Electronic Supplementary Material (ESI) for Chemical Communications.
This journal is © The Royal Society of Chemistry 2022

E_6C_{15} (E = Si-Pb): Polycyclic Aromatic Compounds with Three planar Tetracoordinate Carbons

Diego Inostroza,[a,b] Luis Leyva-Parra[a,b], Alejandro Vásquez-Espinal[c] ,Julia Contreras-García[d], Zhong-hua Cui,[e,f] Sudip Pan,[g,*] Venkatesan S. Thimmakondu,[h,*] and William Tiznado.[a,*]

[a] *Computational and Theoretical Chemistry Group, Departamento de Ciencias Químicas, Facultad de Ciencias Exactas, Universidad Andres Bello, República 498, Santiago, Chile. E-mail: wtiznado@unab.cl*
[b] *Doctorado en Fisicoquímica Molecular, Facultad de Ciencias Exactas, Universidad Andres Bello, República 275, Santiago, Chile.*
[c] *Química y Farmacia, Facultad de Ciencias de la Salud, Universidad Arturo Prat, Casilla 121, Iquique 1100000, Chile*
[d] *Sorbonne Universités and CNRS, Laboratoire de Chimie Théorique (LCT), 75005 Paris, France.*
[e] *Institute of Atomic and Molecular Physics, Jilin University, Changchun 130023, China.*
[f] *Key Laboratory of Physics and Technology for Advanced Batteries (Ministry of Education), Jilin University, Changchun 130023, China.*
[g] *Fachbereich Chemie,Philipps-Universitt Marburg Hans-Meerwein-Straße,35043 Marburg, Germany. E-mail: pans@chemie.uni-marburg.de*
[h] *Department of Chemistry and Biochemistry, San Diego State University, San Diego, CA, 92182-1030 USA E-mail: vthimmakondusamy@sdsu.edu*

Contents

Isomerization Energy Decomposition Analysis 4

Scheme S1. The procedure used to explore the potential energy surface using the AUTOMATON program.[7] 5

Figures 6

Figure S1. Putative global minimum and low-lying isomers of Si_6C_{15} with their point group symmetries. Relative energies are shown in kcal·mol^{-1} at PBE0[8]-D3[9]/def2-TZVP[10] level, including zero-point energy (ZPE) corrections. 6

Figure S2. Putative global minimum and low-lying isomers of Ge_6C_{15} with their point group symmetries. Relative energies are shown in kcal·mol^{-1} at PBE0[8]-D3[9]/def2-TZVP [10] level including zero-point energy (ZPE) corrections. 10

Figure S3. Putative global minimum and low-lying isomers of Sn_6C_{15} with their point group symmetries. Relative energies are shown in kcal·mol^{-1} at PBE0[8]-D3[9]/def2-TZVP[10] level including zero-point energy (ZPE) corrections. 14

Figure S4. Putative global minimum and low-lying isomers of Pb_6C_{15} with their point group symmetries. Relative energies are shown in kcal·mol^{-1} at PBE0[8]-D3[9]/def2-TZVP[10] level including zero-point energy (ZPE) corrections. 17

Figure S5. The natural charges (red) for the Si_6C_{15}/Ge_6C_{15} putative global minimum at the PBE0/def2-TZVP level. 21

Figure S6. The natural charges (red) for the Sn_6C_{15}/Pb_6C_{15} putative global minimum at the PBE0/def2-TZVP level. 22

Figure S7. Lowest energy structures of E_6C_{15} at ωB97XD/def2-TZVP level (relative energies in kcal·mol^{-1}, including the zero-point energy (ZPE) corrections). The bond length in Å (black) and WBI values (blue) at ωB97XD [11]/def2-TZVP level. 23

Figure S9. AdNDP [12,13] analysis of the **3**(Ge) system (D_{3h}-Ge_6C_{15}). ON stands for occupation number. Carbon=gray, Germanium=brown. 24

Figure S10. AdNDP analysis of **4**(E) systems (E=Sn, Pb). ON stands for occupation number. Carbon=gray, Silicon=blue. 25

Figure S11. Different detected ring current circuits for the D_{3h}-Si_6C_{15} system (up) and the RCS profiles along the different integration planes (down) were used to estimate their intensity. Computations were performed using the GIMIC program,[14,15] which employs the gauge-including atomic orbital (GIAO)[16] method. To visualize current pathways, we used Paraview 5.10.0 software.[17,18] 26

Figure S12. Different detected ring current circuits for D_{3h}-Ge_6C_{15} system (up) and the RCS profiles along the different integration planes (down) were used to estimate their intensity. 27

Figure S13. Different detected ring current circuits for the C_3-Sn_6C_{15} system (up) and the RCS profiles along the different integration planes (down) were used to estimate their intensity. 28

Figure S14. Different detected ring current circuits for the C_3-Pb_6C_{15} system (up) and the RCS profiles along the different integration planes (down) were used to estimate their intensity. 29

Figure S15. Vector plots visualization of the current density in diverse planes of the D_{3h}-Si_6C_{15} system. Diatropic currents are assumed to circle clockwise. 30

Figure S16. Vector plots visualization of the current density in diverse planes of the D_{3h}-Ge_6C_{15} system. Diatropic currents are assumed to circle clockwise. 31

Figure S17. Vector plots visualization of the current density in diverse planes of the C_3-Sn_6C_{15} system. Diatropic currents are assumed to circle clockwise..... 32

Figure S18. Vector plots visualization of the current density in diverse planes of the C_3-Pb_6C_{15} system. Diatropic currents are assumed to circle clockwise..... 33

Figure S19. The minimum energy geometries of the complex $[3(Si)]_2$ at PBE0-D3/def2-SVP level. The bond dissociation energies at 0 K (D_e) and 298 K, including thermal correction and entropy factors (ΔG^{298K}), are given in kcal·mol^{-1}. 34

Figure S20. Energetic reaction cycle involving the isomerization of E_6C_{15} between isomers **3**(E) (top) and **4**(E) (bottom). 35

Tables 35

Table S1. Results of the IEDA at the PBE0-D3-BJ/ZORA/TZ2P level for the E_6C_{15} systems with E_6^{12+} + C_{15}^{12-} as fragments.[a] 35

Table S2. The HOMO-LUMO energy gaps for **3**(E) and **4**(E) structures. Values in eV. 36

Table S3. Cartesian coordinates of the E_6C_{18} global minima structures at the PBE0-D3/def2-TZVP level. 36

Table S4. Cartesian coordinates of 3(E) and 4(E) optimized structures at the PBE0-D3/def2-TZVP level. 37

Table S5. Cartesian coordinates for 3(Si) complexes optimized at the PBE0-D3/def2-TZVP level, except for sandwich and dimer complexes for which def2-SVP is used. 39

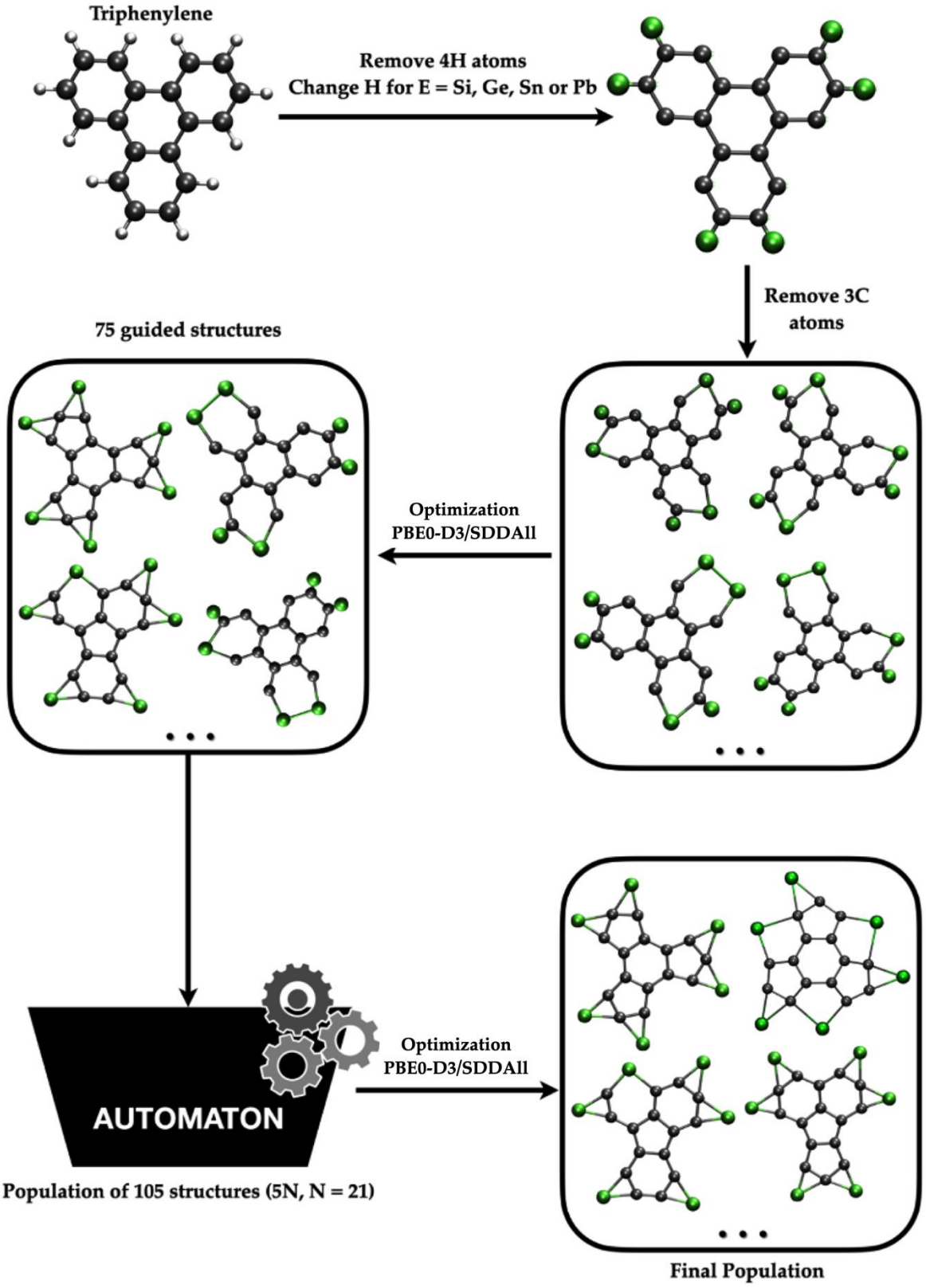
References 43

Isomerization Energy Decomposition Analysis

To gain more insight into the factors that determine the preference of the **3**(E) or **4**(E) isomer, IEDA[1] was performed, which allows decomposing the difference in energy between two isomers (ΔE_{iso}) into two terms: the distortion energy of the fragments (ΔE_{dist}) and the change in the interaction energies between the fragments of each isomer ($\Delta\Delta E_{int}$). The latter term, in turn, is decomposed as the sum of the changes in the orbital ($\Delta\Delta E_{orb}$) and electrostatic ($\Delta\Delta V_{elstat}$) interaction, the Pauli repulsion ($\Delta\Delta E_{Pauli}$) and the dispersion energy ($\Delta\Delta E_{disp}$). This analysis was performed at the PBE0-D3-BJ/TZ2P-ZORA level[2–5] using ADF2012.[6]

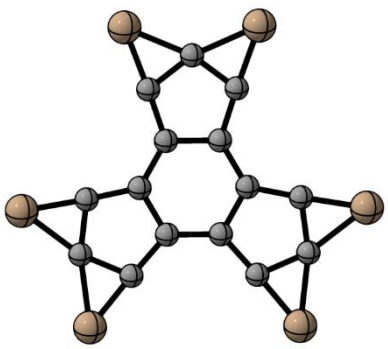
The IEDA results are shown in Table S1, in addition to Figure S20, which shows the thermodynamic cycle that has been considered to perform this analysis where the C_{15}^{12-} and E_6^{12+} (E = Si, Ge, Sn, Pb) species have been selected as interacting fragments. According to Figure S20, positive or negative values in Table S1 indicate that the corresponding term favors the 3(E) and 4(E) isomers, respectively. According to ΔE_{iso} values, for E = Si and Ge, the 3(E) isomer is 44.0 kcal·mol^{-1} and 19.9 kcal·mol^{-1}, respectively, below the 4(E) isomer, while for E = Sn and Pb, it is the 4(E) isomer that is 10.7 kcal·mol^{-1} and 24.2 kcal·mol^{-1} lower in energy, which is in good agreement with the relative energies shown in Figure 1. Note that in all cases, the distortion energy of both the C_{15}^{12-} and E_6^{12+} fragments is positive, i.e., both systems prefer to be in D_{3h} symmetry. On the other hand, for all cases, the interaction energy and the terms into which it decomposes ($\Delta\Delta E_{orb}$, $\Delta\Delta V_{elstat}$, $\Delta\Delta E_{Pauli}$, $\Delta\Delta E_{disp}$) favor the 4(E) isomer (except for the dispersion energy In the Sn_6C_{15} system), so this balance between interaction and distortion energies is what determines the favorability of one isomer over the other. In particular, for E = Si and Ge, the distortion energy is much higher than in their heavier analogs, so the better interaction energy in the 4(E) isomer is not sufficient to compensate for the high energetic cost of deforming the fragments from the D_{3h} symmetry. While for E = Sn and Pb the lower energetic cost of deforming the structure is outweighed by the favorable interaction energy of these fragments in the 4(E) isomer.

Scheme S1. The procedure used to explore the potential energy surface using the AUTOMATON program.[7]



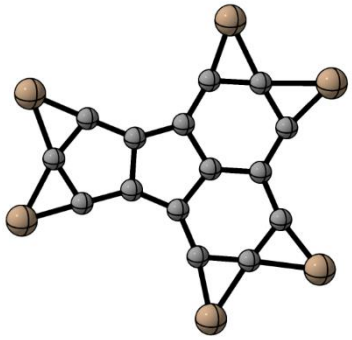
Figures

Figure S1. Putative global minimum and low-lying isomers of Si_6C_{15} with their point group symmetries. Relative energies are shown in kcal·mol^{-1} at PBE0[8]-D3[9]/def2-TZVP[10] level, including zero-point energy (ZPE) corrections.



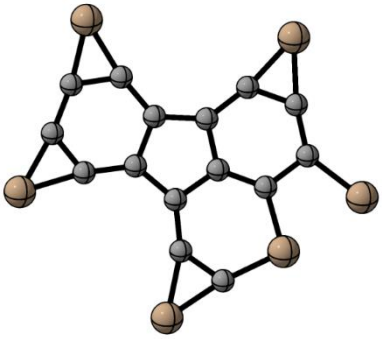
3(Si). D_{3h},^{1}A'$_1$

0.0



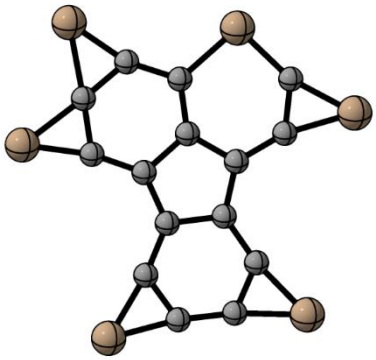
C_{2v},^{1}A$_1$

8.2



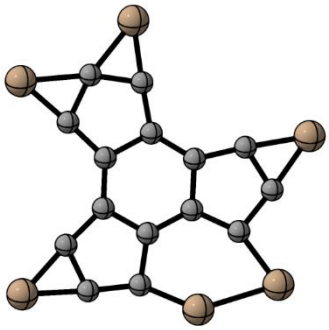
C_s, ^{1}A'

16.8



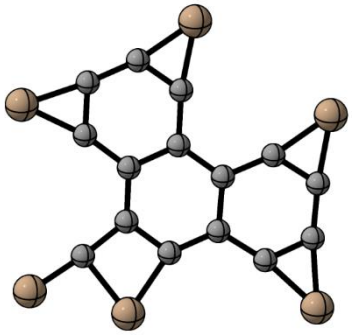
C_s, ^{1}A'

19.4



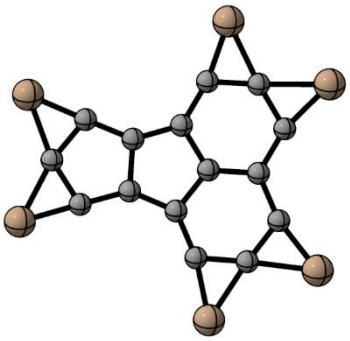
C_s, ^{1}A'

23.0



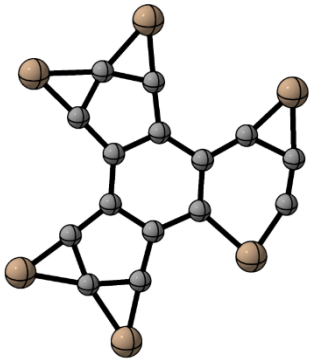
C_s, ^{1}A'

25.6



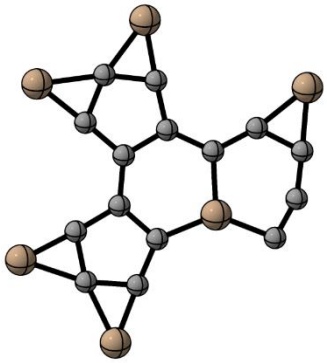
C_{2v},$^3A_1$

25.9



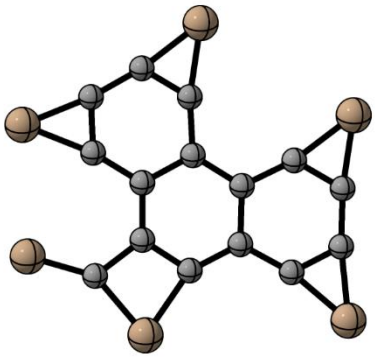
C_s, ^{1}A'

26.2



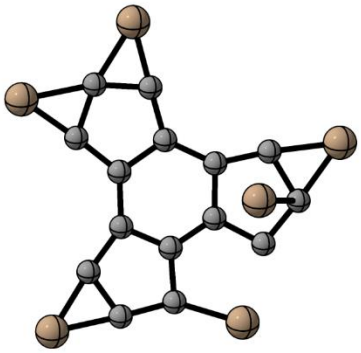
C_s, ^{1}A'

28.7



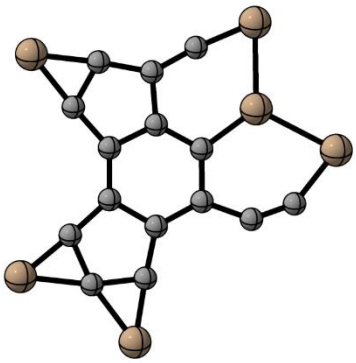
C_s, ^{1}A'

29.2



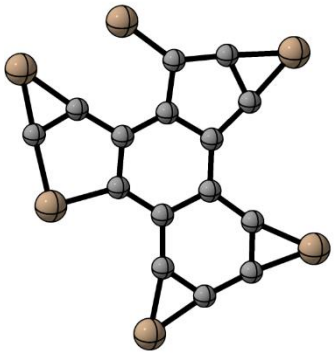
C_1, ^{1}A

30.1



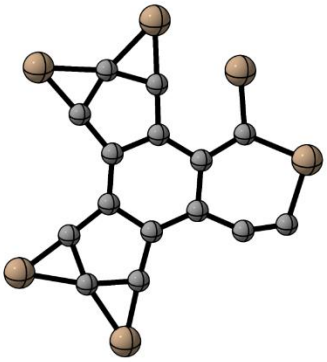
C_s, ^{1}A'

