Supplementary Material (ESI) for Dalton Transactions

Synthesis of star-shaped oligothiophenes with an organosilicon core. Effects of the core structures on their hole mobility

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Supplementary Information

Experimental details for the preparation of Si-linked star-shaped oligothiopehenes, HOMO's of the neutral as well as the SOMO(α)'s and LUMO(β)'s (the two mid-gap orbitals) of the radical cationic **2T**, **2T$_2$Si$_2$C**, and **2T$_2$Si$_2$Ge** from (U)B3LYP calculations, and cartesian coordinates for optimized geometries of all calculated model compounds.

Preparation of Si-linked star-shaped oligothiophenes

General

All reactions were carried out in dry nitrogen. Ether and THF were dried over sodium/benzophenone and distilled immediately before use. Toluene was distilled from sodium and stored over activated molecular sieves before use. Tris[(5'-bromo-2,2'-bithiophenyl)dimethylsilyl]methane[4] was prepares as reported in the literature. Usual work-up described bellow includes hydrolysis of the reaction mixture with water, separation of the organic layer, extraction of the aqueous layer with chloroform, drying the combined organic layer and extracts over anhydrous magnesium sulfate, evaporation of the solvent, and subjecting the residue to silica gel column chromatography, in that order. NMR spectra were recorded on a JEOL model LA-400 spectrometer in $CDCl_3$ at ambient temperature (^{1}H, 400 MHz; ^{13}C, 100 MHz). UV spectra were measured on a Shimadzu model UV-3150 spectrophotometer. MS spectra were measured on a JEOL model SX-102A spectrometer.

Tris[(ethylterthiophenyl)dimethylsilyl]methane (3T$_3$C)

To a solution of 0.50 g (1.4 mmol) of 5-bromo-5"-ethylthiophene in 20 mL of ether was added 0.92 mL (1.4 moL) of a 1.57 M *n*-butyllithium solution in hexane at -80°C and the mixture was stirred at room temperature for 3 hr. The resulting solution of ethylterthiophenyllithium was cooled at -80°C. To this was added 0.14 g (0.48 mmol) of tris(chlorodimethylsilyl)methane in 10 mL of ether and the mixture was stirred for 24

hr at room temperature. After usual work-up, sublimation of the crude product afforded 0.10 g (21% yield) of **3T$_3$C** as a yellow solid. mp 121-123°C. FAB-MS *m/z* 1012 (M^+). ^{1}H NMR: δ 0.33 (s, 1H, HC), 0.38 (s, 18H, CH_3Si), 1.32 (t, 9H, J = 7.6 Hz, CH_3CH_2), 2.82 (br q, 6H, J = 7.6 Hz, CH_2CH_3), 6.66 (dt, 3H, J = 3.6, 1.0 Hz, ring H), 6.90-6.97 (m, 9H, ring H), 6.99 (d, 3H, J = 3.9 Hz, ring H), 7.07 (d, 3H, J = 3.3 Hz, ring H). ^{13}C NMR: δ 2.57 (CH_3Si), 6.10 (HC), 15.84 (CH_3CH_2), 23.51 (CH_2CH_3), 123.27, 123.53, 124.11, 124.27, 124.42, 134.51, 134.52, 134.95, 136.68, 140.75, 142.40, 146.88 (ring carbons). Anal. Calcd for $C_{49}H_{52}S_9Si_3$: C, 58.05; H, 5.17. Found: C, 57.73; H, 5.31.

Tris[(ethylquarterthiophenyl)dimethylsilyl]methane (4T$_3$C)

A mixture of 0.23 g (0.25 mmol) of tris[(bromobithiophenyl)dimethylsilyl]methane, 0.35 g (0.73 mmol) of ethyl(tributylstannyl)bithiophene, 14 mg (0.013 mmol) of $Pd(PPh_3)_4$, 2.4 mg (0.013 mmol) of CuI, 20 mL of toluene was heated at 110°C for 72 hr. After usual work-up, recrystallization of the crude product from hexane gave 54 mg (17% yield) of **4T$_3$C** as a yellow solid. mp 146 – 149°C. ^{1}H NMR: δ 0.33 (s, 1H, HC), 0.40 (s, 18H, CH_3Si), 1.32 (t, 9H, J = 7.7 Hz, CH_3CH_2), 2.82 (q 6H, J = 7.7 Hz, CH_2CH_3), 6.67 (d, 3H, J = 3.3 Hz, ring H), 6.87 – 7.02 (m, 18H, ring H), 7.08 (d, 3H, J = 3.3 Hz, ring H). ^{13}C NMR: δ 2.60 (CH_3Si), 15.82 (CH_3CH_2), 23.53 (CH_2CH_3), 123.39, 123.61, 124.00, 124.11, 124.15, 124.32, 124.51, 134.44, 134.97, 135.30, 136.01, 136.11, 136.75, 140.99, 147.03 (ring carbons), one carbon may overlap. Exact-MS (FAB) Calcd for $C_{61}H_{58}S_{12}Si_3$ (M^+): 1258.0495. Found: 1258.0459.

Tetrakis[(bithiophenyl)dimethylsilyl]silane and germane

To a solution of bithiophenyllithium prepared from 0.98 g (4.0 mmol) of bromobithiophene and 2.4 mL (4.0 mmol) of a 1.66 M hexane solution of *n*-butyllithium in 10 mL of ether was added 0.42 g (1.0 mmol) of tetrakis(chlorodimethylsilyl)silane at -80°C and the resulting mixture was stirred at room temperature for 5 h. Usual work up of the mixture gave 0.20 g (22% yield) of tetrakis[(bithiophenyl)dimethylsilyl]silane as pale green viscous oil. ^{1}H NMR: δ 0.52 (s, 24H, CH_3Si), 6.83 (d, 4H, J = 3.6 Hz, ring H), 6.92 (dd, 4H, J = 3.6 Hz, 5.1 Hz, ring H), 7.04 (dd, 4H, J = 1.0 Hz, 3.6 Hz, ring H), 7.12 (d, 4H, J = 3.6 Hz, ring H), 7.16 (dd, 4H, J = 0.7 Hz, 5.1 Hz, ring protons). ^{13}C NMR: δ 2.50 (CH_3Si), 123.84, 124.20, 124.93, 127.79, 135.91, 137.33, 139.20, 143.00 (ring carbons).

Tetrakis[(bithiophenyl)dimethylsilyl]germane was obtained as pale green viscous oil in 7% yield in a similar fashion to that above. FAB-MS *m/z* 966 (M^+). ^{1}H NMR: δ 0.54 (s, 24H, CH_3Si), 6.85 (d, 4H, J = 2.9 Hz, ring H), 6.92-6.93 (m, 4H, ring

H), 7.04 (d, 4H, *J* = 3.9 Hz, ring H), 7.11 (d, 4H, *J* = 3.9 Hz, ring H), 7.16 (d, 4H, *J* = 3.9 Hz, ring H). ^{13}C NMR: δ 2.89 (CH_3Si), 123.83, 124.21, 124.91, 127.80, 135.72, 137.35, 139.72, 142.91 (ring carbons).

