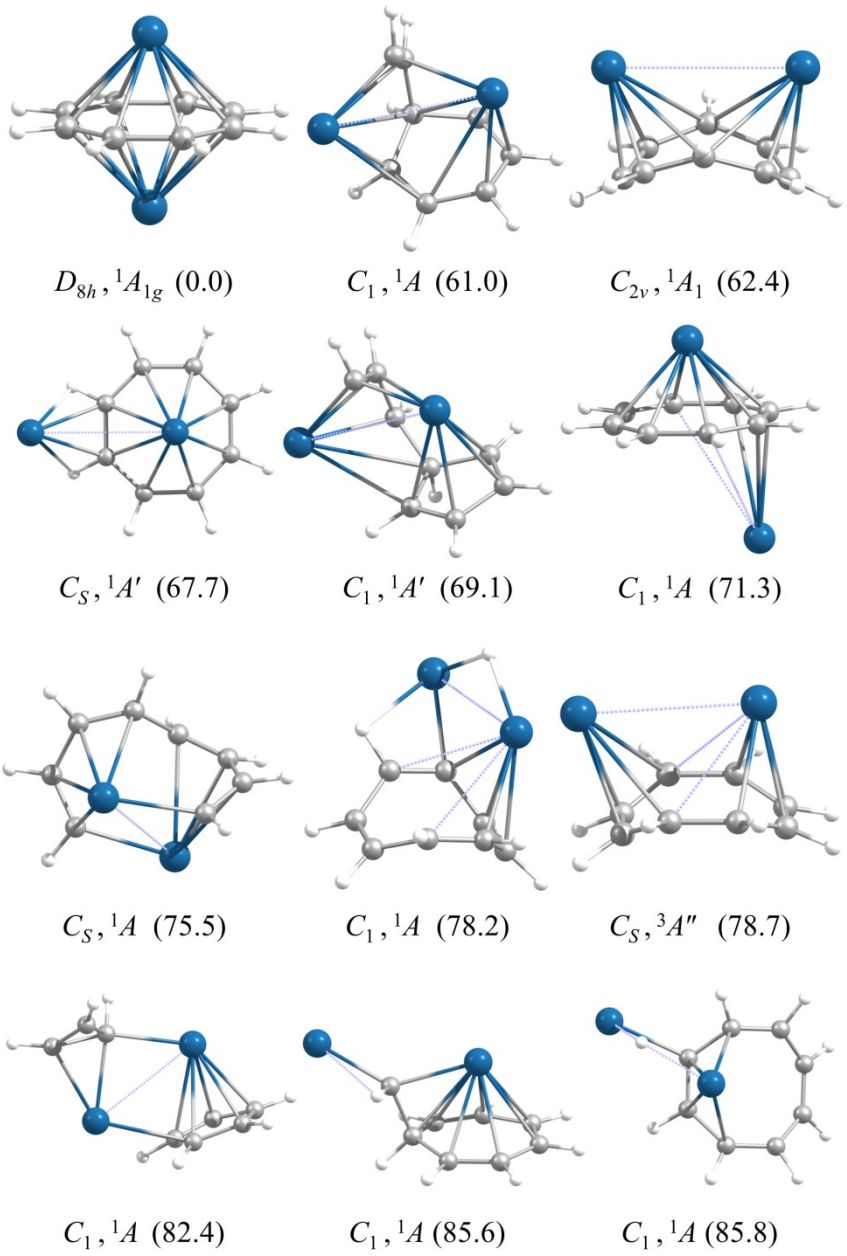

Figure 6-SI. PBE0-D3/def2-TZVP lowest energy structures of the $Ca_2(C_8H_8)^{2+}$ cluster. Relative energies, including the ZPE correction, in kcal/mol with respect to the lowest energy minimum are given in parenthesis.

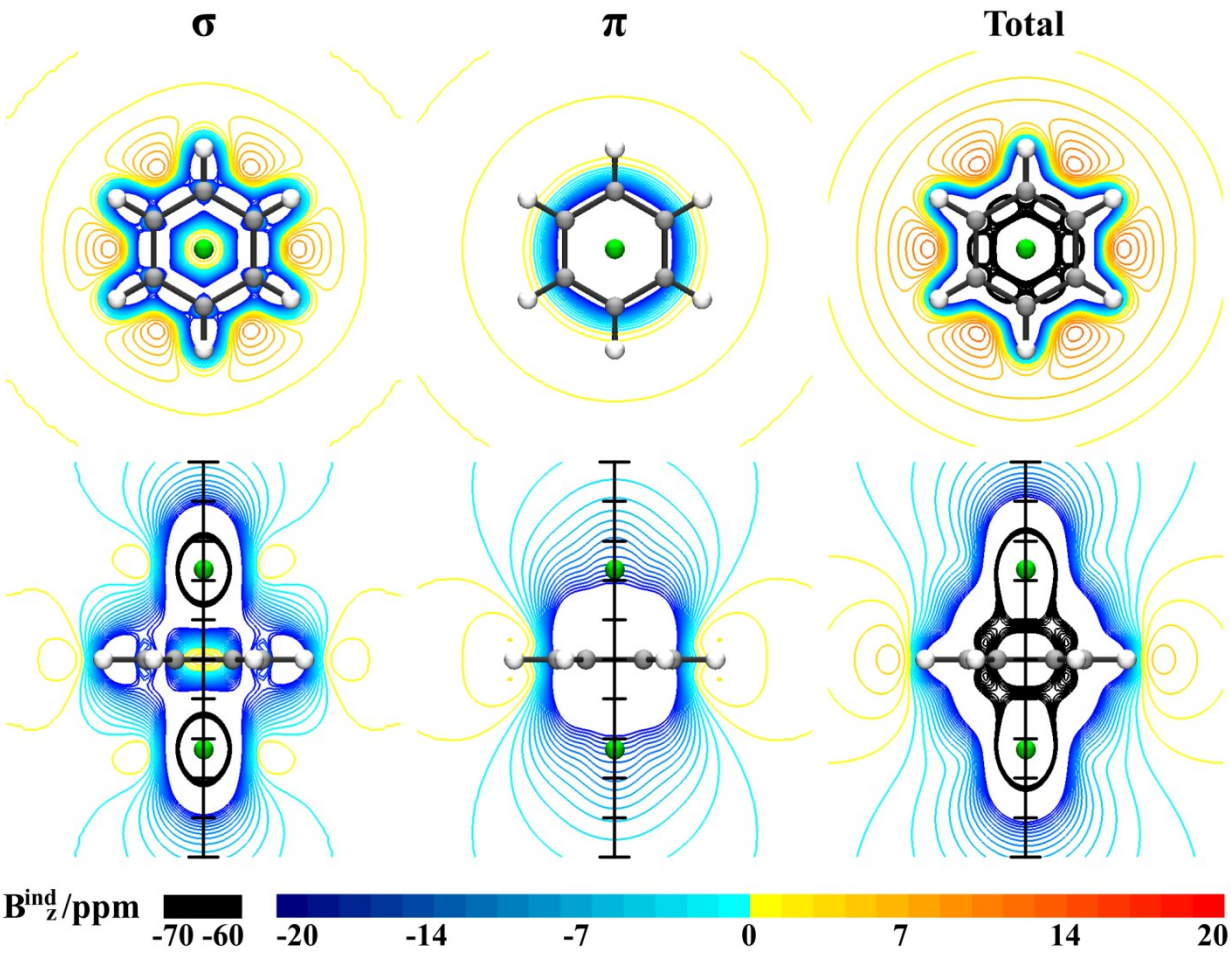

Figure 7-SI. The induced magnetic field of the [Ba-(C_6H_6)-Ba] complex. Blue and red areas denote diatropic and paratropic regions, respectively. The induced magnetic field is given in ppm, which is equivalent to μT.

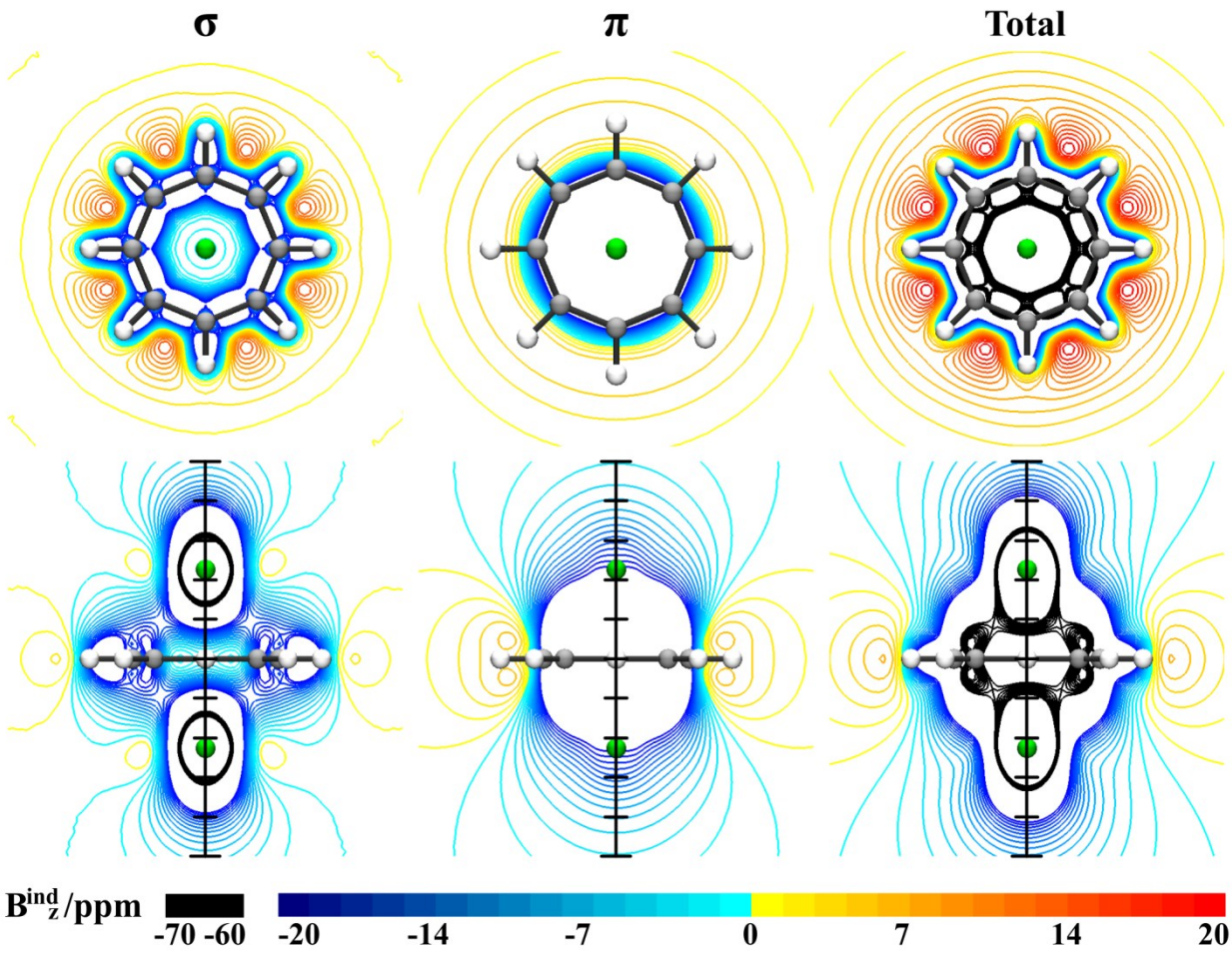

Figure 8-SI. The induced magnetic field of the [Ba-(C_8H_8)-Ba]$^{2+}$ complex. Blue and red areas denote diatropic and paratropic regions, respectively. The induced magnetic field is given in ppm, which is equivalent to μT.

Cartesian Coordinates of all the optimized structures computed at PBE0-D3/def2-TZVP level.

