Supporting information for:

Kinetic Stability of $Si_2C_5H_2$ Isomer with A Planar Tetracoordinate Carbon Atom

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Isomer	Point Group	E a.u	$ZPVE$ a.u	E+$ZPVE$ a.u	ΔE+$ZPVE$ kcal mol^{-1}	NImag	T_1^a
1	C_{2v}	-770.6783795	0.049725	-770.628654	0.00	0	0.015
2	C_s	-770.6473552	0.046621	-770.600734	17.52	0	0.017
3	C_s	-770.6467098	0.046777	-770.599932	18.02	0	0.017
4	C_s	-770.6468126	0.048113	-770.598699	18.80	0	0.026
5	C_s	-770.6405389	0.045596	-770.594943	21.15	0	0.019
6	C_s	-770.6366832	0.047858	-770.588825	24.99	0	0.018
7	C_s	-770.6434194	0.046796	-770.596623	20.10	0	0.023
8	C_s	-770.6366782	0.045878	-770.590800	23.75	0	0.019
9	C_s	-770.6459363	0.046502	-770.599435	18.34	0	0.018
10	C_{2v}	-770.6408517	0.043746	-770.597106	19.80	0	0.018
11	C_{2v}	-770.6388129	0.044781	-770.594032	21.73	0	0.021
12	C_s	-770.6323326	0.046074	-770.586259	26.60	0	0.027
13	C_s	-770.6281327	0.044012	-770.584120	27.95	0	0.020
14	C_{2v}	-770.6303640	0.043823	-770.586541	26.43	0	0.020
15	C_s	-770.6297575	0.045459	-770.584299	27.83	0	0.016
16	C_s	-770.6300475	0.048269	-770.581779	29.41	0	0.027
17	C_s	-770.6253429	0.044247	-770.581096	29.84	0	0.021
18	C_s	-770.6290167	0.046505	-770.582512	28.95	0	0.018
19	C_s	-770.6069905	0.046905	-770.560085	43.03	0	0.019
20	C_1	-770.5890266	0.047443	-770.541583	54.64	0	0.018
21	C_s	-770.5723384	0.044636	-770.527702	63.35	0	0.018
22	C_s	-770.5701316	0.044043	-770.526089	64.36	0	0.018
TS-1	C_1	-770.5720970	0.045511	-770.526586	64.05	1	–
TS-2	C_1	-770.5720971	0.045510	-770.526587	64.05	1	–
TS-3	C_s	-770.6275176	0.047480	-770.580038	30.51	1	–
TS-4	C_s	-770.5762814	0.046193	-770.530088	61.85	1	–
TS-5	C_s	-770.5602569	0.045460	-770.514797	71.45	1	–
TS-6	C_1	-770.5631420	0.044361	-770.518781	68.95	1	–
TS-7	C_s	-770.5716745	0.042955	-770.528720	62.71	1	–

[a] T_1 diagnostic values are calculated at the fc-CCSD/6-311++g(2d,2p)//B3LYP/6-311++G(2d,2p) level of theory.

Table S2: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$-corrected total energy (E+$ZPVE$), net dipole moment (μ), relative energy without ZPVE correction (ΔE) and with ZPVE-correction (ΔE+$ZPVE$), and number of imaginary frequencies (NImag) of $Si_2C_5H_2$ isomers (**1-18** in their respective singlet ground electronic state calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Isomer	Point Group	E a.u	$ZPVE$ kcal mol^{-1}	E+$ZPVE$ a.u	μ Debye	ΔE kcal mol^{-1}	ΔE+$ZPVE$ kcal mol^{-1}	NImag
1	C_{2v}	-769.34455300	31.1338	-769.29493818	0.39	0.00	0.00	0
2	C_s	-769.30700346	28.9567	-769.26085806	0.55	23.56	21.39	0
3	C_s	-769.30622036	29.0254	-769.25996548	0.86	24.05	21.95	0
4	C_s	-769.30650635	30.0193	-769.25866759	1.98	23.87	22.76	0
5	C_s	-769.30080521	28.4226	-769.25551095	1.92	27.45	24.74	0
6	C_s	-769.30228227	29.9493	-769.25455507	3.47	26.53	25.34	0
7	C_s	-769.30051910	29.1418	-769.25407873	1.57	27.63	25.64	0
8	C_s	-769.29942591	28.6063	-769.25383891	0.84	28.32	25.79	0
9	C_s	-769.29751788	28.8234	-769.25158491	0.73	29.51	27.20	0
10	C_{2v}	-769.29225878	26.9136	-769.24936927	1.11	32.82	28.59	0
11	C_{2v}	-769.29227928	27.4920	-769.24846803	0.87	32.80	29.16	0
12	C_s	-769.29198611	28.7788	-769.24612421	1.95	32.99	30.63	0
13	C_s	-769.28807432	27.3746	-769.24445016	2.88	35.44	31.68	0
14	C_{2v}	-769.28676187	26.9674	-769.24378662	2.19	36.26	32.10	0
15	C_s	-769.28745482	28.2094	-769.24250032	0.66	35.83	32.91	0
16	C_s	-769.28988467	30.0366	-769.24201834	2.01	34.30	33.21	0
17	C_s	-769.28351058	27.4983	-769.23968929	1.45	38.30	34.67	0
18	C_s	-769.27766241	28.9700	-769.23149582	1.67	41.97	39.81	0

Table S3: Total energy (E), zero-point vibrational energy ($ZPVE$), $ZPVE$-corrected total energy (E+$ZPVE$), ZPVE-corrected relative energy (ΔE+$ZPVE$), and number of imaginary frequencies (NImag) of $Si_2C_5H_2$ isomers in their respective triplet ground electronic state calculated at the UB3LYP/6-311++G(2d,2p) level of theory.

Isomer	Point Group	E a.u	$ZPVE$ a.u	E+$ZPVE$ a.u	ΔE+$ZPVE$ kcal mol^{-1}	NImag
1	C_{2v}	-770.5593138	0.045813	-770.513501	26.61	3
2	C_s	-770.5919917	0.044217	-770.547775	5.10	0
3	C_s	-770.5908066	0.044335	-770.546471	5.92	0
4	C_s	-770.5998711	0.048020	-770.551851	2.54	0
5	C_s	-770.5493823	0.043089	-770.506293	31.13	0
6	C_s	-770.5901774	0.047850	-770.542327	8.52	1
7	C_s	-770.6028184	0.047091	-770.555728	0.11	0
8	C_s	-770.5458270	0.043819	-770.502008	33.82	0
9	C_s	-770.5973847	0.043930	-770.553455	1.53	1
10	C_{2v}	-770.5654589	0.040228	-770.525231	19.24	1
11	C_{2v}	-770.5879971	0.042225	-770.545772	6.35	2
12	C_s	-770.6031721	0.047273	-770.555899	0.00	0
13	C_s	-770.5530911	0.042905	-770.510186	28.69	0
14	C_{2v}	-770.5734208	0.043028	-770.530392	16.01	0
15	C_s	-770.5775491	0.042831	-770.534718	13.29	1
16	C_s	-770.5800925	0.046639	-770.533453	14.09	0
17	C_s	-770.5485300	0.041919	-770.506611	30.93	1
18	C_s	-770.5896180	0.044982	-770.544636	7.07	1

