

Supporting Information

Reaction Mechanism Study on Reactions of Phenylacetylenes with HSnEt_3 Promoted by $\text{B}(\text{C}_6\text{F}_5)_3$ with/without DABCO

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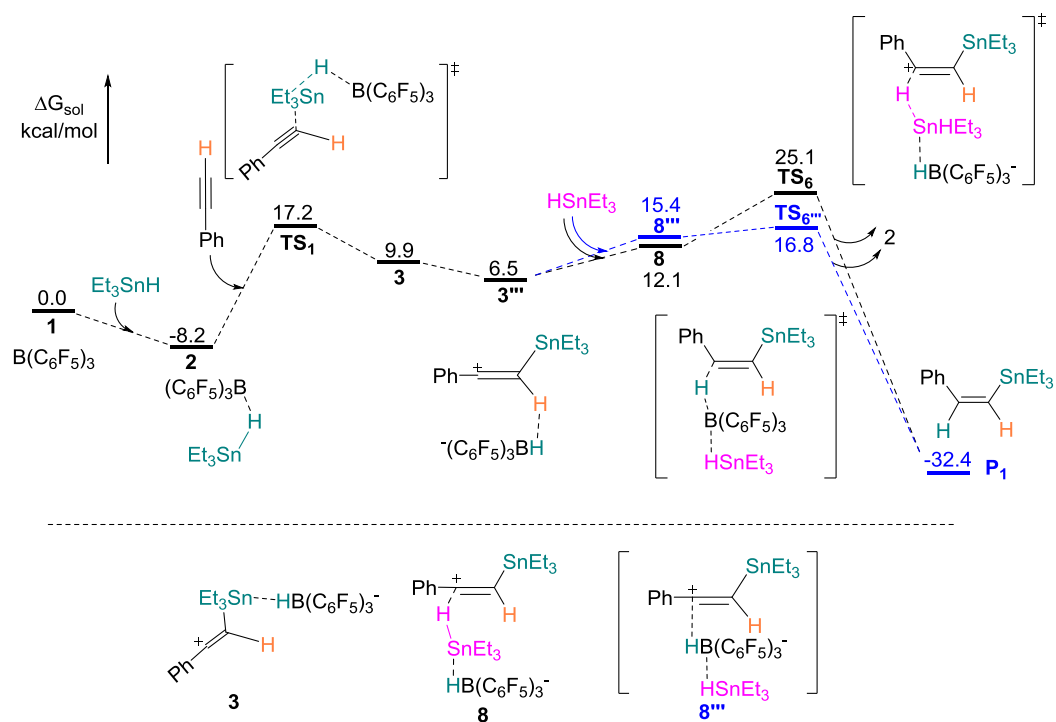


Figure S1. Free energy profile for catalyst $B(C_6F_5)_3$ or $HSnEt_3$ to give P_1 .

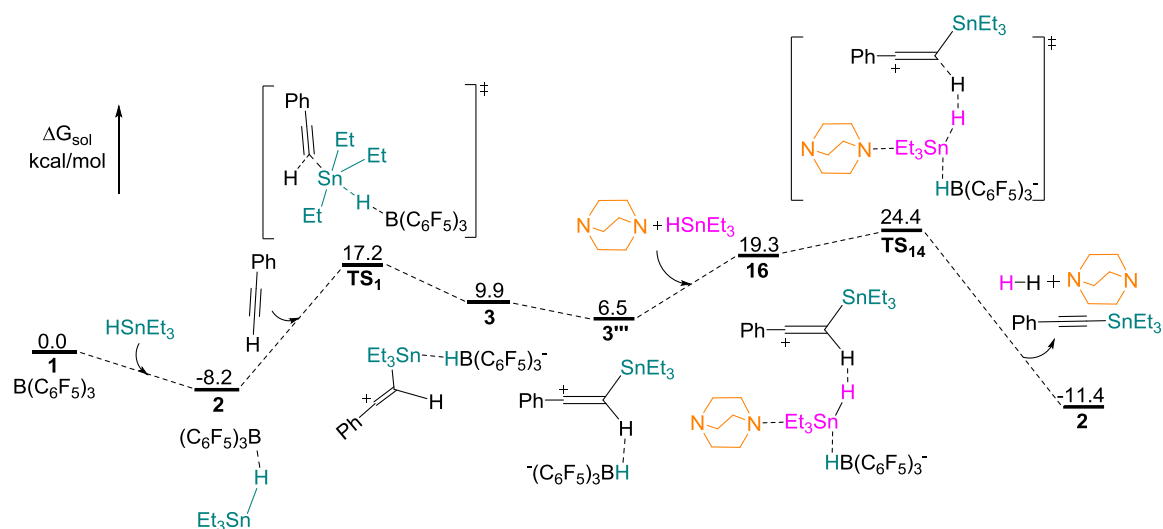


Figure S2. Free energy profile for $HSnEt_3$ which is supported by DABCO to furnish the P_3 .