$Ba_2C_6H_6$ D_{6h} (0.00)

Ba	0.000000000	0.000000000	2.275110000
C	0.000000000	1.457598000	0.000000000
C	1.262317000	0.728799000	0.000000000
C	1.262317000	-0.728799000	0.000000000
C	0.000000000	-1.457598000	0.000000000
C	-1.262317000	-0.728799000	0.000000000
C	-1.262317000	0.728799000	0.000000000
H	0.000000000	2.541484000	0.000000000
H	2.200990000	1.270742000	0.000000000
H	2.200990000	-1.270742000	0.000000000
H	0.000000000	-2.541484000	0.000000000
H	-2.200990000	-1.270742000	0.000000000
H	-2.200990000	1.270742000	0.000000000
Ba	0.000000000	0.000000000	-2.275110000

$Ba_2C_6H_6$ C_{2v} (0.6)

Ba	0.000000000	0.000000000	2.419303000
C	1.254346000	0.706882000	-0.032408000
C	1.254346000	-0.706882000	-0.032408000
C	0.000000000	-1.448023000	-0.077055000
C	-1.254346000	-0.706882000	-0.032408000
C	-1.254346000	0.706882000	-0.032408000
C	0.000000000	1.448023000	-0.077055000
H	2.194167000	1.246329000	-0.007538000
H	2.194167000	-1.246329000	-0.007538000
H	0.000000000	-2.526940000	0.001843000
H	-2.194167000	-1.246329000	-0.007538000
H	-2.194167000	1.246329000	-0.007538000
H	0.000000000	2.526940000	0.001843000
Ba	0.000000000	0.000000000	-2.388430000

$Ba_2C_6H_6$ D_{6h} (3.8)

C	0.000000000	1.425818000	0.000000000
C	-1.234795000	0.712909000	0.000000000
C	-1.234795000	-0.712909000	0.000000000
C	0.000000000	-1.425818000	0.000000000
C	1.234795000	-0.712909000	0.000000000
C	1.234795000	0.712909000	0.000000000
H	0.000000000	2.508550000	0.000000000
H	-2.172468000	1.254275000	0.000000000

H	-2.172468000	-1.254275000	0.000000000
H	0.000000000	-2.508550000	0.000000000
H	2.172468000	-1.254275000	0.000000000
H	2.172468000	1.254275000	0.000000000
Ba	0.000000000	0.000000000	2.562684000
Ba	0.000000000	0.000000000	-2.562684000

$Ba_2C_6H_6$ C_{2v} (8.5)

Ba	-1.937059000	0.000000000	-0.241729000
Ba	1.937059000	0.000000000	-0.241729000
C	0.000000000	1.795720000	0.742054000
C	0.000000000	1.692353000	-0.661865000
C	0.000000000	-1.692353000	-0.661865000
C	0.000000000	-1.795720000	0.742054000
C	0.000000000	-0.735801000	1.706722000
C	0.000000000	0.735801000	1.706722000
H	0.000000000	2.768286000	1.245856000
H	0.000000000	2.670594000	-1.157721000
H	0.000000000	-2.670594000	-1.157721000
H	0.000000000	-2.768286000	1.245856000
H	0.000000000	-1.105788000	2.727255000
H	0.000000000	1.105788000	2.727255000

$Ba_2C_6H_6$ C_1 (12.3)

Ba	-2.301783000	0.014608000	-0.003269000
C	1.425487000	1.546427000	-1.361508000
C	0.206290000	1.596504000	-0.722507000
C	0.094123000	1.328215000	0.743219000
C	1.385379000	1.421217000	1.418181000
C	2.573783000	1.326544000	0.757316000
C	2.625797000	1.215698000	-0.691203000
H	1.455552000	1.758010000	-2.426347000
H	-0.617760000	2.033313000	-1.281595000
H	-0.692916000	1.889367000	1.265925000
H	1.389756000	1.549364000	2.496274000
H	3.500004000	1.369960000	1.321142000
H	3.573601000	1.306510000	-1.204327000
Ba	1.257615000	-1.095218000	-0.015161000

$Ba_2C_6H_6$ C_S (15.3)

C	1.174471000	3.262700000	0.000000000
C	0.003766000	4.007977000	0.000000000
C	-1.221489000	3.355816000	0.000000000
C	-1.263876000	1.964929000	0.000000000

C	-0.107509000	1.165491000	0.000000000
C	1.108610000	1.872662000	0.000000000
H	2.136925000	3.765705000	0.000000000
H	0.045711000	5.091921000	0.000000000
H	-2.141829000	3.932241000	0.000000000
H	-2.244040000	1.485879000	0.000000000
H	1.572141000	-1.246185000	0.000000000
H	2.045455000	1.312901000	0.000000000
Ba	0.003766000	-0.965356000	1.804648000
Ba	0.003766000	-0.965356000	-1.804648000

$Ba_2C_6H_6$ C_1 (19.7)

C	2.614701000	1.031243000	1.218530000
C	1.319805000	1.550983000	1.223916000
C	0.632089000	1.785684000	0.000958000
C	1.318256000	1.551681000	-1.222944000
C	2.613083000	1.031747000	-1.219525000
C	3.279967000	0.752143000	-0.000962000
H	3.127661000	0.870493000	2.160334000
H	0.844525000	1.801720000	2.164486000
H	-0.267145000	2.393072000	0.001716000
H	0.841825000	1.803043000	-2.162770000
H	3.124808000	0.871446000	-2.162072000
H	4.310099000	0.419633000	-0.001704000
Ba	-2.574875000	0.137917000	0.000002000
Ba	1.098997000	-1.108994000	0.000001000

$Ba_2C_6H_6$ C_1 (23.9)

Ba	-1.705220000	-1.023299000	-0.026341000
C	0.194499000	1.132559000	0.509432000
C	-0.879814000	1.349590000	1.403956000
C	-2.161164000	1.771668000	0.945982000
C	-2.407373000	1.878082000	-0.413349000
C	-1.400518000	1.577512000	-1.346101000
C	-0.101765000	1.257179000	-0.853906000
H	3.265499000	0.604843000	-2.010464000
H	-0.716900000	1.277553000	2.475858000
H	-2.948194000	2.014849000	1.653599000
H	-3.388399000	2.185954000	-0.761464000
H	-1.584747000	1.697313000	-2.407667000
H	0.685026000	1.132363000	-1.612900000
Ba	2.512801000	-0.096565000	0.047536000

$Ba_2C_6H_6$ C_S (28.5)

Ba	1.154526000	1.352030000	0.000000000
C	-1.469654000	0.213374000	0.708781000
C	-1.469654000	0.213374000	-0.708781000
C	-1.363455000	1.441647000	-1.410737000
C	-1.363455000	2.661624000	-0.699819000
C	-1.363455000	2.661624000	0.699819000
C	-1.363455000	1.441647000	1.410737000
H	-1.801023000	-0.661505000	1.272813000
H	-1.801023000	-0.661505000	-1.272813000
H	-1.380719000	1.440354000	-2.493291000
H	-1.380047000	3.599293000	-1.242622000
H	-1.380047000	3.599293000	1.242622000
H	-1.380719000	1.440354000	2.493291000
Ba	-0.092342000	-2.433388000	0.000000000

$Ba_2C_6H_6$ C_S (29.8)

C	-2.336576000	-3.107993000	0.694677000
C	-2.336576000	-3.107993000	-0.694677000
C	-2.336576000	-1.904031000	-1.389989000
C	-2.338244000	-0.701524000	-0.694510000
C	-2.338244000	-0.701524000	0.694510000
C	-2.336576000	-1.904031000	1.389989000
H	-2.335473000	-4.046887000	1.236287000
H	-2.335473000	-4.046887000	-1.236287000
H	-2.334451000	-1.903330000	-2.473888000
H	-2.333401000	0.240358000	-1.233342000
H	-2.333401000	0.240358000	1.233342000
H	-2.334451000	-1.903330000	2.473888000
Ba	1.513502000	-1.858612000	0.000000000
Ba	0.239059000	3.286867000	0.000000000

$Ba_2C_6H_6$ D_{6h} (32.4)

C	0.000000000	1.390447000	0.000000000
C	1.204162000	0.695223000	0.000000000
C	1.204162000	-0.695223000	0.000000000
C	0.000000000	-1.390447000	0.000000000
C	-1.204162000	-0.695223000	0.000000000
C	-1.204162000	0.695223000	0.000000000
H	0.000000000	2.474149000	0.000000000
H	2.142676000	1.237075000	0.000000000
H	2.142676000	-1.237075000	0.000000000
H	0.000000000	-2.474149000	0.000000000
H	-2.142676000	-1.237075000	0.000000000

H	-2.142676000	1.237075000	0.000000000
Ba	0.000000000	0.000000000	3.937421000
Ba	0.000000000	0.000000000	-3.937421000

$Ba_2C_6H_6$ C_1 (54.3)

Ba	-2.711816000	0.104348000	-0.062798000
Ba	1.263321000	-1.082869000	-0.071174000
C	-0.424797000	1.046636000	0.998486000
C	0.766480000	1.660676000	0.792608000
C	1.301755000	1.888048000	-0.553229000
C	2.593846000	1.730336000	-0.931978000
C	3.651854000	1.165045000	-0.110585000
C	3.426118000	0.194122000	0.810902000
H	-0.650344000	0.962323000	2.081518000
H	1.437169000	1.972778000	1.598284000
H	0.588472000	2.221388000	-1.303310000
H	2.861466000	2.053539000	-1.937804000
H	4.651080000	1.556327000	-0.334423000
H	4.336380000	-0.078381000	1.360953000

$Ba_2C_7H_7^+$ D_{7h} (0.0)

Ba	0.000000000	0.000000000	2.232545000
C	0.000000000	1.651026000	0.000000000
C	1.290824000	1.029398000	0.000000000
C	1.609632000	-0.367388000	0.000000000
C	-1.290824000	1.029398000	0.000000000
C	0.716353000	-1.487523000	0.000000000
C	-1.609632000	-0.367388000	0.000000000
C	-0.716353000	-1.487523000	0.000000000
H	0.000000000	2.735151000	0.000000000
H	2.138427000	1.705338000	0.000000000
H	2.666575000	-0.608628000	0.000000000
H	-2.138427000	1.705338000	0.000000000
H	1.186737000	-2.464285000	0.000000000
H	-2.666575000	-0.608628000	0.000000000
H	-1.186737000	-2.464285000	0.000000000
Ba	0.000000000	0.000000000	-2.232545000

$Ba_2C_7H_7^+$ C_1 (46.9)

Ba	-2.398242000	0.000076000	0.000031000
C	-0.073914000	0.314805000	-1.612242000
C	-0.078935000	1.471987000	-0.730554000
C	-0.064250000	1.494136000	0.666152000
C	-0.065033000	-1.035980000	-1.268967000

C	-0.098843000	0.394515000	1.594617000
C	-0.095226000	-1.642630000	0.042644000
C	-0.063194000	-0.992629000	1.295612000
H	-0.048794000	0.540286000	-2.671714000
H	-0.050997000	2.434431000	-1.226776000
H	-0.042866000	2.478896000	1.120492000
H	-0.040917000	-1.734247000	-2.098298000
H	-0.068893000	0.659680000	2.643536000
H	-0.066698000	-2.724602000	0.061848000
H	-0.042780000	-1.650104000	2.158687000
Ba	2.462498000	-0.000604000	0.001552000

$Ba_2C_7H_7^+$ C_{2v} (68.3)

Ba	1.938999000	0.000000000	-0.270682000
Ba	-1.938999000	0.000000000	-0.270682000
C	0.000000000	0.000000000	1.999851000
C	0.000000000	1.359633000	1.587181000
C	0.000000000	2.150664000	0.367492000
C	0.000000000	-1.359633000	1.587181000
C	0.000000000	1.690909000	-0.919399000
C	0.000000000	-2.150664000	0.367492000
C	0.000000000	-1.690909000	-0.919399000
H	0.000000000	0.000000000	3.085871000
H	0.000000000	1.999129000	2.462692000
H	0.000000000	3.217042000	0.609750000
H	0.000000000	-1.999129000	2.462692000
H	0.000000000	2.488907000	-1.668404000
H	0.000000000	-3.217042000	0.609750000
H	0.000000000	-2.488907000	-1.668404000

$Ba_2C_7H_7^+$ C_1 (73.3)

Ba	2.542179000	0.030702000	0.004118000
C	-2.860993000	1.460890000	0.365305000
C	-2.052322000	1.390996000	1.445411000
C	-0.603809000	1.141466000	1.506567000
C	-2.494005000	1.408086000	-1.065937000
C	0.298311000	1.172765000	0.465449000
C	-1.244413000	1.363159000	-1.598703000
C	0.014717000	1.123566000	-0.928529000
H	-3.910560000	1.662451000	0.552516000
H	-2.538107000	1.530523000	2.408532000
H	-0.213406000	1.102219000	2.520510000
H	-3.316319000	1.561424000	-1.755406000
H	0.956360000	-1.734553000	0.161287000

H	-1.191762000	1.462546000	-2.681794000
H	0.859046000	1.246123000	-1.627473000
Ba	-1.417003000	-1.123493000	-0.016896000

$Ba_2C_7H_7^+$ C_S (74.8)

Ba	-0.241349000	-2.126379000	0.000000000
C	1.396621000	1.524720000	1.247372000
C	1.396621000	0.130868000	1.500827000
C	2.107219000	-0.832930000	0.687134000
C	1.494762000	2.170184000	0.000000000
C	2.107219000	-0.832930000	-0.687134000
C	1.396621000	1.524720000	-1.247372000
C	1.396621000	0.130868000	-1.500827000
H	1.324998000	2.168838000	2.123658000
H	1.331853000	-0.122415000	2.556257000
H	2.697610000	-1.583543000	1.212560000
H	1.609617000	3.250891000	0.000000000
H	2.697610000	-1.583543000	-1.212560000
H	1.324998000	2.168838000	-2.123658000
H	1.331853000	-0.122415000	-2.556257000
Ba	-1.188877000	1.642992000	0.000000000

$Ba_2C_7H_7^+$ C_S (75.6)

C	-1.226651000	0.990989000	1.586053000
C	-1.175534000	-0.166187000	0.747593000
C	-1.175534000	-0.166187000	-0.747593000
C	-1.175534000	2.347130000	1.268853000
C	-1.226651000	0.990989000	-1.586053000
C	-1.097798000	2.968260000	0.000000000
C	-1.175534000	2.347130000	-1.268853000
H	-1.277204000	0.765875000	2.647677000
H	-1.759022000	-0.977353000	1.208393000
H	-1.759022000	-0.977353000	-1.208393000
H	-1.162557000	3.020126000	2.120656000
H	-1.277204000	0.765875000	-2.647677000
H	-1.076822000	4.052112000	0.000000000
H	-1.162557000	3.020126000	-2.120656000
Ba	-0.028683000	-2.497397000	0.000000000
Ba	1.082144000	1.327002000	0.000000000

$Ba_2C_7H_7^+$ C_1 (78.7)

C	-1.406087000	1.747946000	-0.717540000
C	-1.405934000	1.747775000	0.717957000
C	-0.331622000	1.441623000	1.547336000

C	-0.332002000	1.441854000	-1.547214000
C	1.075062000	1.570177000	1.256941000
C	1.074767000	1.570187000	-1.257082000
C	1.622987000	1.862802000	-0.000142000
H	-2.347019000	1.989312000	-1.217541000
H	-2.346763000	1.988999000	1.218221000
H	-0.564846000	1.358531000	2.606383000
H	-0.565457000	1.358987000	-2.606227000
H	1.703740000	1.751911000	2.126514000
H	1.703295000	1.751828000	-2.126782000
H	2.668044000	2.185071000	-0.000270000
Ba	2.117727000	-0.743564000	-0.000018000
Ba	-2.154049000	-0.697129000	-0.000015000