Table S4: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **1** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a_2	191.7	0.0
2	b_1	215.1	14.8
3	a_1	229.4	2.1
4	b_2	420.1	104.2
5	b_2	509.6	17.6
6	a_2	570.6	0.0
7	b_1	600.0	0.0
8	a_1	610.4	42.5
9	a_1	781.9	1.0
10	b_1	825.4	20.7
11	b_2	880.6	0.2
12	a_2	909.4	0.0
13	a_1	984.0	28.7
14	b_2	997.4	16.5
15	a_1	1099.6	2.4
16	b_2	1266.6	12.4
17	a_1	1331.9	47.8
18	a_1	1454.7	4.3
19	b_2	1476.3	9.3
20	b_2	3201.7	1.9
21	a_1	3221.7	21.4

Table S5: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **2** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a''	88.3	0.3
2	a'	90.6	0.4
3	a''	229.9	0.2
4	a'	249.0	5.2
5	a'	324.6	0.6
6	a''	421.2	2.3
7	a'	440.5	7.9
8	a''	463.0	1.4
9	a'	502.2	1.0
10	a''	575.1	51.5
11	a'	633.3	31.2
12	a'	656.1	82.6
13	a'	794.3	7.3
14	a''	797.4	17.2
15	a'	983.4	5.9
16	a'	1188.1	1.9
17	a'	1360.8	24.1
18	a'	1694.8	4.7
19	a'	2141.4	0.7
20	a'	3159.9	3.2
21	a'	3461.4	84.1

Table S6: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **3** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a'	87.7	0.7
2	a''	119.5	1.6
3	a''	186.6	1.0
4	a'	246.3	0.2
5	a'	324.1	0.7
6	a''	389.4	3.1
7	a'	390.2	11.1
8	a''	518.4	2.9
9	a''	580.3	45.6
10	a'	581.3	52.4
11	a'	630.3	25.5
12	a'	702.8	5.5
13	a'	725.3	31.4
14	a''	790.3	9.9
15	a'	995.4	11.2
16	a'	1192.4	20.4
17	a'	1368.3	8.5
18	a'	1689.0	3.0
19	a'	2138.8	0.6
20	a'	3186.0	2.3
21	a'	3461.1	79.0

Table S7: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **4** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a''	138.7	2.7
2	a'	262.9	12.3
3	a''	280.2	0.0
4	a'	383.7	1.5
5	a''	408.7	0.8
6	a'	465.6	7.0
7	a''	526.8	8.3
8	a'	549.4	39.6
9	a'	610.0	2.7
10	a'	715.2	60.9
11	a''	790.5	17.9
12	a'	813.6	0.9
13	a'	891.1	9.3
14	a''	942.9	0.8
15	a'	1150.4	2.2
16	a'	1267.9	74.7
17	a'	1365.4	15.3
18	a'	1489.0	73.2
19	a'	1701.0	5.3
20	a'	3092.9	11.0
21	a'	3153.1	7.9

Table S8: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **5** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a''	146.1	2.0
2	a''	284.6	4.4
3	a'	309.4	14.6
4	a'	366.2	9.5
5	a''	454.0	3.8
6	a''	486.8	14.2
7	a'	494.2	33.5
8	a''	603.8	0.0
9	a'	613.4	10.5
10	a'	715.0	37.4
11	a''	765.5	19.3
12	a'	771.4	51.0
13	a'	821.2	8.6
14	a'	862.7	15.2
15	a'	958.1	19.8
16	a'	1200.8	2.1
17	a'	1309.0	47.0
18	a'	1387.5	70.0
19	a'	1868.7	278.6
20	a'	2275.8	112.0
21	a'	3187.9	0.8

Table S9: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **6** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a''	118.2	0.2
2	a''	213.7	1.6
3	a'	221.4	14.0
4	a'	274.3	18.8
5	a'	336.2	13.2
6	a''	362.6	11.2
7	a'	539.4	4.5
8	a''	561.8	1.5
9	a'	632.6	2.4
10	a'	662.4	41.9
11	a''	788.2	24.8
12	a'	807.7	6.1
13	a''	934.0	0.5
14	a'	967.5	0.3
15	a'	1127.4	0.7
16	a'	1273.2	24.9
17	a'	1404.9	20.7
18	a'	1513.6	3.8
19	a'	1847.3	4.7
20	a'	3153.1	29.7
21	a'	3210.6	3.7

Table S10: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **7** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a''	138.6	1.3
2	a'	236.6	21.6
3	a''	253.7	1.5
4	a'	352.7	6.9
5	a''	427.9	1.0
6	a'	477.4	15.2
7	a'	497.6	12.5
8	a''	530.9	0.2
9	a'	640.7	21.5
10	a''	662.4	14.9
11	a'	696.1	4.9
12	a'	722.5	31.8
13	a''	791.3	28.9
14	a'	877.2	13.0
15	a'	967.5	170.8
16	a'	1191.2	11.1
17	a'	1316.3	23.0
18	a'	1420.1	35.4
19	a'	1824.1	461.2
20	a'	3102.9	3.4
21	a'	3257.2	25.9

Table S11: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **8** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a''	149.5	0.0
2	a''	268.4	18.9
3	a'	306.0	5.9
4	a'	316.1	24.7
5	a''	405.2	2.7
6	a''	489.1	0.2
7	a'	500.3	6.5
8	a'	512.2	25.0
9	a''	606.0	0.3
10	a''	746.9	25.1
11	a'	757.8	25.0
12	a'	794.0	18.8
13	a'	860.2	42.6
14	a'	950.5	127.6
15	a'	1103.4	3.8
16	a'	1138.6	29.4
17	a'	1320.7	6.2
18	a'	1375.6	36.4
19	a'	1876.7	77.3
20	a'	2291.2	81.4
21	a'	3242.1	0.4

Table S12: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **9** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a'	85.7	1.6
2	a''	91.9	1.8
3	a''	225.1	0.1
4	a'	257.0	2.3
5	a'	308.4	5.4
6	a'	364.5	3.0
7	a''	400.9	1.1
8	a'	439.2	6.7
9	a''	480.6	0.7
10	a''	509.0	1.4
11	a'	569.9	20.7
12	a'	691.0	45.1
13	a''	834.5	46.7
14	a'	932.2	4.7
15	a'	1022.8	0.4
16	a'	1307.6	6.4
17	a'	1470.6	0.2
18	a'	1727.0	4.4
19	a'	2088.4	6.4
20	a'	3135.0	1.9
21	a'	3221.2	1.1