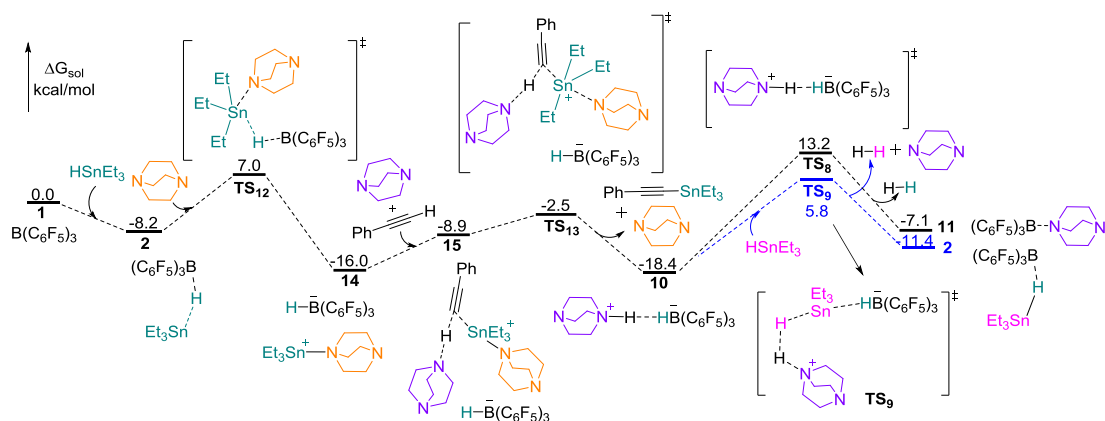


Figure S3. Free energy profile for dehydrogenative stannylation in the presence of two molecule DABCO.

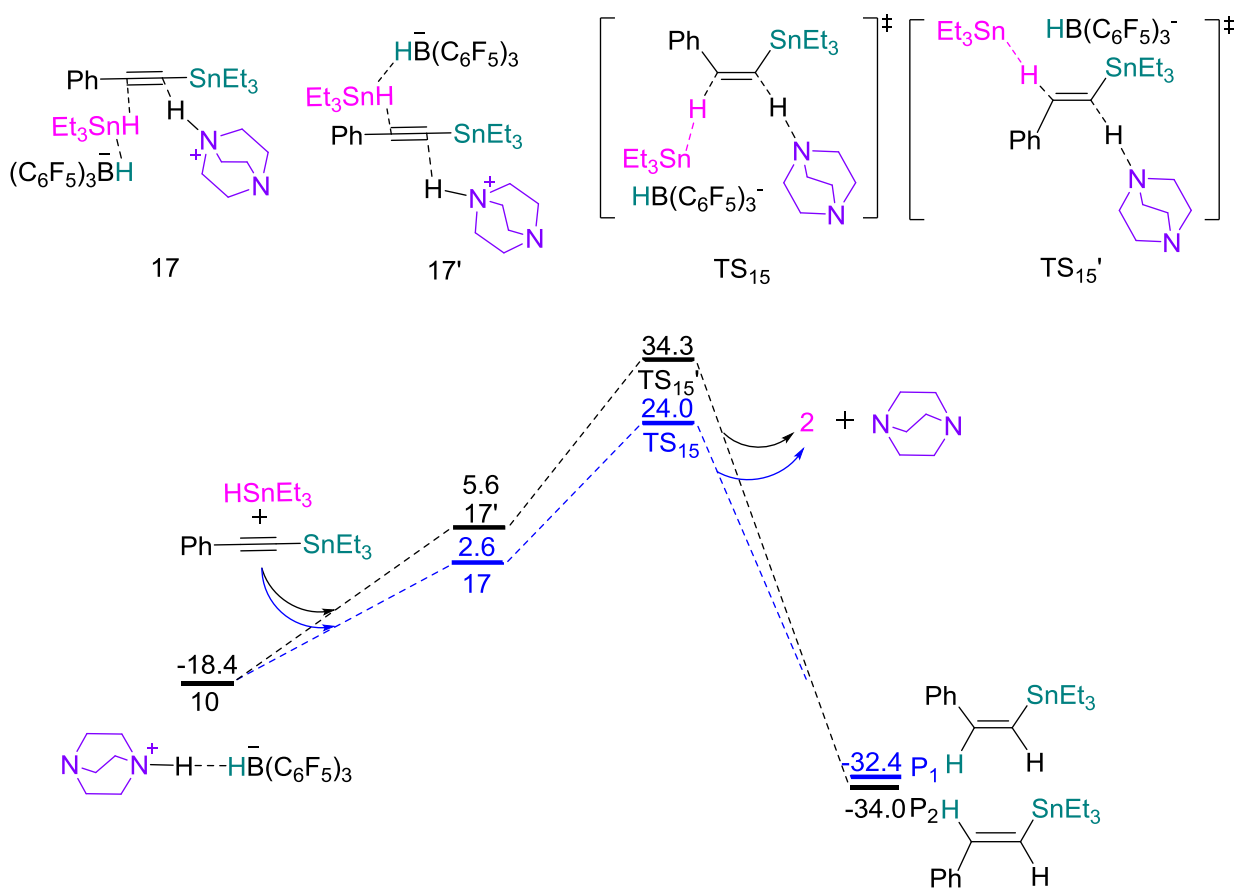


Figure S4. Free energy profile for species **10** to occur the hydrogenation addition reaction to give **P1** and **P2**.