$Ba_2C_7H_7^+$ C_1 (89.9)

C	0.495440000	1.279808000	-0.802279000
C	-0.711840000	1.766400000	-1.208913000
C	-1.799312000	2.080655000	-0.325202000
C	0.289026000	-1.022347000	1.089618000
C	-1.958067000	1.703795000	1.010856000
C	-0.412351000	-0.264876000	2.024949000
C	-1.411582000	0.768316000	1.935041000
H	0.501682000	1.389161000	0.311543000
H	-0.913418000	1.890285000	-2.277600000
H	-2.572076000	2.741896000	-0.707389000
H	0.909933000	-1.770062000	1.619446000
H	-2.803844000	2.213395000	1.466540000
H	-0.308266000	-0.565037000	3.069746000
H	-1.912440000	0.870971000	2.892801000
Ba	-1.781340000	-0.762586000	-0.425214000
Ba	2.498314000	-0.034577000	-0.087635000

$Ba_2C_7H_7^+$ C_S (90.4)

C	3.319886000	-0.359579000	1.601766000
C	3.458767000	-1.501416000	0.673434000
C	3.458767000	-1.501416000	-0.673434000
C	3.319886000	0.968055000	1.266872000
C	3.319886000	-0.359579000	-1.601766000
C	3.142268000	1.600915000	0.000000000
C	3.319886000	0.968055000	-1.266872000
H	3.426723000	-0.604210000	2.651269000
H	3.622288000	-2.459614000	1.156383000
H	3.622288000	-2.459614000	-1.156383000
H	3.365433000	1.654075000	2.109861000

H	3.426723000	-0.604210000	-2.651269000
H	3.170708000	2.682623000	0.000000000
H	3.365433000	1.654075000	-2.109861000
Ba	-3.849157000	0.134443000	0.000000000
Ba	0.919948000	-0.112181000	0.000000000

$Ba_2C_7H_7^+$ D_{7h} (91.2)

Ba	0.000000000	0.000000000	2.680382000
Ba	0.000000000	0.000000000	-2.680382000
C	0.000000000	1.626054000	0.000000000
C	-1.271300000	1.013828000	0.000000000
C	-1.585285000	-0.361831000	0.000000000
C	1.271300000	1.013828000	0.000000000
C	-0.705518000	-1.465024000	0.000000000
C	1.585285000	-0.361831000	0.000000000
C	0.705518000	-1.465024000	0.000000000
H	0.000000000	2.710037000	0.000000000
H	-2.118792000	1.689680000	0.000000000
H	-2.642091000	-0.603040000	0.000000000
H	2.118792000	1.689680000	0.000000000
H	-1.175841000	-2.441659000	0.000000000
H	2.642091000	-0.603040000	0.000000000
H	1.175841000	-2.441659000	0.000000000

$Ba_2C_7H_7^+$ C_1 (101.5)

C	3.428920000	0.879992000	-0.000143000
C	2.831752000	0.999176000	-1.270119000
C	1.497546000	1.318779000	-1.586821000
C	2.831969000	0.999140000	1.269936000
C	0.444638000	1.631606000	-0.702217000
C	1.497815000	1.318721000	1.586880000
C	0.444749000	1.631564000	0.702470000
H	4.490338000	0.656038000	-0.000238000
H	3.493915000	0.855050000	-2.117279000
H	1.266435000	1.395567000	-2.643610000
H	3.494277000	0.854985000	2.116978000
H	-0.477579000	1.967424000	-1.176826000
H	1.266883000	1.395455000	2.643712000
H	-0.477391000	1.967346000	1.177251000
Ba	-2.943282000	0.056682000	0.000000000
Ba	1.319689000	-1.159641000	0.000002000

$Ba_2C_7H_7^+$ C_S (108.9)

Ba	2.342424000	-0.433350000	-0.145843000

Ba	-2.004617000	-0.828707000	-0.061178000
C	1.145165000	1.918577000	0.408739000
C	0.736292000	1.112983000	1.519948000
C	0.288093000	-0.196770000	1.412908000
C	0.554213000	1.811199000	-0.897075000
C	-2.977855000	1.475899000	0.174353000
C	-0.789281000	1.623369000	-1.103698000
C	-1.775399000	2.026230000	-0.074735000
H	1.819959000	2.753804000	0.593089000
H	0.975487000	1.530406000	2.502327000
H	0.156576000	-0.669354000	2.396718000
H	1.177267000	2.000621000	-1.782176000
H	-3.590663000	2.036059000	0.884241000
H	-1.141662000	1.502367000	-2.128534000
H	-1.401478000	2.892351000	0.484862000

$Ba_2C_8H_8^{2+}$ ***D_{8h}*** (0.00)

Ba	0.000000000	0.000000000	-2.258669000
Ba	0.000000000	0.000000000	2.258680000
C	0.000000000	1.847462000	-0.000010000
C	-1.306353000	1.306353000	-0.000010000
C	-1.306353000	-1.306353000	-0.000010000
C	1.306353000	1.306353000	-0.000010000
C	0.000000000	-1.847462000	-0.000010000
C	1.847462000	0.000000000	-0.000010000
C	1.306353000	-1.306353000	-0.000010000
H	0.000000000	2.932144000	-0.000010000
H	-2.073339000	2.073339000	-0.000010000
H	-2.073339000	-2.073339000	-0.000010000
H	2.073339000	2.073339000	-0.000010000
H	0.000000000	-2.932144000	-0.000010000
H	2.932144000	0.000000000	-0.000010000
H	2.073339000	-2.073339000	-0.000010000
C	-1.847462000	0.000000000	-0.000010000
H	-2.932144000	0.000000000	-0.000010000

$Ba_2C_8H_8^{2+}$ ***C_{2v}*** **(66.0)**

Ba	0.000000000	2.439275000	-0.750532000
C	-1.267487000	1.283642000	1.486902000
C	-1.723563000	0.000000000	1.110443000
C	0.000000000	-1.756797000	1.854338000
C	0.000000000	1.756797000	1.854338000
C	1.267487000	-1.283642000	1.486902000
C	1.267487000	1.283642000	1.486902000

C	1.723563000	0.000000000	1.110443000
H	-2.085457000	1.991459000	1.633920000
H	-2.766451000	0.000000000	0.801048000
H	0.000000000	-2.739417000	2.329374000
H	0.000000000	2.739417000	2.329374000
H	2.085457000	-1.991459000	1.633920000
H	2.085457000	1.991459000	1.633920000
H	2.766451000	0.000000000	0.801048000
C	-1.267487000	-1.283642000	1.486902000
H	-2.085457000	-1.991459000	1.633920000
Ba	0.000000000	-2.439275000	-0.750532000

$Ba_2C_8H_8^{2+}$ C_S (77.1)

Ba	-1.085129000	1.568933000	0.000000000
C	1.060361000	0.608281000	1.711791000
C	1.128249000	2.003052000	1.699633000
C	1.230752000	2.987781000	-0.699496000
C	1.092268000	-0.399128000	0.719941000
C	1.128249000	2.003052000	-1.699633000
C	1.092268000	-0.399128000	-0.719941000
C	1.060361000	0.608281000	-1.711791000
H	1.026545000	0.198554000	2.716606000
H	1.100141000	2.423957000	2.699749000
H	1.299607000	3.987935000	-1.115395000
H	1.534386000	-1.298193000	1.176303000
H	1.100141000	2.423957000	-2.699749000
H	1.534386000	-1.298193000	-1.176303000
H	1.026545000	0.198554000	-2.716606000
C	1.230752000	2.987781000	0.699496000
H	1.299607000	3.987935000	1.115395000
Ba	-0.058816000	-2.872939000	0.000000000

$Ba_2C_8H_8^{2+}$ C_1 (79.3)

Ba	3.192122000	-0.033049000	0.000058000
Ba	-2.699549000	-0.322441000	0.000277000
C	-1.042444000	2.105730000	-0.119212000
C	-0.899635000	1.651427000	1.239677000
C	-0.112088000	-0.823072000	1.363891000
C	-0.865921000	1.539593000	-1.359581000
C	0.062106000	-1.398185000	0.116044000
C	-0.453326000	0.246892000	-1.838579000
C	-0.081769000	-0.942219000	-1.244392000
H	-1.373541000	3.138310000	-0.166417000
H	-1.152267000	2.428375000	1.954302000

H	0.077989000	-1.515098000	2.179175000
H	-1.086217000	2.220822000	-2.175243000
H	0.345083000	-2.446595000	0.166437000
H	-0.450078000	0.197271000	-2.923019000
H	0.134292000	-1.729099000	-1.961179000
C	-0.528121000	0.469822000	1.839407000
H	-0.552145000	0.513495000	2.923627000

$Ba_2C_8H_8^{2+}$ C_S (86.9)

C	1.658530000	2.335418000	0.686355000
C	1.658530000	2.335418000	-0.686355000
C	1.360142000	-0.042032000	-1.637917000
C	1.288248000	1.333484000	1.647819000
C	1.926745000	-0.960372000	-0.685996000
C	1.360142000	-0.042032000	1.637917000
C	1.926745000	-0.960372000	0.685996000
H	1.923985000	3.286402000	1.141071000
H	1.923985000	3.286402000	-1.141071000
H	1.169549000	-0.487342000	-2.612749000
H	1.047071000	1.747427000	2.626248000
H	2.452314000	-1.793658000	-1.157670000
H	1.169549000	-0.487342000	2.612749000
H	2.452314000	-1.793658000	1.157670000
C	1.288248000	1.333484000	-1.647819000
H	1.047071000	1.747427000	-2.626248000
Ba	-0.457887000	-2.515282000	0.000000000
Ba	-1.113360000	1.845574000	0.000000000

$Ba_2C_8H_8^{2+}$ C_2 (93.6)

Ba	2.022047000	0.129537000	-0.615737000
C	-0.085552000	1.857721000	-0.239717000
C	-0.712737000	2.252633000	0.896734000
C	-0.712737000	0.181081000	2.312916000
C	0.085552000	-1.857721000	-0.239717000
C	0.712737000	-0.181081000	2.312916000
C	0.712737000	-2.252633000	0.896734000
C	1.285109000	-1.313964000	1.863949000
H	0.214623000	2.731015000	-0.840222000
H	-0.925711000	3.303575000	1.105725000
H	-1.312259000	-0.468014000	2.953775000
H	-0.214623000	-2.731015000	-0.840222000
H	1.312259000	0.468014000	2.953775000
H	0.925711000	-3.303575000	1.105725000
H	2.274379000	-1.556929000	2.258688000

C	-1.285109000	1.313964000	1.863949000
H	-2.274379000	1.556929000	2.258688000
Ba	-2.022047000	-0.129537000	-0.615737000

$Ba_2C_8H_8^{2+}$ C_1 (96.3)

Ba	1.192846000	-1.674396000	-0.154820000
C	-0.168653000	0.961548000	0.161250000
C	0.485141000	0.907426000	-1.148261000
C	2.296157000	2.636675000	-0.916558000
C	0.482818000	0.837864000	1.341338000
C	2.928240000	2.470343000	0.243987000
C	1.916841000	0.609837000	1.606375000
C	2.964732000	1.284970000	1.101054000
H	-1.206671000	-1.547173000	-0.317075000
H	-0.051223000	0.328024000	-1.916294000
H	2.446855000	3.576191000	-1.442437000
H	-0.099699000	0.858790000	2.268214000
H	3.557285000	3.283324000	0.599975000
H	2.144935000	-0.073984000	2.430542000
H	3.950174000	1.033210000	1.490393000
C	1.504295000	1.645321000	-1.639306000
H	1.689235000	1.599235000	-2.711309000
Ba	-2.744423000	0.296154000	0.067297000

$Ba_2C_8H_8^{2+}$ C_{2v} (98.5)

Ba	0.000000000	2.065655000	-0.770031000
C	-1.247444000	1.221483000	1.585939000
C	-1.547694000	0.000000000	0.835177000
C	0.000000000	-1.673486000	2.017735000
C	0.000000000	1.673486000	2.017735000
C	1.247444000	-1.221483000	1.585939000
C	1.247444000	1.221483000	1.585939000
C	1.547694000	0.000000000	0.835177000
H	-2.106591000	1.813305000	1.898392000
H	-2.589809000	0.000000000	0.515045000
H	0.000000000	-2.549493000	2.661149000
H	0.000000000	2.549493000	2.661149000
H	2.106591000	-1.813305000	1.898392000
H	2.106591000	1.813305000	1.898392000
H	2.589809000	0.000000000	0.515045000
C	-1.247444000	-1.221483000	1.585939000
H	-2.106591000	-1.813305000	1.898392000
Ba	0.000000000	-2.065655000	-0.770031000

$Ba_2C_8H_8^{2+}$ C_1 (135.3)

Ba	-2.636673000	-0.162879000	0.054954000
Ba	2.612818000	-0.124377000	-0.077796000
C	0.162958000	-0.114355000	-1.665608000
C	0.079432000	-1.301114000	-0.827048000
C	0.189210000	-0.488099000	1.646165000
C	-0.696830000	1.041715000	-1.498252000
C	0.581158000	0.870453000	1.665294000
C	-0.666991000	1.859027000	-0.287230000
C	0.515450000	1.822977000	0.568602000
H	0.405906000	-0.342226000	-2.701684000
H	0.092581000	-2.253746000	-1.352846000
H	0.147819000	-0.949753000	2.628962000
H	-0.958289000	1.570724000	-2.414413000
H	0.770620000	1.289844000	2.651425000
H	-1.190129000	2.815198000	-0.341676000
H	1.037192000	2.767637000	0.722394000
C	0.023273000	-1.418719000	0.589703000
H	-0.095815000	-2.442608000	0.937218000