31.7



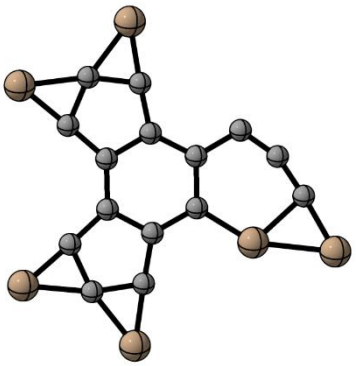
C_s, ^{1}A'

33.1



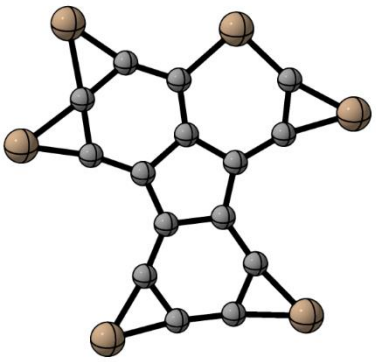
C_s, ^{1}A'

33.5



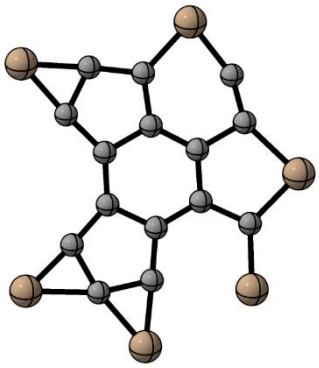
C_s, ^{1}A'

34.2



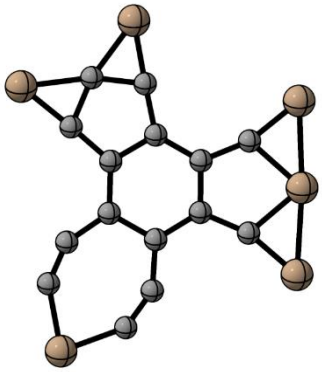
C_s, ^{3}A'

34.7



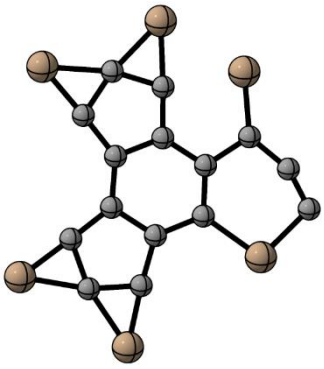
C_s, ^{1}A'

34.9



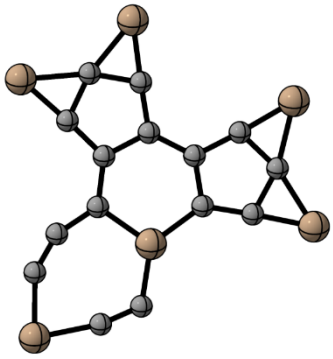
C_s, ^{1}A'

35.0



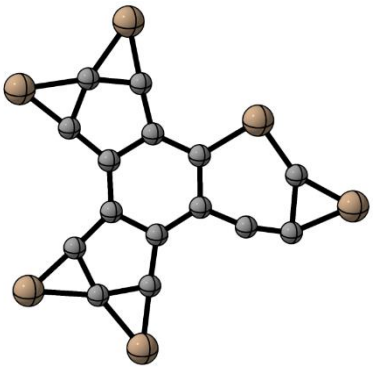
C_s, ^{1}A'

37.5



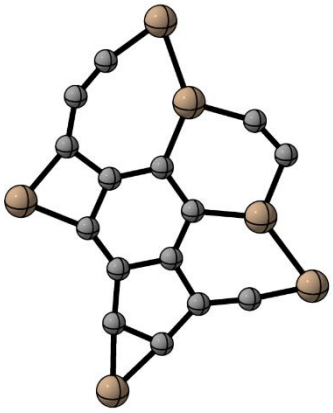
C_s, ^{1}A'

41.3



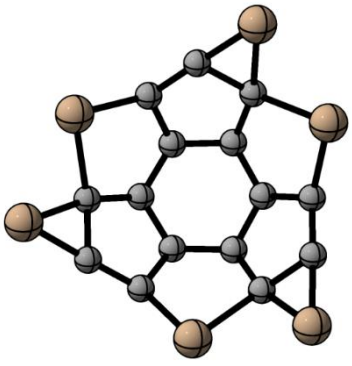
C_s, ^{1}A'

42.3



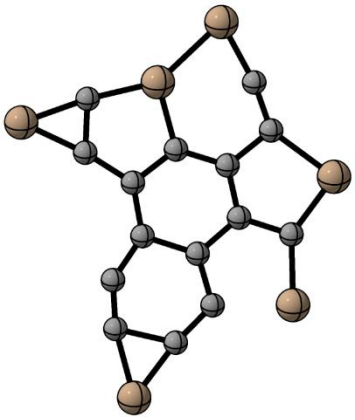
C_s, ^{1}A'

42.5



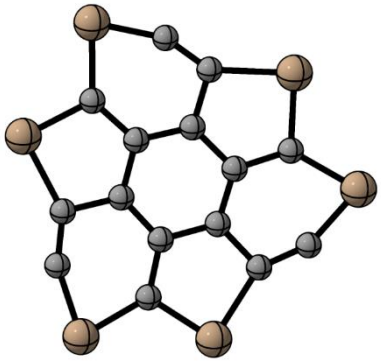
4(Si). C_3, ^{1}A

43.5



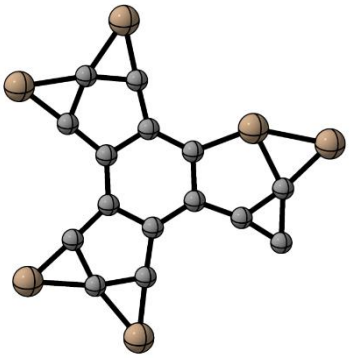
C_s, ^{1}A'

44.1



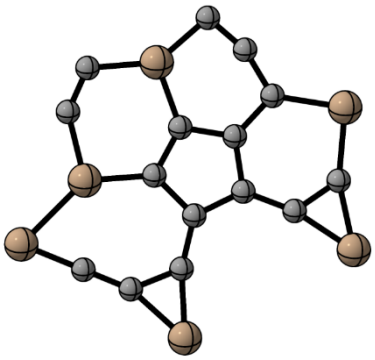
C_{3h}, ^{1}A'

44.4



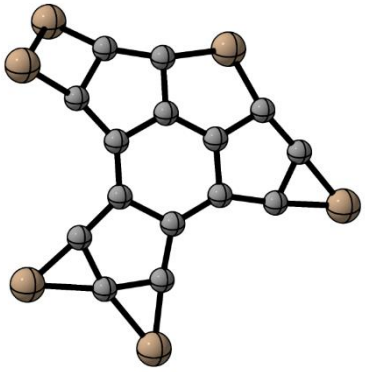
C_s,^{1}A'

45.2



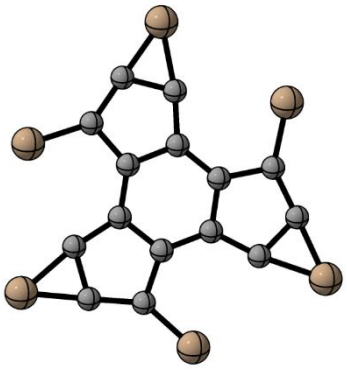
C_s,^{1}A'

46.2



C_s,^{1}A'

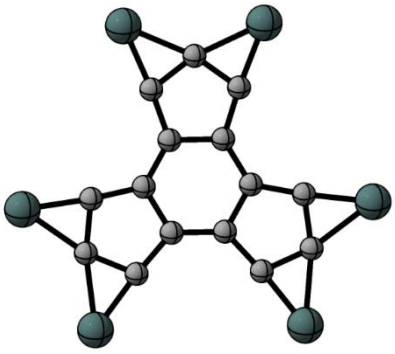
47.3



C_{3h}, ^{1}A'

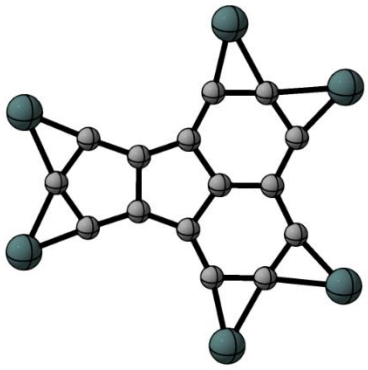
50.6

Figure S2. Putative global minimum and low-lying isomers of Ge_6C_{15} with their point group symmetries. Relative energies are shown in kcal·mol^{-1} at PBE0[8]-D3[9]/def2-TZVP [10] level including zero-point energy (ZPE) corrections.



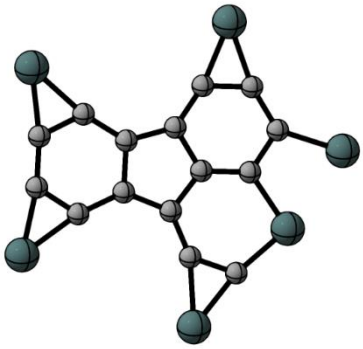
3(Ge). D_{3h}, $^1A'_1$

0.0



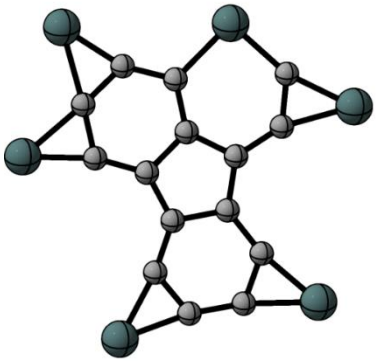
C_{2v}, $^1A_1$

2.8



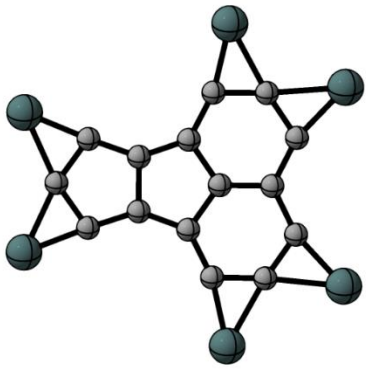
C_s, $^1A'$

8.8



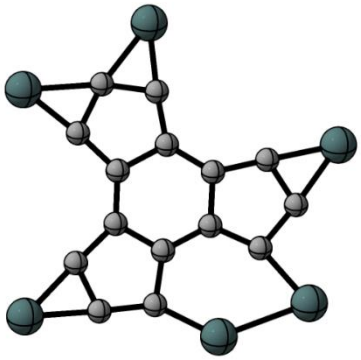
C_s, $^1A'$

11.2



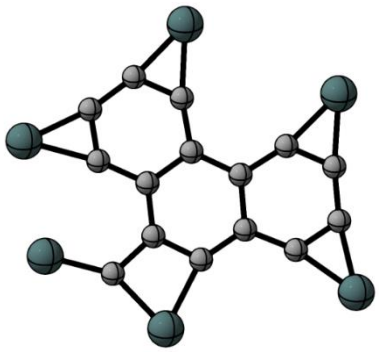
C_{2v}, $^3A_1$

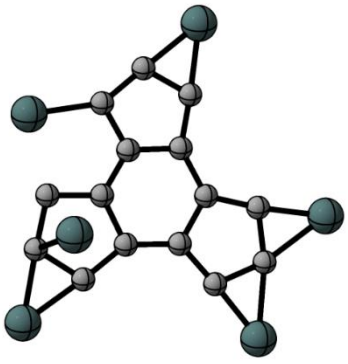
13.1

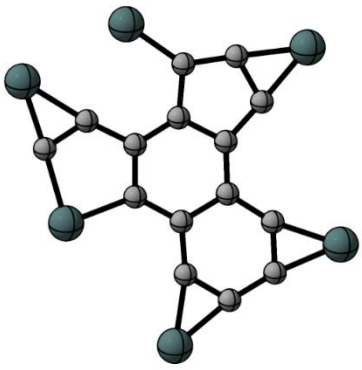


C_s, $^1A'$

13.3

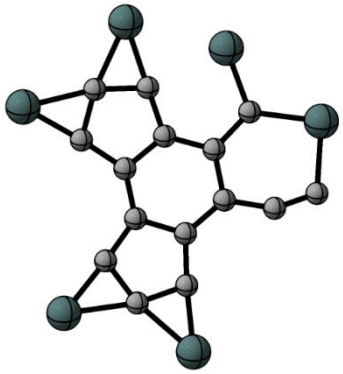






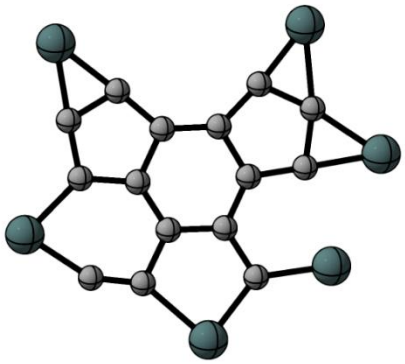
C_s, ^{1}A'

15.6



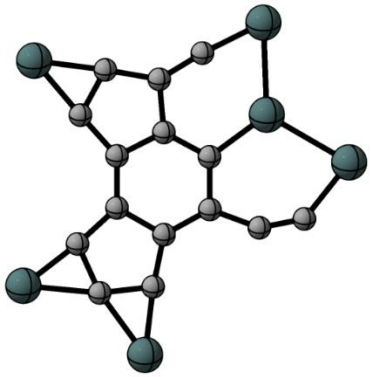
C_1, ^{1}A

15.8



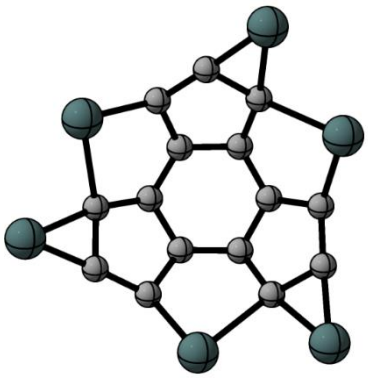
C_s, ^{1}A'

16.6



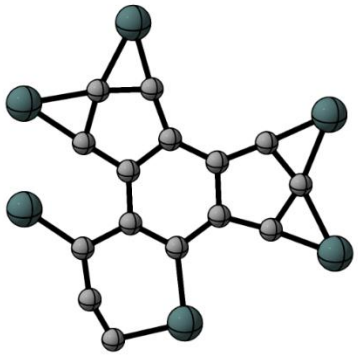
C_s, ^{1}A'

20.4



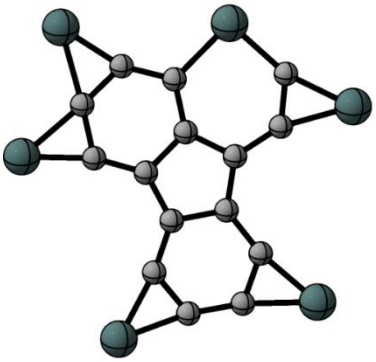
C_s, ^{1}A'

20.4



C_s, ^{1}A'

22.2

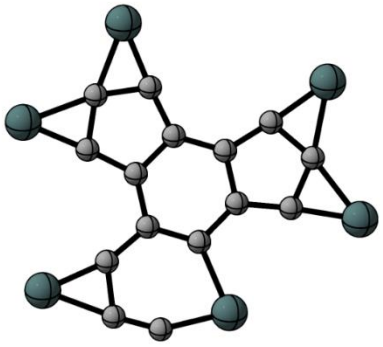


4(Ge). C_3, ^{1}A

23.0

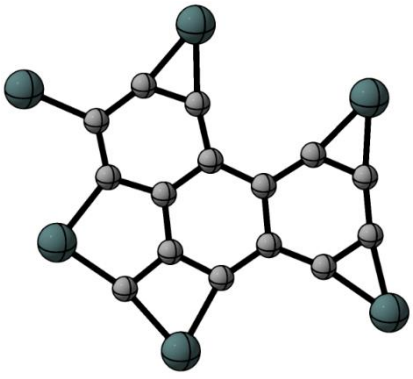
C_s, ^{1}A'

23.4



C_s, ^{3}A'

23.9

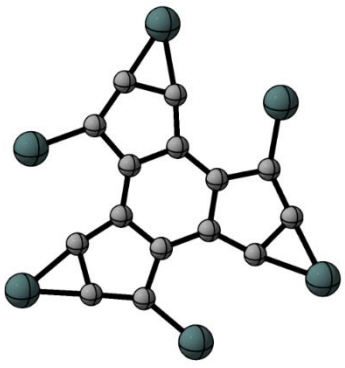


C_s, ^{3}A'

24.5

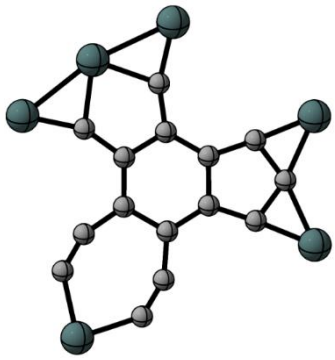
C_s, ^{1}A'

27.3



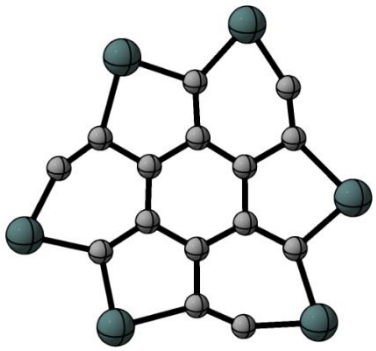
C_{3h}, ^{1}A'

27.8



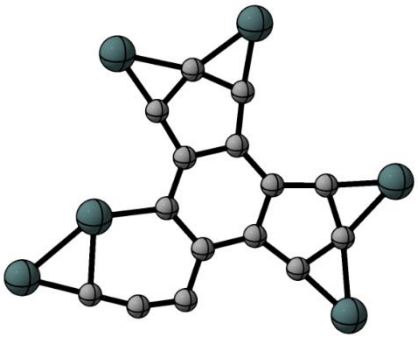
C_s, ^{1}A'

27.9



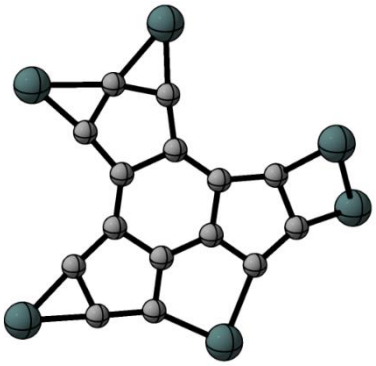
C_{3h}, ^{1}A'

28.7



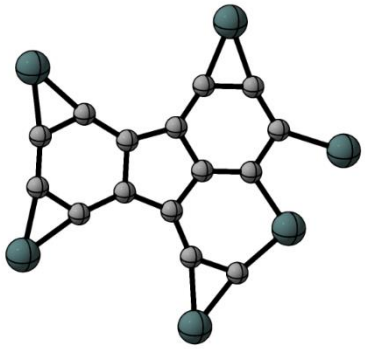
C_s, ^{1}A'

29.7



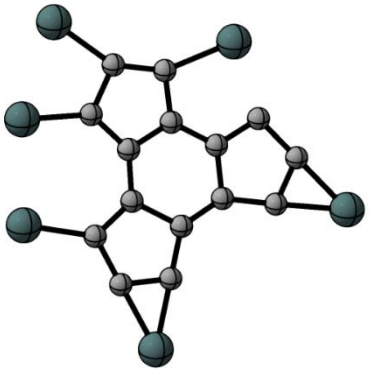
C_1, ^{1}A

31.5



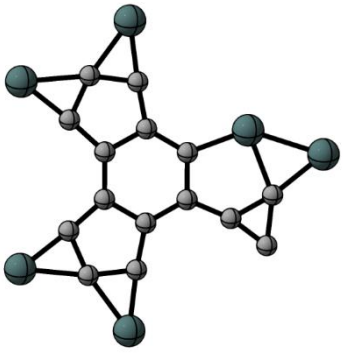
C_s, ^{3}A'