Table S13: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **10** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	b_2	71.5	1.2
2	b_1	92.7	2.4
3	b_2	188.4	2.1
4	b_1	246.5	0.1
5	a_1	351.0	0.0
6	b_2	431.5	0.5
7	b_1	432.8	2.5
8	b_2	481.8	0.1
9	a_1	487.7	2.2
10	b_1	507.4	0.1
11	b_2	591.2	44.9
12	b_1	625.8	37.7
13	b_1	653.9	2.1
14	b_2	786.6	14.2
15	a_1	895.7	0.1
16	b_2	1287.5	283.2
17	a_1	1340.0	5.1
18	a_1	1562.4	8.0
19	a_1	2096.0	0.4
20	a_1	2238.0	33.6
21	a_1	3457.9	119.6

Table S14: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **11** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	b_1	60.4	1.0
2	b_2	73.5	2.1
3	b_1	148.6	2.7
4	b_2	250.3	6.4
5	a_1	321.5	23.5
6	b_1	321.7	0.7
7	b_2	333.8	2.9
8	a_1	398.1	0.0
9	b_2	502.9	0.2
10	b_1	515.1	1.2
11	b_2	595.6	40.3
12	b_1	625.1	42.2
13	b_1	744.3	20.2
14	b_2	792.4	0.5
15	a_1	868.7	18.0
16	b_2	906.7	135.1
17	a_1	966.6	10.9
18	a_1	1964.0	8.9
19	a_1	2136.2	2.5
20	a_1	3254.7	0.9
21	a_1	3451.0	136.7

Table S15: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **12** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a''	113.9	0.2
2	a''	182.6	4.3
3	a'	276.0	0.9
4	a'	287.0	11.8
5	a''	300.0	6.2
6	a'	411.4	15.9
7	a''	422.0	0.3
8	a'	474.1	15.6
9	a'	527.3	26.7
10	a''	594.8	10.6
11	a''	687.6	51.9
12	a'	783.7	24.4
13	a'	871.3	38.4
14	a'	892.9	95.5
15	a'	1060.6	1.4
16	a'	1151.1	28.1
17	a'	1322.4	26.5
18	a'	1404.2	35.8
19	a'	1814.6	101.8
20	a'	3224.5	3.3
21	a'	3329.1	83.3

Table S16: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **13** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a''	143.5	4.7
2	a''	244.7	0.9
3	a'	261.5	6.9
4	a'	299.6	11.4
5	a''	345.9	2.2
6	a'	360.5	32.0
7	a''	476.0	8.5
8	a'	485.2	50.5
9	a''	512.5	0.0
10	a'	517.1	5.9
11	a'	627.1	78.5
12	a''	691.2	23.1
13	a'	745.7	27.8
14	a'	813.6	33.4
15	a'	880.4	13.7
16	a'	1115.9	22.4
17	a'	1244.1	32.8
18	a'	1906.7	78.0
19	a'	1992.7	274.4
20	a'	2297.9	85.4
21	a'	3187.1	1.3

Table S17: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **14** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	b_1	36.6	1.0
2	b_2	107.8	0.2
3	b_1	163.8	2.4
4	b_2	221.9	6.2
5	b_2	311.0	42.7
6	b_1	312.2	7.5
7	a_1	339.0	5.0
8	a_1	438.3	28.1
9	b_2	451.3	0.2
10	b_1	481.9	0.3
11	b_2	542.3	59.3
12	a_1	555.6	11.3
13	b_1	598.6	39.6
14	b_2	607.2	18.9
15	b_1	660.2	32.2
16	b_2	887.0	110.2
17	a_1	1239.8	0.4
18	a_1	1901.8	6.7
19	a_1	2121.3	24.3
20	a_1	3424.1	97.1
21	a_1	3462.5	94.1

Table S18: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **15** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a'	89.4	0.2
2	a''	89.8	0.1
3	a''	161.5	3.0
4	a'	191.6	0.7
5	a'	294.9	25.7
6	a''	391.0	1.4
7	a'	403.3	1.5
8	a''	526.1	0.3
9	a'	552.3	9.3
10	a'	594.2	51.0
11	a''	600.8	45.7
12	a'	685.8	15.7
13	a''	730.3	35.1
14	a'	838.4	30.1
15	a'	928.8	9.6
16	a'	1058.1	62.7
17	a'	1250.7	27.8
18	a'	1511.8	195.7
19	a'	2143.0	23.8
20	a'	3232.3	0.3
21	a'	3458.7	92.6

Table S19: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **16** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a''	117.1	0.6
2	a'	221.3	21.0
3	a''	288.1	0.1
4	a'	351.8	15.5
5	a''	378.0	0.8
6	a'	452.2	73.6
7	a'	481.3	54.6
8	a''	506.7	8.6
9	a'	580.7	24.4
10	a'	647.2	62.0
11	a'	742.9	7.5
12	a''	772.6	25.4
13	a''	970.3	0.7
14	a'	1051.6	15.5
15	a'	1159.6	17.8
16	a'	1327.2	12.9
17	a'	1382.4	0.8
18	a'	1442.6	28.4
19	a'	1846.6	201.1
20	a'	3134.3	9.2
21	a'	3156.5	26.6

Table S20: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **17** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a''	163.9	5.6
2	a''	215.8	3.2
3	a'	225.1	2.1
4	a'	299.5	28.7
5	a''	332.8	2.7
6	a'	406.1	23.2
7	a''	452.6	13.4
8	a'	479.9	10.1
9	a''	550.4	0.7
10	a'	562.0	25.5
11	a'	675.6	43.1
12	a''	684.6	15.4
13	a'	802.5	9.5
14	a'	825.9	17.2
15	a'	875.5	42.8
16	a'	1104.3	44.4
17	a'	1253.1	78.5
18	a'	1894.8	462.8
19	a'	1940.5	77.5
20	a'	2326.5	58.1
21	a'	3164.1	3.6

Table S21: Harmonic vibrational frequencies (cm^{-1}) and IR intensities (km mol^{-1}) of isomer **18** of $Si_2C_5H_2$ calculated at the fc-CCSD(T)/cc-pVTZ level of theory.

