

Persistent Planar Tetracoordinate Carbon in Global Minima Structures of Silicon Rich Silicon-Carbon Clusters

Luis Leyva-Parra ^{1,2}, Diego Inostroza ^{1,2}, Osvaldo Yañez^{3,4}, Julio César Cruz ⁵, Jorge Garza ⁵, Víctor García ^{6,*} and William Tiznado ^{1,*}

¹ Computational and Theoretical Chemistry Group, Departamento de Ciencias Química, Facultad de Ciencias Exactas, Universidad Andres Bello, República 498, Santiago, Chile; wtiznado@unab.cl ; l.leyvaparra@uandresbello.edu ; dinostro92@gmail.com

² Universidad Andres Bello, Programa de Doctorado en Fisicoquímica Molecular, Facultad de Ciencias Exactas, Santiago, Chile; l.leyvaparra@uandresbello.edu ; dinostro92@gmail.com

³ Center of New Drugs for Hypertension (CENDHY), Santiago, Chile; osvyanezosses@gmail.com

⁴ Department of Pharmaceutical Science and Technology, School of Chemical and Pharmaceutical Sciences, Universidad de Chile, Santiago, Chile; osvyanezosses@gmail.com

⁵ Departamento de Química, División de Ciencias Básicas e Ingeniería, Universidad Autónoma Metropolitana-Iztapalapa, San Rafael Atlixco 186, Col. Vicentina, Iztapalapa. C. P. 09340, Ciudad de México, Mexico ; julio.cruz088@gmail.com ; jgo@xanum.uam.mx

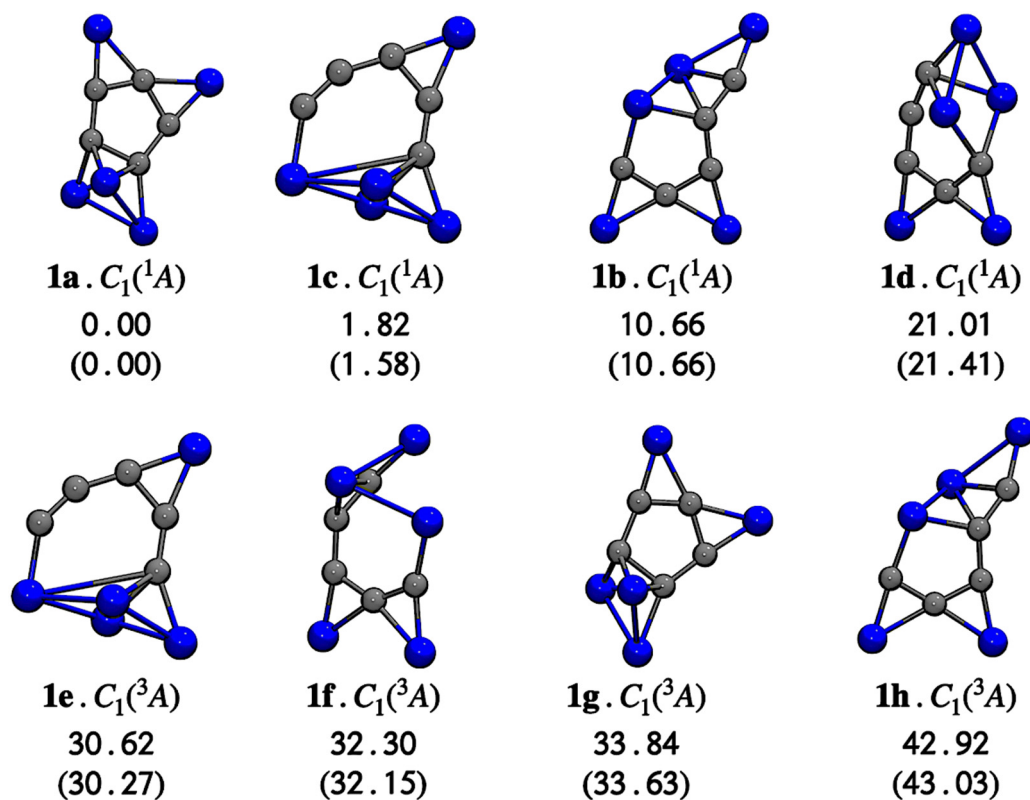
⁶ Facultad de Química e Ingeniería Química, Universidad Nacional Mayor de San Marcos, Lima 15004, Perú; victor.garcia@unmsm.edu.pe

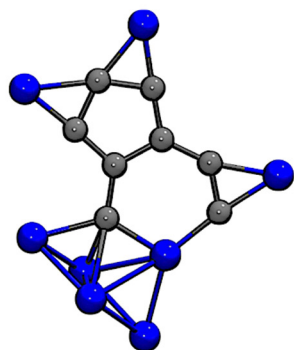
* Correspondence: wtiznado@unab.cl ; Tel.: (optional; include country code; if there are multiple corresponding authors, add author initials)

SUPPORTING INFORMATION

Figures S1-S3. Global minimum and low-lying isomers of Si_nC_n ($n = 5, 8$ and 9), their point group symmetries and spectroscopic states. Relative energies are shown in kcal.mol^{-1} at PBE0/def2-TZVP and PBE0-D3/def2-TZVP (in parentheses) levels including zero-point energy (ZPE) corrections. A number-letter label identifies structure to facilitate their connection with their Cartesian coordinate (at the end of the ESI).