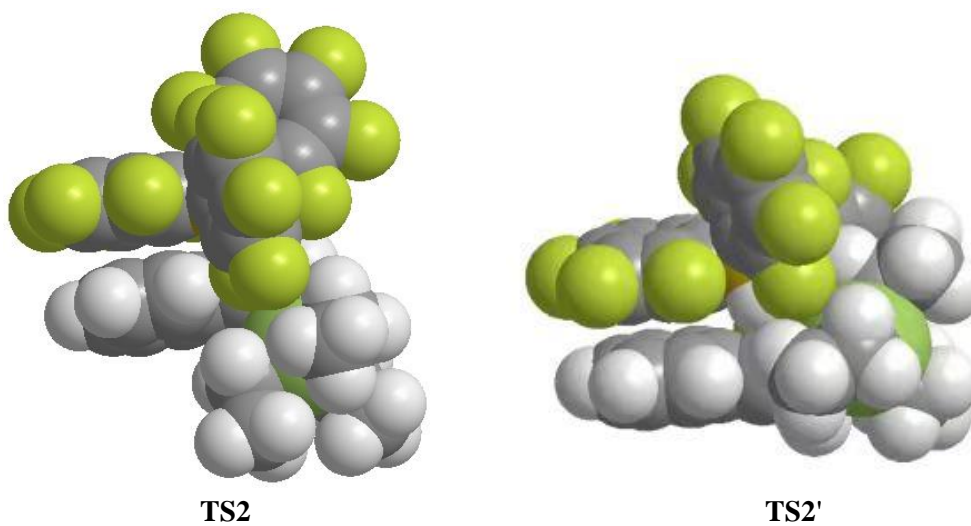
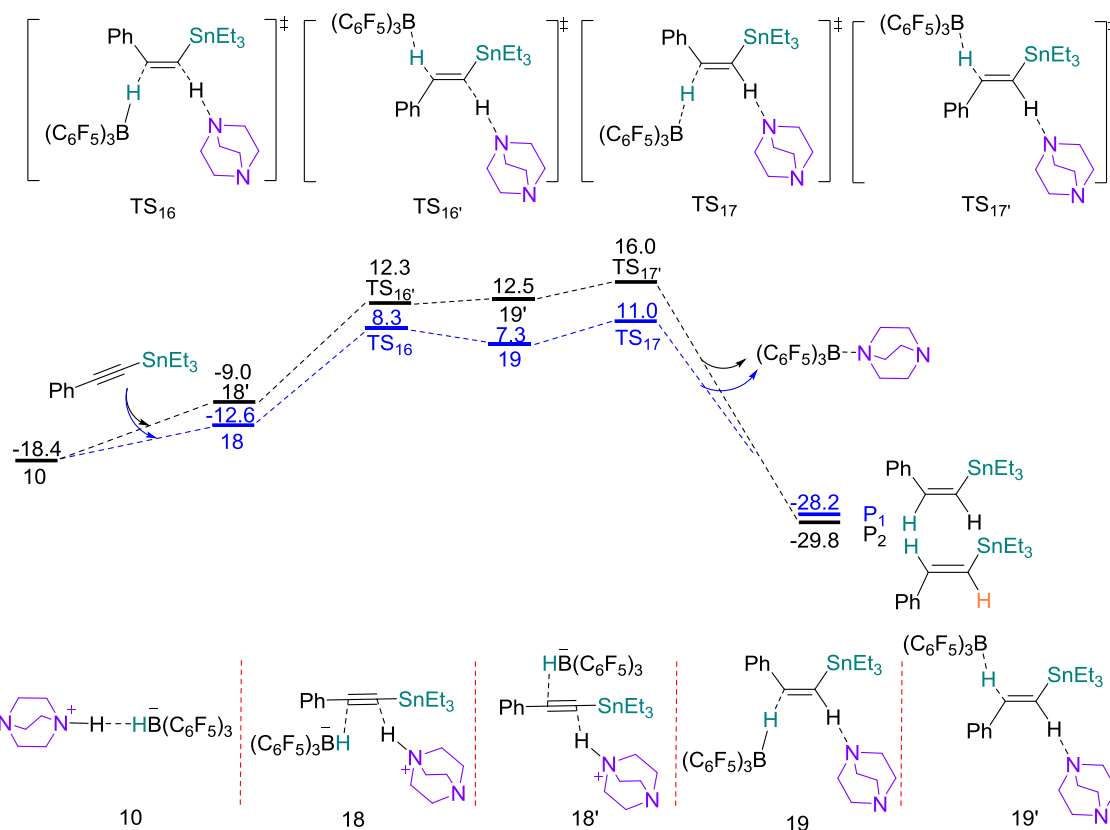


Figure S6. The space filling model of **TS2** and **TS2'**.

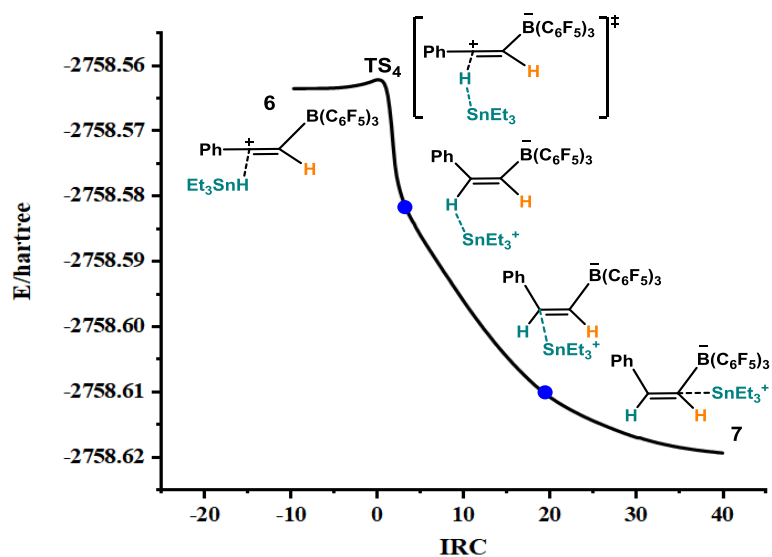


Figure S7. The energy change plot of IRC calculation for **TS4**.