Tetrakis[(bromobithiophenyl)dimethylsilyl]silane and germane

To a solution of 0.052 g (0.056 g) of tetrakis[(bithiophenyl)dimethylsilyl]silane in 10 mL of chloroform was added 0.040 g (0.22 mmol) of NBS at -40°C and the mixture was stirred at this temperature for 2 h. Usual work up of the mixture gave 53 mg (77% yield) of the tetrakis[(bromobithiophenyl)dimethylsilyl]silane as a pale green solid. mp 152-154°C. ^{1}H NMR: δ 0.52 (s, 24H, CH_3Si), 6.73 (d, 4H, *J* = 3.9 Hz, ring H), 6.82 (d, 4H, *J* = 3.6 Hz, ring H), 6.87 (d, 4H, *J* = 3.9 Hz, ring H), 7.04 (br d, 4H, *J* = 3.6 Hz, ring H). ^{13}C NMR: δ 2.48 (CH_3Si), 111.00, 123.75, 124.96, 130.61, 135.83, 138.74, 139.68, 142.13 (ring carbons).

Tetrakis[(bromobithiophenyl)dimethylsilyl]germane was obtained as a pale green solid in 87% yield in a similar fashion to that above. mp 150-153°C. ^{1}H NMR: δ 0.53 (s, 24H, CH_3Si), 6.74 (d, 4H, *J* = 3.9 Hz, ring H), 6.83 (d, 4H, *J* = 3.9 Hz, ring H), 6.87 (d, 4H, *J* = 3.9 Hz, ring H), 7.04 (d, 4H, *J* = 3.9 Hz, ring H). ^{13}C NMR: δ 2.88 (CH_3Si), 111.00, 123.74, 124.94, 130.62, 135.63, 138.75, 140.21, 142.03 (ring carbons).

Tetrakis[(ethylterthiophenyl)dimethylsilyl]silane (3T$_4$Si)

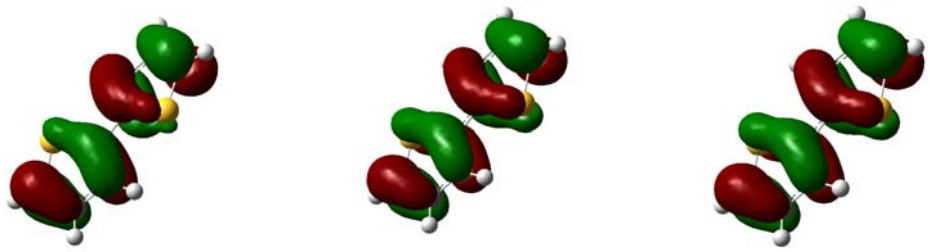
A mixture of 0.21 g (0.17 mmol) of tetrakis[(bromobithiophenyl)dimethylsilyl]silane, 0.27 g (0.68 mmol) of ethyl(tributylstannyl)thiophene, 10 mg (0.0083 mmol) of $Pd(PPh_3)_4$, 1.6 mg (0.0083 mmol) of CuI, and 20 mL of toluene was heated at 110°C for 72 hr. Usual work-up of the mixture gave 50 mg (22% yield) of **3T$_4$Si** as a yellow solid. mp 158 – 160°C. FAB-MS *m/z* 1360 (M^+). ^{1}H NMR: δ 0.55 (s, 24H, CH_3Si), 1.32 (t, 12H, *J* = 7.6 Hz, CH_3CH_2), 2.82 (q 8H, *J* = 7.6 Hz, CH_2CH_3), 6.65 (d, 4H, *J* = 3.9 Hz, ring H), 6.80 – 6.96 (m, 16H, ring H), 7.10 (d, 4H, *J* = 3.3 Hz, ring H). ^{13}C NMR: δ 2.53 (CH_3Si), 15.83 (CH_3CH_2), 23.53 (CH_2CH_3), 123.30, 123.68, 124.11, 124.50, 134.58, 134.54, 135.41, 135.87, 136.64, 139.15, 143.03, 146.85 (ring carbons). Anal. Calcd for $C_{64}H_{68}S_{12}Si_5$: C, 56.42; H, 5.03. Found: C, 56.24; H, 5.27.

Tetrakis[(ethylterthiophenyl)dimethylsilyl]germane (3T$_4$Ge)

A mixture of 0.082 g (0.064 mmol) of tetrakis[(bromobithiophenyl)dimethylsilyl]-germane, 0.082 g (0.064 mmol) of ethyl(tributylstannyl)thiophene, 3.7 mg (0.0032 mmol) of $Pd(PPh_3)_4$, 0.6 mg (0.003 mmol) of CuI, and 5 mL of toluene was heated at 110°C for 72 hr. The usual work-up of teh mixture gave 15 mg (16% yield) of **3T$_4$Ge** as a yellow solid. mp 155 – 157°C. FAB-MS *m/z* 1406 (M^+). ^{1}H NMR:

δ 0.56 (s, 24H, CH_3Si), 1.32 (t, 12H, J = 7.6 Hz, CH_3CH_2), 2.82 (q 8H, J = 7.6 Hz, CH_2CH_3), 6.65 (d, 4H, J = 3.6 Hz, ring H), 6.83–6.95 (m, 16H, ring H), 7.10 (d, 4H, J = 3.3 Hz, ring H). ^{13}C NMR: δ 2.92 (CH_3Si), 15.84 (CH_3CH_2), 23.53 (CH_2CH_3), 123.28, 123.68, 124.11, 124.48, 124.54, 134.53, 135.41, 135.67, 136.62, 139.66, 142.92, 146.85 (ring carbons). Exact-MS (FAB) Calcd for $C_{64}H_{68}GeS_{12}Si_4$ (M^+): 1406.0258. Found: 1406.0262.