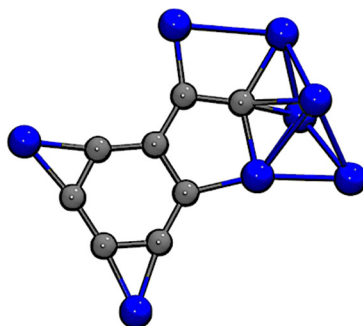
Si_5C_5





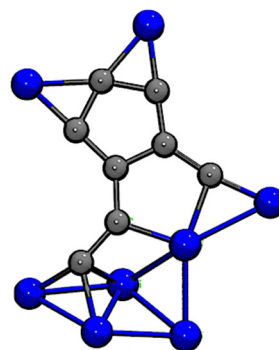
2a . C₁(¹A)

0.00
(0.00)



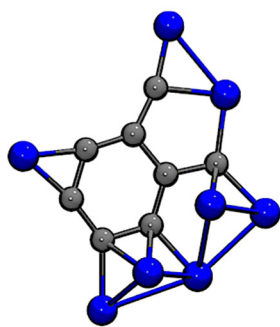
2b . C₁(¹A)

2.48
(2.56)



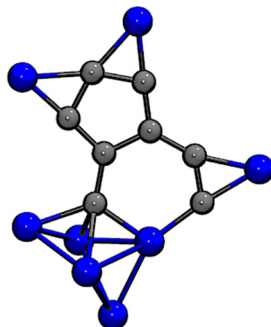
2c . C₁(¹A)

13.92
(13.97)



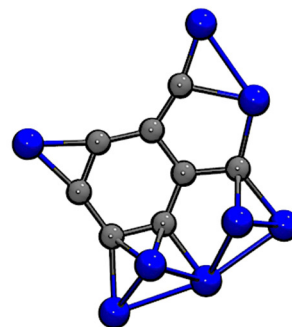
2d . C₁(¹A)

18.60
(18.19)



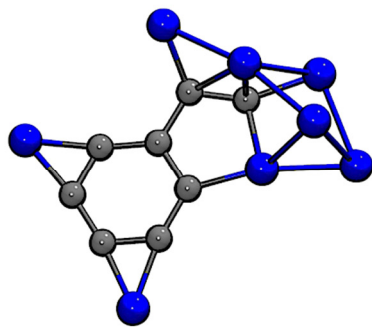
2e . C₁(³A)

22.43
(22.34)



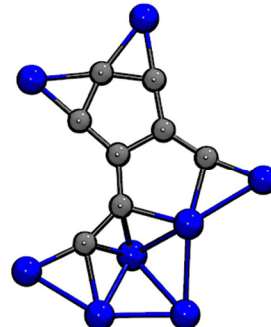
2f . C₁(³A)

25.96
(25.55)



2g . C₁(³A)

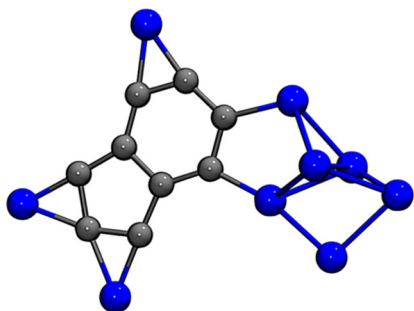
32.70
(32.71)



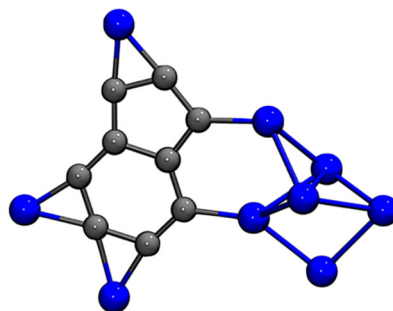
2h . C₁(³A)

49.73
(49.74)

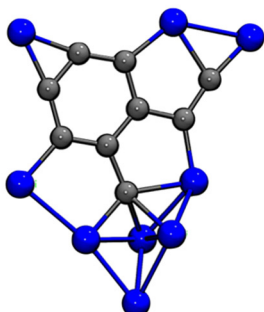
Si₉C₉



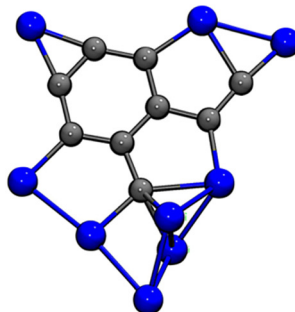
3a. $C_1(^1A)$
0.00
(0.00)



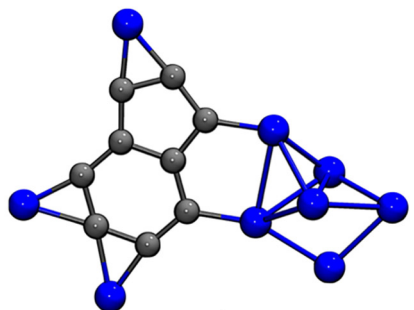
3b. $C_1(^1A)$
12.87
(12.48)