Mode	symmetry	frequency	intensity
1	a'	47.5	0.5
2	a''	72.6	1.4
3	a'	138.7	2.3
4	a''	175.9	5.1
5	a'	311.8	4.0
6	a''	340.0	14.9
7	a'	456.0	1.3
8	a''	497.6	2.7
9	a'	623.0	3.9
10	a'	705.2	7.6
11	a''	706.4	4.9
12	a'	751.1	41.1
13	a''	853.2	33.6
14	a'	988.7	22.5
15	a'	1133.7	84.0
16	a'	1221.5	20.4
17	a'	1397.3	30.5
18	a'	1558.1	186.5
19	a'	1960.5	412.5
20	a'	3141.6	8.2
21	a'	3184.4	8.3

Table S22: Optimized geometries of the singlet and triplet ground electronic states of isomer **1** (C_{2v}) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A_1$; fc-CCSD(T)/cc-pVTZ				$\widetilde{X}^1A_1$; ae-CCSD(T)/cc-pwCVTZ			
C	0.000000	0.000000	0.343912	C	0.000000	0.000000	0.345282
C	0.000000	-1.165613	-0.565033	C	0.000000	-1.161309	-0.560329
C	0.000000	1.165613	-0.565033	C	0.000000	1.161309	-0.560329
Si	0.000000	-1.774151	1.087720	Si	0.000000	-1.760440	1.081244
Si	0.000000	1.774151	1.087720	Si	0.000000	1.760440	1.081244
C	0.000000	-0.693784	-1.908991	C	0.000000	-0.691618	-1.900122
C	0.000000	0.693784	-1.908991	C	0.000000	0.691618	-1.900122
H	0.000000	-1.329561	-2.784451	H	0.000000	-1.326630	-2.774469
H	0.000000	1.329561	-2.784451	H	0.000000	1.326630	-2.774469
$\widetilde{X}^1A_1$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A_2$; UB3LYP/6-311++G(2d,2p)			
C	-0.000000	0.000000	0.392572	C	-0.000000	-0.000000	0.439321
C	0.000000	1.156669	-0.511157	C	0.000000	1.199222	-0.552584
C	-0.000000	-1.156669	-0.511157	C	-0.000000	-1.199222	-0.552584
Si	0.000000	1.785540	1.122541	Si	0.000000	1.767620	1.115511
Si	-0.000000	-1.785540	1.122541	Si	-0.000000	-1.767620	1.115511
C	0.000000	0.690661	-1.850277	C	0.000000	0.716137	-1.829525
C	-0.000000	-0.690661	-1.850277	C	-0.000000	-0.716137	-1.829525
H	0.000000	1.324601	-2.724685	H	0.000000	1.326047	-2.720355
H	-0.000000	-1.324601	-2.724685	H	-0.000000	-1.326047	-2.720355

Table S23: Optimized geometries of the singlet and triplet ground electronic states of isomer **2** (C_s) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
Si	0.691439	1.158966	0.000000
C	-0.316895	-0.487673	0.000000
C	1.030031	-0.785741	0.000000
Si	2.688790	-0.246784	0.000000
C	-1.563408	-1.011548	0.000000
H	-1.687093	-2.089800	0.000000
C	-2.739355	-0.207591	0.000000
C	-3.759169	0.454013	0.000000
H	-4.646218	1.040465	0.000000

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A'$; UB3LYP/6-311++G(2d,2p)			
Si	-0.059076	-1.407903	-0.000000	Si	0.064264	-1.523339	0.000000
C	0.000000	0.522200	0.000000	C	0.096033	0.294258	-0.000000
C	-1.298502	0.111115	-0.000000	C	-1.229855	0.029821	-0.000000
Si	-2.507932	-1.126585	-0.000000	Si	-2.788754	-0.771086	0.000000
C	0.817467	1.591817	0.000000	C	0.851719	1.517148	-0.000000
H	0.376779	2.583437	0.000000	H	0.313015	2.457266	-0.000000
C	2.227129	1.517307	0.000000	C	2.226338	1.550117	-0.000000
C	3.432049	1.495888	0.000000	C	3.443428	1.585626	-0.000000
H	4.492480	1.469432	0.000000	H	4.504205	1.616897	-0.000000

Table S24: Optimized geometries of the singlet and triplet ground electronic states of isomer **3** (C_s) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
Si	1.451954	1.188180	0.000000
C	-0.357869	0.525696	0.000000
C	0.515780	-0.545230	0.000000
Si	2.147121	-1.156508	0.000000
C	-1.663620	0.879436	0.000000
H	-1.932956	1.928289	0.000000
C	-2.718514	-0.080498	0.000000
C	-3.632745	-0.881556	0.000000
H	-4.424743	-1.591158	0.000000

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A'$; UB3LYP/6-311++G(2d,2p)			
Si	-0.026850	-0.000000	0.006411	Si	-1.954476	0.402339	0.000000
C	0.016549	-0.000000	1.931044	C	-0.159490	0.693224	-0.000000
C	1.293286	0.000000	1.449556	C	-0.239535	-0.656087	0.000000
Si	2.439634	0.000000	0.156481	Si	-0.807493	-2.313970	0.000000
C	-0.751818	-0.000000	3.037683	C	0.923664	1.641385	-0.000000
H	-1.829096	-0.000000	2.932200	H	0.682948	2.696442	-0.000000
C	-0.232708	-0.000000	4.352170	C	2.250090	1.278002	-0.000000
C	0.183957	-0.000000	5.482956	C	3.428098	0.968624	-0.000000
H	0.557705	-0.000000	6.475708	H	4.452634	0.692189	-0.000000

Table S25: Optimized geometries of the singlet and triplet ground electronic states of isomer **4** (C_s) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
C	-0.743469	0.860211	0.000000
C	-0.947782	-0.640011	0.000000
C	0.128042	-1.548469	0.000000
C	1.458712	-1.178618	0.000000
Si	2.252163	0.567258	0.000000
C	0.530523	1.069350	0.000000
Si	-2.508735	0.215107	0.000000
H	-0.131110	-2.604105	0.000000
H	2.180881	-1.997591	0.000000

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A$; UB3LYP/6-311++G(2d,2p)			
C	0.019428	-0.000000	0.014500	C	-1.044434	0.125910	-0.002794
C	0.002567	-0.000000	1.512543	C	0.030767	1.065273	0.000601
C	1.184959	-0.000000	2.266316	C	1.395203	0.718997	0.002361
C	2.445403	0.000000	1.725020	C	1.828732	-0.591092	0.000989
Si	2.997594	0.000000	-0.111805	Si	0.575783	-1.922145	-0.002359
C	1.234286	0.000000	-0.385972	C	-1.028957	-1.217283	-0.005806
Si	-1.650346	-0.000000	0.880961	Si	-1.536357	1.946380	-0.000272
H	1.073693	-0.000000	3.346122	H	2.137320	1.513505	0.004682
H	3.275455	0.000000	2.429785	H	2.890797	-0.800291	0.002597

Table S26: Optimized geometries of the singlet and triplet ground electronic states of isomer **5** (C_s) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
C	-0.860033	0.772173	0.000000
C	-0.735059	-0.672713	0.000000
C	0.462664	-1.396431	0.000000
Si	1.958199	-0.413567	0.000000
C	1.652195	1.353212	0.000000
C	0.378683	1.335784	0.000000
Si	-2.479346	-0.058090	0.000000
H	0.455380	-2.479903	0.000000
H	3.313828	-1.001638	0.000000