32.5



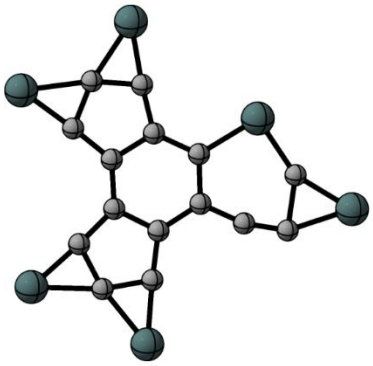
C_1, ^{1}A

34.3



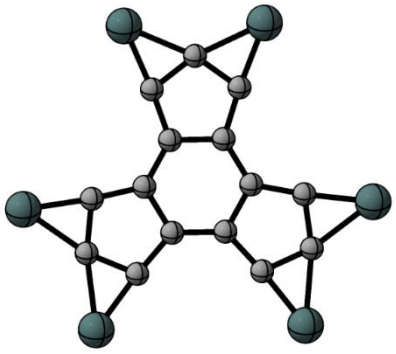
C_s, ^{1}A'

39.3



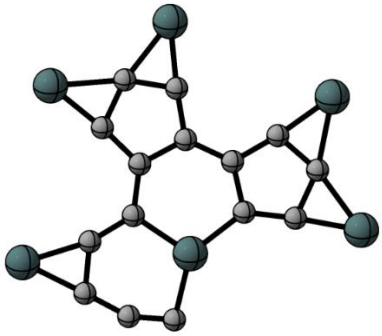
C_s, ^{1}A'

42.0



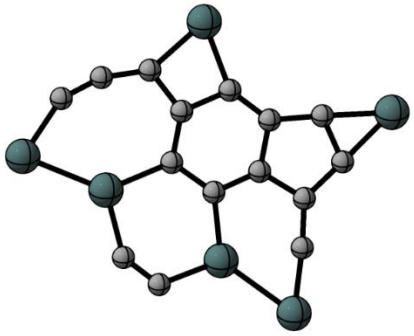
D_{3h}, ^{3}A'$_1$

46.9



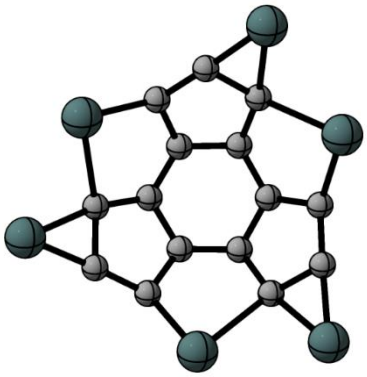
C_s, ^{1}A'

47.7



C_1, ^{1}A

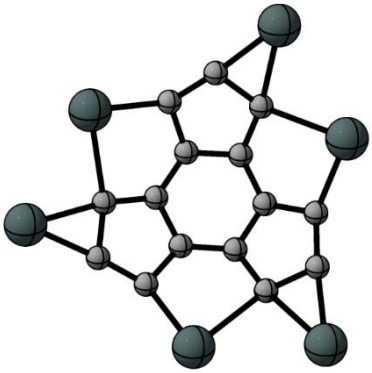
49.7



C_3, ^{3}A

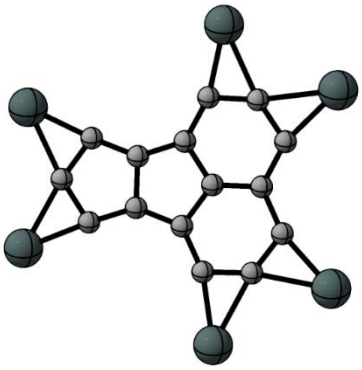
50.0

Figure S3. Putative global minimum and low-lying isomers of Sn_6C_{15} with their point group symmetries. Relative energies are shown in kcal·mol^{-1} at PBE0[8]-D3[9]/def2-TZVP[10] level including zero-point energy (ZPE) corrections.



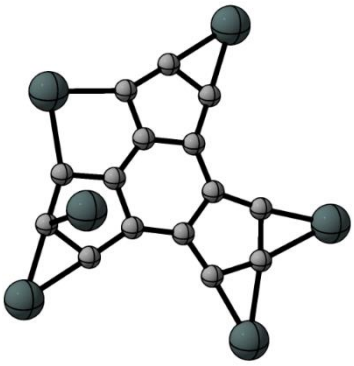
4(Sn). C_3, ^{1}A

0.0



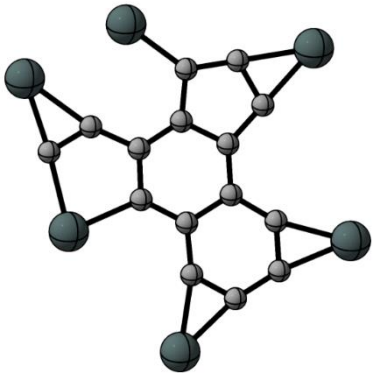
C_{2v}, $^1A_1$

5.5



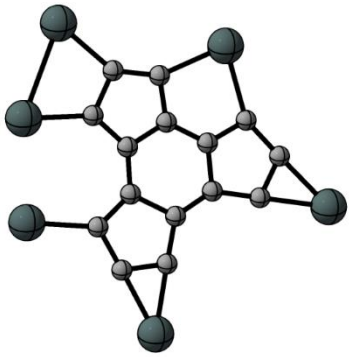
C_1, ^{1}A

5.8



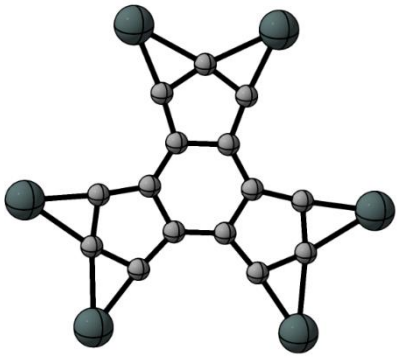
C_s, ^{1}A'

8.6



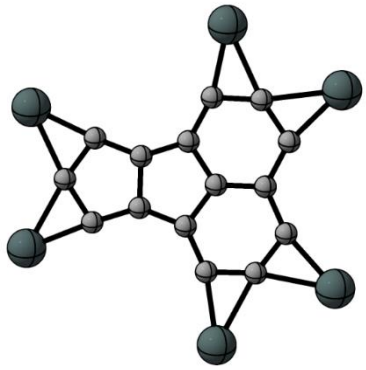
C_s, ^{1}A'

9.2



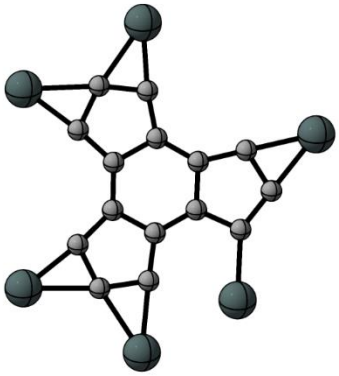
3(Sn). D_{3h}, $^1A'_1$

9.3



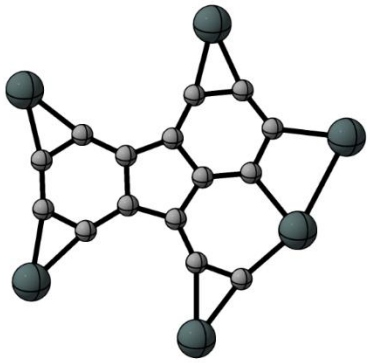
C_{2v}, $^3A_1$

9.5



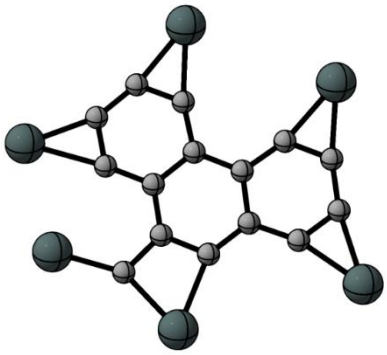
C_s, $^1A'$

10.1



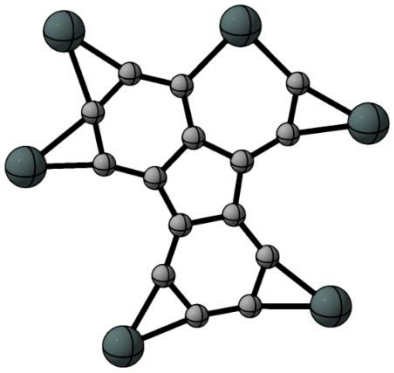
C_s, $^1A'$

10.2



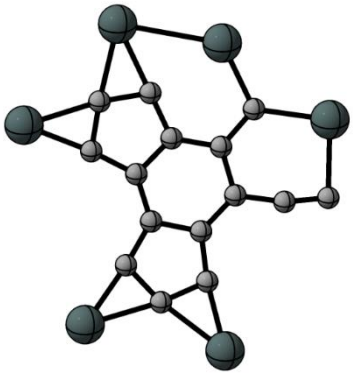
C_s, $^1A'$

11.2



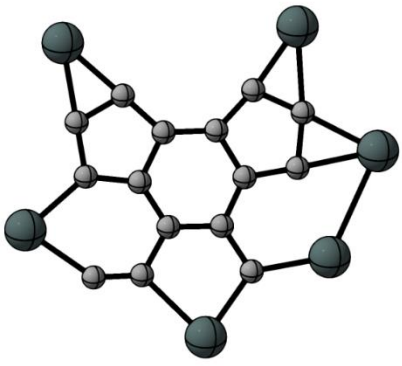
C_s, $^1A'$

11.8



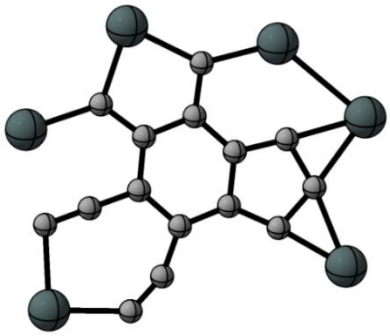
C_s, $^1A'$

12.2



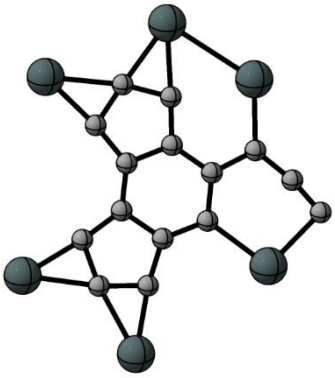
C_s, $^1A'$

12.3



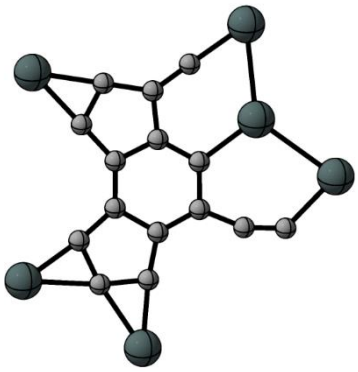
C_s, $^1A'$

12.8



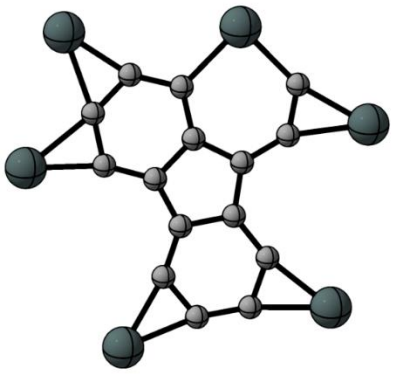
C_s, $^1A'$

13.7



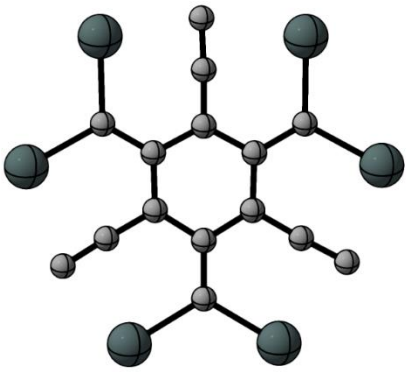
C_s, ^{1}A'

19.7



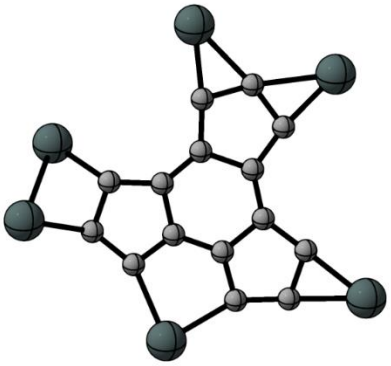
C_s, ^{3}A'

20.5



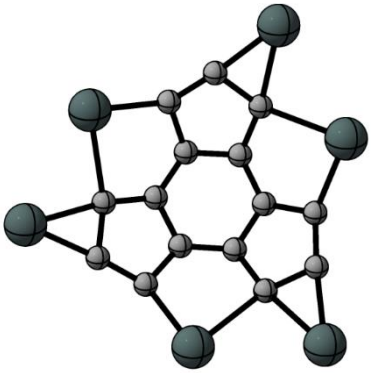
D_{3h}, ^{1}A'$_1$

20.6



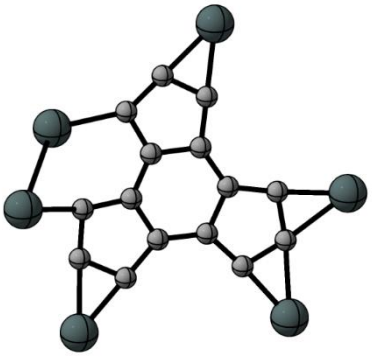
C_1, ^{1}A

20.8



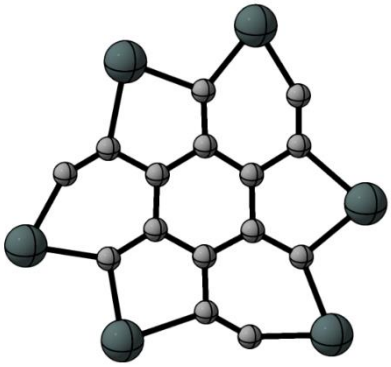
C_3, ^{3}A

24.0



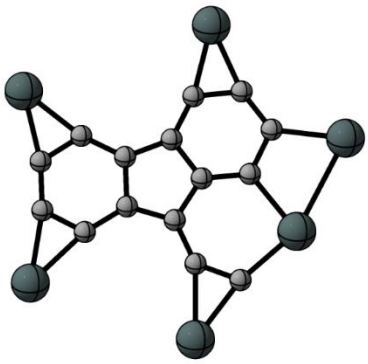
C_1, ^{3}A

26.3



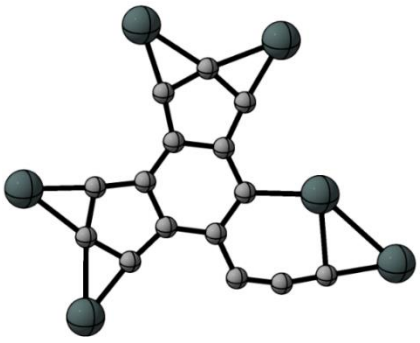
C_{3h}, ^{1}A'

27.6



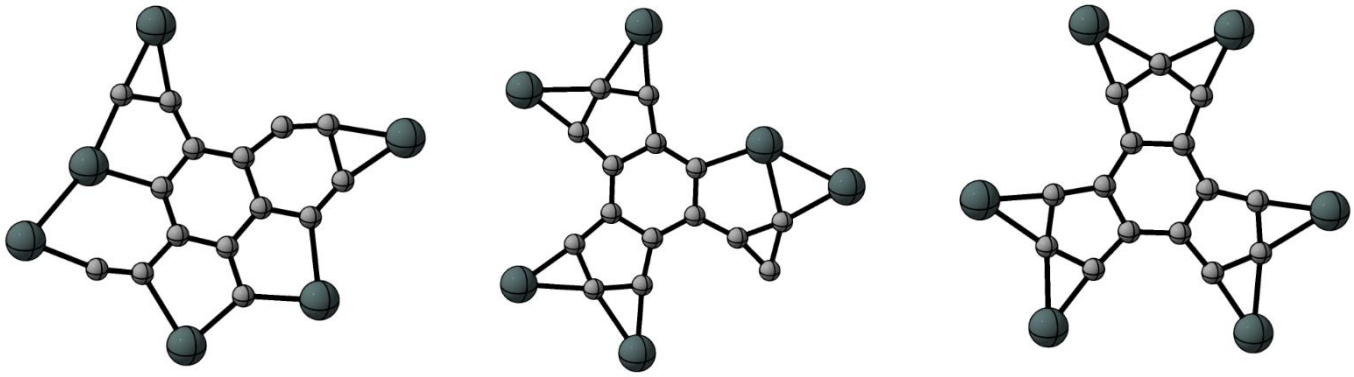
C_s, ^{3}A'

29.0



C_s, ^{1}A'

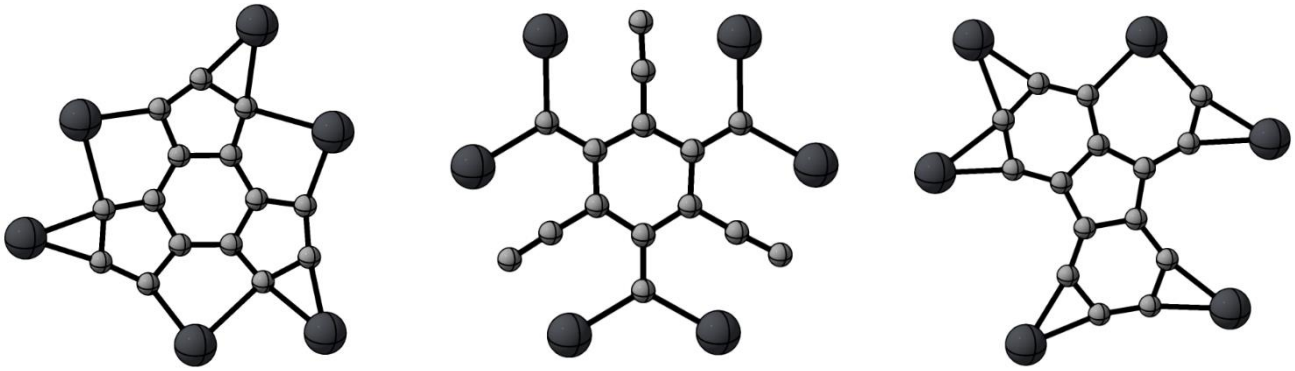
32.9



C_1, ^{1}A | C_s, ^{1}A' | D_{3h}, ^{3}A'$_1$

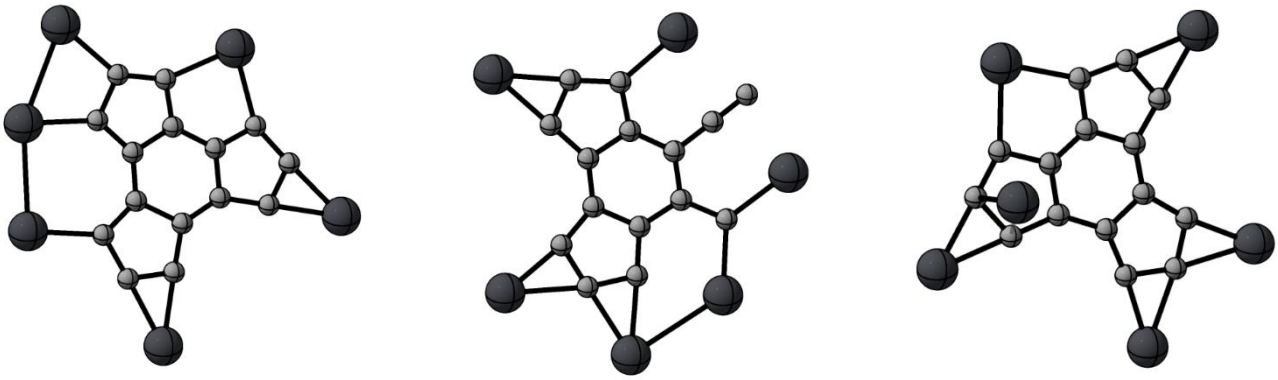
41.2 | **42.2** | **47.5**

Figure S4. Putative global minimum and low-lying isomers of Pb_6C_{15} with their point group symmetries. Relative energies are shown in kcal·mol^{-1} at PBE0[8]-D3[9]/def2-TZVP[10] level including zero-point energy (ZPE) corrections.