2T

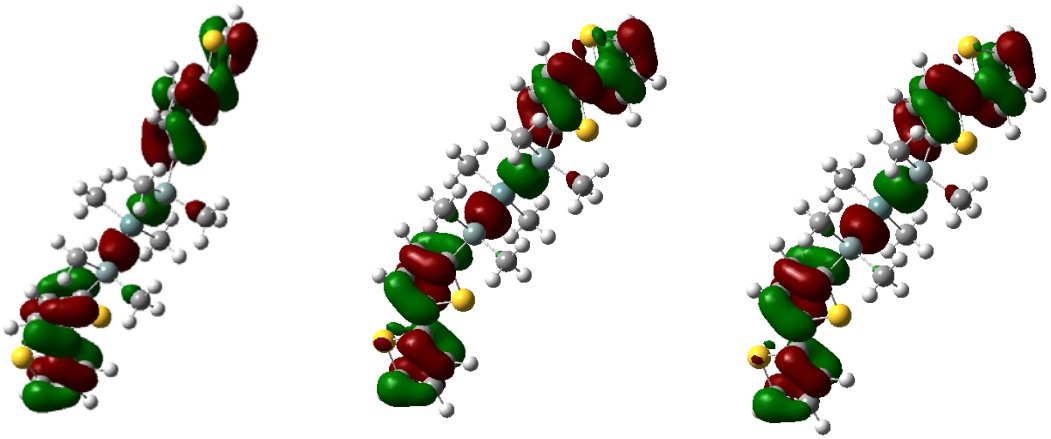


HOMO SOMO(α) LUMO(β)

$2T_2Si_2C$

HOMO SOMO(α) LUMO(β)

$2T_2Si_2Ge$



HOMO SOMO(α) LUMO(β)

Fig S-1 HOMO's of the neutral as well as the SOMO(α)'s and LUMO(β)'s (the two mid-gap orbitals) of the radical cationic 2T, $2T_2Si_2C$, and $2T_2Si_2Ge$ from (U)B3LYP calculations.

Table S-1 Cartesian coordinates for optimized geometries of the model compounds.

2T (*trans*)
B3LYP/6-31G(d): -1104.81670 a.u.
B3LYP/6-311+G(d,p): -1104. 94960 a.u.
Point group: C_2

S	-1.177091	1.855240	-0.226508
C	0.125293	0.714721	0.069009
C	1.309313	1.389537	0.271547
H	2.244062	0.882349	0.486158
C	-0.105055	3.208725	-0.051546
H	-0.487610	4.215983	-0.146767
C	1.177091	2.805913	0.201222
H	2.002710	3.494822	0.343350
C	-0.125293	-0.714721	0.069009
C	-1.309313	-1.389537	0.271547
H	-2.244062	-0.882349	0.486158
S	1.177091	-1.855240	-0.226508
C	-1.177091	-2.805913	0.201222
H	-2.002710	-3.494822	0.343350
C	0.105055	-3.208725	-0.051546
H	0.487610	-4.215983	-0.146767

Radical cation of **2T** (*trans*) calculated at the energy minimum of the ground state geometry.
B3LYP/6-311+G(d,p): -1104. 6704828 a.u.
$\langle S^2 \rangle$ = 0.76351

2T (*trans*) optimized as a radical cation.
B3LYP/6-31G(d): -1104.55562 a.u.
$\langle S^2 \rangle$ = 0.76799
B3LYP/6-311+G(d,p): -1104.67883 a.u.
$\langle S^2 \rangle$ = 0.76463 Point group: C_2

S	1.036724	1.964564	-0.000095
C	-0.180046	0.679580	0.000103
C	-1.481018	1.238566	-0.000042
H	-2.380672	0.632692	0.000081
C	-0.190808	3.162303	-0.000101
H	0.082572	4.210974	0.000004
C	-1.481018	2.629923	0.000223
H	-2.373073	3.244996	0.000341
C	0.180046	-0.679580	0.000103
C	1.481018	-1.238566	-0.000042
H	2.380672	-0.632692	0.000081
S	-1.036724	-1.964564	-0.000095
C	1.481018	-2.629923	0.000223
H	2.373073	-3.244996	0.000341
C	0.190808	-3.162303	-0.000101
H	-0.082572	-4.210974	0.000004

Neutral **2T** (*trans*) calculated at the energy minimum of the radical cation geometry.
B3LYP/6-311+G(d,p): -1104.9426004 a.u.

2T (*cis*)
B3LYP/6-31G(d): -1104.81497 a.u.
B3LYP/6-311+G(d,p): -1104.94771 a.u.
Point group: C_{2v}

S	0.000000	1.628489	1.470764
C	0.000000	0.163673	0.503467
C	0.000000	0.485830	-0.838024
H	0.000000	-0.261982	-1.623221
C	0.000000	1.886492	-1.088687
H	0.000000	2.319044	-2.083392
C	0.000000	2.633519	0.057039
H	0.000000	3.709959	0.161325
C	0.000000	-1.160876	1.100616
C	0.000000	-2.379454	0.453738

H 0.000000 -2.472671 -0.626571
C 0.000000 -3.494760 1.337354
H 0.000000 -4.526570 1.002831
S 0.000000 -1.405974 2.838798
C 0.000000 -3.130856 2.655805
H 0.000000 -3.765490 3.531498

2T$_2$Si

B3LYP/6-31G(d): -2577.80887 a.u.
B3LYP/6-311+G(d,p): -2578.11771 a.u.
Point group: C_1
S 5.62552 -2.13777 -0.88041
C 4.96473 -0.80939 0.06031
C 5.93465 -0.28812 0.88929
H 5.74316 0.5341 1.57063
C 7.17913 -1.97091 -0.12649
H 7.98617 -2.63678 -0.40097
C 7.19156 -0.94825 0.78166
H 8.06566 -0.67637 1.3634
C 3.58254 -0.40049 -0.09963
C 2.5265 -1.10081 -0.64319
H 2.62302 -2.11338 -1.02145
S 3.03932 1.18108 0.42603
C 1.30304 -0.37908 -0.62879
H 0.37145 -0.78468 -1.00995
C 1.3869 0.88194 -0.07663
Si 0.02624 2.16665 0.10892
C -1.61326 1.33768 -0.2749
C -2.37672 1.45266 -1.4187
H -2.08029 2.07062 -2.26044
C -3.57496 0.69053 -1.41045
H -4.27308 0.65636 -2.24051
C -3.75626 -0.02825 -0.24732
S -2.4215 0.26378 0.84857
C -4.84694 -0.91131 0.11912
C -4.88112 -1.89296 1.08603
H -4.02532 -2.13387 1.70778
S -6.39721 -0.81802 -0.70155
C -6.13064 -2.57066 1.166
H -6.33506 -3.37538 1.86382
C -7.04567 -2.1074 0.26103
H -8.06151 -2.44232 0.09998
C 0.28959 3.57383 -1.12391
H 0.28527 3.2116 -2.15796
H 1.25993 4.05424 -0.95102
H -0.48698 4.34143 -1.0263
C 0.02471 2.83716 1.87422
H -0.16407 2.04365 2.60604
H -0.75047 3.60206 1.99937
H 0.99012 3.29347 2.12457

Radical cation of **2T$_2$Si** calculated at the energy minimum of the ground state geometry.
-B3LYP/6-311+G(d,p): -2577.86017 a.u.
$\langle S^2 \rangle$ = 0.75689