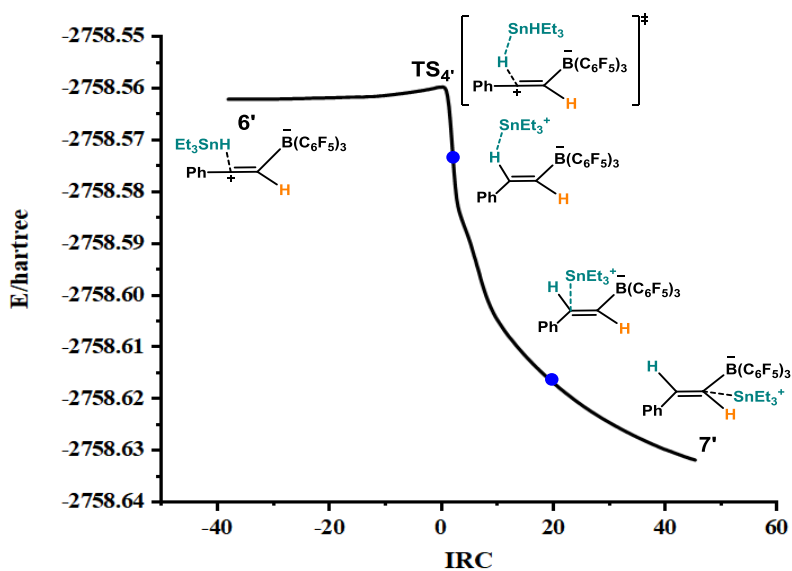


Figure S8. The energy change plot of IRC calculation for **TS4'**.

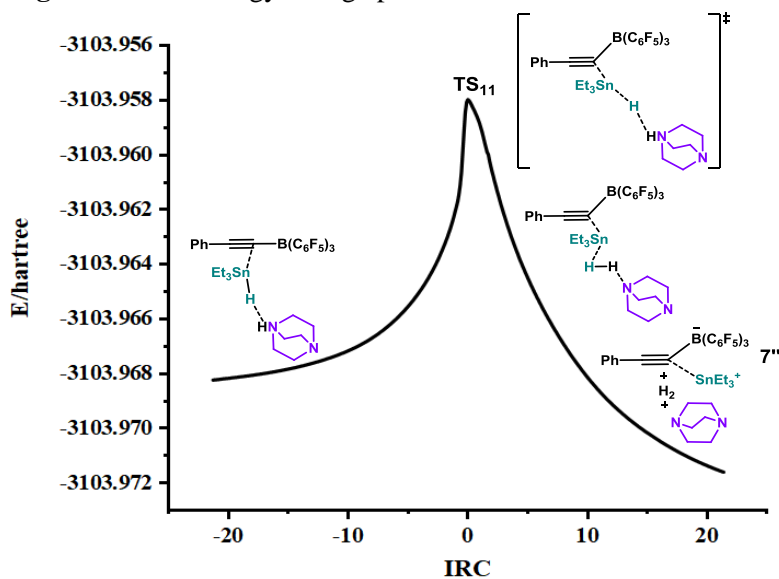


Figure S9. The energy change plot of IRC calculation for **TS11**.

Table S1. ΔE_{gas} , ΔG_{gas} , ΔE_{sol} calculated for species in the **Figure 1**.

species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
1	0.0	0.0	0.0
2	-6.5	-23.0	-24.7
Ts1	14.9	-16.9	-14.5
3	10.8	-20.1	-21.0
3'	10.9	-20.5	-19.8
3''	7.3	-21.3	-21.9
Ts2	10.8	-19.3	-17.7
Ts2'	14.8	-17.4	-15.9
P1	-28.3	-45.6	-41.5
P2	-29.1	-45.1	-41.9

Table S2. ΔE_{gas} , ΔG_{gas} , ΔE_{sol} calculated for species in the **Figure 2**.

species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
4	2.1	-11.8	-9.8
Ts3	8.6	-6.0	-3.5
5	8.6	-5.7	-4.9
6	12.4	-14.1	-10.8
6'	15.6	-14.5	-12.7
Ts4	14.0	-14.5	-11.0
Ts4'	18.4	-13.0	-10.4
7	-19.8	-56.8	-54.9
7'	-25.5	-61.7	-60.5
Ts5	-13.1	-50.5	-45.2
Ts5'	-15.9	-53.9	-47.1

Table S3. ΔE_{gas} , ΔG_{gas} , ΔE_{sol} calculated for species in the **Figure 3**.

species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
3'''	6.4	-22.8	-22.7
8	11.2	-34.3	-33.5
8'	22.5	-23.3	-21.7
Ts6	24.8	-20.0	-19.8
Ts6'	25.5	-21.6	-18.5
P1	-34.8	-68.6	-66.2
P2	-35.6	-68.2	-66.6

Table S4. ΔE_{gas} , ΔG_{gas} , ΔE_{sol} calculated for species in the **Figure 4**.

species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
8''	20.1	-24.6	-25.7
Ts2''	11.8	-14.6	-8.4
Ts6''	21.7	-21.9	-16.5
P3	-6.3	-6.2	-3.1
P3	-12.8	-29.2	-27.8

species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
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6''	11.7	-15.2	-12.1
TS4''	27.7	0.3	-0.2
7''	-10.4	-30.0	-27.6
TS5''	1.2	-19.8	-13.0

Table S5. ΔE_{gas} , ΔG_{gas} , ΔE_{sol} calculated for species in the **Figure 5**.