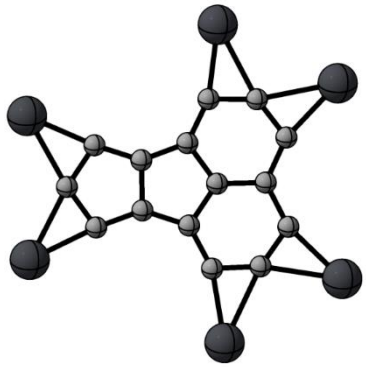
4(Pb). C_3, ^{1}A | D_{3h}, ^{1}A'$_1$ | C_s, ^{3}A'

0.0 | **6.6** | **8.1**



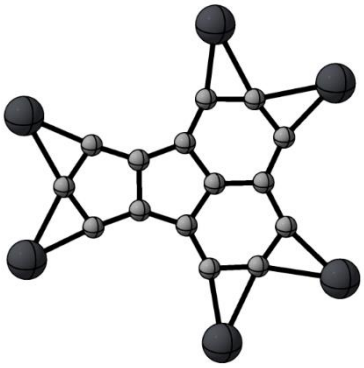
C_s, ^{1}A' | C_s, ^{1}A' | C_1, ^{1}A

9.2 | **9.8** | **11.9**



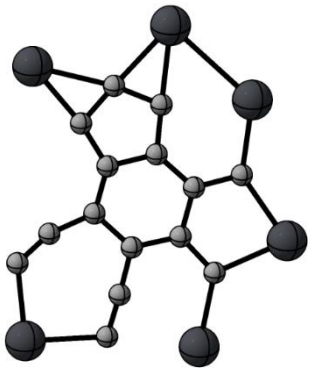
C_{2v}, $^1A_1$

12.2



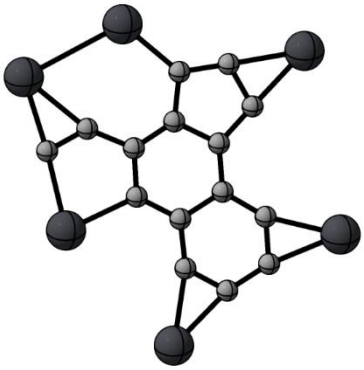
C_{2v}, $^3A_1$

12.2



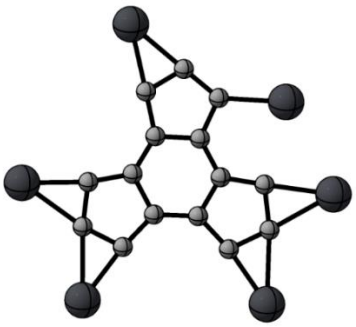
C_s, $^1A'$

13.6



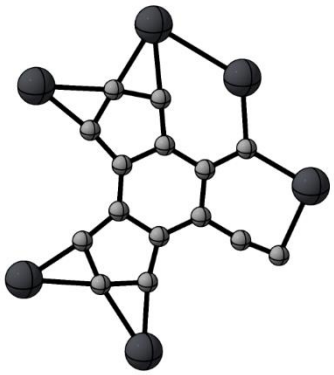
C_s, $^1A'$

13.9



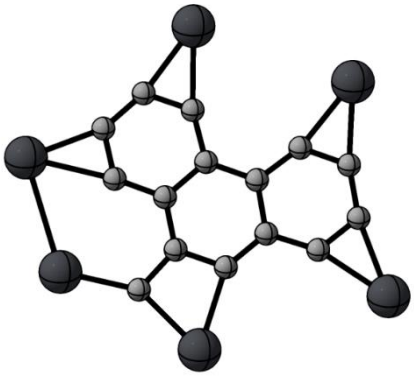
C_s, $^1A'$

17.5



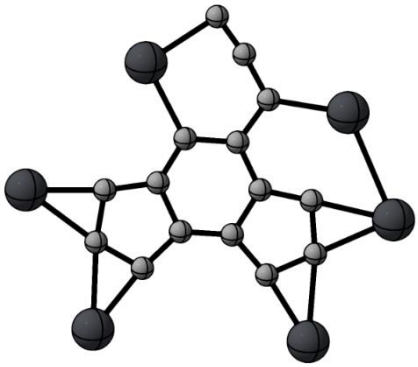
C_s, $^1A'$

18.2



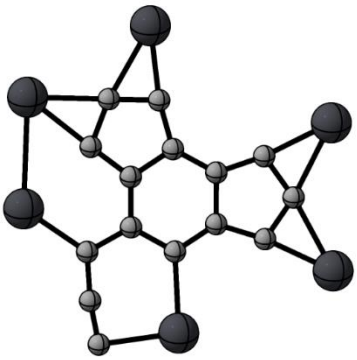
C_s, $^1A'$

18.5



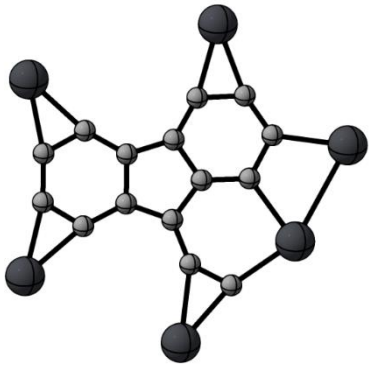
C_s, $^1A'$

18.8



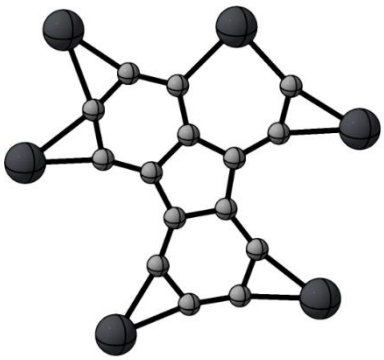
C_s, $^1A'$

18.8



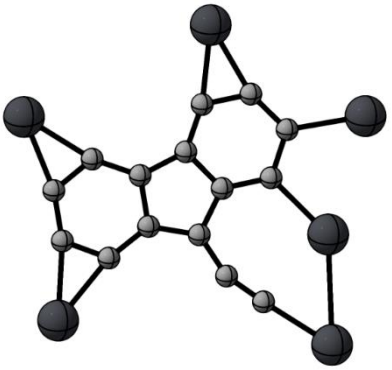
C_s, ^{1}A'

19.7



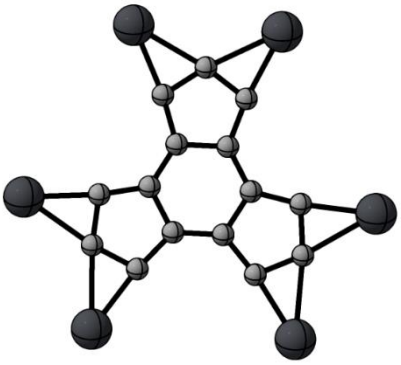
C_s, ^{1}A'

19.9



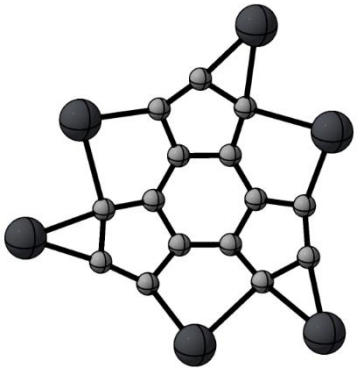
C_s, ^{3}A'

20.7



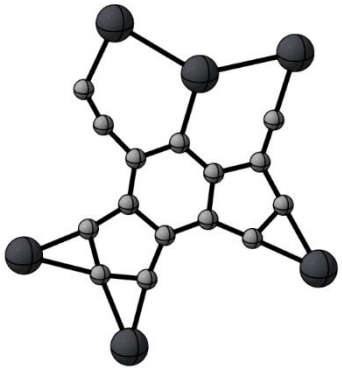
3(Pb). D_{3h}, ^{1}A'$_1$

21.5



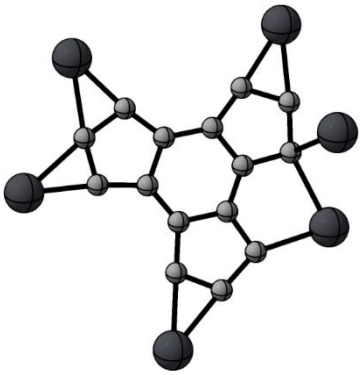
C_3, ^{3}A

22.8



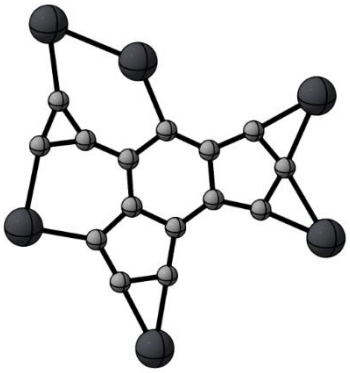
C_s, ^{1}A'

29.3



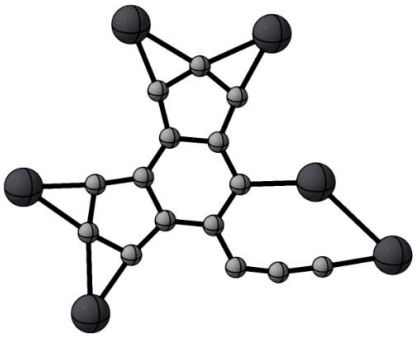
C_1, ^{3}A

29.3



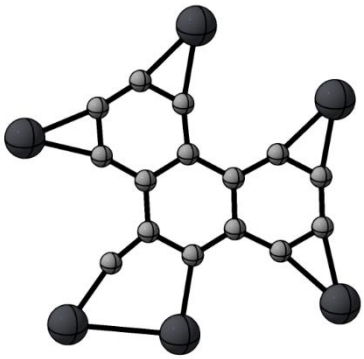
C_s, ^{1}A'

34.0



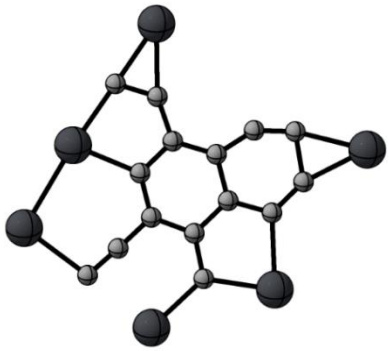
C_s, ^{1}A'

41.6



C_s, ^{3}A'

45.7



C_s, ^{1}A'

46.6

Figure S5. The natural charges (red) for the Si_6C_{15}/Ge_6C_{15} putative global minimum at the PBE0/def2-TZVP level.

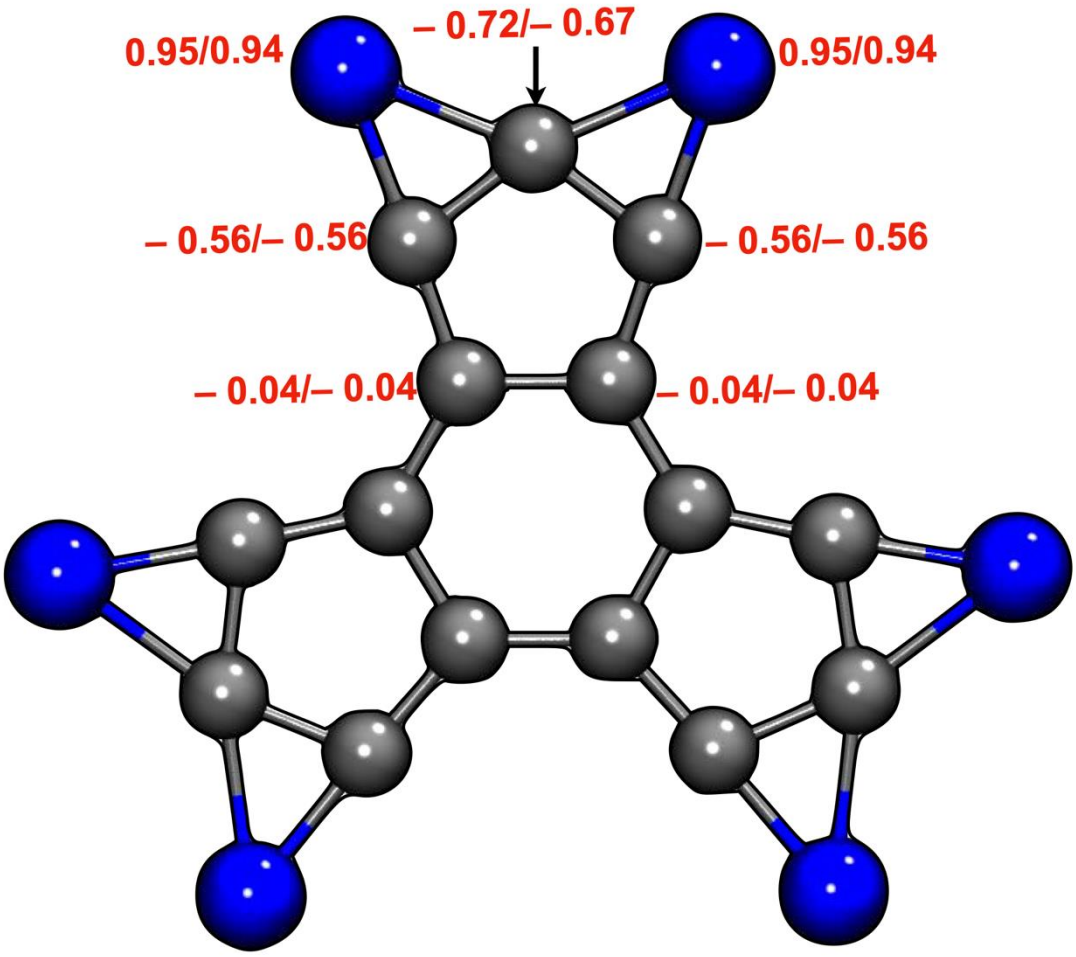


Figure S6. The natural charges (red) for the Sn_6C_{15}/Pb_6C_{15} putative global minimum at the PBE0/def2-TZVP level.

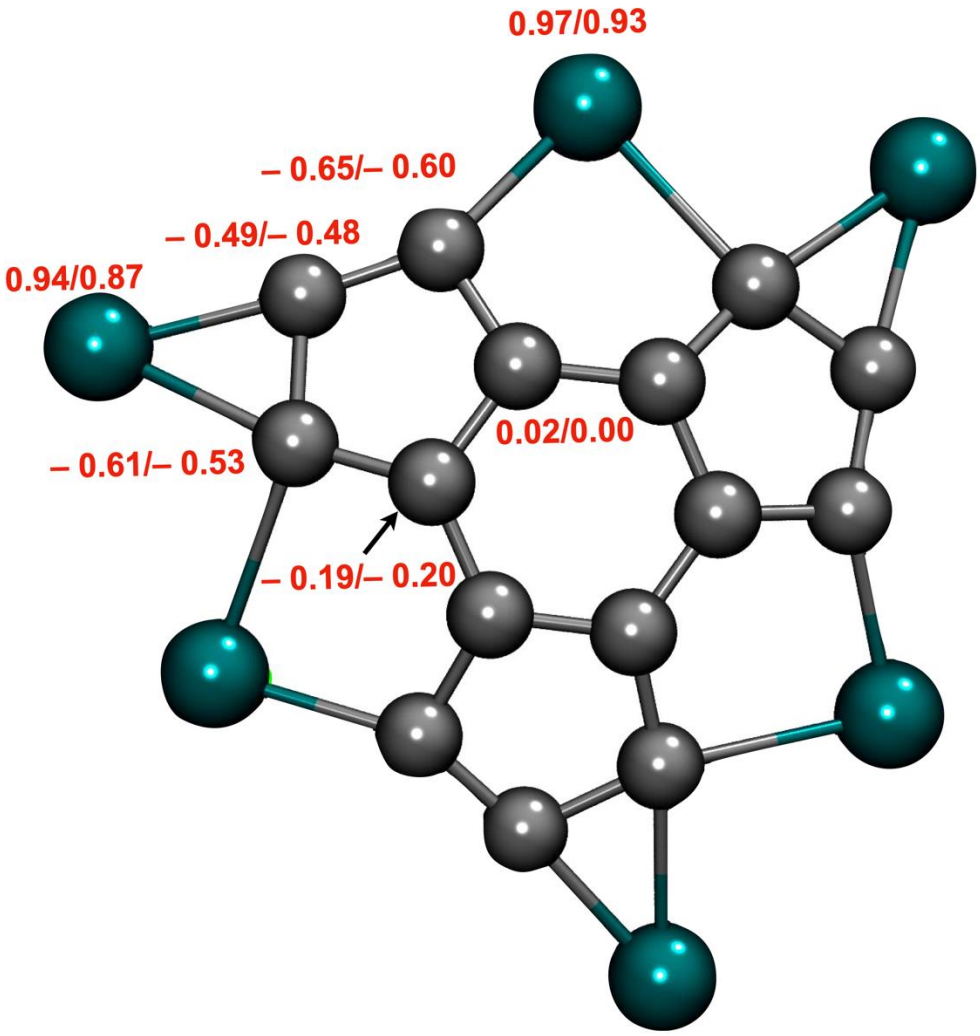


Figure S7. Lowest energy structures of E_6C_{15} at ωB97XD/def2-TZVP level (relative energies in kcal·mol^{-1}, including the zero-point energy (ZPE) corrections). The bond length in Å (black) and WBI values (blue) at ωB97XD [11]/def2-TZVP level.