2T$_2$Si optimized as a radical cation.
B3LYP/6-31G(d): -2577.57007 a.u.
$\langle S^2 \rangle$ = 0.76027
B3LYP/6-311+G(d,p): -2578.11088 a.u.
$\langle S^2 \rangle$ = 0.75678 Point group: C_1
Si -1.254693 2.527884 0.024842
Si 1.972487 2.215866 -0.039082
C 3.457881 1.100362 -0.376996
C 4.153070 0.939209 -1.558385
S 4.135177 0.028493 0.833593
C 5.197097 -0.022948 -1.507171
H 3.917176 1.500883 -2.456918
C 5.325756 -0.626793 -0.274471
H 5.824925 -0.275050 -2.355825

C 6.269010 -1.642107 0.151919
C 6.201983 -2.489540 1.236942
S 7.749871 -1.931441 -0.748348
C 7.317348 -3.368114 1.344171
H 5.364569 -2.493696 1.926633
C 8.231669 -3.191932 0.342416
H 7.428084 -4.106186 2.131215
H 9.159181 -3.723308 0.176977
C -2.740071 1.412362 0.362770
C -3.435221 1.251172 1.544177
S -3.417360 0.340480 -0.847810
C -4.479264 0.289033 1.492961
H -3.199304 1.812825 2.442717
C -4.607970 -0.314767 0.260244
H -5.107083 0.036926 2.341620
C -5.551271 -1.330033 -0.166161
C -5.484290 -2.177440 -1.251206
S -7.032121 -1.619346 0.734130
C -6.599699 -3.055957 -1.358453
H -4.646885 -2.181612 -1.940908
C -7.514004 -2.879759 -0.356686
H -6.710479 -3.793995 -2.145521
H -8.441542 -3.411093 -0.191258
C 1.922495 3.501582 -1.437413
H 1.747643 3.039590 -2.415713
H 1.115397 4.223825 -1.266697
H 2.864144 4.060701 -1.491732
C 2.243460 3.099323 1.621161
H 1.402740 3.761547 1.859640
H 2.345983 2.386538 2.447578
H 3.155342 3.707590 1.591982
C -1.204744 3.813647 1.423132
H -1.029881 3.351693 2.401448
H -0.397667 4.535909 1.252395
H -2.146410 4.372740 1.477430
C -1.525659 3.411281 -1.635434
H -0.684965 4.073540 -1.873906
H -1.628121 2.698468 -2.461835
H -2.437572 4.019503 -1.606299
C 0.294502 1.486374 -0.005820
H 0.309302 0.880379 -0.918929
H 0.309302 0.827711 0.870057

Neutral **2T$_2$Si** calculated at the energy minimum of the radical cation geometry.
B3LYP/6-311+G(d,p): -2577.86904 a.u.

2T$_2$Si$_2$

B3LYP/6-31G(d): -2947.15607 a.u.
B3LYP/6-311+G(d,p): -2947.51516 a.u.
Point group: C_1

S 7.443219 0.782956 0.774431
C 6.195212 -0.083750 -0.107762
C 6.704392 -1.260319 -0.614012
H 6.110958 -1.949367 -1.205622
C 8.618575 -0.445579 0.427701
H 9.632449 -0.339454 0.789373
C 8.080034 -1.464513 -0.308658
H 8.645674 -2.331619 -0.632084
C 4.853170 0.453994 -0.218279
C 4.415737 1.746592 -0.021942
H 5.082826 2.561340 0.240871
S 3.499221 -0.569177 -0.659559
C 3.019671 1.908016 -0.230404
H 2.518473 2.865265 -0.126599
C 2.352916 0.755760 -0.594137
Si 0.508756 0.530503 -0.930731
Si -0.508830 -0.529325 0.931801
C -2.352867 -0.755218 0.594957
C -3.019326 -1.907954 0.232210
H -2.517921 -2.865206 0.129442

C -4.415385 -1.747008 0.023327
H -5.082265 -2.562144 -0.238813
C -4.853106 -0.454302 0.218295
S -3.499442 0.569563 0.658851
C -6.195226 0.083084 0.106977
C -6.704776 1.259962 0.612132
H -6.111637 1.949603 1.203347
S -7.442819 -0.784591 -0.774846
C -8.080380 1.463626 0.306251
H -8.646283 2.330876 0.628825
C -8.618514 0.443989 -0.429433
H -9.632270 0.337367 -0.791290
C 0.228305 -2.255642 1.211270
H -0.242052 -2.747964 2.070689
H 1.303752 -2.183874 1.410356
H 0.098683 -2.904954 0.337882
C -0.288075 0.527422 2.492868
H -0.720324 0.025497 3.366636
H -0.774949 1.504752 2.395947
H 0.775054 0.704734 2.693025
C 0.287419 -0.525771 -2.492024
H 0.774537 -1.503038 -2.395700
H 0.719105 -0.023454 -3.365845
H -0.775780 -0.703226 -2.691672
C -0.227927 2.257107 -1.209663
H -0.098394 2.906048 -0.335985
H -1.303336 2.185660 -1.409078
H 0.242773 2.749663 -2.068761

Radical cation of **2T$_2$Si$_2$** calculated at the energy minimum of the ground state geometry.
B3LYP/6-311+G(d,p): -2947.26745 a.u.
$\langle S^2 \rangle$ = 0.75678

2T$_2$Si$_2$ optimized as a radical cation.
B3LYP/6-31G(d): -2946.92459 a.u.
$\langle S^2 \rangle$ = 0.75913
B3LYP/6-311+G(d,p): -2947.27351 a.u.
$\langle S^2 \rangle$ = 0.75816 Point group: C_1
S 7.449671 1.014377 0.378372
C 6.152687 -0.108104 -0.022021
C 6.654227 -1.404360 -0.120843
H 6.032165 -2.260307 -0.359590
C 8.605400 -0.264943 0.404601
H 9.641925 -0.047596 0.627492
C 8.040141 -1.489850 0.120625
H 8.606603 -2.413147 0.089247
C 4.809367 0.344365 -0.201940
C 4.303884 1.640917 -0.071157
H 4.921136 2.489215 0.204746
S 3.520858 -0.750807 -0.676920
C 2.931238 1.731699 -0.339492
H 2.381009 2.665253 -0.285151
C 2.327080 0.524553 -0.700136
Si 0.510678 0.216417 -1.068683
Si -0.510688 -0.216189 1.068759
C -2.327067 -0.524449 0.700202
C -2.931161 -1.731655 0.339656
H -2.380887 -2.665188 0.285409
C -4.303805 -1.640962 0.071287
H -4.921013 -2.489316 -0.204549
C -4.809353 -0.344424 0.201943
S -3.520905 0.750853 0.676847
C -6.152691 0.107965 0.021961
C -6.654296 1.404204 0.120671
H -6.032281 2.260199 0.359367
S -7.449610 -1.014611 -0.378373
C -8.040209 1.489607 -0.120832
H -8.606717 2.412879 -0.089536