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A''$; UB3LYP/6-311++G(2d,2p)			
C	-0.126697	-0.000000	-0.153140	C	1.248201	0.134149	-0.000000
C	-0.039075	-0.000000	1.291923	C	-0.020774	0.979818	-0.000000
C	1.127923	0.000000	2.041438	C	-1.311774	0.541160	0.000000
Si	2.649640	0.000000	1.109155	Si	-1.580908	-1.245556	0.000000
C	2.371291	0.000000	-0.651895	C	-0.015277	-2.028247	0.000000
C	1.110299	0.000000	-0.687382	C	0.898019	-1.138073	0.000000
Si	-1.760133	-0.000000	0.632386	Si	1.557587	1.927849	-0.000000
H	1.095122	0.000000	3.122377	H	-2.113169	1.268351	0.000000
H	3.984742	0.000000	1.733008	H	-2.896195	-1.897613	0.000000

Table S27: Optimized geometries of the singlet and triplet ground electronic states of isomer **6** (C_s) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
Si	-0.143223	1.138521	0.000000
C	-0.540414	-0.720716	0.000000
C	0.480633	-1.729932	0.000000
C	1.757308	-1.229013	0.000000
C	1.766657	0.190478	0.000000
C	1.742885	1.472321	0.000000
Si	-2.196531	-0.107531	0.000000
H	0.279587	-2.797527	0.000000
H	2.671613	-1.808013	0.000000

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)			
Si	-0.029738	0.000000	-0.015815
C	0.001581	0.000000	1.873199
C	1.203572	-0.000000	2.636611
C	2.364748	-0.000000	1.910583
C	2.132593	-0.000000	0.527065
C	1.745248	-0.000000	-0.671303
Si	-1.745677	0.000000	1.691907
H	1.226369	-0.000000	3.722199
H	3.360837	-0.000000	2.329278

$\widetilde{X}^3A'$; UB3LYP/6-311++G(2d,2p)			
Si	-0.865779	-0.937859	-0.000000
C	-0.145619	0.746296	-0.000000
C	1.273456	0.827809	0.000000
C	2.116055	-0.273518	0.000000
C	1.417809	-1.469423	0.000000
C	0.413857	-2.214088	0.000000
Si	-1.458239	2.037891	-0.000000
H	1.727383	1.814993	0.000000
H	3.191384	-0.198139	0.000000

Table S28: Optimized geometries of the singlet and triplet ground electronic states of isomer **7** (C_s) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
C	-0.961235	0.825952	0.000000
C	-0.733936	-0.656618	0.000000
C	0.489795	-1.296881	0.000000
Si	2.153160	-0.525772	0.000000
C	1.542564	1.347582	0.000000
C	0.242772	1.367906	0.000000
Si	-2.499287	-0.146876	0.000000
H	0.442506	-2.387270	0.000000
H	2.260405	2.152455	0.000000

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)			
C	0.018410	-0.000000	0.020649
C	-0.000994	-0.000000	1.503191
C	1.103972	0.000000	2.319565
Si	2.854978	0.000000	1.803193
C	2.545179	0.000000	-0.148973
C	1.275219	0.000000	-0.357251
Si	-1.656142	-0.000000	0.721751
H	0.904831	0.000000	3.390338
H	3.385188	0.000000	-0.821303

$\widetilde{X}^3A'$; UB3LYP/6-311++G(2d,2p)			
C	-1.136573	0.172843	0.000000
C	0.056091	0.961679	0.000000
C	1.380639	0.609942	0.000000
Si	1.603420	-1.178782	0.000000
C	-0.026750	-2.019017	0.000000
C	-1.109646	-1.207120	0.000000
Si	-1.551909	1.919003	0.000000
H	2.195288	1.318854	0.000000
H	-0.117264	-3.099017	0.000000

Table S29: Optimized geometries of the singlet and triplet ground electronic states of isomer **8** (C_s) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
C	-0.765967	0.755058	0.000000
C	-0.525719	-0.638089	0.000000
Si	1.180065	-1.203662	0.000000
C	2.213735	0.220029	0.000000
C	1.428519	1.224128	0.000000
C	0.183697	1.807333	0.000000
Si	-2.324571	-0.250427	0.000000
H	1.643110	-2.603311	0.000000
H	-0.047018	2.860699	0.000000

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A''$; UB3LYP/6-311++G(2d,2p)			
C	0.381099	-0.000000	0.022527	C	-1.095052	-0.101113	0.000000
C	0.107881	-0.000000	1.396890	C	0.037695	0.849076	0.000000
Si	1.498868	0.000000	2.529710	Si	1.684249	0.188012	0.000000
C	2.953176	0.000000	1.559466	C	1.502760	-1.572993	0.000000
C	2.591216	0.000000	0.352012	C	0.286466	-1.849980	0.000000
C	1.636010	0.000000	-0.623918	C	-1.048305	-1.482542	0.000000
Si	-1.430156	-0.000000	0.400186	Si	-1.591493	1.658029	0.000000
H	1.441939	0.000000	3.998734	H	2.932672	0.955978	0.000000
H	1.789160	0.000000	-1.690116	H	-1.908019	-2.131106	0.000000

Table S30: Optimized geometries of the singlet and triplet ground electronic states of isomer **9** (C_s) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
Si	1.169064	1.235648	0.000000
C	-0.301725	-0.056748	0.000000
C	0.909490	-0.713240	0.000000
Si	2.655794	-0.693076	0.000000
C	-1.617907	-0.136811	0.000000
C	-2.888372	-0.143724	0.000000
C	-4.216949	-0.181335	0.000000
H	-4.747452	-1.126390	0.000000
H	-4.800065	0.732258	0.000000

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A'$; UB3LYP/6-311++G(2d,2p)			
Si	-0.844952	-1.546098	-0.000000	Si	-0.969417	-1.577662	0.000000
C	0.000000	0.237295	0.000000	C	-0.223463	0.093153	0.000000
C	0.935139	-0.748927	0.000000	C	0.839337	-0.742609	0.000000
Si	1.452705	-2.403518	-0.000000	Si	1.811660	-2.204097	0.000000
C	-0.308492	1.507195	0.000000	C	-0.444082	1.466502	0.000000
C	-0.655119	2.719757	0.000000	C	-0.687467	2.667543	0.000000
C	-1.004785	3.989690	0.000000	C	-0.949298	4.008802	0.000000
H	-0.262807	4.778201	0.000000	H	-0.145902	4.731940	0.000000
H	-2.046195	4.286367	0.000000	H	-1.965874	4.376389	0.000000