$Ba_2C_8H_8^{2+}$ C_S (141.1)

C	-2.913054000	-0.888938000	1.834461000
C	-2.929450000	-2.184384000	1.296125000
C	-2.929450000	-2.184384000	-1.296125000
C	-2.913054000	0.406785000	1.296411000
C	-2.913054000	-0.888938000	-1.834461000
C	-2.917609000	0.942315000	0.000000000
C	-2.913054000	0.406785000	-1.296411000
H	-2.926266000	-0.889105000	2.920321000
H	-2.955862000	-2.952658000	2.063166000
H	-2.955862000	-2.952658000	-2.063166000
H	-2.927521000	1.175533000	2.062992000
H	-2.926266000	-0.889105000	-2.920321000
H	-2.926734000	2.027363000	0.000000000
H	-2.927521000	1.175533000	-2.062992000
C	-2.945967000	-2.719897000	0.000000000
H	-2.983038000	-3.805157000	0.000000000
Ba	3.209255000	1.712324000	0.000000000
Ba	-0.284662000	-0.823499000	0.000000000

$Ba_2C_8H_8^{2+}$ C_{2v} (142.9)

Ba	0.000000000	1.993876000	-0.856260000
C	-1.264422000	1.268734000	1.732138000
C	-1.678980000	0.000000000	1.178574000

C	0.000000000	-1.730309000	2.104612000
C	0.000000000	1.730309000	2.104612000
C	1.264422000	-1.268734000	1.732138000
C	1.264422000	1.268734000	1.732138000
C	1.678980000	0.000000000	1.178574000
H	-2.092416000	1.930540000	1.981906000
H	-2.714240000	0.000000000	0.847939000
H	0.000000000	-2.668432000	2.654048000
H	0.000000000	2.668432000	2.654048000
H	2.092416000	-1.930540000	1.981906000
H	2.092416000	1.930540000	1.981906000
H	2.714240000	0.000000000	0.847939000
C	-1.264422000	-1.268734000	1.732138000
H	-2.092416000	-1.930540000	1.981906000
Ba	0.000000000	-1.993876000	-0.856260000

$Ba_2C_8H_8^{2+}$ C_{2h} (144.7)

Ba	3.663551000	1.211085000	0.000000000
Ba	-3.663551000	-1.211085000	0.000000000
C	-0.000023000	-1.829969000	0.000000000
C	0.000000000	-1.294150000	1.295879000
C	0.000000000	1.294150000	1.295879000
C	0.000000000	-1.294150000	-1.295879000
C	0.000023000	1.829969000	0.000000000
C	0.000000000	0.000000000	-1.832243000
C	0.000000000	1.294150000	-1.295879000
H	0.026757000	-2.916591000	0.000000000
H	0.019158000	-2.062455000	2.063776000
H	-0.019158000	2.062455000	2.063776000
H	0.019158000	-2.062455000	-2.063776000
H	-0.026757000	2.916591000	0.000000000
H	0.000000000	0.000000000	-2.918415000
H	-0.019158000	2.062455000	-2.063776000
C	0.000000000	0.000000000	1.832243000
H	0.000000000	0.000000000	2.918415000

$Ca_2C_6H_6$ D_{6h} (0.0)

Ca	0.000000000	0.000000000	2.197615000
Ca	0.000000000	0.000000000	-2.197615000
C	0.000000000	1.431201000	0.000000000
C	-1.239456000	0.715600000	0.000000000
C	-1.239456000	-0.715600000	0.000000000
C	0.000000000	-1.431201000	0.000000000
C	1.239456000	-0.715600000	0.000000000

C	1.239456000	0.715600000	0.000000000
H	0.000000000	2.512820000	0.000000000
H	-2.176166000	1.256410000	0.000000000
H	-2.176166000	-1.256410000	0.000000000
H	0.000000000	-2.512820000	0.000000000
H	2.176166000	-1.256410000	0.000000000
H	2.176166000	1.256410000	0.000000000

$Ca_2C_6H_6$ D_{2h} (1.6)

C	0.000000000	1.436142000	0.000000000
C	0.000000000	0.713566000	1.240553000
C	0.000000000	-0.713566000	1.240553000
C	0.000000000	-1.436142000	0.000000000
C	0.000000000	-0.713566000	-1.240553000
C	0.000000000	0.713566000	-1.240553000
H	0.000000000	2.517369000	0.000000000
H	0.000000000	1.253610000	2.177784000
H	0.000000000	-1.253610000	2.177784000
H	0.000000000	-2.517369000	0.000000000
H	0.000000000	-1.253610000	-2.177784000
H	0.000000000	1.253610000	-2.177784000
Ca	-2.190610000	0.000000000	0.000000000
Ca	2.190610000	0.000000000	0.000000000

$Ca_2C_6H_6$ C_s (3.5)

C	-0.871384000	-1.691402000	1.199610000
C	-0.866511000	-2.398716000	0.000000000
C	-0.871384000	-1.691402000	-1.199610000
C	-0.871384000	-0.294945000	-1.184054000
C	-0.861949000	0.473227000	0.000000000
C	-0.871384000	-0.294945000	1.184054000
H	-0.865920000	-2.228581000	2.142606000
H	-0.844883000	-3.481892000	0.000000000
H	-0.865920000	-2.228581000	-2.142606000
H	-0.859140000	0.210261000	-2.149515000
H	1.799945000	1.452035000	0.000000000
H	-0.859140000	0.210261000	2.149515000
Ca	1.630926000	-0.676383000	0.000000000
Ca	0.058025000	2.749163000	0.000000000

$Ca_2C_6H_6$ C_s (5.0)

Ca	-0.071068000	-1.637484000	1.714029000
Ca	-0.071068000	-1.637484000	-1.714029000
C	1.366652000	1.058078000	0.000000000

C	0.279226000	0.167846000	0.000000000
C	-0.991460000	0.775151000	0.000000000
C	-1.177975000	2.154130000	0.000000000
C	-0.071068000	2.988750000	0.000000000
C	1.204229000	2.437471000	0.000000000
H	2.380904000	0.663891000	0.000000000
H	-0.997564000	-2.531769000	0.000000000
H	-1.892334000	0.150315000	0.000000000
H	-2.178632000	2.574040000	0.000000000
H	-0.199643000	4.065463000	0.000000000
H	2.072390000	3.088890000	0.000000000

$Ca_2C_6H_6$ C_{2v} (5.8)

Ca	-1.535553000	0.000000000	-1.167357000
C	-1.204486000	0.681301000	1.258473000
C	0.000000000	1.303782000	0.683195000
C	1.204486000	0.681301000	1.258473000
C	1.204486000	-0.681301000	1.258473000
C	0.000000000	-1.303782000	0.683195000
C	-1.204486000	-0.681301000	1.258473000
H	-1.983998000	1.264272000	1.742747000
H	0.000000000	2.391276000	0.660803000
H	1.983998000	1.264272000	1.742747000
H	1.983998000	-1.264272000	1.742747000
H	0.000000000	-2.391276000	0.660803000
H	-1.983998000	-1.264272000	1.742747000
Ca	1.535553000	0.000000000	-1.167357000

$Ca_2C_6H_6$ C_1 (6.8)

Ca	-0.322455000	1.379991000	-0.182871000
Ca	2.515589000	-0.022855000	-0.015894000
C	-2.156723000	-0.130936000	0.757997000
C	-2.138506000	-0.126342000	-0.704730000
C	-1.094166000	-0.925552000	-1.267578000
C	0.036332000	-1.259821000	-0.566434000
C	0.239381000	-0.769991000	0.839424000
C	-1.054188000	-0.469375000	1.479233000
H	-3.074351000	0.129544000	1.275105000
H	-3.071845000	-0.024539000	-1.241732000
H	-1.190860000	-1.272983000	-2.291419000
H	0.712580000	-1.983555000	-1.013541000
H	0.876823000	-1.417825000	1.456714000
H	-1.107806000	-0.481268000	2.562686000

$Ca_2C_6H_6$ C_{2v} (7.9)

C	0.000000000	1.444282000	0.107522000
C	-1.247948000	0.743477000	-0.076641000
C	-1.247948000	-0.743477000	-0.076641000
C	0.000000000	-1.444282000	0.107522000
C	1.247948000	-0.743477000	-0.076641000
C	1.247948000	0.743477000	-0.076641000
H	0.000000000	2.527038000	0.083559000
H	-2.184422000	1.275459000	0.026870000
H	-2.184422000	-1.275459000	0.026870000
H	0.000000000	-2.527038000	0.083559000
H	2.184422000	-1.275459000	0.026870000
H	2.184422000	1.275459000	0.026870000
Ca	0.000000000	0.000000000	-2.010467000
Ca	0.000000000	0.000000000	2.024192000

$Ca_2C_6H_6$ C_s (8.3)

C	2.099870000	0.701911000	1.221190000
C	1.989900000	1.436161000	0.000000000
C	2.099870000	0.701911000	-1.221190000
C	2.099870000	-0.674586000	-1.221177000
C	1.989948000	-1.408767000	0.000000000
C	2.099870000	-0.674586000	1.221177000
H	2.163620000	1.236297000	2.162401000
H	2.038431000	2.515884000	0.000000000
H	2.163620000	1.236297000	-2.162401000
H	2.163580000	-1.208982000	-2.162384000
H	2.037350000	-2.488521000	0.000000000
H	2.163580000	-1.208982000	2.162384000
Ca	-0.185541000	0.013704000	0.000000000
Ca	-4.164766000	-0.042417000	0.000000000

$Ca_2C_6H_6$ C_{2v} (9.2)

C	0.000000000	0.740174000	1.458025000
C	0.000000000	-0.740174000	1.458025000
C	0.000000000	-1.791671000	0.481085000
C	0.000000000	-1.672795000	-0.921605000
C	0.000000000	1.672795000	-0.921605000
C	0.000000000	1.791671000	0.481085000
H	0.000000000	1.110467000	2.475951000
H	0.000000000	-1.110467000	2.475951000
H	0.000000000	-2.768011000	0.976495000
H	0.000000000	-2.635506000	-1.435141000
H	0.000000000	2.635506000	-1.435141000

H	0.000000000	2.768011000	0.976495000
Ca	-1.570356000	0.000000000	-0.406117000
Ca	1.570356000	0.000000000	-0.406117000

$Ca_2C_6H_6$ C_1 (9.8)

Ca	2.502759000	-0.207826000	-0.007741000
Ca	-0.228172000	1.458344000	-0.292738000
C	-0.345831000	-1.142880000	-0.930289000
C	-1.700213000	-0.771619000	-1.126072000
C	-2.410427000	-0.214563000	-0.072923000
C	-1.814709000	-0.106256000	1.191649000
C	-0.519622000	-0.633708000	1.389950000
C	0.279205000	-1.116452000	0.336861000
H	0.204506000	-1.500001000	-1.797536000
H	-2.165714000	-0.874441000	-2.101061000
H	-3.425906000	0.138257000	-0.222991000
H	-2.372940000	0.322341000	2.017466000
H	-0.108048000	-0.592331000	2.394650000
H	1.445949000	1.408677000	0.983981000

$Ca_2C_6H_6$ C_s (10.4)

Ca	1.663851000	-0.715721000	0.000000000
C	-0.934406000	-0.319436000	1.182035000
C	-0.934406000	-1.712458000	1.198839000
C	-0.884441000	-2.420858000	0.000000000
C	-0.934406000	-1.712458000	-1.198839000
C	-0.934406000	-0.319436000	-1.182035000
C	-0.879571000	0.451120000	0.000000000
H	-0.921931000	0.182619000	2.148462000
H	-0.938961000	-2.249326000	2.142298000
H	-0.847217000	-3.503728000	0.000000000
H	-0.938961000	-2.249326000	-2.142298000
H	-0.921931000	0.182619000	-2.148462000
H	-0.413055000	4.602960000	0.000000000
Ca	0.235742000	2.677488000	0.000000000

$Ca_2C_6H_6$ C_1 (10.7)

C	0.184116000	-0.031151000	0.004681000
C	0.944467000	0.124210000	1.178208000
C	2.333742000	0.068901000	1.189805000
C	3.022493000	-0.148062000	0.004333000
C	2.317848000	-0.306269000	-1.181210000
C	0.929059000	-0.244635000	-1.169658000
H	-2.099610000	-3.508654000	0.223414000

H	0.438270000	0.299655000	2.129754000
H	2.879909000	0.193040000	2.119455000
H	4.106138000	-0.191597000	0.003856000
H	2.851693000	-0.473850000	-2.111160000
H	0.411571000	-0.359789000	-2.124147000
Ca	-1.480575000	1.866597000	-0.116891000
Ca	-1.868341000	-1.503435000	0.096985000

$Sr_2C_6H_6$ D_{6h} (0.0)

C	0.000000000	1.429685000	0.000000000
C	-1.238143000	0.714842000	0.000000000
C	-1.238143000	-0.714842000	0.000000000
C	0.000000000	-1.429685000	0.000000000
C	1.238143000	-0.714842000	0.000000000
C	1.238143000	0.714842000	0.000000000
H	0.000000000	2.511863000	0.000000000
H	-2.175337000	1.255931000	0.000000000
H	-2.175337000	-1.255931000	0.000000000
H	0.000000000	-2.511863000	0.000000000
H	2.175337000	-1.255931000	0.000000000
H	2.175337000	1.255931000	0.000000000
Sr	0.000000000	0.000000000	2.383799000
Sr	0.000000000	0.000000000	-2.383799000

$Sr_2C_6H_6$ C_{2h} (4.8)