Table S6. ΔE_{gas} , ΔG_{gas} , ΔE_{sol} calculated for species in the **Figure 6**.

species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
9	-4.2	-48.0	-44.5
TS7	2.3	-39.8	-39.3
10	-11.9	-39.0	-45.6
TS8	9.7	-12.6	-9.0
TS9	5.9	-33.5	-33.6
11	-6.3	-6.2	-3.1
2	-12.8	-29.2	-27.8

Table S7. ΔE_{gas} , ΔG_{gas} , ΔE_{sol} calculated for species in the **Figure 7**.

species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
12	-17.3	-42.3	-18.8
TS10	8.9	-19.1	-13.6
13	-10.7	-41.1	-46.1
TS11	12.4	-31.6	-29.8

Table S8. ΔE_{gas} , ΔG_{gas} , ΔE_{sol} calculated for species in the **Figure S1-S5**.

species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
8'''	14.7	-28.5	-27.8
TS6'''	15.9	-27.7	-26.9
16	17.5	-41.5	-39.7
TS14	19.1	-40.4	-35.1
TS12	5.8	-29.7	-28.6
14	-8.8	-41.2	-48.4
15	-8.7	-67.9	-68.1
TS13	-5.9	-64.2	-60.8
17	9.8	-49.0	-56.2
17'	15.3	-43.2	-52.9
TS15	19.5	-38.5	-34.0
TS15'	32.5	-26.2	-24.5
18	-10.5	-57.1	-59.2
18'	-3.9	-49.1	-54.2
TS16	5.2	-39.1	-36.1
TS16'	9.3	-34.0	-31.0
19	3.8	-39.3	-35.8
19'	8.9	-34.0	-30.3
TS17	5.7	-39.2	-33.9
TS17'	10.5	-33.8	-28.3

Table S9. Absolute Calculation Energies and imaginary frequencies.

species	E(gas-B3LYP-D3) ¹	G(corr-B3LYP-D3) ²	H(corr-B3LYP-D3) ³	E(soln-CAM-B3LYP-D3) ⁴	IF ⁵
1	-2208.43470566	0.092578	0.183928	-2208.28539508	-
2	-2450.14971461	0.279839	0.403493	-2449.88174779	-
Ts1	-2758.56597500	0.383328	0.521449	-2758.17492438	-67.22
3	-2758.57103272	0.381952	0.523208	-2758.18514938	-
3'	-2758.57173642	0.382710	0.523119	-2758.18321949	-
3''	-2758.57173642	0.382710	0.523119	-2758.18321949	-
Ts2	-2758.56987930	0.380735	0.521875	-2758.17991809	-24.41
Ts2'	-2758.56674676	0.383977	0.521760	-2758.17708661	-20.23
P1	-550.176967787	0.267677	0.339769	-549.932557365	-
P2	-550.176278276	0.265746	0.339841	-549.933086503	-
4	-2516.87953582	0.193831	0.303084	-2516.61032132	-
Ts3	-2516.87030830	0.195064	0.301447	-2516.60024630	-167.40
5	-2516.86982692	0.194485	0.302573	-2516.60246117	-
6	-2758.56144967	0.374789	0.520431	-2758.16891812	-
6'	-2758.56213193	0.380715	-2758.181417	-2758.17190830	-
Ts4	-2758.56217085	0.378110	0.519361	-2758.16924419	-129.13
Ts4'	-2758.55980761	0.382737	0.519142	-2758.16837704	-130.40
7	-2758.62953813	0.391657	0.526946	-2758.23917343	-
7'	-2758.63744037	0.390470	0.527014	-2758.24809047	-
Ts5	-2758.61948295	0.392285	0.525557	-2758.22378507	-101.67
Ts5'	-2758.62501313	0.393357	0.525829	-2758.22679814	-77.59
3'''	-2758.57538578	0.379231	0.523136	-2758.18788372	-
8	-3000.27211480	0.566318	0.741539	-2999.76211109	-
8'	-3000.25451623	0.566729	0.741416	-2999.74332779	-
Ts6	-3000.24928601	0.565144	0.740096	-2999.74030366	-104.04
Ts6'	-3000.25172679	0.568642	0.739927	-2999.73824837	-193.89
8''	3000.25650271	0.564842	0.741251	-2999.74977987	-
Ts2''	-2758.56234552	0.374770	0.515076	-2758.16518607	-246.04
Ts6''	-3000.25224502	0.563075	0.736591	-2999.73507930	-476.25
P3	-548.938625079	0.241398	0.316877	-548.700604631	-
6''	-2758.56325739	0.375589	0.520441	-2758.17095411	-
TS4''	-2758.53863462	0.376398	0.516681	-2758.15205248	-48.52
7'''	-2757.41121506	0.365187	0.503313	-2757.02491184	-
TS5''	-2757.39505387	0.367521	0.501975	-2757.00179287	-99.72
9	-2862.29663437	0.365576	0.496856	-2861.88361130	-
TS7	-3103.97108231	0.553921	0.714551	-3103.47324701	-1036.40
10	-2555.03112924	0.288565	0.402029	-2554.78268326	-
TS8	-2554.98897524	0.280760	0.391782	-2554.72445574	-136.73
TS9	-2796.70063835	0.469095	0.612877	-2796.32072305	-563.07
11	-2553.83672355	0.278104	0.380069	-2553.58215730	-
12	-2862.29663437	0.365576	0.496856	-2861.88361130	-
TS10	-2862.25971997	0.370442	0.495662	-2861.87537023	-135.64
13	-2862.29483426	0.374283	0.501000	-2861.92710123	-
TS11	-3103.95797380	0.556919	0.713098	-3103.45822473	-573.98