Table S31: Optimized geometries of the singlet and triplet ground electronic states of isomer **10** (C_{2v}) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
C	0.000000	0.000000	0.778391
C	0.000000	0.000000	-0.619049
Si	0.000000	-1.284841	2.044500
Si	0.000000	1.284841	2.044500
H	0.000000	0.000000	3.131377
C	0.000000	0.000000	-1.844027
C	0.000000	0.000000	-3.216068
C	0.000000	0.000000	-4.433679
H	0.000000	0.000000	-5.497310

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A'$; UB3LYP/6-311++G(2d,2p)			
C	-0.026977	0.000000	1.000000	C	0.042226	0.000000	1.000000
C	1.350532	-0.000000	1.000000	C	1.338449	-0.000000	1.000000
Si	-1.289967	0.000000	2.283106	Si	-1.352000	0.000000	2.246173
Si	-1.289967	-0.000000	-0.283106	Si	-1.352000	-0.000000	-0.246173
H	-2.372387	0.000000	1.000000	H	-2.393715	0.000000	1.000000
C	2.570216	-0.000000	1.000000	C	2.611915	-0.000000	1.000000
C	3.926495	-0.000000	1.000000	C	3.926479	-0.000000	1.000000
C	5.135052	-0.000000	1.000000	C	5.158252	-0.000000	1.000000
H	6.195738	-0.000000	1.000000	H	6.219129	-0.000000	1.000000

Table S32: Optimized geometries of the singlet and triplet ground electronic states of isomer **11** (C_{2v}) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
C	0.000000	0.000000	-0.223235
C	0.000000	0.000000	-1.470293
C	0.000000	0.000000	-2.835014
C	0.000000	0.000000	-4.054860
Si	0.000000	-1.317636	1.325584
Si	0.000000	1.317636	1.325584
C	0.000000	0.000000	2.529340
H	0.000000	0.000000	3.608102
H	0.000000	0.000000	-5.119075

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A'$; UB3LYP/6-311++G(2d,2p)			
C	-0.006949	-0.000000	1.000000	C	-0.094000	-0.000000	1.000000
C	1.231265	-0.000000	1.000000	C	1.210891	-0.000000	1.000000
C	2.579903	-0.000000	1.000000	C	2.521208	-0.000000	1.000000
C	3.790849	-0.000000	1.000000	C	3.756194	-0.000000	1.000000
Si	-1.545559	0.000000	2.310676	Si	-1.466786	0.000000	2.307506
Si	-1.545559	-0.000000	-0.310676	Si	-1.466786	-0.000000	-0.307506
C	-2.741106	0.000000	1.000000	C	-2.701439	0.000000	1.000000
H	-3.817127	0.000000	1.000000	H	-3.778469	0.000000	1.000000
H	4.851935	-0.000000	1.000000	H	4.816839	-0.000000	1.000000

Table S33: Optimized geometries of the singlet and triplet ground electronic states of isomer **12** (C_{2v}) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
C	-0.537753	0.578102	0.000000
C	-0.804350	-0.804659	0.000000
C	0.209080	-1.784215	0.000000
C	1.441659	-1.187514	0.000000
C	2.303213	-0.234157	0.000000
Si	1.106532	1.358773	0.000000
Si	-2.350048	0.217578	0.000000
H	0.063968	-2.854406	0.000000
H	3.356845	-0.035139	0.000000

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A'$; UB3LYP/6-311++G(2d,2p)			
C	-0.071837	0.000000	0.043245	C	-0.057498	0.000000	-0.073040
C	-0.002149	0.000000	1.436443	C	0.102114	0.000000	1.318558
C	1.202782	-0.000000	2.160810	C	1.208293	-0.000000	2.163325
C	2.254022	-0.000000	1.301511	C	2.427742	-0.000000	1.521086
C	2.860636	-0.000000	0.181776	C	2.795889	-0.000000	0.197241
Si	1.341100	-0.000000	-1.105051	Si	1.479602	-0.000000	-1.026571
Si	-1.742811	0.000000	0.814644	Si	-1.677468	0.000000	0.730951
H	1.299031	-0.000000	3.235407	H	1.115306	-0.000000	3.239567
H	3.837904	-0.000000	-0.254005	H	3.845748	-0.000000	-0.074038

Table S34: Optimized geometries of the singlet and triplet ground electronic states of isomer **13** (C_s) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
Si	-2.299516	0.167156	0.000000
C	0.145859	-1.515898	0.000000
C	1.509642	-1.299187	0.000000
Si	1.919374	0.438863	0.000000
C	0.517818	1.526533	0.000000
C	-0.688624	1.168867	0.000000
C	-1.066128	-1.193528	0.000000
H	2.250482	-2.089879	0.000000
H	3.318355	0.903176	0.000000

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)			
Si	-0.686703	0.000000	-0.870736
C	0.099128	0.000000	1.981935
C	1.272966	-0.000000	2.681540
Si	2.702508	-0.000000	1.616117
C	2.331932	-0.000000	-0.106467
C	1.188594	-0.000000	-0.599768
C	-0.603619	0.000000	0.957498
H	1.343841	-0.000000	3.761203
H	4.066658	-0.000000	2.164209

$\widetilde{X}^3A'$; UB3LYP/6-311++G(2d,2p)			
Si	0.103836	-0.000000	0.191295
C	-0.032617	-0.000000	2.923810
C	0.956720	-0.000000	3.903619
Si	2.602597	0.000000	3.295186
C	2.729301	0.000000	1.524157
C	1.856541	0.000000	0.647411
C	-0.624066	-0.000000	1.842844
H	0.736441	-0.000000	4.961719
H	3.766103	0.000000	4.187351

Table S35: Optimized geometries of the singlet and triplet ground electronic states of isomer **14** (C_{2v}) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
C	0.000000	0.000000	-0.862419
C	0.000000	0.000000	-2.270101
C	0.000000	0.000000	-3.488455
H	0.000000	0.000000	-4.551348
Si	0.000000	-1.329243	0.347438
Si	0.000000	1.329243	0.347438
C	0.000000	0.000000	1.896780
C	0.000000	0.000000	3.133634
H	0.000000	0.000000	4.200338

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A'$; UB3LYP/6-311++G(2d,2p)			
Si	1.871386	0.796348	1.001197	Si	0.395394	-1.412866	-0.089340
Si	2.042813	-1.844166	0.997939	Si	0.488885	1.211377	-0.082961
C	3.162856	-0.445633	0.999936	C	-0.826672	-0.063061	0.008202
C	4.550271	-0.355290	1.000081	C	-2.202825	0.005355	0.011830
C	5.756896	-0.276886	1.000171	C	-3.413553	0.067256	0.025358
H	6.814865	-0.208009	1.000336	H	-4.472787	0.120336	0.036783
C	-0.806270	-0.703587	1.000109	C	3.096492	-0.229912	0.029142
C	0.414640	-0.624216	0.999795	C	1.794345	-0.158111	0.007026
H	-1.867188	-0.772531	1.000442	H	3.930423	0.459598	0.055535