Sr	0.000000000	0.000000000	2.371265000
C	0.000000000	1.418464000	0.000000000
C	1.228891000	0.753566000	0.000000000
C	1.228522000	-0.753979000	0.000000000
C	0.000000000	-1.418464000	0.000000000
C	-1.228891000	-0.753566000	0.000000000
C	-1.228522000	0.753979000	0.000000000
H	0.000170000	2.505085000	0.000000000
H	2.160193000	1.300870000	0.000000000
H	2.159721000	-1.301535000	0.000000000
H	-0.000170000	-2.505085000	0.000000000
H	-2.160193000	-1.300870000	0.000000000
H	-2.159721000	1.301535000	0.000000000
Sr	0.000000000	0.000000000	-2.371265000

$Sr_2C_6H_6$ C_s (5.1)

Sr	-0.297957000	2.575093000	0.000000000
C	-1.161711000	0.108975000	0.000000000
C	-1.171943000	-0.660047000	1.182451000

C	-1.171943000	-2.056264000	1.199342000
C	-1.165008000	-2.763927000	0.000000000
C	-1.171943000	-2.056264000	-1.199342000
C	-1.171943000	-0.660047000	-1.182451000
H	1.588093000	1.204122000	0.000000000
H	-1.164579000	-0.155360000	2.148933000
H	-1.172431000	-2.593500000	2.142707000
H	-1.151245000	-3.847570000	0.000000000
H	-1.172431000	-2.593500000	-2.142707000
H	-1.164579000	-0.155360000	-2.148933000
Sr	1.517012000	-1.083866000	0.000000000

$Sr_2C_6H_6$ C_{2v} (5.2)

Sr	0.000000000	0.000000000	-2.218112000
C	1.255263000	0.707735000	-0.009888000
C	0.000000000	1.450792000	-0.123106000
C	-1.255263000	0.707735000	-0.009888000
C	-1.255263000	-0.707735000	-0.009888000
C	0.000000000	-1.450792000	-0.123106000
C	1.255263000	-0.707735000	-0.009888000
H	2.193150000	1.249188000	0.013927000
H	0.000000000	2.525029000	0.002169000
H	-2.193150000	1.249188000	0.013927000
H	-2.193150000	-1.249188000	0.013927000
H	0.000000000	-2.525029000	0.002169000
H	2.193150000	-1.249188000	0.013927000
Sr	0.000000000	0.000000000	2.261653000

$Sr_2C_6H_6$ C_s (6.8)

Sr	-1.687316000	1.504816000	0.000000000
Sr	-0.629202000	-3.295469000	0.000000000
C	2.095896000	0.417656000	0.694411000
C	2.095896000	1.619891000	1.389600000
C	2.097776000	2.823154000	0.694456000
C	2.097776000	2.823154000	-0.694456000
C	2.095896000	1.619891000	-1.389600000
C	2.095896000	0.417656000	-0.694411000
H	2.087670000	-0.523096000	1.234186000
H	2.091920000	1.619256000	2.473486000
H	2.096844000	3.762040000	1.236045000
H	2.096844000	3.762040000	-1.236045000
H	2.091920000	1.619256000	-2.473486000
H	2.087670000	-0.523096000	-1.234186000

$Sr_2C_6H_6$ C_1 (8.1)

C	-0.201669000	-1.456056000	-0.666731000
C	-0.060003000	-1.102600000	0.781042000
C	-1.375124000	-1.010386000	1.431210000
C	-2.514708000	-0.744288000	0.735700000
C	-2.505671000	-0.610649000	-0.718491000
C	-1.366224000	-1.199534000	-1.345513000
H	0.557886000	-2.039711000	-1.181120000
H	0.644855000	-1.732116000	1.340509000
H	-1.425973000	-1.129986000	2.508712000
H	-3.454769000	-0.649711000	1.269804000
H	-3.446621000	-0.584680000	-1.251460000
H	-1.417238000	-1.453468000	-2.399914000
Sr	2.341089000	-0.072238000	-0.006222000
Sr	-0.849450000	1.238836000	-0.035616000

$Sr_2C_6H_6$ C_1 (8.3)

C	2.994004000	0.386465000	-0.728653000
C	3.007640000	0.398777000	0.709835000
C	1.963470000	1.005023000	1.395238000
C	0.847823000	1.519526000	0.728794000
C	0.851516000	1.539357000	-0.708727000
C	1.940621000	1.019147000	-1.394619000
H	3.838118000	-0.003286000	-1.281749000
H	3.858251000	0.004036000	1.250590000
H	1.993588000	1.041575000	2.479528000
H	0.056208000	2.006863000	1.282055000
H	0.050912000	2.027430000	-1.249755000
H	1.952279000	1.066845000	-2.478802000
Sr	0.846616000	-1.244758000	-0.000424000
Sr	-2.988190000	0.156515000	0.000080000

$Sr_2C_6H_6$ C_{2v} (9.0)

Sr	1.667875000	0.000000000	-0.859883000
Sr	-1.667875000	0.000000000	-0.859883000
C	-1.201702000	0.681179000	1.698144000
C	0.000000000	1.313812000	1.133494000
C	1.201702000	0.681179000	1.698144000
C	1.201702000	-0.681179000	1.698144000
C	0.000000000	-1.313812000	1.133494000
C	-1.201702000	-0.681179000	1.698144000
H	-1.985517000	1.260128000	2.181793000
H	0.000000000	2.401849000	1.133275000
H	1.985517000	1.260128000	2.181793000

H	1.985517000	-1.260128000	2.181793000
H	0.000000000	-2.401849000	1.133275000
H	-1.985517000	-1.260128000	2.181793000

$Sr_2C_6H_6$ C_{2v} (9.9)

C	0.000000000	1.435431000	0.089200000
C	1.243789000	0.743170000	-0.074568000
C	1.243789000	-0.743170000	-0.074568000
C	0.000000000	-1.435431000	0.089200000
C	-1.243789000	-0.743170000	-0.074568000
C	-1.243789000	0.743170000	-0.074568000
H	0.000000000	2.518941000	0.100777000
H	2.178727000	1.279456000	0.023124000
H	2.178727000	-1.279456000	0.023124000
H	0.000000000	-2.518941000	0.100777000
H	-2.178727000	-1.279456000	0.023124000
H	-2.178727000	1.279456000	0.023124000
Sr	0.000000000	0.000000000	2.233109000
Sr	0.000000000	0.000000000	-2.221920000

$Sr_2C_6H_6$ C_1 (10.0)

Sr	0.786488000	-1.358484000	0.063474000
C	0.661053000	1.318415000	1.103430000
C	2.053315000	1.111241000	1.190883000
C	2.774500000	0.835925000	0.035221000
C	2.128459000	0.862767000	-1.204431000
C	0.765378000	1.202446000	-1.267682000
C	-0.034259000	1.386389000	-0.121288000
H	0.116142000	1.437920000	2.038364000
H	2.554704000	1.123263000	2.153834000
H	3.835279000	0.613406000	0.089205000
H	2.691699000	0.660212000	-2.110284000
H	0.308234000	1.260909000	-2.252149000
H	-0.980076000	-1.149101000	-1.335625000
Sr	-2.329031000	0.194018000	0.015470000

$Sr_2C_6H_6$ C_1 (12.7)

Sr	-1.129056000	1.693635000	-0.069634000
C	3.676509000	-0.093526000	0.082976000
C	3.045154000	-0.222651000	-1.146659000
C	1.655978000	-0.217897000	-1.212911000
C	0.836181000	-0.090143000	-0.076534000
C	1.524735000	0.036608000	1.145271000
C	2.913317000	0.037317000	1.234587000

H	4.759662000	-0.094322000	0.142749000
H	3.637133000	-0.323969000	-2.051274000
H	1.192494000	-0.315001000	-2.195484000
H	-1.606840000	0.118320000	1.533993000
H	0.948307000	0.133962000	2.066621000
H	3.401357000	0.137142000	2.199499000
Sr	-1.351033000	-1.597698000	0.020779000

$Sr_2C_6H_6$ C_{2v} (13.7)

C	0.000000000	0.739312000	1.603060000
C	0.000000000	1.800334000	0.634544000
C	0.000000000	1.706526000	-0.770197000
C	0.000000000	-1.706526000	-0.770197000
C	0.000000000	-1.800334000	0.634544000
C	0.000000000	-0.739312000	1.603060000
H	0.000000000	1.107303000	2.622738000
H	0.000000000	2.770850000	1.142491000
H	0.000000000	2.684266000	-1.259266000
H	0.000000000	-2.684266000	-1.259266000
H	0.000000000	-2.770850000	1.142491000
H	0.000000000	-1.107303000	2.622738000
Sr	1.742873000	0.000000000	-0.297642000
Sr	-1.742873000	0.000000000	-0.297642000

$Ca_2C_7H_7^+$ D_{7h} (0.0)

Ca	0.000000000	0.000000000	1.838855000
Ca	0.000000000	0.000000000	-1.838855000
C	0.000000000	1.653965000	0.000000000
C	1.293122000	1.031231000	0.000000000
C	1.612497000	-0.368042000	0.000000000
C	-1.293122000	1.031231000	0.000000000
C	0.717629000	-1.490171000	0.000000000
C	-1.612497000	-0.368042000	0.000000000
C	-0.717629000	-1.490171000	0.000000000
H	0.000000000	2.736359000	0.000000000
H	2.139372000	1.706092000	0.000000000
H	2.667753000	-0.608897000	0.000000000
H	-2.139372000	1.706092000	0.000000000
H	1.187262000	-2.465374000	0.000000000
H	-2.667753000	-0.608897000	0.000000000
H	-1.187262000	-2.465374000	0.000000000

$Ca_2C_7H_7^+$ C_1 (40.5)

C	-0.024913000	-1.316097000	-0.989645000

C	-0.014550000	-0.018302000	-1.643865000
C	-0.016301000	1.252179000	-1.068676000
C	-0.013408000	-1.589024000	0.393335000
C	-0.021316000	1.610862000	0.344693000
C	-0.029207000	-0.683020000	1.496829000
C	-0.013324000	0.754578000	1.454762000
H	-0.018572000	-2.172499000	-1.649849000
H	-0.007682000	-0.050609000	-2.726264000
H	-0.009423000	2.088973000	-1.755356000
H	-0.008236000	-2.639375000	0.660392000
H	-0.013983000	2.672057000	0.554060000
H	-0.022819000	-1.128636000	2.481655000
H	-0.007351000	1.241781000	2.422623000
Ca	2.044179000	-0.002925000	0.003142000
Ca	-1.999870000	-0.001013000	0.001265000

$Ca_2C_7H_7^+$ C_2 (64.9)

C	1.635648000	0.000883000	-1.168405000
C	-1.635648000	-0.000883000	-1.168405000
C	-2.135065000	0.000953000	0.098595000
C	2.135065000	-0.000953000	0.098595000
C	-1.357233000	0.001224000	1.332361000
C	1.357233000	-0.001224000	1.332361000
C	0.000000000	0.000000000	1.748582000
H	2.385213000	0.000393000	-1.959668000
H	-2.385213000	-0.000393000	-1.959668000
H	-3.205622000	0.002453000	0.319606000
H	3.205622000	-0.002453000	0.319606000
H	-2.002336000	0.002128000	2.202402000
H	2.002336000	-0.002128000	2.202402000
H	0.000000000	0.000000000	2.833209000
Ca	0.000000000	1.573316000	-0.440000000
Ca	0.000000000	-1.573316000	-0.440000000

$Ca_2C_7H_7^+$ C_1 (65.9)

C	2.074182000	1.112558000	-0.262758000
C	2.478572000	-0.309896000	-0.264019000
C	1.721469000	-1.407356000	-0.477673000
C	0.859907000	1.623472000	-0.620353000
C	0.260067000	-1.498311000	-0.707015000
C	-0.392368000	0.934689000	-0.800437000
C	-0.621382000	-0.488212000	-0.978596000
H	2.881219000	1.818369000	-0.109463000
H	3.541314000	-0.471449000	-0.116849000

H	2.246670000	-2.358402000	-0.474237000
H	0.811576000	2.708252000	-0.693813000
H	-0.100754000	-2.521058000	-0.769565000
H	-1.154829000	1.605869000	-1.220303000
H	-1.694041000	-0.149706000	1.791174000
Ca	-2.658150000	-0.011379000	-0.062504000
Ca	0.417458000	-0.010298000	1.375412000

$Ca_2C_7H_7^+$ C_1 (67.4)

Ca	-1.205536000	1.456840000	-0.042054000
Ca	1.961611000	0.843951000	-0.026982000
C	1.079594000	-1.349354000	0.739980000
C	0.111913000	-0.523289000	1.464281000
C	-1.301151000	-0.716285000	1.257667000
C	1.088845000	-1.417738000	-0.625094000
C	-1.928971000	-0.914061000	0.020631000
C	0.126856000	-0.692249000	-1.444514000
C	-1.283953000	-0.800074000	-1.224132000
H	1.800953000	-1.926556000	1.316515000
H	0.359432000	-0.370692000	2.512466000
H	-1.937770000	-0.689702000	2.139283000
H	1.826043000	-2.038774000	-1.131932000
H	-3.001216000	-1.086446000	0.018209000
H	0.388785000	-0.625239000	-2.497560000
H	-1.916520000	-0.800094000	-2.109173000

$Ca_2C_7H_7^+$ C_1 (68.6)

Ca	0.365526000	1.714136000	-0.085095000
C	1.397560000	-0.229776000	-1.305012000
C	-1.611905000	0.940940000	-1.038380000
C	-2.067972000	0.144825000	-0.040574000
C	2.001628000	-0.301799000	-0.072499000
C	-1.359281000	-0.139904000	1.231348000
C	1.323445000	-0.346359000	1.207555000
C	-0.032621000	-0.272300000	1.675748000
H	2.080441000	-0.129496000	-2.148611000
H	-2.259260000	0.991593000	-1.914719000
H	-2.992215000	-0.452303000	-0.025412000
H	3.087349000	-0.323604000	0.055442000
H	-2.055805000	-0.293632000	2.050062000
H	2.000126000	-0.519899000	2.035054000
H	-0.027807000	-0.426375000	2.749983000
Ca	-0.252424000	-1.595139000	-0.552451000