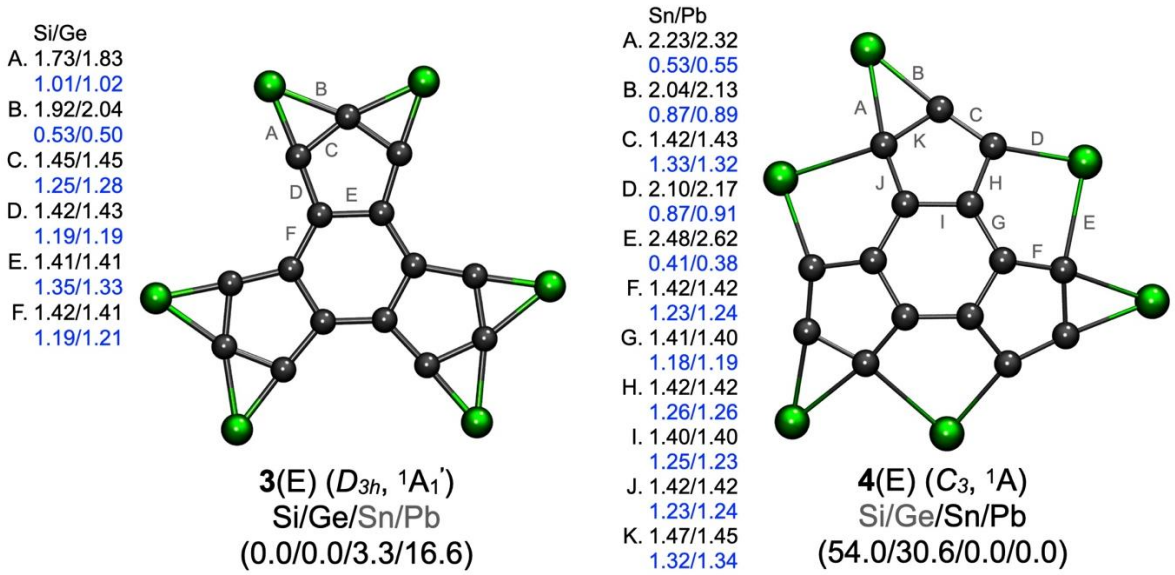


Figure S8. Lowest energy structures of E_6C_{15} at MP2/def2-TZVP level (relative energies in kcal·mol^{-1}). The bond length in Å (black) and WBI values (blue) at MP2/def2-TZVP level.

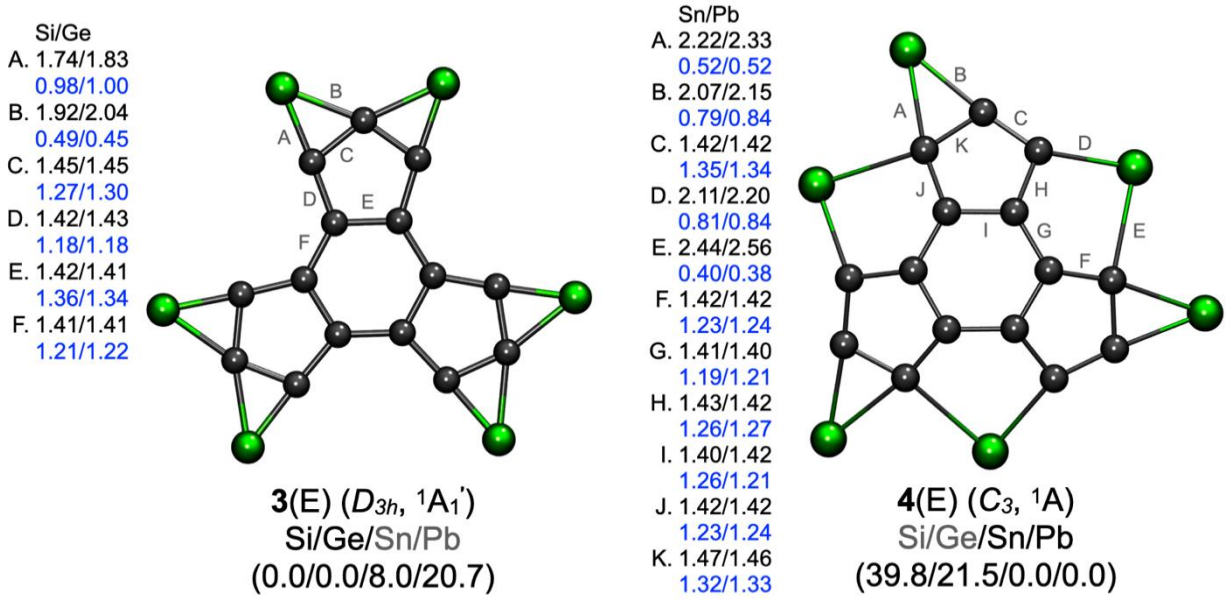


Figure S9. AdNDP [12,13] analysis of the **3**(Ge) system (D_{3h}-Ge_6C_{15}). ON stands for occupation number. Carbon=gray, Germanium=brown.

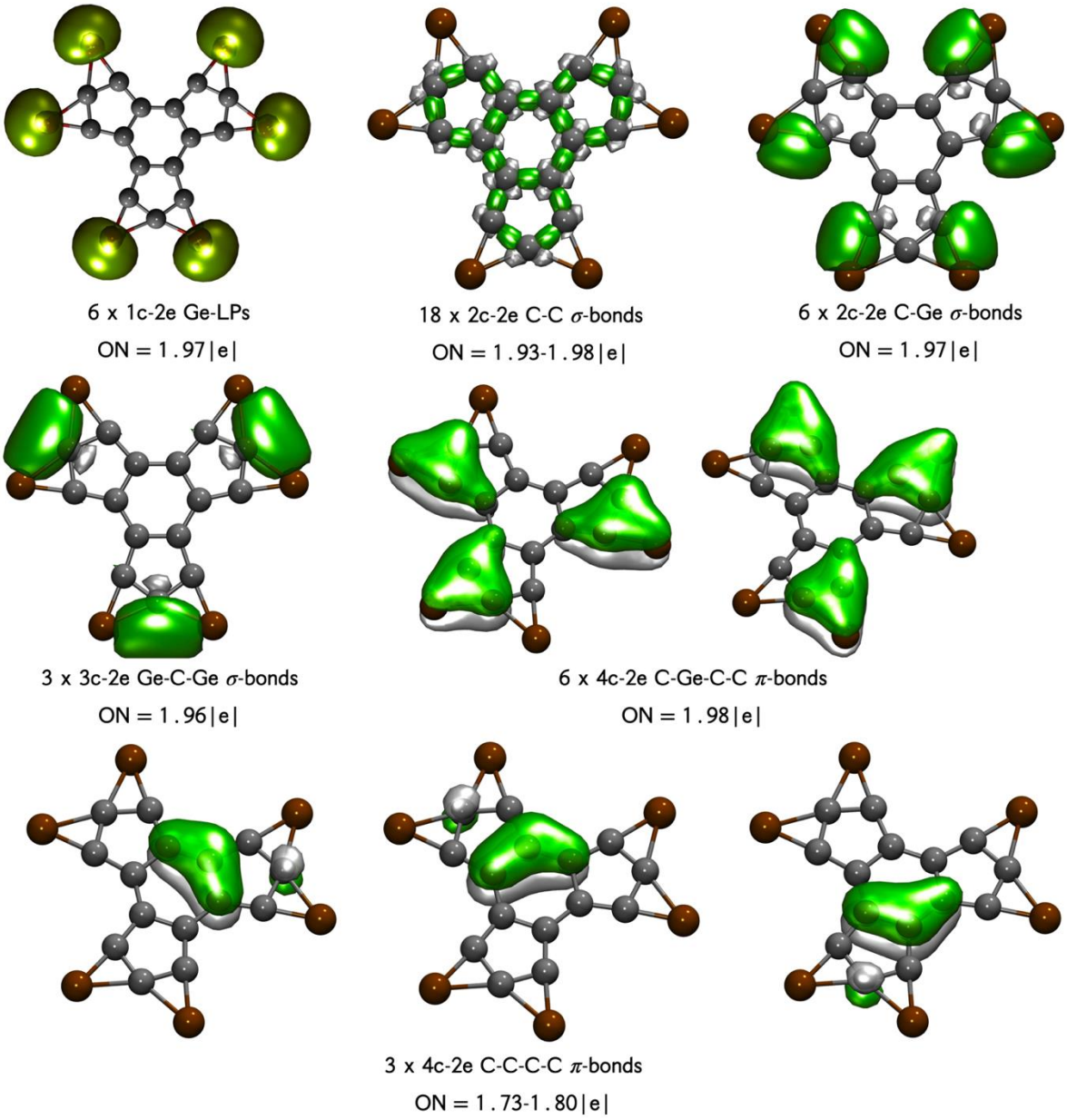


Figure S10. AdNDP analysis of **4**(E) systems (E=Sn, Pb). ON stands for occupation number. Carbon=gray, Silicon=blue.

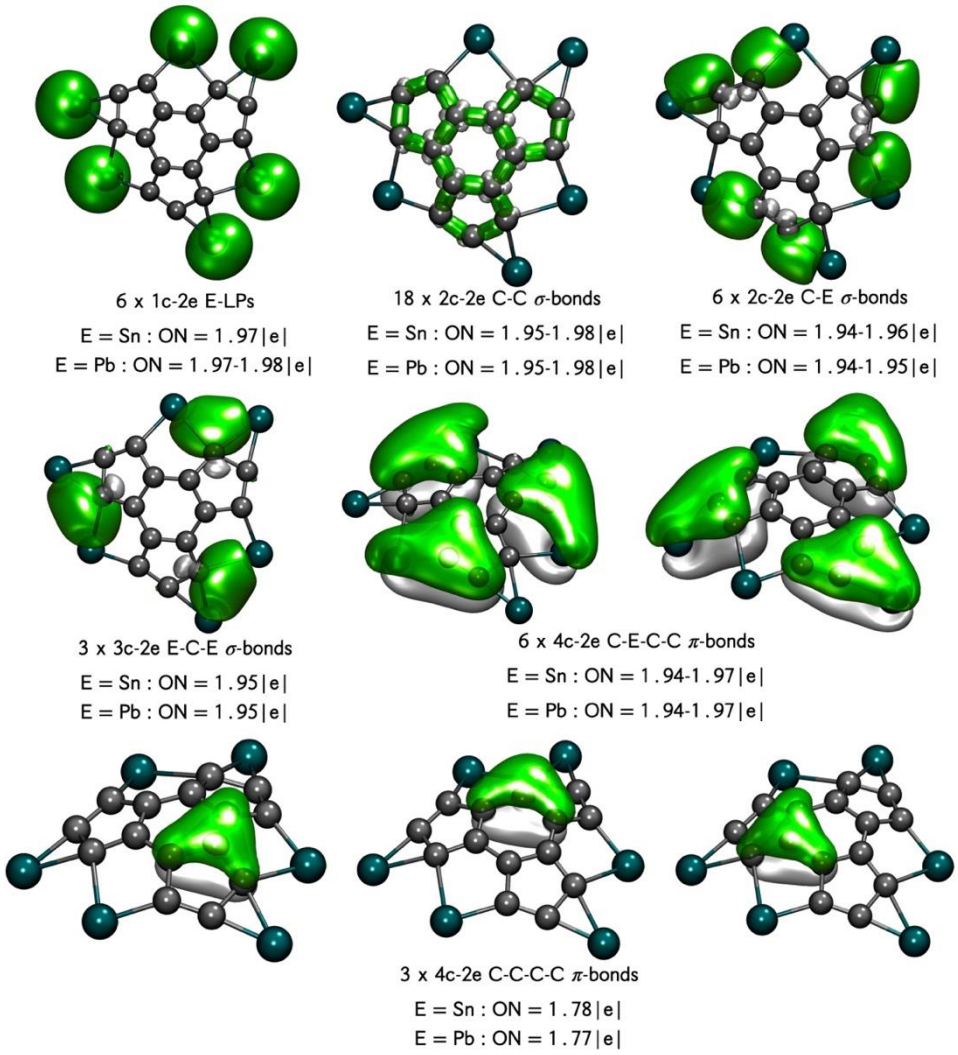


Figure S11. Different detected ring current circuits for the D_{3h}-Si_6C_{15} system (up) and the RCS profiles along the different integration planes (down) were used to estimate their intensity. Computations were performed using the GIMIC program,[14,15] which employs the gauge-including atomic orbital (GIAO)[16] method. To visualize current pathways, we used Paraview 5.10.0 software.[17,18]

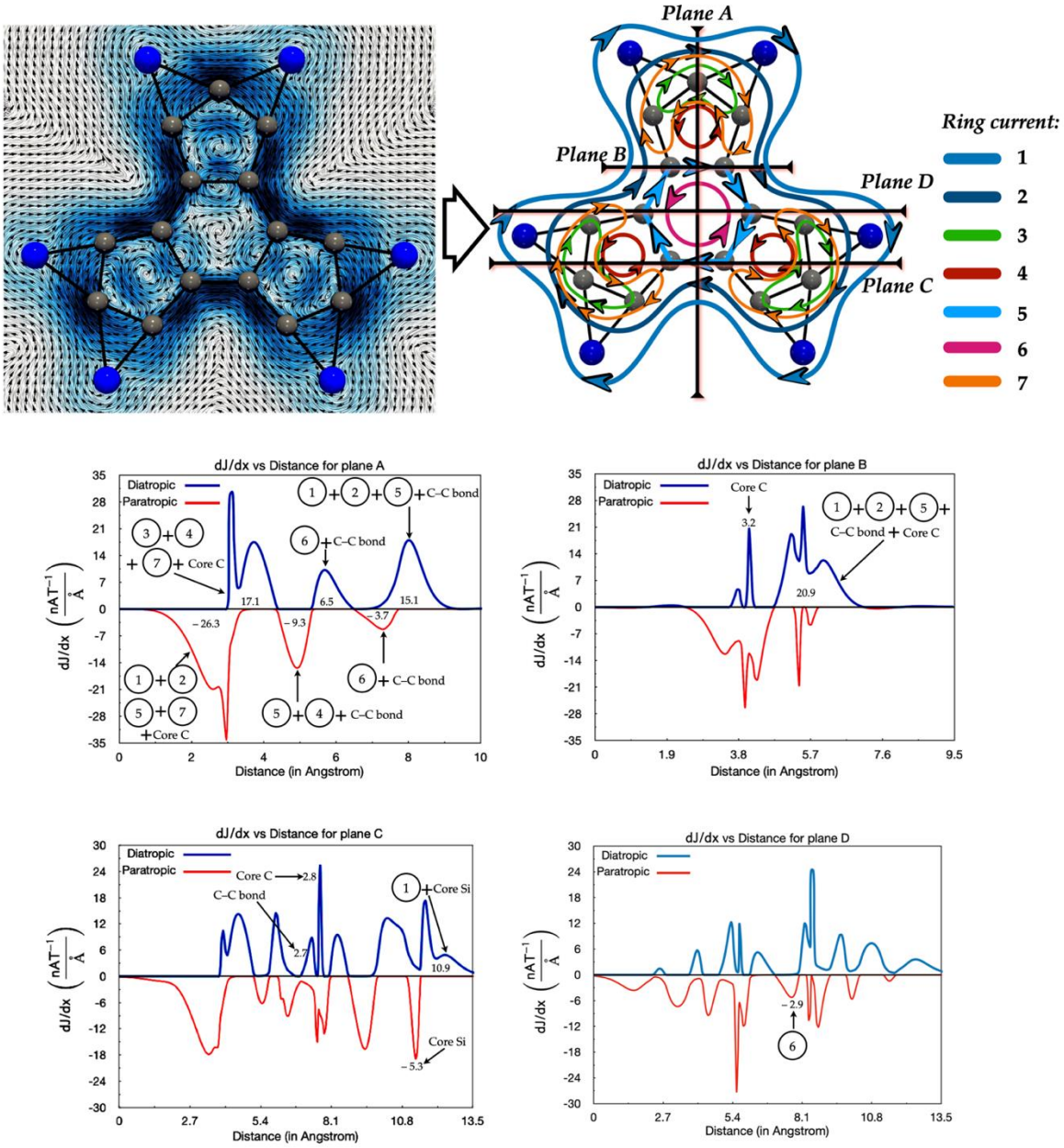


Figure S12. Different detected ring current circuits for D_{3h}-Ge_6C_{15} system (up) and the RCS profiles along the different integration planes (down) were used to estimate their intensity.

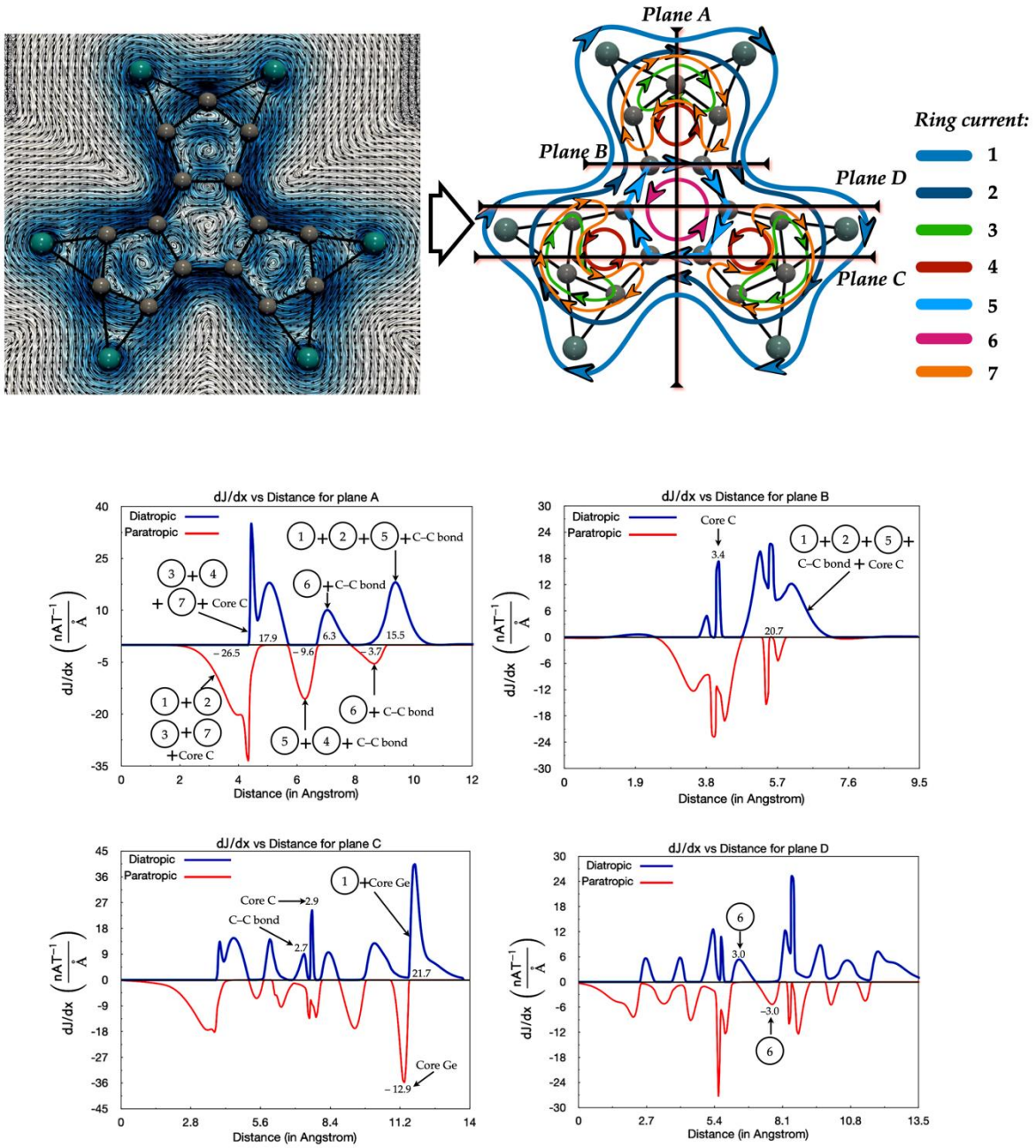


Figure S13. Different detected ring current circuits for the C_3-Sn_6C_{15} system (up) and the RCS profiles along the different integration planes (down) were used to estimate their intensity.