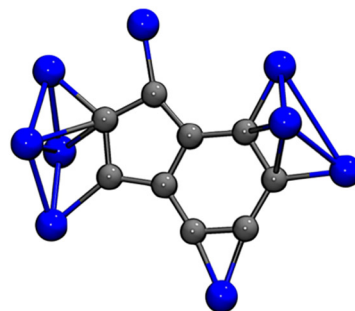
3c. $C_1(^1A)$
18.26
(17.14)



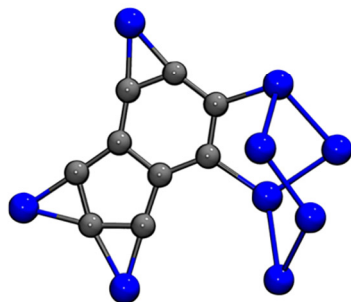
3d. $C_1(^3A)$
18.92
(17.73)



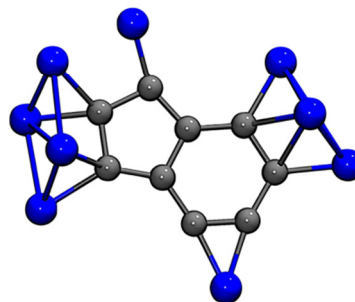
3e. $C_1(^3A)$
21.63
(21.44)



3f. $C_1(^1A)$
41.23
(39.84)



3g. $C_1(^3A)$
43.94
(42.43)



3h. $C_1(^3A)$
67.03
(65.66)

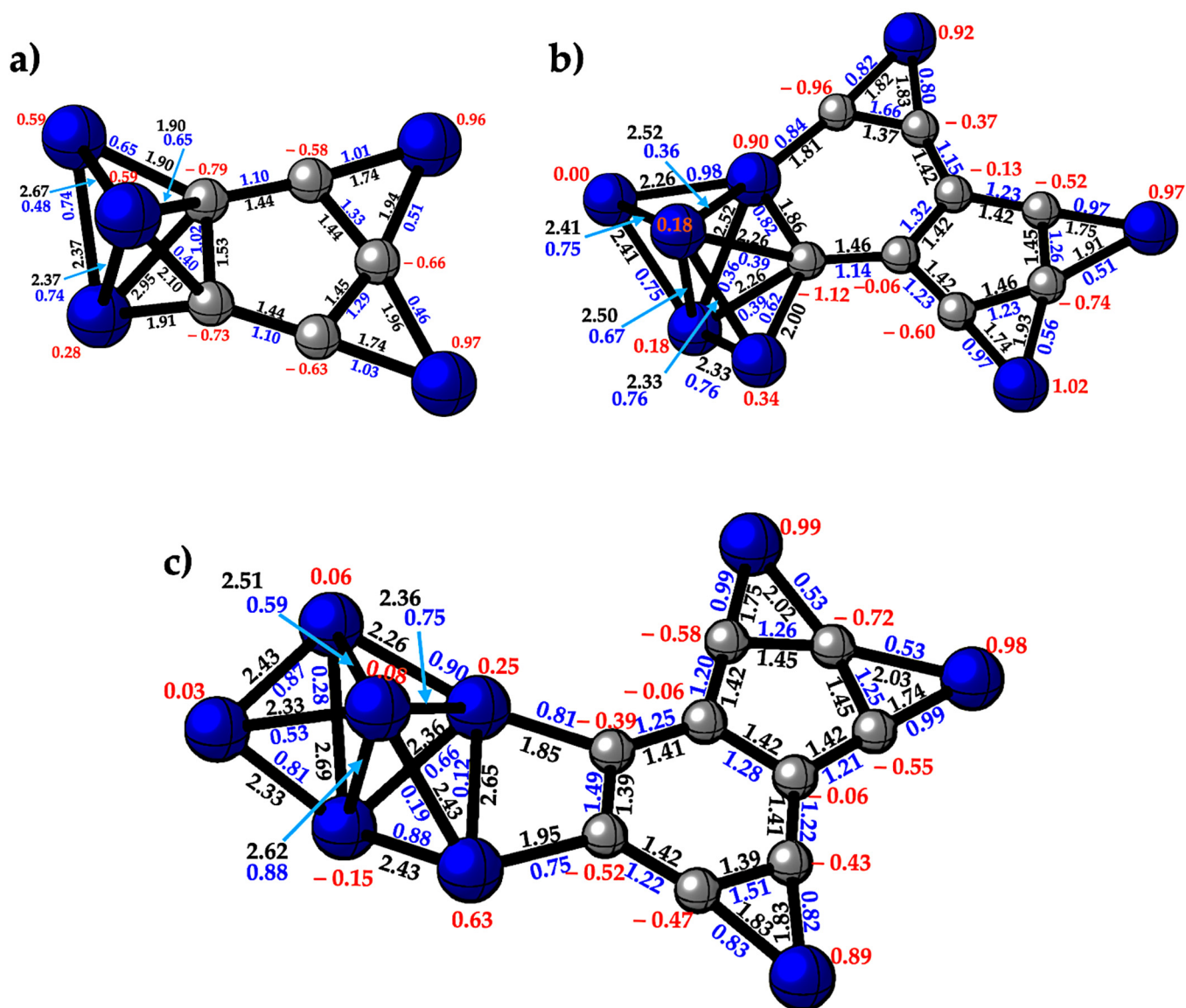


Figure S4. Bond length in Å (**black**), natural charges (**red**) and Wiberg bond indices (**blue**) for the a) Si_5C_5 , b) Si_8C_8 and c) Si_9C_9 global minimum at the PBE0/def2-TZVP level.