C -8.605402 0.264650 -0.404725
H -9.641912 0.047236 -0.627620
C 0.227739 -1.774384 1.845234
H -0.247743 -1.984042 2.810225
H 1.300631 -1.638661 2.022411
H 0.106743 -2.658356 1.209852
C -0.330117 1.288123 2.199172
H -0.789786 1.092681 3.174989
H -0.799598 2.185323 1.780611
H 0.728755 1.514547 2.367261
C 0.330000 -1.287844 -2.199147
H 0.799493 -2.185070 -1.780653
H 0.789608 -1.092372 -3.174986
H -0.728887 -1.514242 -2.367172
C -0.227660 1.774687 -1.845095
H -0.106652 2.658618 -1.209659
H -1.300551 1.639017 -2.022320
H 0.247866 1.984380 -2.810056

Neutral **2T$_2$Si$_2$** calculated at the energy minimum of the radical cation geometry.
B3LYP/6-311+G(d,p): -2947.51052 a.u.

2T$_2$Si$_3$ (*cis*)
B3LYP/6-31G(d): -3316.50243 a.u.
B3LYP/6-311+G(d,p): -3316.91107 a.u.
Point group: C_1
C -2.744138 0.558303 1.367017
C -3.896501 1.136295 1.859179
H -3.881727 1.945144 2.582823
C -5.102954 0.592738 1.341852
H -6.090201 0.948277 1.619158
C -4.900147 -0.424291 0.433757
S -3.180493 -0.706727 0.235197
C -5.878805 -1.212783 -0.289156
C -5.706981 -1.996060 -1.410246
H -4.751108 -2.098056 -1.913075
S -7.554296 -1.272818 0.236684
C -6.902483 -2.631401 -1.851161
H -6.954611 -3.278508 -2.720040
C -7.983637 -2.332242 -1.068826
H -9.006062 -2.668459 -1.176608
Si -0.956544 1.011205 1.775225
Si 0.000205 2.274698 0.001289
C -0.000512 -0.581780 2.167070
H 1.051244 -0.368705 2.390940
H -0.020735 -1.289166 1.330172
H -0.438668 -1.085755 3.037085
C -1.016546 2.091250 3.339007
H -1.550583 3.033742 3.172407
H -1.512734 1.562496 4.161590
H -0.001060 2.342850 3.666447
C -1.370197 3.398848 -0.716751
H -0.977654 4.038085 -1.516656
H -1.783866 4.054699 0.058985
H -2.198900 2.811400 -1.126849
C 1.370792 3.397580 0.720944
H 1.784953 4.054151 -0.053918
C 2.744310 0.559844 -1.366950
C 3.896823 1.137160 -1.859549
H 3.882244 1.946030 -2.583170
C 5.103161 0.592880 -1.342702
H 6.090507 0.947844 -1.620388
C 4.900110 -0.424026 -0.434525
S 3.180367 -0.705432 -0.235281
C 5.878566 -1.213049 0.288080
C 5.706645 -1.996253 1.409208
H 4.750856 -2.097771 1.912295
S 7.553884 -1.273933 -0.238210
C 6.901943 -2.632195 1.849805
H 6.953976 -3.279329 2.718671

C 7.983042 -2.333568 1.067192
H 9.005328 -2.670295 1.174704
Si 0.956808 1.013715 -1.774495
H 2.199152 2.809357 1.130623
H 0.978232 4.036051 1.521452
C 0.000472 -0.578466 -2.168856
H 0.438719 -1.081345 -3.039459
H -1.051193 -0.364876 -2.392672
H 0.020355 -1.287017 -1.332933
C 1.017006 2.096363 -3.336461
H 0.001538 2.348669 -3.663425
H 1.513081 1.568993 -4.159999
H 1.551153 3.038508 -3.168248

2T$_2$Si$_3$ (*cis*) calculated at the energy minimum of the ground state geometry.
B3LYP/6-311+G(d,p): -3316.66384 a.u.
$\langle S^2 \rangle$ = 0.75003

2T$_2$Si$_3$ (*cis*) optimized as a radical cation.
B3LYP/6-31G(d): -3316.27003 a.u.
$\langle S^2 \rangle$ = 0.75697
B3LYP/6-311+G(d,p): -3316.66873 a.u.
$\langle S^2 \rangle$ = 0.75594 Point group: C_1
C 2.7626 0.52205 -1.32431
C 3.8688 1.32493 -1.60207
H 3.78908 2.25248 -2.15894
C 5.08932 0.82985 -1.11673
H 6.04154 1.32945 -1.26015
C 4.963 -0.38178 -0.43575
S 3.2768 -0.88177 -0.4248
C 5.98603 -1.17366 0.17204
C 5.86237 -2.38526 0.84901
H 4.91023 -2.88451 0.99272
S 7.67418 -0.67212 0.13253
C 7.08982 -2.89269 1.32131
H 7.19266 -3.82221 1.86889
C 8.1562 -2.07633 1.01073
H 9.20043 -2.22685 1.25187
Si 0.96039 0.86768 -1.7654
Si 0.00002 2.17786 0.00006
C 0.06947 -0.77553 -2.06849
H -0.9928 -0.60846 -2.2803
H 0.1336 -1.45273 -1.20979
H 0.50556 -1.29004 -2.93285
C 0.95988 1.91761 -3.34519
H 1.48912 2.86834 -3.21778
H 1.43341 1.37373 -4.17052
H -0.0681 2.15209 -3.64378
C 1.34468 3.28965 0.76552
H 0.92013 3.92905 1.54825
H 1.78106 3.95027 0.00668
H 2.15992 2.70794 1.2087
C -1.34463 3.28973 -0.76532
H -1.78101 3.9503 -0.00643
C -2.76259 0.52198 1.32431
C -3.86878 1.32486 1.60211
H -3.78905 2.25238 2.15902
C -5.08931 0.82982 1.11676
H -6.04152 1.32941 1.26022
C -4.96301 -0.38178 0.43573
S -3.27681 -0.88177 0.4247
C -5.98605 -1.17364 -0.17207
C -5.86241 -2.3852 -0.84911
H -4.91027 -2.88444 -0.99288
S -7.6742 -0.6721 -0.13251
C -7.08986 -2.89262 -1.32139
H -7.19272 -3.82211 -1.86902
C -8.15625 -2.07628 -1.01074
H -9.20048 -2.22679 -1.25185
Si -0.96037 0.86756 1.76541
H -2.15988 2.70806 -1.20855

H -0.92008 3.92917 -1.54801
C -0.06947 -0.77568 2.06839
H -0.50556 -1.29024 2.93272
H 0.99281 -0.60864 2.28019
H -0.13362 -1.45282 1.20964
C -0.95985 1.91738 3.34528
H 0.06814 2.15183 3.64389
H -1.43338 1.37344 4.17057
H -1.48908 2.86812 3.21794

Neutral **2T$_2$Si$_3$** (*cis*) calculated at the energy minimum of the radical cation geometry.