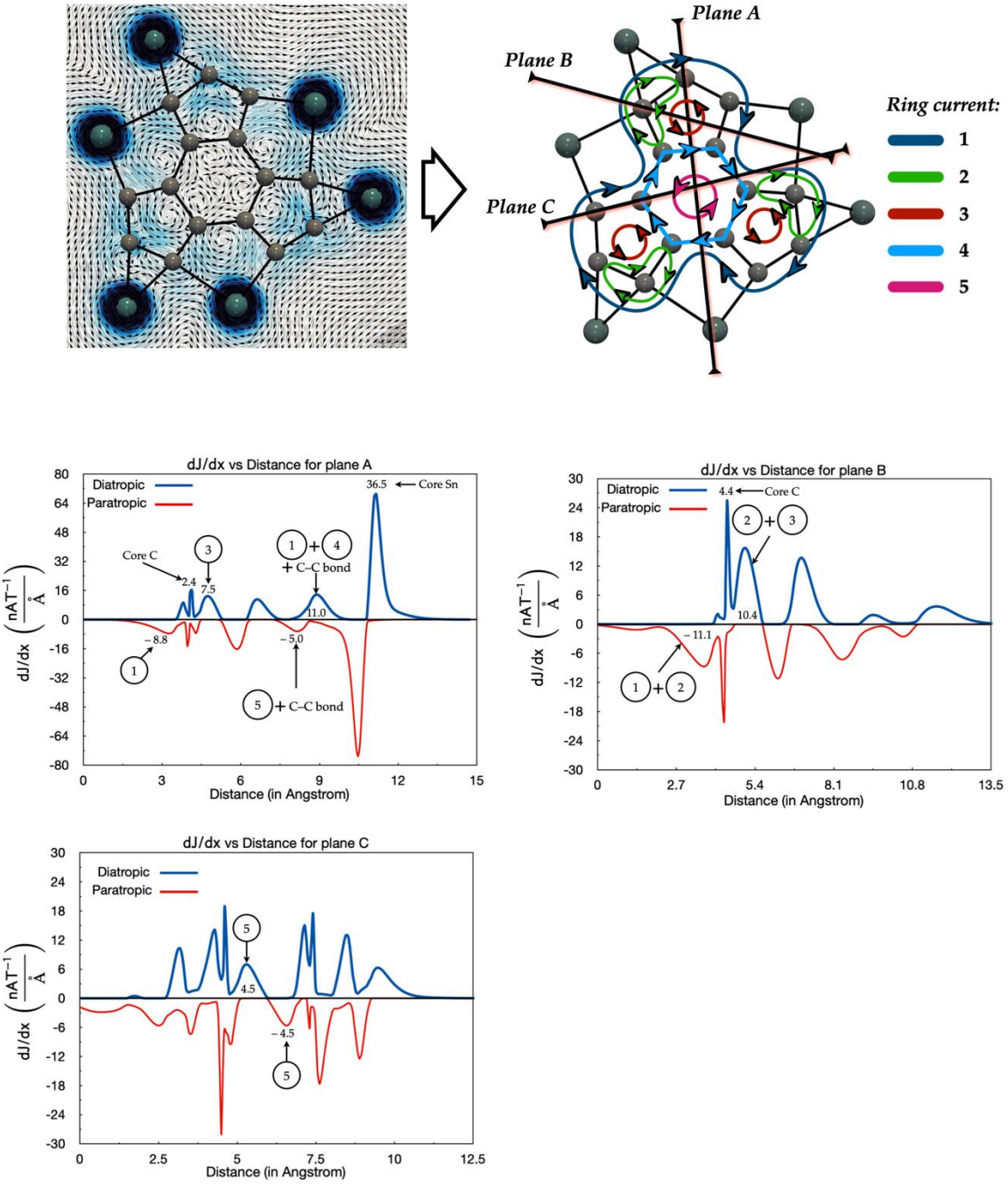


Figure S14. Different detected ring current circuits for the C_3-Pb_6C_{15} system (up) and the RCS profiles along the different integration planes (down) were used to estimate their intensity.

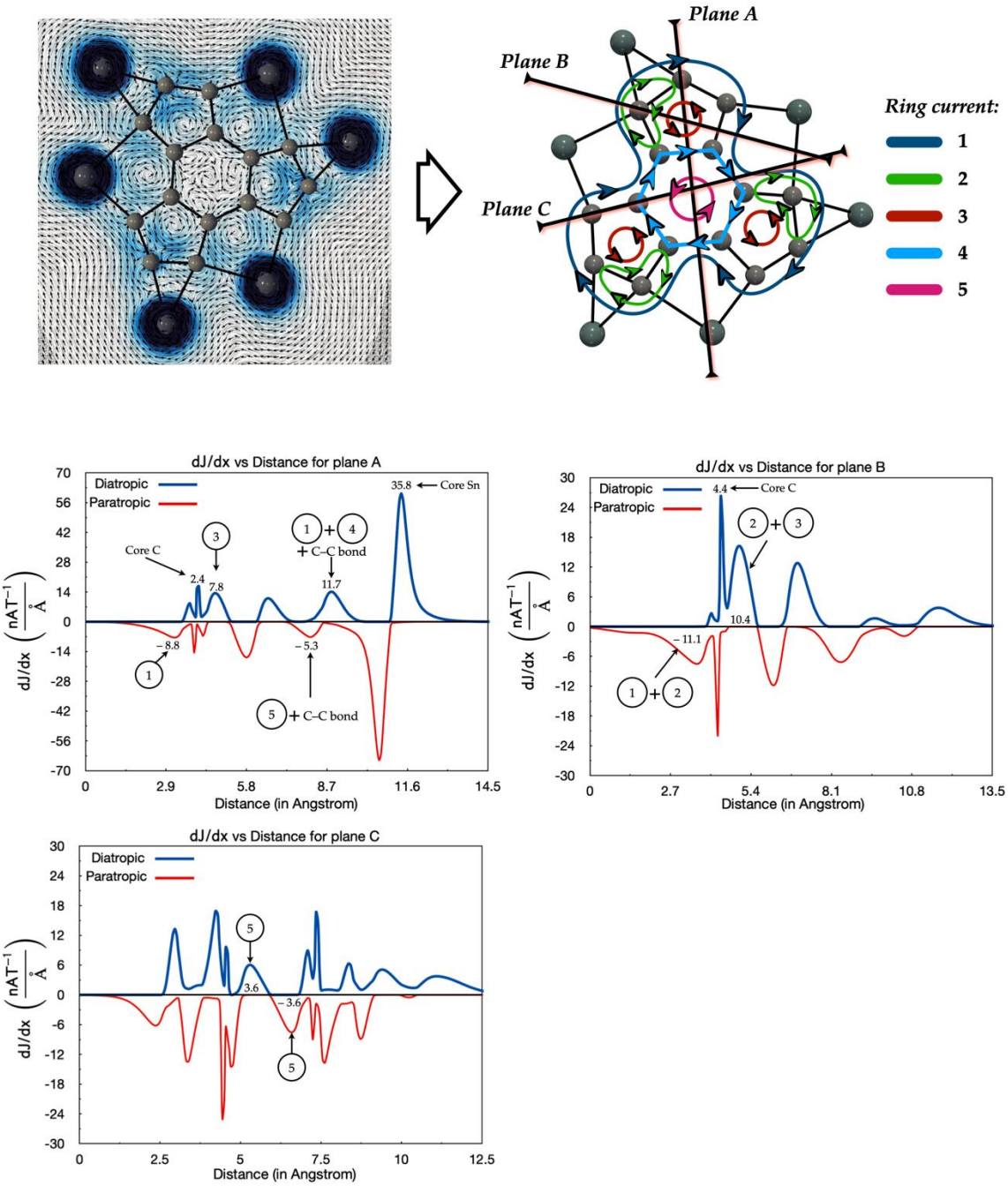
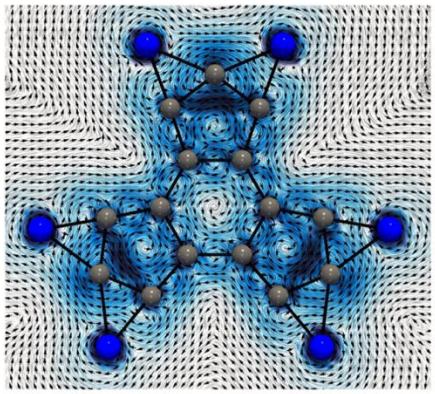
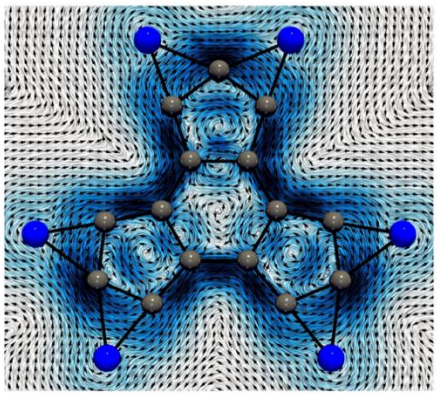


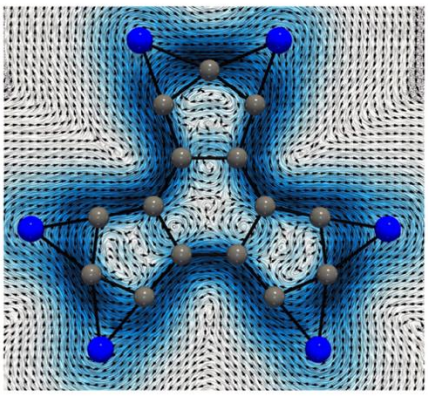
Figure S15. Vector plots visualization of the current density in diverse planes of the D_{3h}-Si_6C_{15} system. Diatropic currents are assumed to circle clockwise.



0.0Å



0.5Å



1.0Å

Figure S16. Vector plots visualization of the current density in diverse planes of the D_{3h}-Ge_6C_{15} system. Diatropic currents are assumed to circle clockwise.

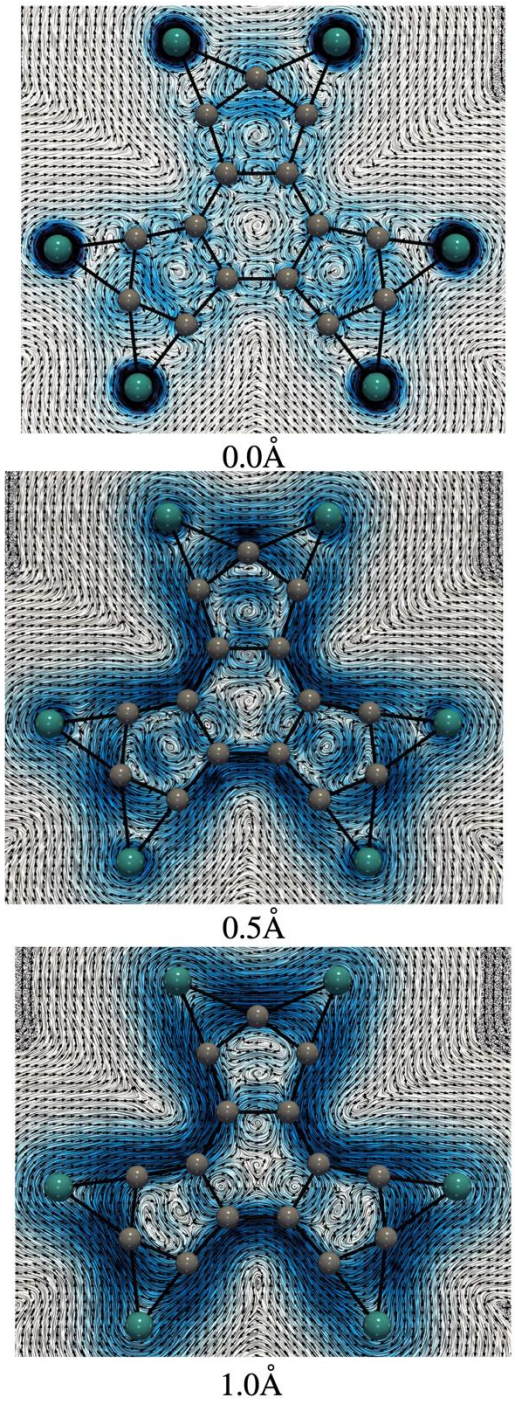
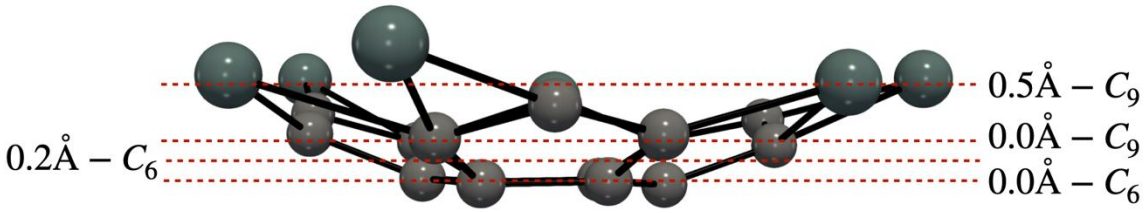
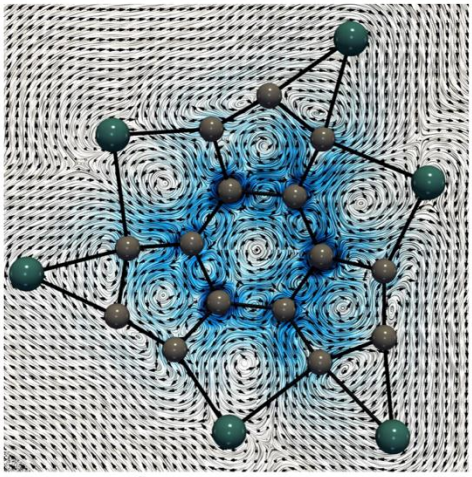
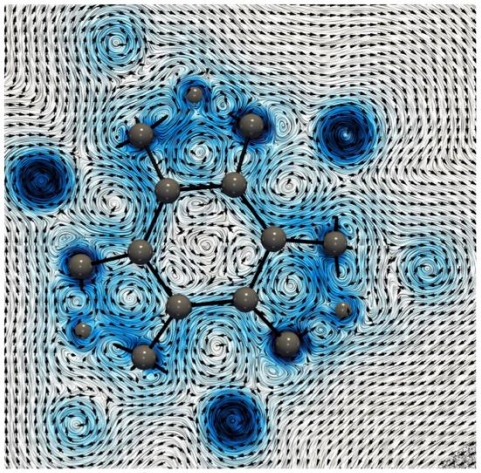


Figure S17. Vector plots visualization of the current density in diverse planes of the C_3-Sn_6C_{15} system. Diatropic currents are assumed to circle clockwise.

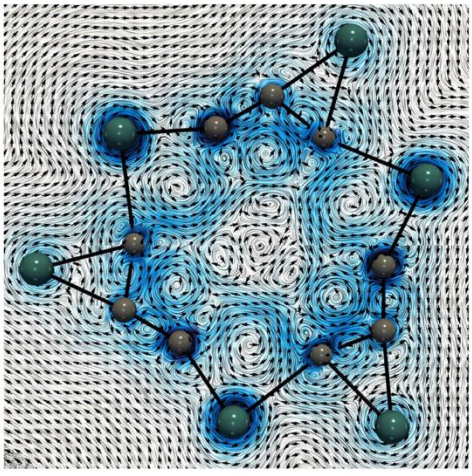




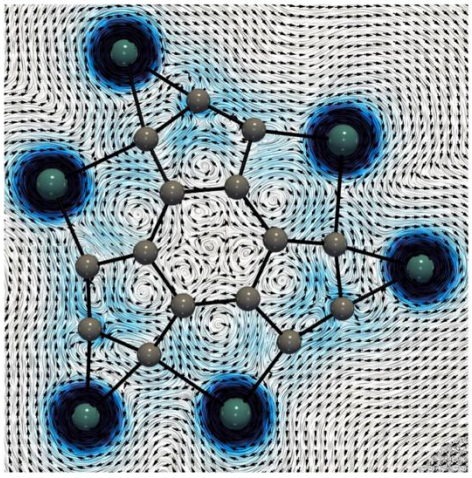
0.0Å above C_6-plane



0.0Å above C_9-plane

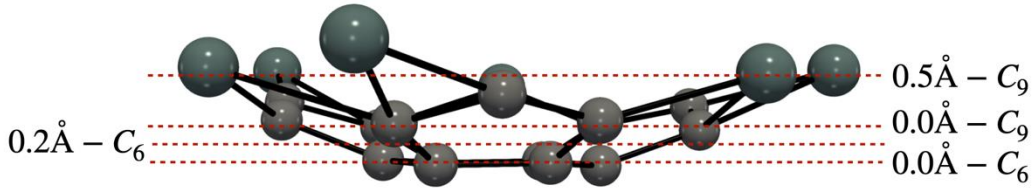


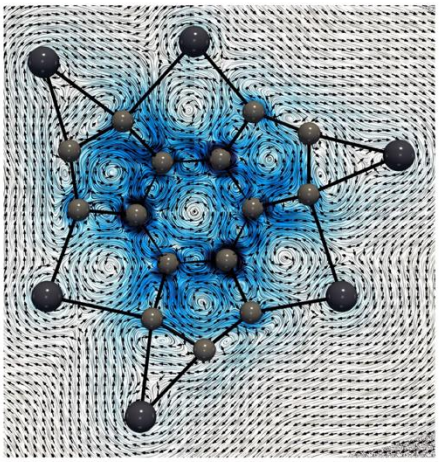
0.2Å above C_6-plane



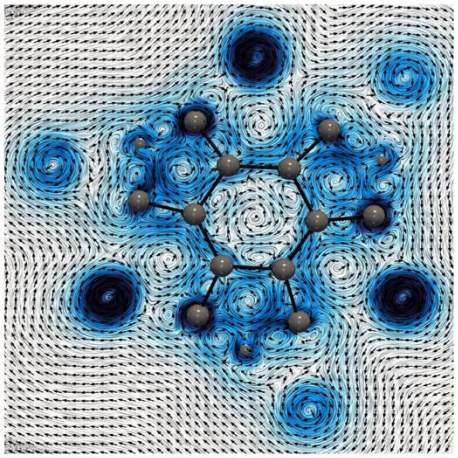
0.5Å above C_9-plane

Figure S18. Vector plots visualization of the current density in diverse planes of the C_3-Pb_6C_{15} system. Diatropic currents are assumed to circle clockwise.