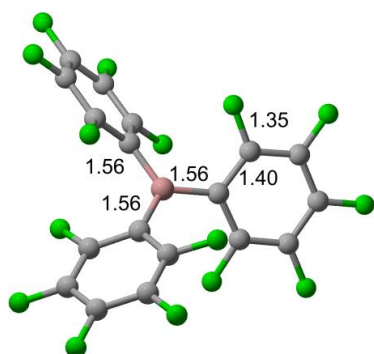
8'''	-3000.26277871	0.562587	0.741305	-2999.75309868	-
TS6'''	-3000.26157209	0.563233	0.740176	-2999.75157394	-19.03
16	-3345.65212146	0.741781	0.936285	-3345.03097348	-
TS14	-3345.65024441	0.742484	0.933003	-3345.02359685	-39.87
TS12	-2795.52893243	0.464252	0.597843	-2795.14692541	-25.13
14	-2795.54724547	0.459222	0.600013	-2795.17850283	-
15	-3449.38439655	0.735085	0.914358	-3448.77816541	-
TS13	-3449.37848408	0.733634	0.910344	-3448.76658456	-1010.82
17	-3345.66394176	0.741340	0.939772	-3345.05725996	-
17'	-3345.65476587	0.740910	0.939719	-3345.05202456	-
TS15	-3345.64722552	0.740157	0.933795	-3345.02197431	-127.30
TS15'	-3345.62767986	0.741317	0.933292	-3345.00673810	-265.75
18	-3103.99865989	0.560977	0.721789	-3103.50510304	-
18'	-3103.98585688	0.558793	0.721931	-3103.49708932	-
TS16	-3103.96989944	0.557370	0.715088	-3103.46814222	-15.63
TS16'	-3103.96169314	0.555678	0.714782	-3103.46007798	-50.37
19	-3103.97016270	0.555352	0.716509	-3103.46774606	-
19'	-3103.96170410	0.554957	0.716167	-3103.45900916	-
TS17	-3103.97003995	0.558259	0.715561	-3103.46471797	-27.47
TS17-1	-3103.96150146	0.557342	0.715047	-3103.45574023	-57.27

¹The electronic energy calculated by B3LYP-D3 in gas phase. ²The thermal correction to Gibbs free energy calculated by B3LYP-D3 in gas phase. ³The thermal correction to enthalpy calculated by B3LYP-D3 in gas phase. ⁴The electronic energy calculated by CAM-B3LYP-D3 in toluene solvent. ⁵The B3LYP-D3 calculated imaginary frequencies for the transition states.

Table S10. TOFs for the pathway in **Figure1-7**.

TOF/s ⁻¹	Figure 1	Figure 2	Figure 3	Figure 4	Figure 5	Figure 6	Figure 7
Blue line	1.41×10 ⁻⁶	8.52×10 ⁻⁷	2.25×10 ⁻¹²	3.66×10 ⁻⁷	—	1.07×10 ⁻⁵	—
Black line	1.41×10 ⁻⁶	2.3×10 ⁻⁹	7.19×10 ⁻¹⁵	9.08×10 ⁻¹⁴	6.47×10 ⁻¹⁴	3.98×10 ⁻¹¹	8.34×10 ⁻¹⁰

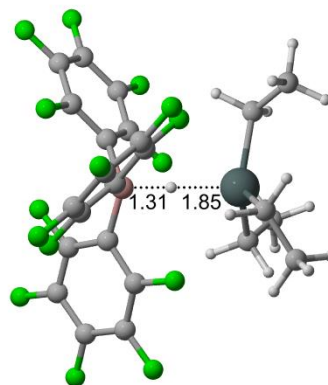
Cartesian coordinates for the complexes calculated in this study: [gas phase results optimized at the level of B3LYP-D3/6-31+G* (LanI2dz for Sn)]:



1

B	-2.04264900	0.43117400	0.00007900
C	-2.82436800	1.78364900	-0.00008900
C	-3.99384100	1.97083100	0.75058600
C	-2.40199300	2.89017300	-0.75072700
C	-4.69575700	3.16992500	0.77248200
C	-3.08970500	4.09747100	-0.77250700
C	-4.24169700	4.23801900	0.00002800
C	-2.82229000	-0.92248700	0.00590900
C	-2.39284100	-2.02834300	0.75351000
C	-3.99685600	-1.11146000	-0.73631500
C	-3.07855300	-3.23667800	0.78028000
C	-4.69710300	-2.31161200	-0.75311300
C	-4.23587400	-3.37899000	0.01607700
C	-0.48045300	0.43236600	-0.00556800
C	0.26441900	-0.48861600	-0.75590000
C	0.26841500	1.35452200	0.73932600
C	1.65374700	-0.49573700	-0.78287900
C	1.65788800	1.36382600	0.75618800
C	2.35365800	0.43459300	-0.01588700
F	2.33149400	2.25091400	1.49864900
F	-0.35695400	2.26627200	1.50857100
F	-0.36509400	-1.40133100	-1.52060500
F	2.32331900	-1.38176000	-1.53024400
F	3.68709800	0.43564600	-0.02074400
F	-1.28603100	-1.93839600	1.51567900
F	-4.47787100	-0.11408400	-1.50302600
F	-5.80378100	-2.45273800	-1.49286900
F	-4.90091600	-4.53472300	0.02086900
F	-2.64182200	-4.25978100	1.52487300

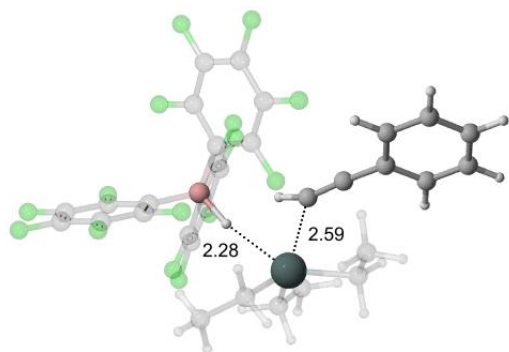
F	-4.46782800	0.97270500	1.52069200
F	-5.79728600	3.30935800	1.52020100
F	-4.90849500	5.39274900	0.00007700
F	-2.65989500	5.12125600	-1.52018500
F	-1.30056500	2.80193000	-1.52085000



2

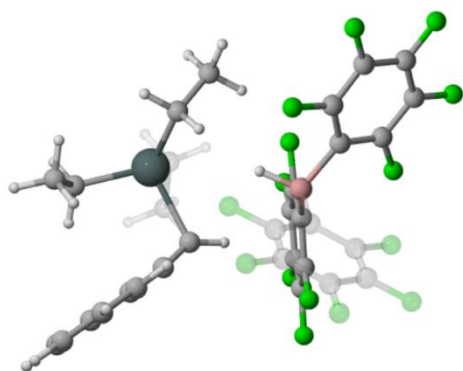
C	-0.21673400	1.31144200	2.23140500
C	0.86501400	2.19129700	2.23271200
C	-0.28705900	0.46516300	3.33880600
C	1.82888900	2.24064500	3.23198400
C	0.65045500	0.48111800	4.37012400
C	1.71873600	1.37222700	4.31522300
C	-2.16430800	2.65990900	0.87600600
C	-2.47604200	3.52060100	1.92929100
C	-2.68974000	3.03143900	-0.36101800
C	-3.24520600	4.67198200	1.76959700
C	-3.45476800	4.17160300	-0.57262800
C	-3.73522600	5.00279800	0.50912800
C	-2.05542200	-0.06433200	0.75676900
C	-3.42565400	-0.25215000	0.94267900
C	-1.36229800	-1.19221100	0.31895400
C	-4.06704800	-1.46641300	0.70392700
C	-1.95647100	-2.42099500	0.06010200
C	-3.32859300	-2.55818700	0.25554200
H	-0.49644800	1.39978700	-0.02742000
C	0.50333200	3.60306200	-1.94477300
H	0.03727200	3.71603300	-2.93030800
H	-0.19052900	4.03920800	-1.21774300
C	1.86375200	4.31399400	-1.88337800
H	2.57746800	3.90269000	-2.60793000