$Ca_2C_7H_7^+$ C_1 (68.9)

Ca	0.413744000	-0.026115000	1.315262000
Ca	-2.652372000	0.002857000	0.137540000
C	-0.553057000	-0.711367000	-0.934326000
C	0.570942000	-1.583887000	-0.714275000
C	1.867645000	-1.278384000	-0.319003000
C	-0.475476000	0.753596000	-1.024279000
C	2.472979000	0.007085000	-0.146030000
C	0.569530000	1.603893000	-0.668003000
C	1.890614000	1.271551000	-0.239182000
H	-1.284237000	-1.169079000	-1.611941000
H	0.346115000	-2.640257000	-0.819943000
H	2.520084000	-2.127067000	-0.150589000
H	-1.281982000	1.257200000	-1.567994000
H	3.518975000	-0.011148000	0.139398000
H	0.359658000	2.664639000	-0.749209000
H	2.534882000	2.115942000	-0.025180000

$Ca_2C_7H_7^+$ C_1 (70.4)

Ca	-2.227377000	-0.396468000	-0.002301000
C	0.587531000	1.030632000	-1.315318000
C	1.809580000	0.810052000	-0.636230000
C	2.035258000	0.501666000	0.719749000
C	-0.537100000	1.695799000	-0.694908000
C	1.009157000	0.032671000	1.592984000
C	-0.686191000	1.467827000	0.641913000
C	-0.312835000	0.160605000	1.196910000
H	0.673760000	1.111581000	-2.396544000
H	2.698215000	0.837519000	-1.266111000
H	3.072117000	0.401698000	1.030525000
H	-1.018173000	2.518000000	-1.225333000
H	1.323027000	-0.663410000	2.380950000
H	-1.030802000	2.241488000	1.328816000
H	-1.186689000	-1.999144000	-0.903835000
Ca	0.829185000	-1.535694000	-0.396652000

$Ca_2C_7H_7^+$ C_s (71.2)

Ca	-1.106519000	2.478810000	0.000000000
Ca	-1.082288000	-0.857328000	0.000000000
C	0.697666000	0.808589000	0.759316000
C	0.697666000	0.808589000	-0.759316000
C	0.936435000	-0.300421000	-1.576975000
C	0.936435000	-0.300421000	1.576975000
C	0.936435000	-1.676476000	-1.270889000

C	0.936435000	-1.676476000	1.270889000
C	0.957626000	-2.283805000	0.000000000
H	1.041859000	1.743710000	1.209481000
H	1.041859000	1.743710000	-1.209481000
H	1.041297000	-0.066920000	-2.631720000
H	1.041297000	-0.066920000	2.631720000
H	1.003142000	-2.346550000	-2.119405000
H	1.003142000	-2.346550000	2.119405000
H	1.011360000	-3.367590000	0.000000000

$Ca_2C_7H_7^+$ C_1 (71.6)

Ca	-4.135290000	-0.000546000	-0.004980000
C	1.778690000	-1.590044000	0.351610000
C	1.808601000	-1.254281000	-1.019205000
C	1.818899000	0.026913000	-1.611497000
C	1.751517000	-0.727210000	1.468617000
C	1.802105000	1.288859000	-0.979362000
C	1.747554000	0.684161000	1.490606000
C	1.770187000	1.581407000	0.401135000
H	1.781911000	-2.650602000	0.576339000
H	1.832512000	-2.091195000	-1.707941000
H	1.849828000	0.043983000	-2.695048000
H	1.737399000	-1.212872000	2.437786000
H	1.822429000	2.146880000	-1.641709000
H	1.731062000	1.139304000	2.474433000
H	1.769111000	2.634418000	0.658889000
Ca	-0.234189000	-0.002892000	-0.030729000

$Ca_2C_7H_7^+$ C_1 (74.5)

C	2.175720000	-1.522781000	0.345910000
C	-0.243481000	0.973950000	1.342050000
C	-1.220426000	0.086700000	1.670123000
C	1.095378000	-1.571864000	-0.266132000
C	-1.842130000	-0.909653000	0.794008000
C	-0.072096000	-1.416721000	-0.972173000
C	-1.374936000	-1.501407000	-0.344668000
H	0.641246000	1.709110000	-1.567813000
H	-0.072485000	1.682225000	2.162393000
H	-1.715129000	0.145824000	2.641344000
H	2.888478000	-2.131963000	0.871137000
H	-2.839501000	-1.214651000	1.098968000
H	-0.022032000	-1.740704000	-2.009566000
H	-2.098966000	-2.104919000	-0.890759000
Ca	-1.231724000	1.052296000	-0.877739000

Ca	1.837234000	0.888991000	-0.008281000

$Ca_2C_7H_7^+$ C_1 (74.6)

Ca	-1.343973000	-1.706604000	0.000000000
Ca	-1.090741000	1.784560000	0.000000000
C	0.987036000	-1.485840000	0.722015000
C	0.762208000	-0.394663000	1.537718000
C	0.987036000	1.018660000	1.250325000
C	0.987036000	-1.485840000	-0.722015000
C	1.356664000	1.525444000	0.000000000
C	0.762208000	-0.394663000	-1.537718000
C	0.987036000	1.018660000	-1.250325000
H	1.091304000	-2.450829000	1.220171000
H	0.647253000	-0.616271000	2.595774000
H	1.238744000	1.613479000	2.123718000
H	1.091304000	-2.450829000	-1.220171000
H	1.764334000	2.537573000	0.000000000
H	0.647253000	-0.616271000	-2.595774000
H	1.238744000	1.613479000	-2.123718000

$Sr_2C_7H_7^+$ D_{7h} (0.0)

Sr	0.000000000	0.000000000	2.029190000
C	0.000000000	1.653710000	0.000000000
C	1.292923000	1.031071000	0.000000000
C	1.612248000	-0.367985000	0.000000000
C	-1.292923000	1.031071000	0.000000000
C	0.717518000	-1.489941000	0.000000000
C	-1.612248000	-0.367985000	0.000000000
C	-0.717518000	-1.489941000	0.000000000
H	0.000000000	2.736754000	0.000000000
H	2.139681000	1.706338000	0.000000000
H	2.668138000	-0.608985000	0.000000000
H	-2.139681000	1.706338000	0.000000000
H	1.187433000	-2.465730000	0.000000000
H	-2.668138000	-0.608985000	0.000000000
H	-1.187433000	-2.465730000	0.000000000
Sr	0.000000000	0.000000000	-2.029190000

$Sr_2C_7H_7^+$ C_1 (47.6)

Sr	-0.916575000	-1.282275000	0.078601000
C	-2.821308000	0.568957000	-0.868157000
C	-2.861877000	0.780730000	0.532264000
C	-1.733249000	1.107814000	1.245940000
C	-1.649048000	0.968585000	-1.531510000

C	0.766476000	0.839546000	1.261541000
C	-0.505902000	1.295341000	-0.829576000
C	-0.423947000	1.171961000	0.620087000
H	-3.723847000	0.347599000	-1.420982000
H	-3.804124000	0.659835000	1.057594000
H	-1.784806000	1.218941000	2.324533000
H	-1.637193000	1.007724000	-2.615971000
H	1.197455000	-1.527155000	-0.794046000
H	0.360687000	1.647758000	-1.384376000
H	0.656011000	0.798186000	2.353054000
Sr	2.603653000	0.109894000	-0.133952000

$Sr_2C_7H_7^+$ C_1 (65.0)

C	-0.001021000	0.006517000	1.897728000
C	-0.003685000	-1.353659000	1.486164000
C	-0.003097000	-2.148934000	0.262195000
C	0.002174000	1.364776000	1.481152000
C	-0.000624000	-1.687962000	-1.021671000
C	0.002766000	2.153145000	0.252532000
C	0.001798000	1.683308000	-1.027990000
H	-0.001696000	0.008236000	2.982809000
H	-0.006228000	-1.992787000	2.361078000
H	-0.005593000	-3.214654000	0.507004000
H	0.003213000	2.007677000	2.353312000
H	-0.000136000	-2.476438000	-1.776598000
H	0.003378000	3.220574000	0.490114000
H	0.001467000	2.466033000	-1.788847000
Sr	1.742347000	-0.003109000	-0.329980000
Sr	-1.741933000	-0.000096000	-0.330797000

$Sr_2C_7H_7^+$ C_1 (67.7)

Sr	-0.954371000	-1.257140000	-0.023642000
Sr	2.515023000	0.095860000	0.007207000
C	-0.536282000	0.927434000	1.516184000
C	-2.012964000	0.908173000	1.432013000
C	-2.801174000	0.835680000	0.338219000
C	0.368812000	1.114277000	0.502327000
C	-2.407503000	0.827418000	-1.087065000
C	0.111977000	1.012113000	-0.914329000
C	-1.158360000	1.021983000	-1.597098000
H	-0.166221000	0.936029000	2.537843000
H	-2.528730000	0.961251000	2.387328000
H	-3.872990000	0.846555000	0.506999000
H	1.295361000	-1.779823000	0.110588000

H	-3.231360000	0.821371000	-1.790634000
H	0.919061000	1.334198000	-1.589483000
H	-1.106929000	1.126587000	-2.679601000

$Sr_2C_7H_7^+$ C_1 (68.2)

Sr	2.504511000	0.001068000	-0.002632000
C	0.145164000	-1.270541000	-0.740468000
C	0.246711000	-1.136587000	0.714166000
C	-0.877371000	-0.976653000	1.601720000
C	-0.935284000	-1.019529000	-1.579547000
C	-2.205719000	-0.695732000	1.313962000
C	-2.285719000	-0.696878000	-1.233117000
C	-2.848977000	-0.606156000	0.036531000
H	0.986293000	-1.750858000	-1.251589000
H	1.017066000	-1.770019000	1.172854000
H	-0.628663000	-1.045310000	2.656206000
H	-0.740015000	-1.121870000	-2.641399000
H	-2.855601000	-0.567935000	2.172135000
H	-2.962407000	-0.577023000	-2.071250000
H	-3.916390000	-0.416583000	0.069601000
Sr	-0.881698000	1.200565000	-0.018053000

$Sr_2C_7H_7^+$ C_s (70.3)

Sr	-0.879193000	1.203429000	0.000000000
C	1.116031000	-0.512230000	0.753172000
C	1.329015000	0.591330000	1.573200000
C	1.329015000	1.974477000	1.270332000
C	1.116031000	-0.512230000	-0.753172000
C	1.373222000	2.577440000	0.000000000
C	1.329015000	0.591330000	-1.573200000
C	1.329015000	1.974477000	-1.270332000
H	1.435949000	-1.450250000	1.211880000
H	1.442369000	0.356408000	2.626981000
H	1.413891000	2.642086000	2.119121000
H	1.435949000	-1.450250000	-1.211880000
H	1.456615000	3.659936000	0.000000000
H	1.442369000	0.356408000	-2.626981000
H	1.413891000	2.642086000	-2.119121000
Sr	-0.793677000	-2.436692000	0.000000000

$Sr_2C_7H_7^+$ C_s (71.4)

Sr	0.787093000	-1.165927000	0.000000000
Sr	1.064740000	2.723721000	0.000000000
C	-1.296679000	-2.230812000	1.268318000

C	-1.339495000	-2.819429000	0.000000000
C	-1.296679000	-2.230812000	-1.268318000
C	-1.504685000	-0.832707000	1.570495000
C	-1.504685000	-0.832707000	-1.570495000
C	-1.504685000	0.250796000	0.745107000
C	-1.504685000	0.250796000	-0.745107000
H	-1.315061000	-2.902945000	2.116207000
H	-1.311888000	-3.906509000	0.000000000
H	-1.315061000	-2.902945000	-2.116207000
H	-1.624683000	-0.613719000	2.627271000
H	-1.624683000	-0.613719000	-2.627271000
H	-1.734376000	1.206459000	1.204875000
H	-1.734376000	1.206459000	-1.204875000

$Sr_2C_7H_7^+$ C_s (75.4)

Sr	-0.837473000	-1.950022000	0.000000000
Sr	-1.024068000	1.855797000	0.000000000
C	1.606287000	-1.366941000	0.726300000
C	1.295516000	-0.315093000	1.552043000
C	1.295516000	1.111493000	1.256081000
C	1.606287000	-1.366941000	-0.726300000
C	1.572651000	1.659027000	0.000000000
C	1.295516000	-0.315093000	-1.552043000
C	1.295516000	1.111493000	-1.256081000
H	1.831184000	-2.315246000	1.215958000
H	1.240918000	-0.550658000	2.612212000
H	1.478134000	1.742257000	2.121699000
H	1.831184000	-2.315246000	-1.215958000
H	1.834371000	2.720198000	0.000000000
H	1.240918000	-0.550658000	-2.612212000
H	1.478134000	1.742257000	-2.121699000

$Sr_2C_7H_7^+$ C_1 (76.0)

Sr	-1.376375000	-1.360391000	-0.118254000
Sr	2.080077000	-0.570945000	-0.082005000
C	0.814089000	1.733087000	0.893801000
C	0.789914000	2.195915000	-0.375454000
C	-0.221286000	1.831223000	-1.362901000
C	-0.049354000	0.656486000	1.415115000
C	-1.512445000	1.524327000	-1.100006000
C	-1.454771000	1.016704000	1.340249000
C	-2.133444000	1.353470000	0.204394000
H	1.528408000	2.192273000	1.578560000
H	1.472818000	2.991070000	-0.660801000