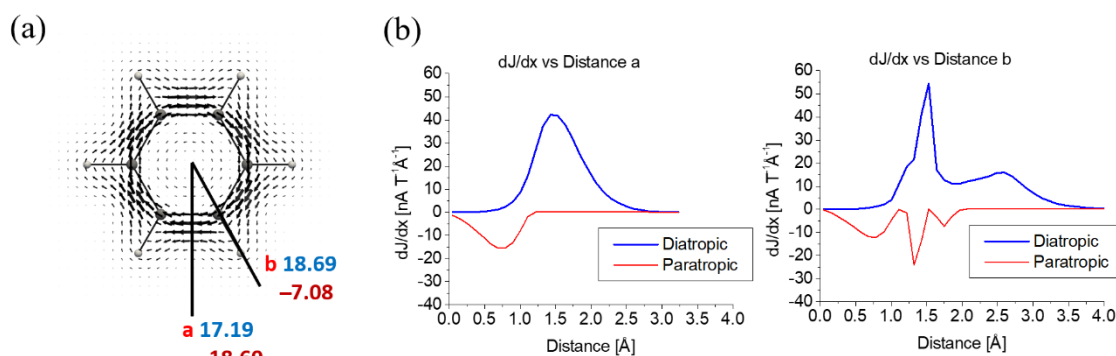


Figure S5. (a) Vector plot visualization of the current density of C_6H_6 in a plane placed 0.5 \AA above the molecular plane and top view of integration planes. The intensities of the diatropic currents are indicated in blue while the intensity of the paratropic currents in red. The intensity of the total current susceptibility is the sum of the paratropic and diatropic contribution. (b) Integration profiles along the integration planes of C_6H_6 .

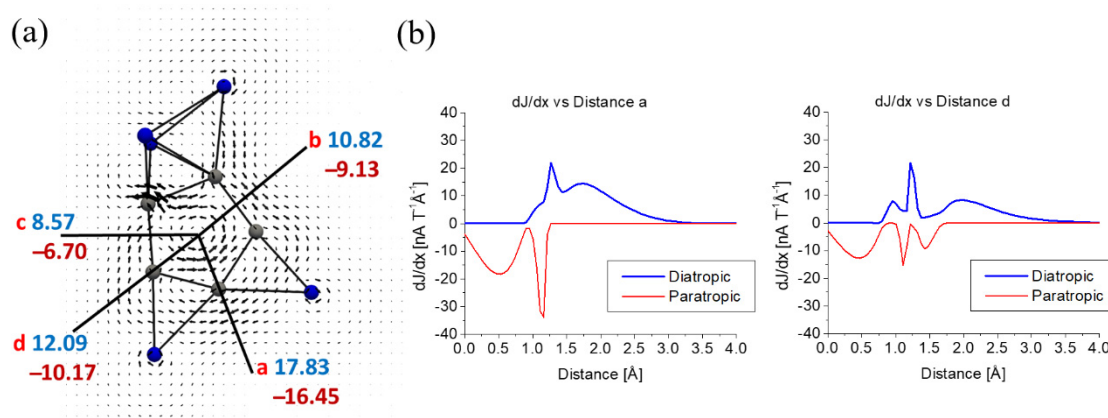


Figure S6. (a) Vector plot visualization of the current density of Si_5C_5 in a plane placed 0.5 \AA above the molecular plane and top view of integration planes. The intensities of the diatropic currents are indicated in blue while the intensity of the paratropic currents in red. The intensity of the total current susceptibility is the sum of the paratropic and diatropic contribution. (b) Integration profiles along the integration planes of Si_5C_5 .