Table S36: Optimized geometries of the singlet and triplet ground electronic states of isomer **15** (C_s) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
Si	0.141314	1.662813	0.000000
C	-0.969719	0.283997	0.000000
C	0.271573	-0.369496	0.000000
C	-2.264282	-0.276001	0.000000
C	-3.388080	-0.740726	0.000000
H	-4.369058	-1.151207	0.000000
C	0.983910	-1.564024	0.000000
H	0.594006	-2.570637	0.000000
Si	2.296544	-0.385118	0.000000

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A'$; UB3LYP/6-311++G(2d,2p)			
Si	-0.029022	0.000000	0.024034	Si	0.144050	0.000000	0.093227
C	0.011744	0.000000	1.788884	C	0.142924	0.000000	2.031841
C	1.375243	-0.000000	1.498810	C	1.494095	-0.000000	1.939607
C	-0.647526	0.000000	3.020268	C	-0.736227	0.000000	3.085344
C	-1.233849	0.000000	4.074056	C	-1.566121	0.000000	3.972105
H	-1.750123	0.000000	5.000387	H	-2.284795	0.000000	4.752898
C	2.669503	-0.000000	1.976594	C	2.810182	-0.000000	1.932754
H	3.004106	-0.000000	3.001263	H	3.548252	-0.000000	2.721260
Si	2.985876	-0.000000	0.252192	Si	2.621461	-0.000000	0.039203

Table S37: Optimized geometries of the singlet and triplet ground electronic states of isomer **16** (C_s) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
C	-0.664105	0.872165	0.000000
Si	-0.318731	-1.073408	0.000000
C	1.519565	-1.163280	0.000000
C	2.377375	-0.058519	0.000000
C	1.849571	1.268628	0.000000
C	0.577637	1.347097	0.000000
Si	-2.304444	0.187692	0.000000
H	1.976624	-2.150158	0.000000
H	3.448778	-0.244587	0.000000

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A'$; UB3LYP/6-311++G(2d,2p)			
C	-0.145076	-0.000000	0.099404	C	-1.014204	-0.696996	-0.000000
Si	-0.110507	-0.000000	2.071770	Si	0.023532	0.954240	-0.000000
C	1.683990	0.000000	2.434448	C	1.781900	0.633637	0.000000
C	2.688750	0.000000	1.471483	C	2.264939	-0.704917	0.000000
C	2.376418	0.000000	0.083591	C	1.312319	-1.693389	0.000000
C	1.138088	0.000000	-0.179908	C	0.017242	-1.449398	0.000000
Si	-1.869927	-0.000000	0.495449	Si	-2.327320	0.648575	-0.000000
H	1.984929	0.000000	3.476619	H	2.487587	1.453217	0.000000
H	3.719600	0.000000	1.814365	H	3.326647	-0.918934	0.000000

Table S38: Optimized geometries of the singlet and triplet ground electronic states of isomer **17** (C_s) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
C	-0.485880	1.252938	0.000000
Si	-2.145665	0.406106	0.000000
C	-1.325857	-1.295400	0.000000
C	0.014322	-1.446154	0.000000
C	1.289202	-1.358074	0.000000
Si	1.992442	0.229631	0.000000
C	0.743502	1.502077	0.000000
H	-1.978803	-2.163113	0.000000
H	3.430678	0.525310	0.000000

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A'$; UB3LYP/6-311++G(2d,2p)			
C	0.391344	0.000000	0.579925	C	-0.200052	-0.000000	-0.061983
Si	-0.455863	0.000000	2.231267	Si	0.079814	-0.000000	1.696724
C	1.196056	0.000000	3.148187	C	1.979853	0.000000	1.989246
C	2.368914	-0.000000	2.509345	C	2.665214	0.000000	0.863616
C	3.327753	-0.000000	1.683278	C	3.069375	0.000000	-0.346100
Si	2.993658	-0.000000	-0.010274	Si	2.051302	-0.000000	-1.722086
C	1.245290	-0.000000	-0.317955	C	0.361986	-0.000000	-1.169106
H	1.141214	0.000000	4.230320	H	2.372165	0.000000	2.993203
H	3.992876	-0.000000	-1.079321	H	2.441602	-0.000000	-3.130886

Table S39: Optimized geometries of the singlet and triplet ground electronic states of isomer **18** (C_s) of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) at different levels.

$\widetilde{X}^1A'$; fc-CCSD(T)/cc-pVTZ			
C	-2.923384	0.649573	0.000000
Si	-2.504456	-1.133042	0.000000
C	-1.575362	0.465096	0.000000
C	-0.401696	1.308356	0.000000
C	0.828795	0.779693	0.000000
C	2.000416	0.261197	0.000000
Si	3.539687	-0.493412	0.000000
H	-3.575487	1.514871	0.000000
H	-0.500407	2.390756	0.000000

$\widetilde{X}^1A'$; B3LYP/6-311++G(2d,2p)				$\widetilde{X}^3A'$; UB3LYP/6-311++G(2d,2p)			
Si	-2.905346	0.000000	0.887836	Si	-2.683731	2.622144	-0.000000
C	-0.031880	0.000000	1.642476	C	-0.038995	1.107344	-0.000000
C	1.258862	-0.000000	1.965611	C	1.162605	0.454914	0.000000
C	2.308513	-0.000000	0.988390	C	1.293360	-0.968710	0.000000
C	3.660537	-0.000000	1.009445	C	2.324888	-1.845283	0.000000
Si	3.048902	-0.000000	-0.703089	Si	0.711854	-2.721082	0.000000
C	-1.264190	0.000000	1.337280	C	-1.118756	1.728501	-0.000000
H	1.507577	-0.000000	3.024392	H	2.071085	1.055287	0.000000
H	4.407601	-0.000000	1.792496	H	3.403168	-1.749738	0.000000

Table S40: Optimized geometries of isomers **19** to **22** and **TS-1** of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) obtained at the B3LYP/6-311++G(2d,2p) level of theory.