H	0.048959000	1.971315000	-2.405738000
H	0.227903000	0.374621000	2.430961000
H	-2.180506000	1.460223000	-1.957009000
H	-2.042238000	0.955009000	2.256331000
H	-3.192221000	1.578971000	0.276355000

$Sr_2C_7H_7^+$ D_{7h} (78.5)

C	0.000000000	1.627830000	0.000000000
C	1.272688000	1.014935000	0.000000000
C	1.587016000	-0.362226000	0.000000000
C	-1.272688000	1.014935000	0.000000000
C	0.706289000	-1.466624000	0.000000000
C	-1.587016000	-0.362226000	0.000000000
C	-0.706289000	-1.466624000	0.000000000
H	0.000000000	2.711712000	0.000000000
H	2.120101000	1.690725000	0.000000000
H	2.643723000	-0.603413000	0.000000000
H	-2.120101000	1.690725000	0.000000000
H	1.176568000	-2.443168000	0.000000000
H	-2.643723000	-0.603413000	0.000000000
H	-1.176568000	-2.443168000	0.000000000
Sr	0.000000000	0.000000000	2.534926000
Sr	0.000000000	0.000000000	-2.534926000

$Sr_2C_7H_7^+$ C_1 (79.5)

C	-1.028245000	0.721335000	1.892588000
C	-1.744586000	1.533993000	0.907274000
C	-1.453509000	1.819594000	-0.394651000
C	-0.172285000	-0.307051000	1.649530000
C	-0.269525000	1.534451000	-1.177857000
C	2.156556000	1.907876000	-0.291030000
C	0.993043000	1.813310000	-0.716663000
H	-1.349199000	0.940311000	2.913554000
H	-2.669550000	1.968655000	1.278091000
H	-2.243353000	2.328544000	-0.947441000
H	0.094360000	-0.810009000	2.589623000
H	-0.382946000	1.620847000	-2.256857000
H	0.366061000	-1.799694000	-1.179937000
H	2.914968000	2.632216000	-0.056695000
Sr	1.894237000	-0.662921000	0.068497000
Sr	-1.568422000	-0.942919000	-0.425220000

$Sr_2C_7H_7^+$ C_1 (80.6)

Sr	1.073384000	-1.022327000	-0.005356000

Sr	-1.351093000	1.309696000	0.001408000
C	2.484459000	1.242780000	0.000405000
C	1.290317000	1.719492000	-0.012617000
C	-1.085272000	-0.786956000	-1.467674000
C	3.585549000	0.501013000	0.014204000
C	-1.883062000	-1.604572000	-0.734521000
C	-1.073947000	-0.784251000	1.472362000
C	-1.877340000	-1.603200000	0.746820000
H	4.121029000	0.288017000	-0.906691000
H	1.223865000	2.813940000	-0.027222000
H	-1.208787000	-0.907822000	-2.547513000
H	4.110036000	0.305974000	0.945262000
H	-2.578755000	-2.312482000	-1.192233000
H	-1.189203000	-0.903195000	2.553327000
H	-2.569432000	-2.310299000	1.211193000

$Ca_2C_8H_8^{2+}$ D_{8h} (0.0)

C	-1.306995000	-1.306996000	0.000000000
C	-1.848370000	-0.000001000	0.000000000
C	0.000000000	1.848369000	0.000000000
C	0.000000000	-1.848361000	0.000000000
C	1.306995000	1.306993000	0.000000000
C	1.306995000	-1.306996000	0.000000000
C	1.848370000	-0.000001000	0.000000000
H	-2.073341000	-2.073342000	0.000000000
H	-2.932147000	-0.000001000	0.000000000
H	0.000000000	2.932147000	0.000000000
H	0.000000000	-2.932148000	0.000000000
H	2.073341000	2.073341000	0.000000000
H	2.073341000	-2.073342000	0.000000000
H	2.932147000	-0.000001000	0.000000000
C	-1.306995000	1.306994000	0.000000000
H	-2.073341000	2.073341000	0.000000000
Ca	0.000000000	-0.000001000	1.835958000
Ca	0.000000000	-0.000001000	-1.835958000

$Ca_2C_8H_8^{2+}$ C_1 (61.0)

C	-0.015628000	0.653185000	1.412119000
C	-0.552180000	1.482994000	0.247703000
C	1.471645000	1.026831000	-1.076552000
C	-0.481321000	-0.794565000	1.482984000
C	2.168883000	0.776650000	0.171060000
C	-0.936790000	-1.524503000	0.431898000
C	1.509647000	0.581945000	1.337323000

H	-0.280363000	1.126476000	2.362922000
H	-1.203048000	2.330840000	0.482395000
H	2.049032000	1.301499000	-1.952493000
H	-0.348611000	-1.237656000	2.474267000
H	3.257050000	0.783061000	0.171292000
H	-1.160946000	-2.565445000	0.695752000
H	2.057198000	0.489146000	2.268494000
C	0.186157000	1.586429000	-0.920872000
H	-0.186025000	2.222271000	-1.723595000
Ca	-2.454754000	0.060704000	-0.461684000
Ca	1.240416000	-1.419903000	-0.702967000

$Ca_2C_8H_8^{2+}$ C_{2v} (62.4)

Ca	0.000000000	2.060758000	1.173411000
C	1.672717000	0.000000000	-0.400194000
C	1.256498000	-1.288671000	-0.832745000
C	-1.256498000	-1.288671000	-0.832745000
C	1.256498000	1.288671000	-0.832745000
C	-1.672717000	0.000000000	-0.400194000
C	0.000000000	1.759977000	-1.235404000
C	-1.256498000	1.288671000	-0.832745000
H	2.694051000	0.000000000	-0.024523000
H	2.087680000	-1.982619000	-0.963754000
H	-2.087680000	-1.982619000	-0.963754000
H	2.087680000	1.982619000	-0.963754000
H	-2.694051000	0.000000000	-0.024523000
H	0.000000000	2.740905000	-1.709668000
H	-2.087680000	1.982619000	-0.963754000
C	0.000000000	-1.759977000	-1.235404000
H	0.000000000	-2.740905000	-1.709668000
Ca	0.000000000	-2.060758000	1.173411000

$Ca_2C_8H_8^{2+}$ C_s (67.7)

C	0.760036000	2.413604000	0.697791000
C	0.760036000	2.413604000	-0.697791000
C	0.548105000	0.040620000	-1.721203000
C	0.637111000	1.431503000	1.704564000
C	0.548105000	-0.974489000	-0.729780000
C	0.548105000	0.040620000	1.721203000
C	0.548105000	-0.974489000	0.729780000
H	0.815064000	3.414325000	1.112616000
H	0.815064000	3.414325000	-1.112616000
H	0.480825000	-0.367219000	-2.724535000
H	0.587630000	1.858534000	2.700278000

H	1.000123000	-1.876175000	-1.177882000
H	0.480825000	-0.367219000	2.724535000
H	1.000123000	-1.876175000	1.177882000
C	0.637111000	1.431503000	-1.704564000
H	0.587630000	1.858534000	-2.700278000
Ca	-0.631835000	-2.993028000	0.000000000
Ca	-1.152542000	0.943338000	0.000000000

$Ca_2C_8H_8^{2+}$ C_1 (69.1)

Ca	2.424433000	-0.480748000	-0.620722000
Ca	-1.027731000	1.597750000	-0.276401000
C	1.243022000	1.422878000	0.058070000
C	1.257988000	0.654292000	1.231881000
C	-0.416249000	-1.230405000	0.586468000
C	-1.741334000	-0.764835000	1.120994000
C	-0.639698000	-1.154003000	-0.904006000
C	-2.611807000	-0.554076000	0.103655000
C	-1.929577000	-0.825316000	-1.161277000
H	1.763948000	2.383475000	0.144441000
H	1.807425000	1.002161000	2.113125000
H	-0.434968000	-2.319701000	0.784198000
H	-1.948945000	-0.689280000	2.181259000
H	0.025477000	-1.542512000	-1.671106000
H	-3.663440000	-0.307659000	0.199873000
H	-2.408368000	-0.834666000	-2.133403000
C	0.826702000	-0.688705000	1.308830000
H	0.990560000	-1.190826000	2.256381000

$Ca_2C_8H_8^{2+}$ C_1 (71.3)

C	0.928049000	-1.511169000	-1.052936000
C	1.329408000	-0.288910000	-1.705477000
C	0.527247000	1.819321000	-0.405347000
C	0.229809000	-1.824825000	0.093268000
C	-0.170291000	1.516229000	0.745985000
C	-0.414697000	-1.061360000	1.132267000
C	-0.572495000	0.293788000	1.402571000
H	1.292595000	-2.387279000	-1.579106000
H	1.915724000	-0.482789000	-2.597413000
H	0.658796000	2.886315000	-0.551555000
H	0.165845000	-2.891798000	0.278488000
H	-0.454918000	2.393672000	1.317818000
H	-0.812075000	-1.697905000	1.917350000
H	-1.051457000	0.483874000	2.359225000
C	1.165267000	1.051224000	-1.446251000

H	1.649164000	1.690312000	-2.177313000
Ca	-3.036403000	0.000104000	-0.381362000
Ca	1.961530000	0.001886000	0.803763000

$Ca_2C_8H_8^{2+}$ C_1 (75.5)

Ca	1.186835000	-0.947383000	-1.191198000
C	-1.261620000	-0.765839000	-1.278688000
C	-2.060820000	0.314867000	-1.088161000
C	-0.639156000	1.780152000	0.370093000
C	1.262478000	-0.767029000	1.278003000
C	0.637170000	1.780569000	-0.368822000
C	2.059630000	0.315545000	1.089363000
C	1.834438000	1.302302000	0.025711000
H	-1.627404000	-1.397819000	-2.097671000
H	-2.980638000	0.461591000	-1.657426000
H	-0.620382000	2.441037000	1.238913000
H	1.628816000	-1.398960000	2.096724000
H	0.618163000	2.441710000	-1.237453000
H	2.978801000	0.463634000	1.659335000
H	2.715942000	1.682129000	-0.493868000
C	-1.836272000	1.301199000	-0.024119000
H	-2.717859000	1.680038000	0.495960000
Ca	-1.185361000	-0.949815000	1.189958000

$Ca_2C_8H_8^{2+}$ C_1 (78.2)

Ca	-2.851308000	0.468016000	-0.042729000
C	1.507411000	-0.901113000	1.273767000
C	0.354223000	-0.269601000	1.597039000
C	-0.248343000	1.414955000	-0.096193000
C	2.195213000	-0.863010000	-0.025540000
C	1.011828000	2.172563000	-0.118404000
C	2.469836000	0.235154000	-0.761043000
C	2.188880000	1.631796000	-0.428784000
H	1.993640000	-1.499797000	2.040557000
H	0.003155000	-0.381075000	2.621517000
H	-0.971245000	1.835185000	-0.828631000
H	2.706736000	-1.780808000	-0.327259000
H	0.944721000	3.248345000	0.019373000
H	3.101536000	0.092676000	-1.636623000
H	3.048901000	2.291229000	-0.525506000
C	-0.580186000	0.360050000	0.667870000
H	-2.235621000	-1.206798000	-1.104793000
Ca	-0.247942000	-1.732202000	-0.602816000

$Ca_2C_8H_8^{2+}$ C_s (78.7)

Ca	2.114734000	-1.370508000	0.000000000
Ca	0.475943000	1.909241000	0.000000000
C	-0.356777000	-0.676976000	1.626779000
C	-1.047188000	0.519345000	1.644178000
C	-1.900598000	1.169960000	-0.687974000
C	-0.356777000	-1.771017000	0.686924000
C	-1.047188000	0.519345000	-1.644178000
C	-0.356777000	-1.771017000	-0.686924000
C	-0.356777000	-0.676976000	-1.626779000
H	0.063372000	-0.937862000	2.596580000
H	-1.045441000	1.006633000	2.618112000
H	-2.617129000	1.847511000	-1.144544000
H	-0.339531000	-2.751482000	1.164657000
H	-1.045441000	1.006633000	-2.618112000
H	-0.339531000	-2.751482000	-1.164657000
H	0.063372000	-0.937862000	-2.596580000
C	-1.900598000	1.169960000	0.687974000
H	-2.617129000	1.847511000	1.144544000

$Ca_2C_8H_8^{2+}$ C_1 (82.4)

C	-2.883017000	1.026639000	0.672655000
C	1.303515000	-1.162534000	-0.583165000
C	2.911490000	0.304358000	0.102266000
C	-3.198524000	0.127161000	-0.220936000
C	2.187890000	-0.096190000	1.242857000
C	-1.802660000	0.923189000	-0.325050000
C	1.195293000	-1.010432000	0.832257000
H	-3.267721000	1.654241000	1.466356000
H	0.878398000	-1.940849000	-1.218037000
H	3.774908000	0.958001000	0.097997000
H	-4.085531000	-0.173375000	-0.768887000
H	2.400851000	0.179787000	2.267242000
H	-1.808236000	1.813614000	-0.989023000
H	0.668337000	-1.645378000	1.545849000
C	2.360645000	-0.339386000	-1.023468000
H	2.728836000	-0.282159000	-2.039369000
Ca	0.641193000	1.417809000	-0.190962000
Ca	-1.328075000	-1.377845000	-0.036369000

$Ca_2C_8H_8^{2+}$ C_1 (85.6)

Ca	3.462750000	0.121497000	-0.068622000
Ca	-0.523851000	-0.134184000	-1.394485000
C	-0.780341000	-1.339011000	1.019690000