B3LYP/6-311+G(d,p): -3316. 90745 a.u.

2T$_2$Si$_3$ (*trans*)

B3LYP/6-31G(d): -3316.50120 a.u.

B3LYP/6-311+G(d,p): -3316.91008 a.u.

Point group: C_1

Si 1.972380 2.216178 -0.038688
Si -1.972411 2.216232 0.038704
C -3.457847 1.100734 0.376529
C -4.153083 0.939738 1.557919
S -4.134752 0.028333 -0.833788
C -5.196913 -0.022637 1.506875
H -3.917406 1.501734 2.456306
C -5.325356 -0.626841 0.274328
H -5.824782 -0.274614 2.355536
C -6.268409 -1.642406 -0.151897
C -6.201193 -2.490037 -1.236754
S -7.749221 -1.931877 0.748409
C -7.316378 -3.368858 -1.343831
H -5.363766 -2.494170 -1.926427
C -8.230792 -3.192613 -0.342172
H -7.426945 -4.107108 -2.130731
H -9.158226 -3.724107 -0.176677
C 3.457819 1.100693 -0.376533
C 4.153097 0.939760 -1.557906
S 4.134714 0.028266 0.833767
C 5.196953 -0.022587 -1.506863
H 3.917430 1.501779 -2.456281
C 5.325372 -0.626833 -0.274333
H 5.824857 -0.274516 -2.355512
C 6.268439 -1.642390 0.151884
C 6.201210 -2.490063 1.236706
S 7.749290 -1.931785 -0.748383
C 7.316415 -3.368858 1.343788
H 5.363760 -2.494245 1.926351
C 8.230860 -3.192547 0.342169
H 7.426977 -4.107135 2.130663
H 9.158315 -3.724007 0.176685
C -1.922745 3.502154 1.436867
H -1.747381 3.040430 2.415201
H -1.116151 4.224878 1.265823
H -2.864729 4.060703 1.491327
C -2.243175 3.099609 -1.621622
H -1.402463 3.761849 -1.860068
H -2.345672 2.386812 -2.448031
H -3.155071 3.707868 -1.592489
C 1.922696 3.502121 -1.436835
H 1.747441 3.040401 -2.415190
H 1.116022 4.224765 -1.265832
H 2.864630 4.060761 -1.491222
C 2.243142 3.099550 1.621639
H 1.402372 3.761700 1.860127
H 2.345751 2.386756 2.448036

H	3.154973	3.707903	1.592464
C	0.021020	-0.220180	1.552842
H	0.892065	-0.886177	1.548698
H	-0.880653	-0.842302	1.592804
H	0.057477	0.371727	2.474829
C	-0.021056	-0.220189	-1.552844
H	0.880620	-0.842317	-1.592719
H	-0.057389	0.371721	-2.474836
H	-0.892101	-0.886181	-1.548811
Si	-0.000034	0.890031	-0.000005

2T$_2$Si$_2$Ge (*cis*)

B3LYP/6-31G(d): -5102.03280 a.u.

B3LYP/6-3l1+G(d,p): -5104.40553 a.u.

Point group: C_1

Si	1.96029	-2.24294	-0.00464
Si	-1.97188	-2.16174	0.50233
C	-3.50288	-1.16759	0.03707
C	-4.48752	-1.48588	-0.87535
S	-3.8493	0.40633	0.72594
C	-5.49661	-0.49744	-1.02905
H	-4.48638	-2.41498	-1.43658
C	-5.30439	0.6104	-0.23146
H	-6.33057	-0.59119	-1.71725
C	-6.11948	1.80356	-0.11305
C	-5.78725	3.0339	0.41213
S	-7.78568	1.81651	-0.67096
C	-6.84898	3.98115	0.36185
H	-4.80127	3.25634	0.80615
C	-7.98769	3.47455	-0.20134
H	-6.76369	5.00007	0.72365
H	-8.93373	3.97132	-0.36943
C	3.46814	-1.16664	-0.35243
C	4.30425	-1.19489	-1.44998
S	3.98754	0.11339	0.72664
C	5.3482	-0.23147	-1.42699
H	4.17994	-1.90509	-2.26126
C	5.33153	0.56707	-0.30331
H	6.10141	-0.14266	-2.20332
C	6.23206	1.64047	0.06944
C	6.42664	2.22134	1.30424
S	7.27199	2.40113	-1.12505
C	7.40271	3.2579	1.2996
H	5.89575	1.89922	2.19383
C	7.95183	3.4661	0.06445
H	7.6882	3.81921	2.1827
H	8.71266	4.17948	-0.22229
C	-2.05279	-3.79035	-0.46879
H	-1.97776	-3.63013	-1.55004
H	-1.23217	-4.45456	-0.17352
H	-2.9922	-4.31987	-0.26936
C	-1.98702	-2.52504	2.36681
H	-1.08223	-3.06573	2.66939
H	-2.03047	-1.59987	2.95275
H	-2.85562	-3.13468	2.64199
C	2.17077	-3.09693	1.67877
H	2.24604	-2.36769	2.49351
H	1.31905	-3.75248	1.89704
H	3.07998	-3.70938	1.69516
C	1.87128	-3.5366	-1.39071
H	1.0311	-4.22096	-1.22767
H	1.72968	-3.0689	-2.37153
H	2.78723	-4.138	-1.43212
Ge	-0.01359	-0.86908	-0.01542
C	-0.18874	-0.05239	-1.79466
H	0.70168	0.54092	-2.02133
H	-1.06703	0.59796	-1.82749
H	-0.29656	-0.84509	-2.5397
C	0.15758	0.5666	1.32035
H	1.02376	1.19393	1.09252
H	0.28467	0.11744	2.30889

H -0.73676 1.19666 1.32051

Radical cation of **2T$_2$Si$_2$Ge** (*cis*) calculated at the energy minimum of the ground state geometry.
B3LYP/6-311+G(d,p): -5104.16037 a.u.
$\langle S^2 \rangle$ = 0.75467