	19				**20**		
H	0.000000	0.000000	0.000000	C	-0.677775	0.667515	-0.012839
C	0.000000	0.000000	1.103098	C	1.660177	-0.284710	0.495771
C	1.332650	0.000000	1.711192	C	-0.688376	-0.709026	0.041030
H	2.214484	0.000000	1.059275	Si	1.059204	1.467829	0.010783
C	-1.179294	0.000000	1.772606	Si	-2.382709	-0.025542	-0.079199
Si	-2.662238	0.000000	2.628299	C	1.760872	-1.060915	-0.558617
C	1.521588	0.000000	3.047366	C	0.578271	-1.393849	0.305959
C	1.668179	0.000000	4.328173	H	2.125346	-1.204128	-1.563452
Si	1.576783	0.000000	6.051951	H	0.604704	-2.301980	0.893459
	21				**22**		
C	0.644008	-0.558615	-0.000642	C	0.513741	-0.503285	-0.000356
C	-0.327236	0.403937	-0.000652	C	-0.362525	0.544651	-0.000530
C	-3.939570	-0.516277	0.000537	C	-3.065778	-1.338418	-0.000681
Si	1.404902	1.242173	0.000241	Si	1.432621	1.223153	-0.000115
Si	2.298086	-1.060449	0.000194	Si	2.109725	-1.163428	0.000307
C	-1.650122	0.635454	-0.000165	C	-1.663412	0.884413	0.000187
C	-2.643300	-0.417619	-0.000008	C	-2.730520	-0.088947	0.000454
H	-2.018198	1.650542	-0.000116	H	-1.944418	1.926563	0.000421
H	-2.326314	-1.475967	-0.000391	H	-3.797455	0.246813	0.002436
	TS-1						
C	-0.727157	-0.654184	-0.026882				
C	1.817120	0.040503	0.373559				
C	-0.623391	0.723591	0.024932				
Si	0.907192	-1.575874	-0.020424				
Si	-2.381048	0.118763	-0.046579				
C	1.901310	1.117577	-0.345543				
C	0.547294	1.487540	0.155395				
H	2.612248	1.714897	-0.902458				
H	0.530681	2.394489	0.751736				

Table S41: Optimized geometries of **TS-2** to **TS-6** of $Si_2C_5H_2$ in Cartesian coordinates (in Ångström units) obtained at the B3LYP/6-311++G(2d,2p) level of theory.

	TS-2				**TS-3**		
C	0.727150	-0.654245	-0.027267	C	-0.662173	-0.645392	-0.000038
C	-1.817021	0.040519	0.373535	C	0.693962	-0.713153	-0.000019
C	0.623342	0.723612	0.024885	C	-1.147827	0.683274	0.000002
Si	-0.907122	-1.575987	-0.020345	Si	2.389612	-0.668535	0.000040
Si	2.381014	0.118836	-0.046480	Si	-2.501149	-0.512640	-0.000069
C	-1.901417	1.117593	-0.345484	C	1.161448	1.068504	0.000048
C	-0.547270	1.487621	0.155306	C	-0.085370	1.624253	0.000051
H	-2.612508	1.715028	-0.902070	H	2.021854	1.734383	0.000067
H	-0.530685	2.394490	0.751761	H	-0.220571	2.697155	0.000082
	TS-4				**TS-5**		
C	0.935706	-0.297286	0.000013	C	-0.251868	0.312164	-0.000012
C	-1.835352	0.075803	0.000041	C	0.465752	-0.901094	0.000042
C	0.746029	0.980411	-0.000002	C	1.566936	1.508917	-0.000053
Si	-1.662151	-1.608453	-0.000014	Si	-1.295160	-1.365013	-0.000040
Si	2.653068	-0.507128	0.000001	Si	-1.679762	1.264074	0.000029
C	-1.554505	1.387406	0.000002	C	1.825594	-0.912470	0.000069
C	-0.205561	1.933951	-0.000014	C	2.358635	0.422044	0.000006
H	-2.342085	2.137354	-0.000014	H	2.433749	-1.805099	0.000037
H	-0.048635	2.999067	-0.000038	H	3.424867	0.640886	-0.000183
	TS-6				**TS-7**		
C	0.591067	-0.549013	0.071061	C	-0.609216	-0.544027	0.000030
C	-0.381440	0.408409	0.075826	C	0.316741	0.462641	0.000037
C	-3.386217	-0.650962	-0.694578	C	3.852703	-0.725684	-0.000086
Si	1.356144	1.245336	-0.089332	Si	-1.447034	1.223278	-0.000027
Si	2.237349	-1.063167	-0.017355	Si	-2.237366	-1.122188	-0.000006
C	-1.690529	0.666591	0.173350	C	1.630033	0.745606	0.000041
C	-2.707187	-0.421464	0.384792	C	2.669601	-0.240745	0.000028
H	-2.052049	1.681263	0.105515	H	1.964251	1.773199	0.000026
H	-2.811015	-0.953009	1.325385	H	2.458166	-1.375190	0.000147

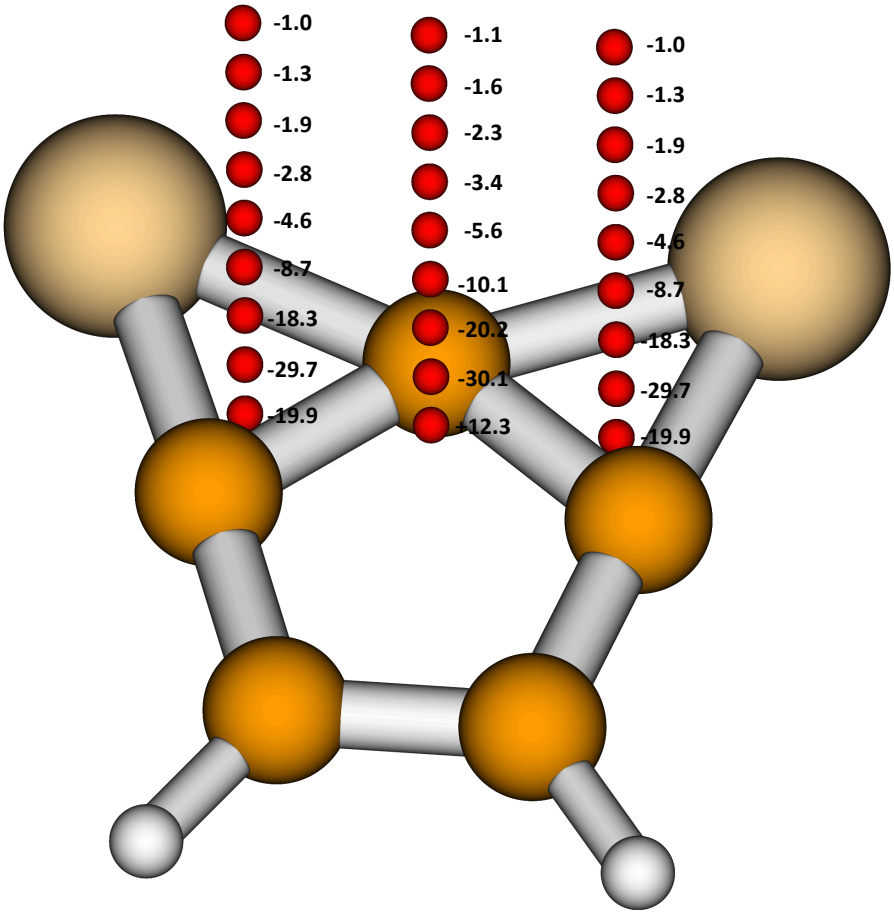

Figure S1: NICS values (in ppm) calculated from 0 to 4 Å with an interval of 0.5 Å.