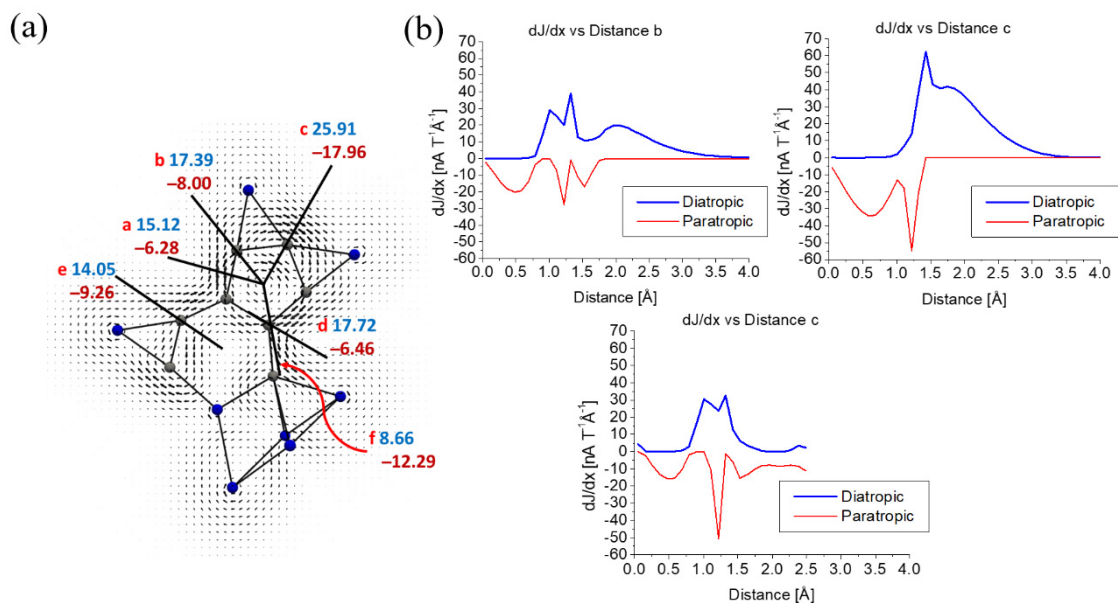


Figure S7. (a) Vector plot visualization of the current density of Si_8C_8 in a plane placed 0.5 \AA above the molecular plane and top view of integration planes. The intensities of the diatropic currents are indicated in blue while the intensity of the paratropic currents in red. The intensity of the total current susceptibility is the sum of the paratropic and diatropic contribution. (b) Integration profiles along the integration planes of Si_8C_8 .

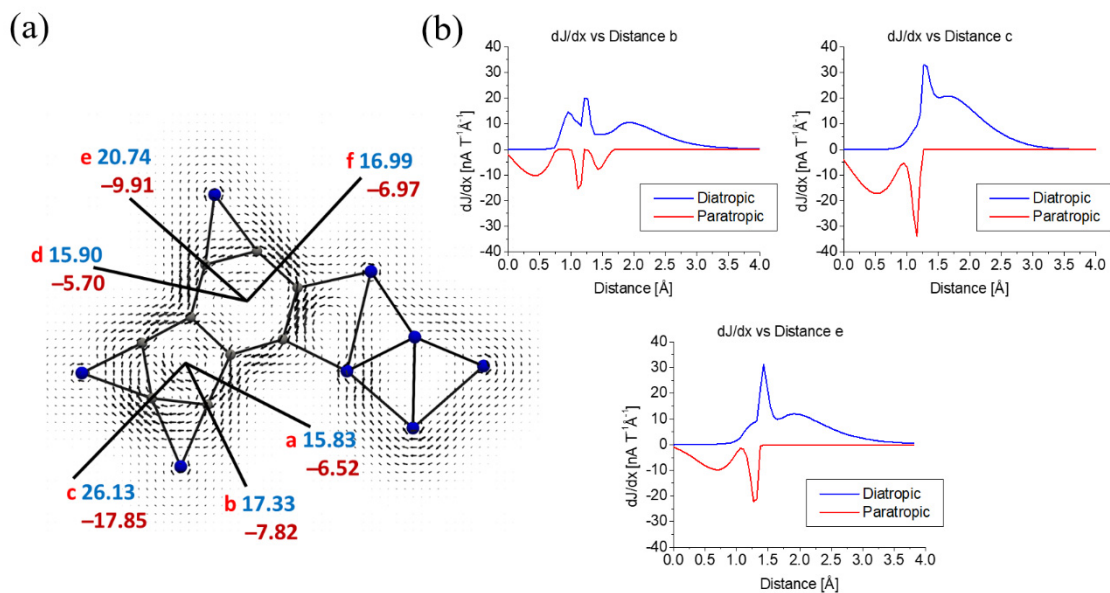


Figure S8. (a) Vector plot visualization of the current density of Si_9C_9 in a plane placed 0.5 \AA above the molecular plane and top view of integration planes. The intensities of the diatropic currents are indicated in blue while the intensity of the paratropic currents in red. The intensity of the total current susceptibility is the sum of the paratropic and diatropic contribution. (b) Integration profiles along the integration planes of Si_9C_9 .

Table S1. Cartesian coordinates of the Si_nC_n (n = 5, 8 and 9) systems and the lowest harmonic vibrational frequencies in parentheses (in cm⁻¹) calculated at the PBE0/def2-TZVP level of theory.