2T$_2$Si$_2$Ge (*cis*) optimized as a radical cation.
B3LYP/6-31G(d): -5101.79898 a.u.
$\langle S^2 \rangle$ = 0.75726
B3LYP/6-31+G(d,p): -5104.16809 a.u.
$\langle S^2 \rangle$ = 0.75004 Point group: C_1
C -3.37335 -1.1587 0.01727
C -4.0381 -1.1334 -1.20991
H -3.8201 -1.83943 -2.00426
C -5.01683 -0.13528 -1.32456
H -5.63397 0.0049 -2.20557
C -5.12959 0.66306 -0.18488
S -3.98557 0.12505 1.03366
C -6.02604 1.75286 0.05337
C -6.11763 2.57481 1.17214
H -5.47233 2.46622 2.03729
S -7.2286 2.22364 -1.14369
C -7.12563 3.55705 1.06741
H -7.34488 4.28646 1.83835
C -7.80727 3.49177 -0.12713
H -8.6205 4.12113 -0.46419
Si -1.93976 -2.25668 0.51183
C -2.03644 -3.87853 -0.45251
H -1.206 -4.53748 -0.17465
H -1.98846 -3.72428 -1.53581
H -2.96861 -4.40817 -0.22532
C -1.91295 -2.52669 2.38187
H -1.89343 -1.58113 2.93475
H -2.79945 -3.08586 2.70245
H -1.02953 -3.10223 2.6798
C -0.23701 -0.23174 -1.96086
H 0.62255 0.38508 -2.23701
H -1.13742 0.3853 -2.02048
H -0.32312 -1.07258 -2.65344
C 0.15133 0.59634 1.10658
H 1.01199 1.21117 0.82917
C 3.32125 -1.08652 -0.40051
C 3.72774 -0.61589 -1.6511
H 3.32131 -1.00371 -2.57941
C 4.71157 0.3825 -1.60854
H 5.14526 0.83927 -2.49168
C 5.08846 0.73312 -0.31078
S 4.1874 -0.22784 0.85056
C 6.06431 1.69362 0.10447
C 6.41116 2.0784 1.39592
H 5.94306 1.66073 2.28085
S 7.02918 2.58056 -1.07125
C 7.42312 3.06109 1.43725
H 7.82217 3.48331 2.35211
C 7.85371 3.4317 0.18286
H 8.61315 4.15938 -0.07167
Si 1.96051 -2.32063 -0.03614
H 0.28585 0.21605 2.12187
H -0.74538 1.22142 1.0656
C 2.1934 -3.07952 1.67723
H 3.13433 -3.63966 1.72776
H 1.38058 -3.77845 1.90446
H 2.20963 -2.32129 2.46793
C 1.8943 -3.61642 -1.41022
H 1.05295 -4.30053 -1.2546
H 2.81313 -4.2134 -1.42367
H 1.77184 -3.16197 -2.39918
Ge -0.01846 -0.91039 -0.13443

2T$_2$Si$_2$Ge (*cis*) calculated at the energy minimum of the radical cation geometry.

B3LYP/6-311+G(d,p):-5104.39933 a.u.

2T$_2$Si$_2$Ge (*trans*)

B3LYP/6-31G(d): -5102.03127 a.u.

B3LYP/6-31+G(d,p): -5104.40416 a.u.

Point group: C_1

Si	1.978087	2.241622	-0.004222
Si	-1.978318	2.241700	0.026767
C	-3.475925	1.141352	0.336855
C	-4.353816	1.164663	1.400933
S	-3.922000	-0.165434	-0.743087
C	-5.359473	0.161512	1.363255
H	-4.276608	1.888231	2.206335
C	-5.272105	-0.660563	0.260090
H	-6.114682	0.038278	2.132937
C	-6.115870	-1.778050	-0.115925
C	-5.864516	-2.792169	-1.014984
S	-7.709690	-1.983502	0.594132
C	-6.929835	-3.729765	-1.129878
H	-4.932209	-2.871415	-1.564036
C	-7.990513	-3.431726	-0.319500
H	-6.902161	-4.594377	-1.784162
H	-8.920342	-3.971760	-0.202030
C	3.475851	1.144494	-0.325079
C	4.354385	1.179185	-1.388310
S	3.921519	-0.173584	0.741257
C	5.360188	0.175858	-1.360660
H	4.277536	1.911230	-2.186053
C	5.272274	-0.657870	-0.266324
H	6.115870	0.060896	-2.131158
C	6.115965	-1.779193	0.098274
C	5.864123	-2.803014	0.986128
S	7.710363	-1.976661	-0.612752
C	6.929527	-3.741613	1.091671
H	4.931412	-2.888356	1.533579
C	7.990759	-3.434639	0.285364
H	6.901519	-4.613258	1.736542
H	8.920780	-3.973201	0.162768
C	-1.923252	3.521226	1.427398
H	-1.771383	3.050497	2.405183
H	-1.099742	4.226871	1.267781
H	-2.852171	4.102317	1.472078
C	-2.172417	3.116620	-1.647953
H	-1.309335	3.757617	-1.863286
H	-2.261709	2.394380	-2.467490
H	-3.071452	3.744005	-1.658568
C	1.923834	3.535742	-1.391408
H	1.772423	3.075213	-2.374116
H	1.100169	4.239610	-1.224843
H	2.852726	4.117312	-1.429599
C	2.171749	3.098951	1.679645
H	1.308524	3.737482	1.901631
H	2.261148	2.368170	2.491564
H	3.070657	3.726367	1.696943
Ge	-0.000148	0.874621	0.003745
C	0.000816	-0.275762	1.598768
H	0.860509	-0.951623	1.585725
H	-0.915275	-0.872189	1.628236
H	0.048673	0.357591	2.488568
C	-0.001023	-0.258827	-1.603343
H	0.914979	-0.855071	-1.638774
H	-0.048470	0.383850	-2.486452
H	-0.860844	-0.934628	-1.597671

2T$_2$Si$_2$C (*cis*)

B3LYP/6-31G(d): -2986.48303 a.u.

B3LYP/6-311+G(d,p): -2986.85532 a.u.

Point group: C_1

C	8.419920	-0.326501	-0.908393
H	9.253707	0.317241	-1.166958
C	8.477299	-1.691874	-0.962864
H	9.308588	-2.319317	-1.254902
C	7.156027	0.157650	-0.465959
H	6.925675	1.210119	-0.338874
C	6.249791	-0.841832	-0.184386
S	6.973735	-2.414161	-0.484772
C	4.882562	-0.729973	0.286303
C	4.095186	-1.679319	0.901660
H	4.447487	-2.680212	1.129634
C	2.795835	-1.206624	1.230688
H	2.054410	-1.825977	1.725629
C	2.553023	0.105765	0.882547
S	3.981034	0.763108	0.107752
Si	0.980460	1.114423	1.146782
C	1.398165	2.610951	2.228428
H	1.803838	2.287064	3.193847
H	0.514157	3.228075	2.426033
H	2.151433	3.250928	1.753408
C	-0.253228	-0.006675	2.037261
H	0.159512	-0.368029	2.986561
H	-0.531425	-0.876549	1.432747
H	-1.178457	0.535361	2.263648
C	0.352218	1.695370	-0.548249
H	0.478825	0.862603	-1.255318
H	1.040395	2.478689	-0.901509
Si	-1.410301	2.354488	-0.766052
C	-1.902455	3.598669	0.573449
H	-1.904037	3.155744	1.575504
H	-2.906753	3.998969	0.388383
H	-1.210846	4.449861	0.585150
C	-1.546591	3.204011	-2.453802
H	-2.569139	3.553109	-2.639829
H	-1.276673	2.519904	-3.266587
H	-0.879626	4.073441	-2.512756
C	-2.603521	0.895114	-0.708750
C	-2.413052	-0.392827	-1.165772
H	-1.477498	-0.727879	-1.603937
C	-3.541151	-1.245349	-1.029736
H	-3.557164	-2.279692	-1.357945
C	-4.630709	-0.622809	-0.457703
S	-4.230648	1.040066	-0.077467
C	-5.941981	-1.166777	-0.161043
C	-7.123119	-0.500589	0.085350
H	-7.200997	0.581297	0.065598
C	-8.224396	-1.366852	0.338536
H	-9.230137	-1.016900	0.544482
C	-7.883735	-2.690300	0.283784
H	-8.517593	-3.554825	0.428038
S	-6.197648	-2.902337	-0.066662