C	1.320755000	-0.464166000	0.034128000
C	-0.269678000	1.188203000	1.005220000
C	-2.015312000	-1.392238000	0.465690000
C	-1.398392000	1.698271000	0.467919000
C	-2.845705000	-0.312608000	-0.032684000
C	-2.574933000	1.016157000	-0.048128000
H	-0.393100000	-2.282279000	1.396398000
H	1.628581000	-1.536502000	0.083577000
H	0.441907000	1.918078000	1.382717000
H	-2.479858000	-2.372534000	0.426751000
H	-1.470243000	2.781367000	0.447829000
H	-3.812438000	-0.617458000	-0.420914000
H	-3.348254000	1.668843000	-0.439609000
C	0.228511000	-0.228175000	1.130291000
H	0.665994000	-0.304370000	2.132636000

$Ca_2C_8H_8^{2+}$ C_1 (85.8)

C	2.383694000	-0.802395000	-0.735246000
C	1.139953000	-1.163210000	-1.109434000
C	-0.578640000	0.627463000	-0.463988000
C	2.883732000	0.557479000	-0.542672000
C	0.000427000	0.976214000	0.845394000
C	2.392036000	1.506971000	0.250680000
C	1.252152000	1.387984000	1.153532000
H	3.145417000	-1.581118000	-0.727079000
H	1.028369000	-2.190288000	-1.472383000
H	-2.374802000	-0.965169000	0.836924000
H	3.808083000	0.763482000	-1.078215000
H	-0.721537000	1.130100000	1.660581000
H	2.938817000	2.443748000	0.325774000
H	1.411112000	1.794205000	2.151492000
C	-0.036007000	-0.288098000	-1.306372000
H	-0.556634000	-0.516599000	-2.240185000
Ca	-0.326614000	-1.518167000	1.041846000
Ca	-2.938532000	0.633526000	-0.442260000

$Sr_2C_8H_8^{2+}$ D_{8h} (0.0)

Sr	2.043519000	0.000000000	-0.000002000
C	0.000000000	1.307436000	-1.307439000
C	0.000000000	1.848994000	-0.000002000
C	0.000000000	0.000000000	1.848992000
C	0.000000000	0.000000000	-1.848944000
C	0.000000000	-1.307436000	1.307434000
C	0.000000000	-1.307436000	-1.307439000

C	0.000000000	-1.848994000	-0.000002000
H	0.000000000	2.073914000	-2.073916000
H	0.000000000	2.932957000	-0.000002000
H	0.000000000	0.000000000	2.932955000
H	0.000000000	0.000000000	-2.932959000
H	0.000000000	-2.073914000	2.073911000
H	0.000000000	-2.073914000	-2.073916000
H	0.000000000	-2.932957000	-0.000002000
C	0.000000000	1.307436000	1.307434000
H	0.000000000	2.073914000	2.073911000
Sr	-2.043519000	0.000000000	-0.000002000

$Sr_2C_8H_8^{2+}$ C_{2v} (66.1)

C	1.262029000	1.286430000	1.218135000
C	1.697159000	0.000000000	0.809124000
C	0.000000000	-1.756417000	1.606324000
C	0.000000000	1.756417000	1.606324000
C	-1.262029000	-1.286430000	1.218135000
C	-1.262029000	1.286430000	1.218135000
C	-1.697159000	0.000000000	0.809124000
H	2.087779000	1.985217000	1.361812000
H	2.729564000	0.000000000	0.465668000
H	0.000000000	-2.736648000	2.084459000
H	0.000000000	2.736648000	2.084459000
H	-2.087779000	-1.985217000	1.361812000
H	-2.087779000	1.985217000	1.361812000
H	-2.729564000	0.000000000	0.465668000
C	1.262029000	-1.286430000	1.218135000
H	2.087779000	-1.985217000	1.361812000
Sr	0.000000000	-2.246642000	-0.904843000
Sr	0.000000000	2.246642000	-0.904843000

$Sr_2C_8H_8^{2+}$ C_1 (67.3)

Sr	-2.465418000	-0.323308000	-0.256066000
Sr	1.812501000	-1.117649000	-0.251750000
C	1.344678000	1.274379000	-1.297624000
C	-0.034812000	1.567427000	-1.228198000
C	-0.031518000	1.317678000	1.274354000
C	2.071222000	1.554870000	-0.076909000
C	-0.168491000	-0.114248000	1.770888000
C	1.468274000	1.571422000	1.135781000
C	-0.471260000	-1.198682000	1.012658000
H	1.848698000	1.414967000	-2.247747000
H	-0.532863000	1.861067000	-2.152034000

H	-0.404348000	1.968401000	2.072355000
H	3.127637000	1.809083000	-0.145238000
H	0.072073000	-0.211156000	2.834367000
H	2.014573000	1.890911000	2.015996000
H	-0.455220000	-2.129248000	1.597900000
C	-0.729249000	1.656525000	-0.036175000
H	-1.552806000	2.376100000	-0.007247000

$Sr_2C_8H_8^{2+}$ C_s (70.0)

Sr	-1.061195000	1.310825000	0.000000000
C	0.858182000	0.372095000	1.716253000
C	0.858182000	-0.640725000	0.726772000
C	0.858182000	0.372095000	-1.716253000
C	0.939934000	1.765494000	1.701559000
C	0.939934000	1.765494000	-1.701559000
C	1.052518000	2.749545000	0.698895000
C	1.052518000	2.749545000	-0.698895000
H	0.815470000	-0.035919000	2.720992000
H	1.305058000	-1.542753000	1.176365000
H	0.815470000	-0.035919000	-2.720992000
H	0.909322000	2.188344000	2.700104000
H	0.909322000	2.188344000	-2.700104000
H	1.119156000	3.749347000	1.114727000
H	1.119156000	3.749347000	-1.114727000
C	0.858182000	-0.640725000	-0.726772000
H	1.305058000	-1.542753000	-1.176365000
Sr	-0.328379000	-2.881219000	0.000000000

$Sr_2C_8H_8^{2+}$ C_s (80.8)

Sr	-1.313469000	1.534293000	0.000000000
C	1.112764000	-0.140805000	1.635563000
C	1.743243000	-1.021707000	0.686781000
C	1.112764000	-0.140805000	-1.635563000
C	0.943990000	1.228117000	1.647537000
C	0.943990000	1.228117000	-1.647537000
C	1.233824000	2.257086000	0.687442000
C	1.233824000	2.257086000	-0.687442000
H	0.949360000	-0.598059000	2.609783000
H	2.313917000	-1.822895000	1.159146000
H	0.949360000	-0.598059000	-2.609783000
H	0.669608000	1.620758000	2.625700000
H	0.669608000	1.620758000	-2.625700000
H	1.415925000	3.227100000	1.142738000
H	1.415925000	3.227100000	-1.142738000

C	1.743243000	-1.021707000	-0.686781000
H	2.313917000	-1.822895000	-1.159146000
Sr	-0.557676000	-2.395506000	0.000000000

$Sr_2C_8H_8^{2+}$ C_2 (84.1)

Sr	0.152431000	1.834381000	-0.736749000
Sr	-0.152431000	-1.834381000	-0.736749000
C	-0.152431000	0.720759000	2.092138000
C	-1.253150000	1.343405000	1.628566000
C	-1.841592000	0.130473000	-0.463139000
C	0.152431000	-0.720759000	2.092138000
C	1.841592000	-0.130473000	-0.463139000
C	1.253150000	-1.343405000	1.628566000
C	2.210332000	-0.808807000	0.653202000
H	0.512163000	1.289947000	2.744730000
H	-1.453137000	2.344783000	2.015481000
H	-2.719042000	-0.131267000	-1.070382000
H	-0.512163000	-1.289947000	2.744730000
H	2.719042000	0.131267000	-1.070382000
H	1.453137000	-2.344783000	2.015481000
H	3.248836000	-1.089331000	0.842042000
C	-2.210332000	0.808807000	0.653202000
H	-3.248836000	1.089331000	0.842042000

$Sr_2C_8H_8^{2+}$ C_s (95.2)

C	1.684540000	1.987575000	0.672757000
C	0.544067000	2.102715000	1.592366000
C	-0.583536000	4.155950000	0.665094000
C	1.684540000	1.987575000	-0.672757000
C	-0.583536000	4.155950000	-0.665094000
C	0.544067000	2.102715000	-1.592366000
C	-0.443072000	3.016472000	-1.571976000
H	2.641630000	1.824934000	1.163131000
H	0.602559000	1.471716000	2.483215000
H	-0.771253000	5.099195000	1.173216000
H	2.641630000	1.824934000	-1.163131000
H	-0.771253000	5.099195000	-1.173216000
H	0.602559000	1.471716000	-2.483215000
H	-1.144053000	3.003584000	-2.405566000
C	-0.443072000	3.016472000	1.571976000
H	-1.144053000	3.003584000	2.405566000
Sr	-0.486213000	-0.017740000	0.000000000
Sr	0.036693000	-4.138876000	0.000000000

$Sr_2C_8H_8^{2+}$ C_1 (124.1)

Sr	2.529958000	0.449668000	0.142201000
Sr	-1.614577000	-1.042816000	0.344057000
C	-1.432241000	1.862031000	0.787254000
C	-2.667370000	1.783100000	0.065591000
C	1.120748000	-1.543952000	0.557758000
C	-0.247186000	1.253447000	0.374183000
C	0.909394000	-1.560597000	-0.810056000
C	-0.043226000	0.810225000	-0.976481000
C	0.473410000	-0.382825000	-1.522271000
H	-1.464536000	2.338811000	1.760127000
H	-3.525777000	2.276978000	0.533940000
H	1.369106000	-2.521139000	0.981143000
H	0.427511000	1.039359000	1.206733000
H	1.048464000	-2.442613000	-1.440740000
H	-0.504486000	1.464933000	-1.711165000
H	0.445189000	-0.439721000	-2.605632000
C	-2.918160000	1.090743000	-1.054872000
H	-3.752193000	0.949984000	-1.728849000

$Sr_2C_8H_8^{2+}$ D_{8h} (127.1)

C	-1.832024000	0.000138000	0.000000000
C	-1.295246000	1.295571000	0.000000000
C	1.295999000	1.295601000	0.000000000
C	-1.295537000	-1.295448000	0.000000000
C	1.832131000	-0.000052000	0.000000000
C	-0.000090000	-1.832080000	0.000000000
C	1.295469000	-1.295503000	0.000000000
H	-2.918278000	0.000268000	0.000000000
H	-2.063156000	2.063729000	0.000000000
H	2.063904000	2.063714000	0.000000000
H	-2.063619000	-2.063439000	0.000000000
H	2.918415000	-0.000249000	0.000000000
H	-0.000131000	-2.918334000	0.000000000
H	2.063504000	-2.063532000	0.000000000
C	0.000263000	1.832024000	0.000000000
H	0.000377000	2.918291000	0.000000000
Sr	-0.000090000	-0.000026000	3.583351000
Sr	-0.000090000	-0.000026000	-3.583351000

$Sr_2C_8H_8^{2+}$ C_1 (127.9)

Sr	2.477354000	-0.346169000	-0.314980000
Sr	-1.851429000	-1.118673000	-0.242549000
C	0.945040000	1.239964000	1.281687000

C	0.625970000	-0.089083000	1.682990000
C	-2.210317000	1.215295000	1.266635000
C	0.838701000	1.829482000	0.005569000
C	-2.400227000	1.552665000	-0.009820000
C	-0.080792000	1.694908000	-1.061990000
C	-1.462926000	1.507132000	-1.104943000
H	1.447703000	1.846228000	2.032517000
H	0.737631000	-0.255866000	2.756131000
H	-2.747792000	1.303000000	2.200413000
H	1.540295000	2.649872000	-0.177185000
H	-3.409241000	1.886564000	-0.286509000
H	0.314768000	2.019104000	-2.024731000
H	-1.907272000	1.671063000	-2.082159000
C	0.395203000	-1.173960000	0.833971000
H	0.334823000	-2.114368000	1.403028000

$Sr_2C_8H_8^{2+}$ C_{2v} (134.6)

Sr	0.000000000	2.669365000	-1.282022000
C	1.692077000	-0.699371000	1.669848000
C	0.701469000	-1.683254000	1.789201000
C	-1.692077000	-0.699371000	1.669848000
C	1.692077000	0.699371000	1.669848000
C	-1.692077000	0.699371000	1.669848000
C	0.701469000	1.683254000	1.789201000
C	-0.701469000	1.683254000	1.789201000
H	2.695730000	-1.114659000	1.657594000
H	1.122145000	-2.675795000	1.946536000
H	-2.695730000	-1.114659000	1.657594000
H	2.695730000	1.114659000	1.657594000
H	-2.695730000	1.114659000	1.657594000
H	1.122145000	2.675795000	1.946536000
H	-1.122145000	2.675795000	1.946536000
C	-0.701469000	-1.683254000	1.789201000
H	-1.122145000	-2.675795000	1.946536000
Sr	0.000000000	-2.669365000	-1.282022000

$Sr_2C_8H_8^{2+}$ C_{2v} (137.4)

Sr	0.000000000	1.830695000	-1.021595000
C	0.000000000	-1.737395000	1.777394000
C	-1.265783000	-1.271935000	1.409323000
C	-1.265783000	1.271935000	1.409323000
C	1.265783000	-1.271935000	1.409323000
C	0.000000000	1.737395000	1.777394000
C	1.672675000	0.000000000	0.846339000

C	1.265783000	1.271935000	1.409323000
H	0.000000000	-2.675058000	2.327729000
H	-2.096437000	-1.928063000	1.664056000
H	-2.096437000	1.928063000	1.664056000
H	2.096437000	-1.928063000	1.664056000
H	0.000000000	2.675058000	2.327729000
H	2.706042000	0.000000000	0.510500000
H	2.096437000	1.928063000	1.664056000
C	-1.672675000	0.000000000	0.846339000
H	-2.706042000	0.000000000	0.510500000
Sr	0.000000000	-1.830695000	-1.021595000