1a (88.6)				1b (82.6)			
6	0.448483	-1.624707	0.000000	6	-0.849026	2.546393	-0.000959
6	-0.941430	-1.261804	0.000000	6	-1.700212	1.634041	0.000955
6	-1.045056	0.177559	0.000000	6	-2.225489	0.367619	0.000608
6	1.235842	-0.408725	0.000000	6	-1.250441	-0.632901	-0.000030
6	0.374596	0.750770	0.000000	6	0.173791	-0.464346	-0.000189
14	2.408441	-1.692128	0.000000	14	-2.950576	-1.298457	-0.000452
14	-0.910536	-3.003978	0.000000	14	1.624615	0.047131	-1.416657
14	-1.045056	1.528551	1.332836	14	1.562764	-1.795127	0.000372
14	0.561162	2.653393	0.000000	14	0.647027	1.519821	-0.000370
14	-1.045056	1.528551	-1.332836	14	1.623903	0.047714	1.416942
1c (68.2)				1d (82.1)			
6	-1.583087	-1.017064	-0.091059	6	-1.607764000	-1.021827000	-0.323335000
6	-1.669582	0.414778	-0.030473	6	-0.391807000	-1.422634000	-0.374650000
6	-0.433899	1.113368	-0.298773	6	0.967099000	-1.378957000	-0.427185000
6	0.643408	0.218607	-0.639147	6	1.417994000	-0.033310000	-0.077086000
6	1.997958	0.493524	-0.542489	6	0.409116000	0.959396000	0.217089000
14	-3.266953	-0.881804	0.340722	14	2.731058000	-1.355285000	-0.467708000
14	-1.682343	2.270089	0.049062	14	2.074768000	1.653611000	0.424175000
14	0.082061	-1.647681	-0.665944	14	-1.166977000	0.940291000	-1.017887000
14	1.710072	-0.717218	0.906966	14	-3.097058000	0.009028000	0.068845000
14	3.605107	0.452379	0.055739	14	-1.083605000	0.111488000	1.359402000
1e (49.3)				1f (70.4)			
6	-0.023753	2.293833	-0.051549	6	-1.412255	-0.733084	-0.726868
6	-1.151259	1.788827	-0.071050	6	-0.454884	-1.476048	-0.136277
6	-2.062410	0.770674	-0.045134	6	0.977627	-1.288421	-0.185797
6	-1.478794	-0.516620	0.006690	6	1.455835	0.027824	-0.092259
6	-0.158657	-0.917647	0.014556	6	0.726436	1.223528	0.101103
14	-3.325149	-0.495162	0.035096	14	2.703435	-1.489556	-0.255267
14	1.693201	1.719849	0.076979	14	2.387877	1.766227	0.028407
14	1.241935	-0.224728	-1.314895	14	-1.139800	1.304281	0.312246
14	1.225417	-0.313767	1.327553	14	-2.893140	0.227102	-0.934353
14	1.253826	-2.151506	-0.061953	14	-1.612412	-0.845397	1.294722
1g (83.9)				1h (67.4)			
6	0.415682	-1.557472	0.000000	6	-2.512954	2.328639	-16.039202
6	-0.964323	-1.176426	0.000000	6	-1.738997	2.826377	-14.940195
6	-1.099592	0.290191	0.000000	6	-1.859955	2.294211	-13.613445
6	1.243439	-0.373987	0.000000	6	-2.800037	1.230336	-13.490480
6	0.386840	0.796801	0.000000	6	-3.585605	0.750047	-12.457127
14	2.369030	-1.708613	0.000000	14	-1.657642	3.625277	-16.798812
14	-0.982817	-2.917819	0.000000	14	-0.594036	3.519677	-13.574223
14	-0.799851	1.275734	1.589916	14	-3.433150	0.919118	-15.301748
14	0.276225	2.740087	0.000000	14	-4.903786	1.803290	-13.546797
14	-0.799851	1.275734	-1.589916	14	-5.040549	0.153954	-11.753648

2a (32.4)				2b (35.1)			
6	-2.124452	0.872470	0.000000	6	2.414875	1.207734	-0.015072
6	0.907593	3.027848	0.000000	6	3.563381	0.453278	-0.038873
6	-0.535474	2.863109	0.000000	6	3.467190	-0.966876	-0.029878
6	-0.840075	1.478228	0.000000	6	2.206363	-1.540285	0.002028
6	-2.439516	-0.464943	0.000000	6	1.019387	-0.779098	0.020506
6	1.440101	1.670587	0.000000	6	1.101932	0.637957	0.011531
6	0.368829	0.736613	0.000000	6	-0.122397	1.362946	0.021193
6	0.500727	-0.717857	0.000000	6	-1.316152	0.535874	0.032999
14	2.814460	2.742546	0.000000	14	3.930111	2.240076	-0.010338
14	-0.203401	4.579901	0.000000	14	3.574188	-2.773670	0.019865
14	-3.929621	0.587255	0.000000	14	-0.761562	-1.252512	0.041985
14	-1.090963	-1.672899	0.000000	14	-0.803610	3.002077	0.065124
14	-0.656438	-3.894299	0.000000	14	-3.052814	1.547616	-0.061632
14	2.417465	-1.298988	0.000000	14	-2.643886	-0.385300	-1.323235