Radical cation of **2T$_2$Si$_2$C** (*cis*) calculated at the energy minimum of the ground state geometry.
B3LYP/6-311+G(d,p): -2986.60314 a.u.
$\langle S^2 \rangle$ = 0.75683

2T$_2$Si$_2$C (*cis*) optimized as a radical cation.
B3LYP/6-31G(d): -2986.24626 a.u.
$\langle S^2 \rangle$ = 0.75802
B3LYP/6-311+G(d,p): -2986.61007 a.u.
$\langle S^2 \rangle$ = 0.75003 Point group: C_1

C	-8.530716	-0.115563	0.421889
H	-9.367103	0.571696	0.471484
C	-8.653757	-1.473682	0.636855
H	-9.552187	-2.028431	0.874568
C	-7.208117	0.269510	0.133637
H	-6.908698	1.292709	-0.065514
C	-6.307664	-0.797374	0.125902
S	-7.149678	-2.303033	0.488145

C	-4.903475	-0.774125	-0.125615
C	-4.003046	-1.843115	-0.140717
H	-4.301477	-2.868561	0.050062
C	-2.686998	-1.454523	-0.434861
H	-1.863772	-2.158651	-0.493086
C	-2.519755	-0.088030	-0.658317
S	-4.053613	0.720826	-0.493517
Si	-0.908111	0.851345	-1.033752
C	-1.325576	2.228981	-2.252977
H	-1.760706	1.817759	-3.170868
H	-0.431597	2.795036	-2.536617
H	-2.045439	2.943327	-1.835733
C	0.297479	-0.393628	-1.777203
H	-0.123060	-0.864211	-2.672860
H	0.564703	-1.187634	-1.070476
H	1.229382	0.101786	-2.073235
C	-0.301479	1.542764	0.624540
H	-0.333740	0.728231	1.362230
H	-1.044315	2.278564	0.969277
Si	1.398538	2.384265	0.797129
C	1.794690	3.559985	-0.623276
H	1.872681	3.049674	-1.590085
H	2.741115	4.083930	-0.446470
H	1.014387	4.324333	-0.717576
C	1.445590	3.297253	2.450109
H	2.423110	3.762358	2.618444
H	1.242167	2.628038	3.293802
H	0.689488	4.091523	2.468519
C	2.736396	1.038838	0.858118
C	2.904886	0.048663	1.824334
H	2.240080	-0.056306	2.675920
C	4.008496	-0.794139	1.613949
H	4.280608	-1.609152	2.276290
C	4.734810	-0.473842	0.465716
S	3.996393	0.906251	-0.335714
C	5.910532	-1.101446	-0.049142
C	6.642108	-0.776733	-1.191298
H	6.372230	0.042245	-1.849159
C	7.757955	-1.611008	-1.398751
H	8.444538	-1.511680	-2.231286
C	7.888403	-2.576338	-0.421904
H	8.651553	-3.339417	-0.340624
S	6.645368	-2.477818	0.769823

Neutral **$2T_2Si_2C$** (*cis*) calculated at the energy minimum of the radical cation geometry.

B3LYP/6-311+G(d,p): -2986.85046 a.u.

$2T_2Si_2C$ (*trans*)

B3LYP/6-31G(d): -2986.481328 a.u.

B3LYP/6-311+G(d,p): -2986.85348 a.u.

Point group: C_1

Si	0.872314	-1.409380	2.275251
Si	-0.872314	1.409380	2.275251
C	-1.254979	2.782846	1.041339
C	-2.486369	3.252623	0.634838
S	0.000000	3.674936	0.204487
C	-2.436761	4.292120	-0.333238
H	-3.420041	2.852393	1.017533
C	-1.153242	4.645498	-0.690542
H	-3.317976	4.752178	-0.768685
C	-0.710994	5.650915	-1.637542
C	0.511239	5.777733	-2.261820
S	-1.782208	6.949705	-2.139708
C	0.589727	6.895722	-3.140074
H	1.323219	5.074818	-2.108521
C	-0.570431	7.618519	-3.186073
H	1.472187	7.144752	-3.719469
H	-0.789263	8.503053	-3.768947
C	1.254979	-2.782846	1.041339
C	2.486369	-3.252623	0.634838

S	0.000000	-3.674936	0.204487
C	2.436761	-4.292120	-0.333238
H	3.420041	-2.852393	1.017533
C	1.153242	-4.645498	-0.690542
H	3.317976	-4.752178	-0.768685
C	0.710994	-5.650915	-1.637542
C	-0.511239	-5.777733	-2.261820
S	1.782208	-6.949705	-2.139708
C	-0.589727	-6.895722	-3.140074
H	-1.323219	-5.074818	-2.108521
C	0.570431	-7.618519	-3.186073
H	-1.472187	-7.144752	-3.719469
H	0.789263	-8.503053	-3.768947
C	0.000000	0.000000	1.353157
H	0.749775	0.446270	0.682890
H	-0.749775	-0.446270	0.682890
C	-2.525378	0.827001	2.988622
H	-3.178962	0.412281	2.212316
H	-2.373276	0.045607	3.741803
H	-3.060848	1.651909	3.472864
C	0.207459	2.121741	3.657704
H	1.177640	2.466980	3.281280
H	-0.286885	2.979532	4.128086
H	0.399718	1.377458	4.440126
C	2.525378	-0.827001	2.988622
H	3.178962	-0.412281	2.212316
H	2.373276	-0.045607	3.741803
H	3.060848	-1.651909	3.472864
C	-0.207459	-2.121741	3.657704
H	-0.399718	-1.377458	4.440126
H	-1.177640	-2.466980	3.281280
H	0.286885	-2.979532	4.128086