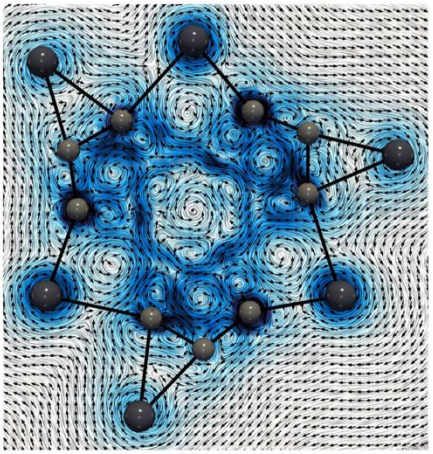




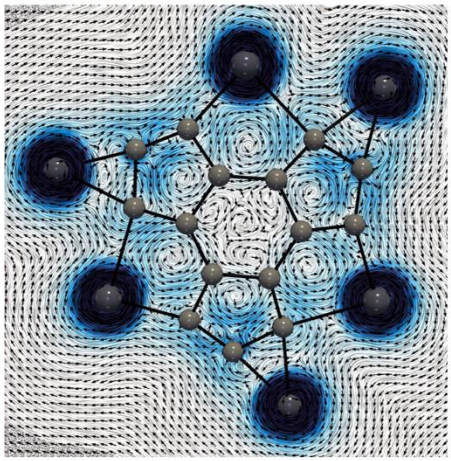
0.0Å above C_6-plane



0.0Å above C_9-plane

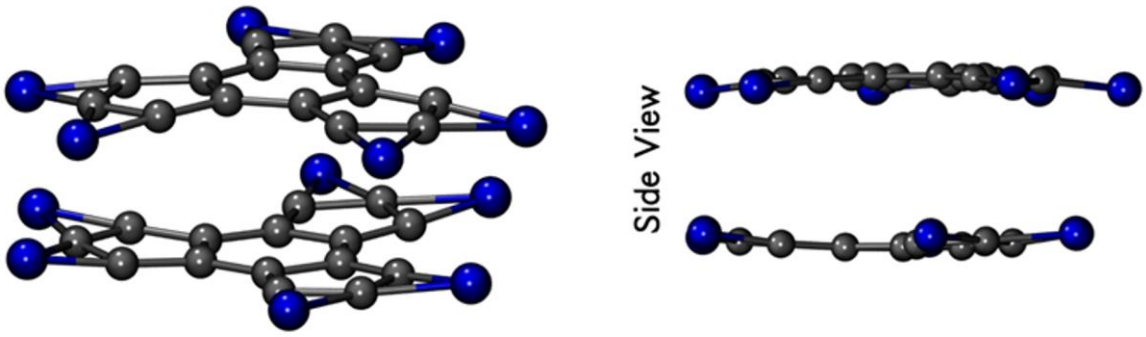


0.2Å above C_6-plane



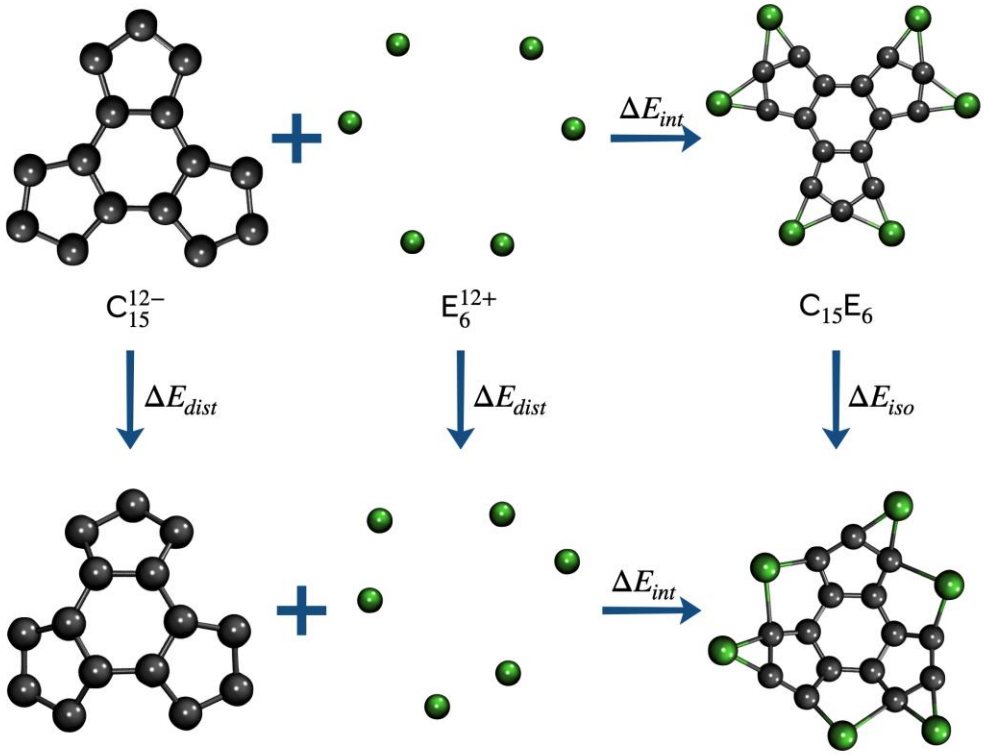
0.5Å above C_9-plane

Figure S19. The minimum energy geometries of the complex $[3(Si)]_2$ at PBE0-D3/def2-SVP level. The bond dissociation energies at 0 K (D_e) and 298 K, including thermal correction and entropy factors (ΔG^{298K}), are given in kcal·mol^{-1}.



$2[\mathbf{3}(Si)] \rightarrow [\mathbf{3}(Si)]_2$; D_e =23.8; ΔG^{298K} = 10.4

Figure S20. Energetic reaction cycle involving the isomerization of E_6C_{15} between isomers **3**(E) (top) and **4**(E) (bottom).



Tables

Table S1. Results of the IEDA at the PBE0-D3-BJ/ZORA/TZ2P level for the E_6C_{15} systems with E_6^{12+} + C_{15}^{12-} as fragments.[a]

System	Si_6C_{15}	Ge_6C_{15}	Sn_6C_{15}	Pb_6C_{15}
ΔE_{iso}	44.0	19.9	-10.7	-24.2
ΔE_{dist} (E_6^{12+})	729.7	563.9	384.4	337.5
ΔE_{dist} (C_{15}^{12-})	283.1	198.9	94.6	72.6
$\Delta\Delta E_{int}$	-968.8	-742.9	-489.7	-434.3
$\Delta\Delta E_{orb}$	-442.7	-352.1	-282.4	-209.2
$\Delta\Delta V_{elstat}$	-252.7	-144.8	-116.7	-96.5
$\Delta\Delta E_{Pauli}$	-271.1	-244.4	-90.6	-127.2
$\Delta\Delta E_{disp}$	-2.3	-1.7	0.0	-1.4

[a] Values in kcal·mol^{-1}. Positive values of the components favor the **3**(E) isomer.

Table S2. The HOMO-LUMO energy gaps for **3**(E) and **4**(E) structures. Values in eV.

Δ_{H-L}	**Si**	**Ge**	**Sn**	**Pb**
3(E)	4.03	3.63	2.90	2.59
4(E)	2.71	2.78	2.35	2.13

Table S3. Cartesian coordinates of the E_6C_{18} global minima structures at the PBE0-D3/def2-TZVP level.

Si_6C_{15}				Ge_6C_{15}			
6	0.000000000	1.414123000	0.000000000	6	0.000000000	1.415253000	0.000000000
6	-1.226308000	0.704678000	0.000000000	6	-1.228927000	0.702000000	0.000000000
6	1.223472000	0.709294000	0.000000000	6	1.222415000	0.713207000	0.000000000
6	-1.224935000	-0.707283000	0.000000000	6	-1.225703000	-0.707661000	0.000000000
6	1.224799000	-0.707418000	0.000000000	6	1.225659000	-0.707687000	0.000000000
6	0.002582000	-1.414448000	0.000000000	6	0.006457000	-1.415292000	0.000000000
6	-2.294516000	1.648690000	0.000000000	6	-2.297916000	1.647257000	0.000000000
6	2.574984000	1.162504000	0.000000000	6	2.575520000	1.166351000	0.000000000
6	-2.291258000	-1.653248000	0.000000000	6	-2.290342000	-1.657803000	0.000000000
6	2.577186000	-1.157937000	0.000000000	6	2.580822000	-1.154648000	0.000000000
6	-0.280955000	-2.811382000	0.000000000	6	-0.277658000	-2.813677000	0.000000000
6	-0.285773000	2.810735000	0.000000000	6	-0.290477000	2.812342000	0.000000000
6	-1.728763000	2.987816000	0.000000000	6	-1.727323000	2.976080000	0.000000000
6	-1.723838000	-2.991977000	0.000000000	6	-1.713767000	-2.984057000	0.000000000
6	3.452341000	0.002973000	0.000000000	6	3.441064000	0.007798000	0.000000000
14	-0.575257000	4.525149000	0.000000000	32	-0.533618000	4.630790000	0.000000000
14	-3.636488000	2.754014000	0.000000000	32	-3.756266000	2.760373000	0.000000000
14	4.202778000	1.773072000	0.000000000	32	4.268587000	1.872926000	0.000000000
14	-3.631878000	-2.760237000	0.000000000	32	-3.743652000	-2.777471000	0.000000000
14	4.206767000	-1.764368000	0.000000000	32	4.277205000	-1.853305000	0.000000000
14	-0.565500000	-4.526395000	0.000000000	32	-0.512222000	-4.633214000	0.000000000
Sn_6C_{15}				Pb_6C_{15}			
6	-2.926230000	-1.387299000	-0.009582000	6	-2.706566000	1.834821000	0.293921000
6	2.664551000	-1.840540000	-0.009582000	6	2.942284000	1.426544000	0.293921000
6	0.261679000	3.227839000	-0.009582000	6	-0.235718000	-3.261365000	0.293921000
6	-1.733460000	-2.107657000	-0.273631000	82	-4.733040000	1.296450000	-0.202368000
6	-2.734615000	0.035687000	-0.340336000	6	-1.410248000	2.365341000	0.532100000
6	-0.814595000	-1.136005000	-0.778737000	6	-2.718771000	0.405209000	0.574834000
6	-1.403911000	0.135117000	-0.819128000	6	-0.626608000	1.258182000	0.964244000
6	1.336401000	-2.386090000	-0.340336000	6	-1.407398000	0.076670000	0.998083000
6	2.692015000	-0.447391000	-0.273631000	82	3.489279000	3.450708000	-0.202368000
6	0.584941000	-1.283381000	-0.819128000	6	1.710307000	2.151920000	0.574834000
6	1.391107000	-0.137457000	-0.778737000	6	2.753570000	0.038640000	0.532100000
6	1.398214000	2.350403000	-0.340336000	6	0.770097000	1.180507000	0.998083000
6	-0.958555000	2.555049000	-0.273631000	6	1.402922000	-0.086432000	0.964244000
6	0.818970000	1.148264000	-0.819128000	82	1.243762000	-4.747158000	-0.202368000
6	-0.576512000	1.273462000	-0.778737000	6	1.008464000	-2.557129000	0.574834000
50	2.790789000	-3.842392000	0.501676000	6	-1.343322000	-2.403982000	0.532100000
50	-0.568763000	-3.766387000	0.312923000	6	0.637301000	-1.257177000	0.998083000
50	-4.723003000	-0.495698000	0.501676000	6	-0.776313000	-1.171750000	0.964244000
50	-2.977406000	2.375757000	0.312923000	82	0.000000000	3.955609000	-0.043718000
50	1.932215000	4.338090000	0.501676000	82	3.425658000	-1.977804000	-0.043718000
50	3.546168000	1.390631000	0.312923000	82	-3.425658000	-1.977804000	-0.043718000

Table S4. Cartesian coordinates of 3(E) and 4(E) optimized structures at the PBE0-D3/def2-TZVP level.

3(Si)				4(Si)			
6	0.000000000	1.414123000	0.000000000	6	0.000000000	2.943260000	-0.126176000
6	-1.226308000	0.704678000	0.000000000	6	2.548938000	-1.471630000	-0.126176000
6	1.223472000	0.709294000	0.000000000	6	-2.548938000	-1.471630000	-0.126176000
6	-1.224935000	-0.707283000	0.000000000	6	1.145756000	2.265962000	0.329519000
6	1.224799000	-0.707418000	0.000000000	6	-1.236579000	2.279069000	0.422730000
6	0.002582000	-1.414448000	0.000000000	6	0.675096000	1.213211000	1.164402000
6	-2.294516000	1.648690000	0.000000000	6	-0.727302000	1.220778000	1.233242000
6	2.574984000	1.162504000	0.000000000	6	2.592021000	-0.068625000	0.422730000
6	-2.291258000	-1.653248000	0.000000000	6	1.389503000	-2.125235000	0.329519000
6	2.577186000	-1.157937000	0.000000000	6	1.420876000	0.019473000	1.233242000
6	-0.280955000	-2.811382000	0.000000000	6	0.713123000	-1.191256000	1.164402000
6	-0.285773000	2.810735000	0.000000000	6	-1.355442000	-2.210444000	0.422730000
6	-1.728763000	2.987816000	0.000000000	6	-2.535259000	-0.140727000	0.329519000
6	-1.723838000	-2.991977000	0.000000000	6	-0.693574000	-1.240251000	1.233242000
6	3.452341000	0.002973000	0.000000000	6	-1.388219000	-0.021955000	1.164402000
14	-0.575257000	4.525149000	0.000000000	14	-2.517192000	-3.085320000	-0.854075000
14	-3.636488000	2.754014000	0.000000000	14	3.930561000	-0.637292000	-0.854075000
14	4.202778000	1.773072000	0.000000000	14	-1.413369000	3.722612000	-0.854075000
14	-3.631878000	-2.760237000	0.000000000	14	0.184225000	-3.313707000	-0.441803000
14	4.206767000	-1.764368000	0.000000000	14	2.777642000	1.816397000	-0.441803000
14	-0.565500000	-4.526395000	0.000000000	14	-2.961867000	1.497310000	-0.441803000
3(Ge)				4(Ge)			
6	0.000000000	1.415253000	0.000000000	6	0.000000000	3.067487000	0.160571000
6	-1.228927000	0.702000000	0.000000000	6	2.656522000	-1.533743000	0.160571000
6	1.222415000	0.713207000	0.000000000	6	-2.656522000	-1.533743000	0.160571000
6	-1.225703000	-0.707661000	0.000000000	6	1.164490000	2.346958000	0.546869000
6	1.225659000	-0.707687000	0.000000000	6	-1.204097000	2.358665000	0.619983000
6	0.006457000	-1.415292000	0.000000000	6	0.684677000	1.213539000	1.262183000
6	-2.297916000	1.647257000	0.000000000	6	-0.721175000	1.218288000	1.321383000
6	2.575520000	1.166351000	0.000000000	6	2.644712000	-0.136554000	0.619983000
6	-2.290342000	-1.657803000	0.000000000	6	1.450280000	-2.181957000	0.546869000
6	2.580822000	-1.154648000	0.000000000	6	1.415655000	0.015412000	1.321383000
6	-0.277658000	-2.813677000	0.000000000	6	0.708618000	-1.199717000	1.262183000
6	-0.290477000	2.812342000	0.000000000	6	-1.440616000	-2.222111000	0.619983000
6	-1.727323000	2.976080000	0.000000000	6	-2.614770000	-0.165001000	0.546869000
6	-1.713767000	-2.984057000	0.000000000	6	-0.694481000	-1.233699000	1.321383000
6	3.441064000	0.007798000	0.000000000	6	-1.393294000	-0.013822000	1.262183000
32	-0.533618000	4.630790000	0.000000000	32	-2.781928000	-3.277881000	-0.492752000
32	-3.756266000	2.760373000	0.000000000	32	4.229692000	-0.770280000	-0.492752000
32	4.268587000	1.872926000	0.000000000	32	-1.447764000	4.048161000	-0.492752000
32	-3.743652000	-2.777471000	0.000000000	32	0.276163000	-3.483950000	-0.240558000
32	4.277205000	-1.853305000	0.000000000	32	2.879107000	1.981139000	-0.240558000
32	-0.512222000	-4.633214000	0.000000000	32	-3.155271000	1.502810000	-0.240558000
3(Sn)				4(Sn)			
6	-1.234780000	-0.699640000	0.000000000	6	-2.926230000	-1.387299000	-0.009582000
6	0.000000000	-1.419194000	0.000000000	6	2.664551000	-1.840540000	-0.009582000
6	-1.229078000	0.709621000	0.000000000	6	0.261679000	3.227839000	-0.009582000
6	1.223301000	-0.719498000	0.000000000	6	-1.733460000	-2.107657000	-0.273631000
6	0.011473000	1.419159000	0.000000000	6	-2.734615000	0.035687000	-0.340336000
6	1.229077000	0.709595000	0.000000000	6	-0.814595000	-1.136005000	-0.778737000
6	-0.287770000	-2.816625000	0.000000000	6	-1.403911000	0.135117000	-0.819128000
6	-2.295377000	1.657593000	0.000000000	6	1.336401000	-2.386090000	-0.340336000
6	2.573731000	-1.179891000	0.000000000	6	2.692015000	-0.447391000	-0.273631000
6	-0.264987000	2.818869000	0.000000000	6	0.584941000	-1.283381000	-0.819128000
6	2.583178000	1.159065000	0.000000000	6	1.391107000	-0.137457000	-0.778737000

6	-2.308722000	-1.638949000	0.000000000	6	1.398214000	2.350403000	-0.340336000
6	-1.719769000	-2.951148000	0.000000000	6	-0.958555000	2.555049000	-0.273631000
6	3.415766000	-0.013801000	0.000000000	6	0.818970000	1.148264000	-0.819128000
6	-1.695848000	2.965017000	0.000000000	6	-0.576512000	1.273462000	-0.778737000
50	-3.958736000	-2.821621000	0.000000000	50	2.790789000	-3.842392000	0.501676000
50	-0.503134000	-4.835236000	0.000000000	50	-0.568763000	-3.766387000	0.312923000
50	-3.935870000	2.853400000	0.000000000	50	-4.723003000	-0.495698000	0.501676000
50	4.422802000	-2.017787000	0.000000000	50	-2.977406000	2.375757000	0.312923000
50	-0.463994000	4.839154000	0.000000000	50	1.932215000	4.338090000	0.501676000
50	4.438910000	1.982069000	0.000000000	50	3.546168000	1.390631000	0.312923000
		3(Pb)				4(Pb)	
6	1.237990000	0.696692000	0.000000000	6	-2.706566000	1.834821000	0.293921000
6	0.000000000	1.420545000	0.000000000	6	2.942284000	1.426544000	0.293921000
6	1.230246000	-0.710426000	0.000000000	6	-0.235718000	-3.261365000	0.293921000
6	-1.222452000	0.723680000	0.000000000	82	-4.733040000	1.296450000	-0.202368000
6	-0.015616000	-1.420622000	0.000000000	6	-1.410248000	2.365341000	0.532100000
6	-1.230341000	-0.710356000	0.000000000	6	-2.718771000	0.405209000	0.574834000
6	0.293717000	2.818499000	0.000000000	6	-0.626608000	1.258182000	0.964244000
6	2.294039000	-1.663783000	0.000000000	6	-1.407398000	0.076670000	0.998083000
6	-2.575003000	1.183166000	0.000000000	82	3.489279000	3.450708000	-0.202368000
6	0.262731000	-2.821723000	0.000000000	6	1.710307000	2.151920000	0.574834000
6	-2.587873000	-1.154927000	0.000000000	6	2.753570000	0.038640000	0.532100000
6	2.312206000	1.638299000	0.000000000	6	0.770097000	1.180507000	0.998083000
6	1.718359000	2.938866000	0.000000000	6	1.402922000	-0.086432000	0.964244000
6	-3.404518000	0.018664000	0.000000000	82	1.243762000	-4.747158000	-0.202368000
6	1.685964000	-2.957770000	0.000000000	6	1.008464000	-2.557129000	0.574834000
82	4.060888000	2.830282000	0.000000000	6	-1.343322000	-2.403982000	0.532100000
82	0.474525000	4.927006000	0.000000000	6	0.637301000	-1.257177000	0.998083000
82	4.029668000	-2.874553000	0.000000000	6	-0.776313000	-1.171750000	0.964244000
82	-4.481293000	2.102073000	0.000000000	82	0.000000000	3.955609000	-0.043718000
82	0.420523000	-4.932076000	0.000000000	82	3.425658000	-1.977804000	-0.043718000
82	-4.504271000	-2.052644000	0.000000000	82	-3.425658000	-1.977804000	-0.043718000

Table S5. Cartesian coordinates for 3(Si) complexes optimized at the PBE0-D3/def2-TZVP level, except for sandwich and dimer complexes for which def2-SVP is used.