14	0.907593	-2.550198	1.252226	14	-2.756627	-2.423509	0.025813
14	0.907593	-2.550198	-1.252226	14	-2.772048	-0.345433	1.240518
2c (51.7)				2d (44.5)			
6	3.267955	-0.578372	-0.027656	6	1.059966	5.616077	-16.750028
6	2.015443	-1.293990	-0.253948	6	0.934669	4.752703	-15.629901
6	0.971031	-0.338363	-0.270854	6	0.847928	5.438357	-14.392703
6	1.512717	0.947143	-0.065830	6	0.793028	6.876150	-14.283131
6	2.923212	0.831887	0.084782	6	0.902157	7.724081	-15.436480
6	-0.448952	-0.368435	-0.491794	6	1.056162	7.001753	-16.662491
6	0.650024	2.074853	-0.032803	6	0.908288	3.350797	-15.480712
14	3.290740	-2.486020	-0.234512	14	0.857977	2.831610	-13.573231
14	4.654295	0.706473	0.277857	6	0.832765	4.668358	-13.177425
14	-1.157848	1.345568	-0.488974	14	0.863366	1.639128	-15.673971
14	-0.152914	3.560772	0.084053	14	1.296087	6.420527	-18.384053
6	-1.438334	-1.360978	-0.571061	14	0.869323	9.518244	-14.799714
14	-3.454976	1.174552	0.059865	14	2.613814	8.105017	-14.194484
14	-3.278090	-1.056907	-0.704090	14	0.853356	7.660327	-12.575647
14	-2.053119	-2.786980	0.457930	14	2.661586	5.761262	-13.177068
14	-1.901474	-0.420757	1.250140	14	0.875056	5.473570	-11.468126
2e (43.1)				2f (39.2)			
6	-2.102937	0.833810	0.000000	6	0.883305	5.624049	-16.804226
6	0.921392	2.998722	0.000000	6	0.811657	4.765822	-15.667199
6	-0.519705	2.830291	0.000000	6	0.753210	5.443301	-14.426853
6	-0.817080	1.443862	0.000000	6	0.773665	6.858054	-14.341050
6	-2.448686	-0.495863	0.000000	6	1.029084	7.701053	-15.451808
6	1.464242	1.645402	0.000000	6	1.015915	7.005341	-16.711839
6	0.396259	0.712786	0.000000	6	0.955738	3.366236	-15.507210
6	0.522916	-0.741725	0.000000	14	1.225527	2.888319	-13.628555
14	2.825958	2.736764	0.000000	6	0.924823	4.717418	-13.212175
14	-0.193843	4.549621	0.000000	14	1.068337	1.666126	-15.725037
14	-3.913416	0.591479	0.000000	14	0.982535	6.425646	-18.443207
14	-1.094955	-1.711480	0.000000	14	1.121463	9.471436	-14.536077
14	-0.277247	-3.898343	0.000000	14	2.755732	7.721969	-14.327503
14	2.313417	-1.547727	0.000000	14	0.760080	7.749365	-12.697558
14	0.682694	-2.267338	1.546162	14	2.565688	5.804718	-12.726072
14	0.682694	-2.267338	-1.546162	14	0.598766	5.629109	-11.452796
2g (34.9)				2h (36.7)			
6	2.280073	1.060213	0.149592	6	-0.257041	2.653411	-9.305461
6	3.410117	0.293670	-0.033780	6	-0.052526	3.874922	-8.519433
6	3.280853	-1.122413	-0.078521	6	-0.014293	3.503667	-7.158029
6	2.020210	-1.678177	0.070637	6	-0.148946	2.097071	-7.046705
6	0.854131	-0.905657	0.268439	6	-0.316304	1.557254	-8.351979
6	0.977331	0.509116	0.315348	6	0.128602	4.213378	-5.912766
6	-0.225245	1.288368	0.514426	6	-0.033896	1.527485	-5.756839
6	-1.375241	0.455895	0.670050	14	-0.105903	4.337790	-10.204109
14	3.807703	2.068022	-0.041956	14	-0.514622	0.866299	-9.946535
14	3.336713	-2.933555	-0.179561	14	0.226450	2.943328	-4.474406
14	-0.935585	-1.365321	0.470498	14	0.301443	0.571552	-4.341542
14	-0.458585	3.135669	0.196523	6	0.159102	5.586377	-5.599111
14	-1.915658	1.626997	-0.913844	14	-0.631985	4.330515	-2.573002
14	-2.257555	-0.656368	-1.443370	14	-0.158521	6.316480	-3.779705
14	-3.165719	-2.121818	0.259080	14	0.453993	7.334102	-5.798330
14	-3.220840	0.288796	0.848549	14	-1.566704	4.649502	-4.785000

3a (37.8)				3b (43.7)			
6	-0.254944	0.101129	-0.000569	6	-3.389416	-0.370136	-0.031620
6	-1.610292	-0.296088	-0.000514	6	-2.529435	0.722238	0.002661
6	-2.204797	-1.590101	-0.000632	6	-1.072392	0.468756	0.060222
6	0.125358	1.436388	-0.000371	6	-0.517738	-0.811808	0.090786
6	-0.924157	2.389822	-0.000276	6	-1.397680	-1.906936	0.049891
6	-2.265160	2.036162	-0.000217	6	-2.804510	-1.672149	-0.004532
6	-2.644883	0.681005	-0.000346	6	-2.676095	2.120385	-0.023644
6	-3.900123	0.009003	0.000035	6	-1.372795	2.696456	0.010493
6	-3.649542	-1.423355	-0.000777	6	-0.366802	1.701803	0.062346
14	-5.460447	-0.769786	0.001824	14	-2.728718	3.927948	-0.064381
14	-2.899877	-3.191331	-0.000861	14	-4.724402	-1.551822	-0.049294
14	-2.020445	3.849598	0.000013	14	-2.156121	-3.504608	0.015673
14	2.026160	1.857742	-0.000156	14	1.467735	1.985183	0.043402

14	1.404918	-0.718678	-0.000634	14	1.336813	-0.783162	0.136350
14	3.114959	-2.192886	0.000733	14	2.958853	0.336153	1.367839
14	4.941563	-0.587494	0.000590	14	2.820729	0.360834	-1.280116
14	3.159671	0.159740	1.311926	14	4.726165	-0.068389	-0.129930
14	3.160481	0.159732	-1.311770	14	3.210458	-1.965827	-0.132373
3c (48.5)				3d (50.2)			
6	2.360225	1.994565	-0.069589	6	2.120550	2.130526	0.001928
6	2.421635	0.588110	-0.018962	6	2.311339	0.733761	-0.015377
6	1.160386	-0.055775	0.017043	6	1.128087	-0.023184	-0.028322
6	-0.061775	0.654960	0.008671	6	-0.158514	0.555770	0.009252
6	-0.120447	2.049560	-0.047802	6	-0.370145	1.941315	-0.036259
6	1.155649	2.693392	-0.086729	6	0.845950	2.688268	-0.036375
14	3.827703	-0.643249	0.005112	14	3.794558	-0.366409	0.144591
6	2.428144	-2.039614	0.045960	6	2.535524	-1.931097	-0.115282
6	1.153457	-1.473329	0.048908	6	1.248860	-1.451503	-0.025779
14	3.868149	-3.004952	0.051587	14	4.074078	-2.666085	-0.376750
14	2.598683	3.806267	-0.137479	14	2.155349	3.958771	0.018628
14	-1.699935	3.020220	-0.087585	14	-2.074179	2.758992	-0.087105
14	-2.867105	0.770329	0.077156	14	-2.968739	0.499031	0.062143
14	-0.549586	-2.119755	0.063016	14	-0.402861	-2.333991	0.106568
6	-1.274872	-0.166507	0.044554	6	-1.279722	-0.360587	0.086377
14	-2.329312	-1.330616	1.361091	14	-2.151137	-1.489892	1.431733
14	-4.336924	-1.068754	0.043309	14	-4.182984	-1.595176	0.158859
14	-2.330178	-1.306194	-1.267305	14	-2.234344	-1.584807	-1.175882
3e (44.4)				3f (31.4)			
6	-2.958885	5.404511	-18.704779	6	-2.690615	5.477147	-18.622463
6	-2.781016	4.639809	-17.543931	6	-2.620176	4.852205	-17.324763
6	-2.521039	5.306856	-16.298028	6	-2.560141	5.589724	-16.129668
6	-2.434106	6.718261	-16.190857	6	-2.608511	6.995751	-16.210183
6	-2.612918	7.484937	-17.350402	6	-2.691944	7.621758	-17.439720
6	-2.866045	6.828919	-18.589675	6	-2.703980	6.920269	-18.681164
6	-2.799972	3.237850	-17.269197	6	-2.575544	3.462900	-17.029918
6	-2.556103	3.053892	-15.892765	6	-2.470880	3.358919	-15.606253
6	-2.376398	4.320611	-15.265431	6	-2.475274	4.679959	-14.995162
14	-2.798587	1.507164	-16.796734	14	-2.711695	1.775646	-17.595197
14	-3.186248	5.994324	-20.356329	14	-2.691639	8.816523	-16.074182
14	-2.777617	8.760780	-18.570605	14	-4.440017	6.020457	-19.757378
14	-2.071683	4.760508	-13.555788	14	-2.810137	4.504442	-20.228583
14	-2.140633	7.210643	-14.464524	14	-2.836632	7.626851	-20.415627
14	-0.485181	6.494305	-12.803835	14	-2.440970	1.546635	-14.877966
14	-3.205593	6.612267	-12.371722	14	-2.392621	5.001578	-13.057105
14	-1.573615	7.343592	-10.881231	14	-3.683813	3.200092	-13.805478
14	-1.778096	8.693008	-12.833592	14	-1.089757	3.231045	-13.911662
3g (27.3)				3h (31.9)			
6	-0.114996	0.325998	0.292494	6	-2.634350	5.482785	-18.634635
6	1.216254	-0.150162	0.141086	6	-2.552246	4.845966	-17.337886
6	1.692023	-1.488530	0.056717	6	-2.578251	5.591627	-16.127646
6	-0.356336	1.707370	0.336372	6	-2.663856	6.997969	-16.208120
6	0.760949	2.566921	0.228431	6	-2.756996	7.620899	-17.435436
6	2.067642	2.112803	0.120077	6	-2.729543	6.922124	-18.685370
6	2.329081	0.730826	0.066043	6	-2.444880	3.475146	-17.043080
6	3.513948	-0.046090	-0.063644	6	-2.375809	3.369689	-15.611693
6	3.139738	-1.452301	-0.075971	6	-2.502312	4.705278	-15.007707
14	4.989437	-0.962790	-0.231410	14	-2.633442	1.696679	-17.254683
14	2.218345	-3.147048	-0.057400	14	-2.815395	8.814022	-16.070195
14	1.963202	3.935607	0.112570	14	-4.439731	6.013605	-19.771256
14	-2.185505	2.212539	0.202197	14	-2.700216	4.572904	-20.272700
14	-1.583635	-0.788252	0.776111	14	-2.914881	7.683873	-20.392507
14	-3.425256	-1.338571	-0.881541	14	-2.694571	1.479635	-14.860321
14	-2.108309	-2.986522	0.137199	14	-2.189453	4.905219	-13.052153
14	-2.219409	0.517794	-1.463900	14	-3.757165	3.436489	-13.921928
14	-3.544920	0.426614	0.900932	14	-1.111251	3.067992	-14.075157