$3Si\cdot(BH_3)_6$				3Si·[12]CPP			
6	2.709464000	-2.124520000	-0.035132000	6	-3.760809000	7.411456000	0.180845000
6	-3.194280000	-1.283525000	-0.016376000	6	-2.986370000	7.346962000	-0.978565000
6	0.485754000	3.408554000	0.000987000	6	-1.666012000	7.753769000	-0.978610000
14	2.225295000	-3.950683000	-0.042930000	6	-1.062057000	8.242838000	0.180784000
14	4.367607000	-1.219301000	-0.032095000	6	-1.880982000	8.453968000	1.292907000
6	1.300967000	-2.503686000	-0.034830000	6	-3.202609000	8.046840000	1.292929000
6	2.742031000	-0.666333000	-0.027576000	6	0.407864000	8.271743000	0.261794000
6	0.528114000	-1.313332000	-0.027667000	6	1.213855000	8.511649000	-0.853326000
6	1.401794000	-0.199388000	-0.023179000	6	2.550871000	8.159238000	-0.856032000
14	-3.239308000	-3.172297000	-0.025538000	6	3.139505000	7.555808000	0.257780000
14	-4.533776000	0.048609000	-0.004216000	6	2.370397000	7.456150000	1.417591000
6	-1.947689000	-2.041001000	-0.024653000	6	1.033190000	7.805870000	1.419213000
6	-2.818396000	0.125606000	-0.009834000	6	4.423822000	6.839342000	0.180066000
6	-0.873163000	-1.113728000	-0.023139000	6	4.726053000	6.105048000	-0.967689000
6	-1.401020000	0.199810000	-0.014228000	6	5.738672000	5.164831000	-0.967713000
14	-1.127267000	4.391890000	0.014067000	6	6.493338000	4.917760000	0.180022000
14	2.309328000	3.902471000	-0.004526000	6	6.278740000	5.745558000	1.284419000
6	-0.793275000	2.707658000	-0.001448000	6	5.265260000	6.686589000	1.284440000
6	1.518432000	2.378424000	-0.007612000	6	7.302958000	3.690028000	0.257676000
6	-0.527557000	1.313562000	-0.009968000	6	7.948189000	3.147652000	-0.856176000
6	0.874038000	1.113950000	-0.013940000	6	8.398630000	1.840390000	-0.853456000
5	-1.924644000	6.176792000	-0.115660000	6	8.219201000	1.018893000	0.261713000
5	3.570958000	5.395760000	0.127607000	6	7.708401000	1.608058000	1.419161000
5	6.313181000	-1.425078000	0.076802000	6	7.260647000	2.915696000	1.417531000
5	2.892089000	-5.790670000	0.054504000	6	8.299158000	-0.449141000	0.180731000
5	-4.398512000	-4.750435000	0.054120000	6	7.856181000	-1.087702000	-0.978639000
5	-6.458909000	0.392032000	0.120035000	6	7.548244000	-2.434557000	-0.978522000
1	3.437988000	5.639201000	1.308311000	6	7.669803000	-3.202033000	0.180941000
1	4.603549000	4.845618000	-0.172203000	6	8.262101000	-2.598284000	1.293013000
1	3.141140000	6.230241000	-0.626426000	6	8.570293000	-1.250150000	1.292905000
1	-1.742033000	6.361312000	-1.300899000	6	6.959844000	-4.489447000	0.262039000
1	-3.066519000	5.938171000	0.197055000	6	6.764525000	-5.307411000	-0.853059000
1	-1.271734000	6.866335000	0.624001000	6	5.790679000	-6.288948000	-0.855760000
1	-6.625118000	0.109778000	1.287225000	6	4.973776000	-6.496897000	0.258067000
1	-6.492423000	1.571611000	-0.137794000	6	5.272117000	-5.781043000	1.417880000
1	-6.953961000	-0.367027000	-0.673293000	6	6.243679000	-4.797936000	1.419468000
1	-4.790980000	-4.659087000	1.196256000	6	3.711064000	-7.250778000	0.180332000
1	-5.226724000	-4.544818000	-0.797129000	6	2.923950000	-7.145001000	-0.967331000
1	-3.593815000	-5.626821000	-0.154744000	6	1.603395000	-7.551850000	-0.967388000
1	3.221261000	-5.813144000	1.220821000	6	1.012174000	-8.082300000	0.180200000
1	1.888111000	-6.406565000	-0.213298000	6	1.836428000	-8.310601000	1.284502000
1	3.796164000	-5.824926000	-0.740778000	6	3.158118000	-7.903377000	1.284571000
1	6.405410000	-1.724447000	1.247902000	6	-0.455878000	-8.169697000	0.257805000
1	6.569842000	-2.303876000	-0.705704000	6	-1.248111000	-8.457085000	-0.856186000
1	6.671448000	-0.305526000	-0.201428000	6	-2.605425000	-8.193471000	-0.853575000
				6	-3.227226000	-7.627449000	0.261619000
				6	-2.461753000	-7.479996000	1.419199000
				6	-1.105435000	-7.746138000	1.417678000
				6	-4.538518000	-6.962615000	0.180563000
				6	-4.869812000	-6.259521000	-0.978771000
				6	-5.882262000	-5.319430000	-0.978728000
				6	-6.607945000	-5.041139000	0.180619000
				6	-6.381392000	-5.856070000	1.292637000
				6	-5.367947000	-6.797023000	1.292616000
				6	-7.368125000	-3.782715000	0.261655000
				6	-7.978362000	-3.204419000	-0.853633000
				6	-8.341742000	-1.870357000	-0.856211000

	6	-8.114097000	-1.059110000	0.257909000
	6	-7.643951000	-1.675639000	1.417857000
	6	-7.278117000	-3.008538000	1.419344000
	6	-8.135546000	0.411380000	0.180332000
	6	-7.650218000	1.040186000	-0.967240000
	6	-7.342164000	2.387210000	-0.967204000
	6	-7.505950000	3.164380000	0.180420000
	6	-8.115934000	2.564712000	1.284641000
	6	-8.424265000	1.216512000	1.284596000
	6	-6.847534000	4.479403000	0.258063000
	6	-6.700326000	5.309223000	-0.855899000
	6	-5.793360000	6.352874000	-0.853276000
	6	-4.992246000	6.608305000	0.261907000
	6	-5.247242000	5.871601000	1.419465000
	6	-6.155881000	4.830064000	1.417931000
	1	-3.384539000	6.856999000	-1.859407000
	1	-1.061187000	7.572800000	-1.859473000
	1	-1.462670000	8.899873000	2.188681000
	1	-3.799292000	8.180072000	2.188723000
	1	0.775148000	8.936402000	-1.749496000
	1	3.140027000	8.315159000	-1.753112000
	1	2.793204000	6.988717000	2.299559000
	1	0.438081000	7.600860000	2.301650000
	1	4.087380000	6.191817000	-1.839333000
	1	5.872502000	4.534386000	-1.839393000
	1	6.891551000	5.623625000	2.170899000
	1	5.098304000	7.288665000	2.170941000
	1	8.059933000	3.746675000	-1.753310000
	1	8.854597000	1.434310000	-1.749666000
	1	7.548095000	0.999437000	2.301635000
	1	6.763289000	3.302782000	2.299531000
	1	7.631039000	-0.498020000	-1.859593000
	1	7.089144000	-2.867984000	-1.859348000
	1	8.439111000	-3.183413000	2.188847000
	1	8.984012000	-0.799940000	2.188659000
	1	7.351714000	-5.139911000	-1.749247000
	1	5.630992000	-6.877075000	-1.752852000
	1	4.655878000	-5.913399000	2.299844000
	1	6.363710000	-4.179976000	2.301850000
	1	3.318377000	-6.635006000	-1.838840000
	1	0.990438000	-7.352207000	-1.838948000
	1	1.424498000	-8.780629000	2.170866000
	1	3.763069000	-8.060070000	2.170989000
	1	-0.785147000	-8.853306000	-1.753313000
	1	-3.185003000	-8.385132000	-1.749875000
	1	-2.908791000	-7.037028000	2.301707000
	1	-0.521628000	-7.509155000	2.299799000
	1	-4.246394000	-6.359264000	-1.859616000
	1	-6.027823000	-4.704992000	-1.859495000
	1	-6.976790000	-5.716908000	2.188384000
	1	-5.185019000	-7.380473000	2.188357000
	1	-8.126363000	-3.796507000	-1.750028000
	1	-8.770891000	-1.437911000	-1.753421000
	1	-7.451079000	-1.075996000	2.300102000
	1	-6.803573000	-3.421631000	2.301978000
	1	-7.405703000	0.443635000	-1.838747000
	1	-6.862690000	2.818260000	-1.838694000
	1	-8.317000000	3.156439000	2.171031000
	1	-8.862564000	0.770959000	2.170954000
	1	-7.274926000	5.106374000	-1.753036000
	1	-5.669546000	6.950649000	-1.749563000
	1	-4.640079000	6.037234000	2.301963000

				1	-6.242530000	4.205924000	2.300016000
				6	-1.015422000	3.299439000	-0.606194000
				6	-2.348901000	-2.529139000	-0.604943000
				6	3.365483000	-0.769625000	-0.606564000
				14	-2.928771000	3.501918000	-0.637199000
				14	0.452727000	4.543020000	-0.637526000
				6	-1.868293000	2.118761000	-0.585255000
				6	0.353841000	2.802932000	-0.585561000
				6	-1.037131000	0.963604000	-0.558314000
				6	0.316356000	1.380338000	-0.558524000
				14	-4.159967000	-1.879523000	-0.635383000
				14	-1.567556000	-4.287388000	-0.636067000
				6	-2.603548000	-1.095069000	-0.584527000
				6	-0.899960000	-2.677383000	-0.584836000
				6	-1.352804000	-0.416207000	-0.558083000
				6	-0.315148000	-1.379992000	-0.558231000
				14	3.708523000	-2.662800000	-0.637824000
				14	4.497510000	0.786157000	-0.637802000
				6	2.250915000	-1.707234000	-0.585716000
				6	2.769429000	0.559305000	-0.585803000
				6	1.037640000	-0.963479000	-0.558530000
				6	1.353463000	0.417049000	-0.558627000
$3Si{\cdot}(Coronene)_2$				$3Si_2$			
6	1.962622000	1.269658000	2.270607000	6	-1.943170000	3.409271000	1.158353000
6	-1.956331000	1.279353000	-2.262374000	6	1.686707000	-1.224159000	2.252433000
6	-0.001626000	-3.922806000	-0.003081000	6	-3.981298000	-2.188301000	0.565148000
14	1.773364000	3.197378000	2.122536000	14	-0.319952000	4.438460000	1.460489000
14	2.974031000	0.112732000	3.448948000	14	-3.715143000	3.877714000	0.525137000
6	1.088305000	1.838397000	1.257518000	6	-0.728260000	2.733471000	1.578183000
6	1.861608000	-0.175657000	2.125773000	6	-2.925131000	2.360553000	0.914867000
6	0.472912000	0.772272000	0.535591000	6	-0.960997000	1.326804000	1.577149000
6	0.947196000	-0.461407000	1.067042000	6	-2.309293000	1.097747000	1.179984000
14	-1.764323000	3.206233000	-2.108841000	14	2.997859000	0.182765000	2.542820000
14	-2.969948000	0.127283000	-3.443807000	14	1.811738000	-3.148678000	2.144143000
6	-1.080894000	1.843832000	-1.247875000	6	1.281863000	0.175557000	2.190056000
6	-1.857177000	-0.166519000	-2.122120000	6	0.500106000	-2.002258000	1.934995000
6	-0.466752000	0.774624000	-0.529421000	6	-0.096615000	0.228602000	1.832622000
6	-0.942861000	-0.456753000	-1.064534000	6	-0.576850000	-1.105138000	1.679275000
14	-1.216803000	-4.672532000	-1.310853000	14	-3.409549000	-4.050017000	0.545484000
14	1.211460000	-4.678605000	1.303033000	14	-5.612267000	-1.293035000	0.015578000
6	-0.775973000	-3.040305000	-0.866426000	6	-2.638139000	-2.534599000	1.003607000
6	0.774890000	-3.044206000	0.862355000	6	-4.056137000	-0.735746000	0.611680000
6	-0.473102000	-1.686103000	-0.531209000	6	-1.923250000	-1.331627000	1.285852000
6	0.475259000	-1.688488000	0.530360000	6	-2.791599000	-0.229302000	1.046020000
6	-4.263944000	-3.255348000	0.366486000	6	1.941693000	3.409683000	-1.158612000
6	-3.447592000	-2.588270000	1.320685000	6	3.982242000	-2.186972000	-0.565299000
6	-3.416729000	-1.171187000	1.323087000	6	-1.686273000	-1.225376000	-2.251956000
6	-4.190423000	-0.440624000	0.376023000	14	3.713425000	3.878845000	-0.525131000
6	-4.987880000	-1.132073000	-0.571219000	14	0.318326000	4.438280000	-1.461802000
6	-5.004205000	-2.553748000	-0.549533000	6	2.923989000	2.361367000	-0.914772000
6	-2.607889000	-0.477718000	2.267925000	6	0.727099000	2.733324000	-1.578529000
6	-4.155869000	0.983764000	0.375838000	6	2.308673000	1.098271000	-1.179710000
6	-3.351525000	1.677212000	1.325672000	6	0.960355000	1.326736000	-1.577100000
6	-2.580423000	0.945865000	2.274240000	14	5.612907000	-1.291017000	-0.015736000
6	-3.312848000	3.094865000	1.323737000	14	3.411934000	-4.048973000	-0.546027000
6	-4.077624000	3.799086000	0.354148000	6	4.056424000	-0.734400000	-0.611529000
6	-4.853843000	3.131423000	-0.562629000	6	2.639240000	-2.533990000	-1.003584000
6	-4.918493000	1.711871000	-0.574075000	6	2.791565000	-0.228560000	-1.045672000
6	-5.702714000	0.995663000	-1.518077000	6	1.923730000	-1.331294000	-1.285549000
6	-5.735662000	-0.378298000	-1.516669000	14	-1.810742000	-3.149836000	-2.143335000
1	-6.346554000	-0.912252000	-2.249353000	14	-2.998063000	0.180952000	-2.542535000
1	-6.283761000	1.557960000	-2.253580000	6	-0.499392000	-2.002995000	-1.934494000

1	-4.289536000	-4.348581000	0.372160000	6	-1.282034000	0.174514000	-2.189872000
1	-5.621699000	-3.082734000	-1.280142000	6	0.577209000	-1.105397000	-1.678939000
1	-4.042706000	4.891749000	0.349952000	6	0.096438000	0.228139000	-1.832471000
1	-5.435541000	3.690243000	-1.300276000				
6	-2.652495000	-3.293150000	2.264924000				
6	-1.867657000	-2.625599000	3.168911000				
6	-1.826032000	-1.205212000	3.200209000				
1	-2.670174000	-4.386064000	2.253659000				
1	-1.254160000	-3.182536000	3.881538000				
6	-1.026955000	-0.488765000	4.131646000				
6	-1.008285000	0.881754000	4.144435000				
6	-1.781263000	1.635508000	3.220203000				
1	-0.416463000	-1.053572000	4.840623000				
1	-0.384417000	1.416456000	4.865313000				
6	-2.506110000	3.762293000	2.285969000				
1	-2.481103000	4.855109000	2.282654000				
6	-1.771910000	3.057382000	3.204088000				
1	-1.158780000	3.585336000	3.939643000				
6	2.646713000	-3.288759000	-2.274607000				
6	3.442176000	-2.586866000	-1.328468000				
6	3.413011000	-1.169737000	-1.327824000				
6	2.605653000	-0.473268000	-2.271685000				
6	1.823697000	-1.197820000	-3.206196000				
6	1.863434000	-2.618314000	-3.177809000				
6	4.187263000	-0.442172000	-0.378910000				
6	2.579694000	0.950348000	-2.274766000				
6	3.350818000	1.678701000	-1.323904000				
6	4.154101000	0.982232000	-0.375391000				
6	3.313528000	3.096387000	-1.318652000				
6	2.508257000	3.766873000	-2.279999000				
6	1.774295000	3.064851000	-3.200534000				
6	1.782211000	1.643002000	-3.219939000				
6	1.009308000	0.892177000	-4.146620000				
6	1.026379000	-0.478393000	-4.136835000				
1	0.415919000	-1.040917000	-4.847657000				
1	0.386764000	1.429188000	-4.866930000				
1	2.662947000	-4.381714000	-2.265561000				
1	1.249750000	-3.172977000	-3.892048000				
1	2.484350000	4.859702000	-2.274152000				
1	1.162481000	3.595146000	-3.935500000				
6	4.257613000	-3.256970000	-0.375610000				
6	4.998801000	-2.558250000	0.541838000				
6	4.984103000	-1.136608000	0.566659000				
1	4.281806000	-4.350218000	-0.383592000				
1	5.615733000	-3.089554000	1.271239000				
6	5.732844000	-0.385808000	1.513702000				
6	5.701161000	0.988183000	1.518402000				
6	4.917425000	1.707334000	0.576261000				
1	6.343466000	-0.922087000	2.244915000				
1	6.282891000	1.548209000	2.255100000				
6	4.078598000	3.797563000	-0.347105000				
1	4.044697000	4.890245000	-0.340284000				
6	4.854036000	3.126979000	0.568227000				
1	5.436186000	3.683517000	1.307243000				

References

1 M. Contreras, E. Osorio, F. Ferraro, G. Puga, K. J. Donald, J. G. Harrison, G. Merino and W. Tiznado, *Chemistry-A European Journal*, 2013, **19**, 2305–2310.

2 C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158.

3 S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456–1465.

4 E. van Lenthe, E. J. Baerends and J. G. Snijders, *J. Chem. Phys.*, 1994, **101**, 9783–9792.

5 E. van Lenthe and E. J. Baerends, *J. Comput. Chem.*, 2003, **24**, 1142–1156.

6 ADF2012, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam The Netherlands, Http://www.scm.com.

7 O. Yañez, R. Báez-Grez, D. Inostroza, W. A. Rabanal-León, R. Pino-Rios, G. Garza, W. Tiznado, J. Garza and W. Tiznado, *J. Chem. Theory Comput.*, 2018, **15**, 1463–1475.

8 C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158–6170.

9 S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J Chem Phys*, 2010, **132**, 154104.

10 F. Weigend and R. Ahlrichs, *Physical Chemistry Chemical Physics*, 2005, **7**, 3297–3305.

11 J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615–6620.

12 D. Y. Zubarev and A. I. Boldyrev, *Phys. Chem. Chem. Phys.*, 2008, **10**, 5207–5217.

13 D. Y. Zubarev and A. I. Boldyrev, *J. Org. Chem.*, 2008, **73**, 9251–9258.

14 H. Fliegl, S. Taubert, O. Lehtonen and D. Sundholm, *Phys. Chem. Chem. Phys.*, 2011, **13**, 20500–20518.

15 J. Jusélius, D. Sundholm and J. Gauss, *J. Chem. Phys.*, 2004, **121**, 3952–3963.

16 K. Wolinski, J. F. Hinton and P. Pulay, *J. Am. Chem. Soc.*, 1990, **112**, 8251–8260.

17 Ahrens, J., Geveci, B. and Law, C. (2005) Paraview: An End-User Tool for Large Data Visualization. The Visualization Handbook, 717-731.

18 U. Ayachit, *The ParaView Guide: A Parallel Visualization Application*, Kitware, Inc., USA, 2015.

19 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian 16, Revis. B.01, Gaussian, Inc.*, Wallingford CT, 2016.