H	1.75448500	5.38246700	-2.10749300	C	-0.78233500	1.65861400	1.96188700
H	2.31535700	4.23272100	-0.88888600	C	-0.05003200	2.84820400	1.99116100
C	-0.40626000	0.19177900	-2.86834700	C	-1.43493400	1.35929100	3.16061400
H	0.25463800	-0.66063800	-3.06293900	C	0.07734700	3.66402700	3.10971200
H	-1.27683100	-0.20181300	-2.33222000	C	-1.33878100	2.14551900	4.30815200
C	-0.84236900	0.87219600	-4.17488200	C	-0.57180800	3.30516300	4.28705700
H	0.01059700	1.27255900	-4.73678400	C	-1.63832500	1.78027400	-0.50618900
H	-1.35630500	0.15908400	-4.83150400	C	-2.96802100	2.16415000	-0.31493400
H	-1.53430600	1.70002800	-3.98607600	C	-1.00403200	2.40665300	-1.57396400
C	2.45734100	0.79243800	-0.68792300	C	-3.64307100	3.06138800	-1.13547000
H	3.17896800	1.61642800	-0.72829900	C	-1.63380300	3.31463200	-2.42156700
H	2.27115400	0.59021100	0.37259100	C	-2.96766200	3.64034000	-2.20768900
C	3.00089700	-0.46276000	-1.38731500	C	-1.48578800	-0.69820500	0.74545200
H	2.29814500	-1.29975900	-1.31526900	C	-2.54990500	-1.28111800	0.05112100
H	3.20265300	-0.28782800	-2.45138500	C	-0.83723700	-1.56939100	1.62885200
B	-1.28130300	1.32183900	1.02368600	C	-2.95589300	-2.60644700	0.22666600
F	2.85448800	3.10441600	3.16130100	C	-1.19885200	-2.89363600	1.83322200
F	2.63114100	1.39595600	5.29443400	C	-2.27628100	-3.42073500	1.12382700
F	0.53380400	-0.35238000	5.41407400	H	0.26936100	0.61995500	0.14025300
F	-1.30725400	-0.40936700	3.46814400	C	3.09827600	-0.01825500	-2.92459700
F	-1.22944800	-3.46264000	-0.37507500	H	4.12210400	-0.34200900	-2.68290200
F	-3.93041200	-3.72954000	0.01542300	H	2.70004800	-0.74833500	-3.63512000
F	1.01465900	3.06342500	1.19713400	C	3.12279600	1.39169700	-3.53145700
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F	-4.47021800	6.10837400	0.33763200	H	3.54209400	2.12487800	-2.83263000
F	-3.91669200	4.47714200	-1.79583000	C	2.15029600	-2.13391800	-0.15754600
F	-2.44674900	2.24897900	-1.44930800	H	3.23463600	-2.32562100	-0.15195400
F	-4.19940100	0.75700100	1.39571300	H	1.84976600	-2.04076300	0.88889400
F	-5.38719400	-1.59369900	0.90180800	C	1.41724900	-3.28881600	-0.84631600
F	-0.01769100	-1.10975900	0.11667700	H	1.66665700	-3.36204000	-1.91118900
H	3.94350800	-0.78596800	-0.92814300	H	1.67829200	-4.24559200	-0.37692300
Sn	0.60805200	1.50515900	-1.50904500	H	0.33064000	-3.18331600	-0.76967000
				C	2.94893400	1.32793100	0.21550500
				H	3.98378200	1.39929400	-0.15049900
				H	2.46862300	2.28586300	0.00987300
				C	2.91380200	0.99392600	1.71067900
				H	1.89179600	0.85268800	2.07046100
				H	3.47138500	0.07731400	1.93816500
				B	-0.89726400	0.81232000	0.56954000
				F	0.81484900	4.78795400	3.06417300
				F	-0.46581700	4.07181600	5.38228300
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TS1

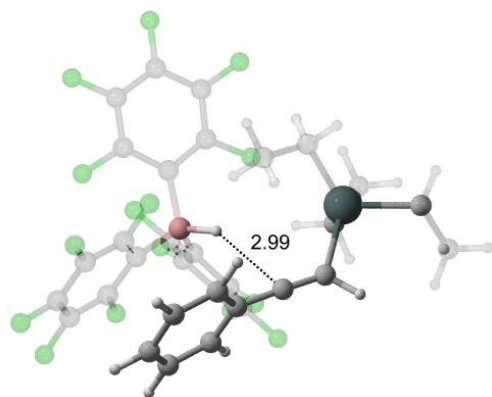
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F	0.58548100	3.27128500	0.86938600	C	-2.84349700	1.61005400	0.21400700
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F	-4.92723800	3.37879700	-0.90771700	C	-3.62747600	2.44221600	-0.57814100
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F	-3.23791700	-0.58504100	-0.88254100	C	-2.07715800	-1.81844700	0.32826300
F	-3.98380500	-3.10396000	-0.47974200	C	-0.37204300	-2.02936500	1.92265700
F	0.22010800	-1.11990900	2.34839100	C	-2.36130500	-3.18359100	0.42597400
H	3.36145600	1.80508600	2.29936800	C	-0.61469100	-3.38987200	2.05363400
C	0.64948300	-1.15147500	-5.66994000	C	-1.62575500	-3.97761500	1.29575900
C	0.83553600	-0.81635500	-7.00686800	H	0.51585600	0.33534700	0.52418000
C	0.47774600	0.45747200	-7.46556600	C	3.93800500	-1.47821200	-2.77152000
C	-0.07130300	1.39874600	-6.58762900	H	4.84881400	-2.00905400	-2.46312000
C	-0.26235400	1.07528900	-5.24817100	H	3.37912200	-2.18159300	-3.40071600
C	0.10149400	-0.20422200	-4.77795100	C	4.30304100	-0.21156600	-3.56218000
H	0.91939800	-2.13584900	-5.30048800	H	4.90483300	-0.45656700	-4.44662100
H	1.25755800	-1.54417900	-7.69331100	H	3.41349100	0.32338100	-3.91149400
H	0.62581900	0.71564400	-8.51029400	H	4.88676500	0.49008800	-2.95521000
H	-0.34799700	2.38537400	-6.94638900	C	2.71965500	-2.84896100	0.30258900
H	-0.67693300	1.80138800	-4.56029800	H	3.76811800	-3.09846700	0.51717200
C	-0.09061500	-0.54333800	-3.41920200	H	2.27149900	-2.54133500	1.25068400
C	-0.16017800	-0.81025000	-2.22262600	C	1.99273100	-4.06247700	-0.29147800
H	-0.69309700	-1.18994200	-1.37069900	H	2.45283700	-4.39832100	-1.22880500
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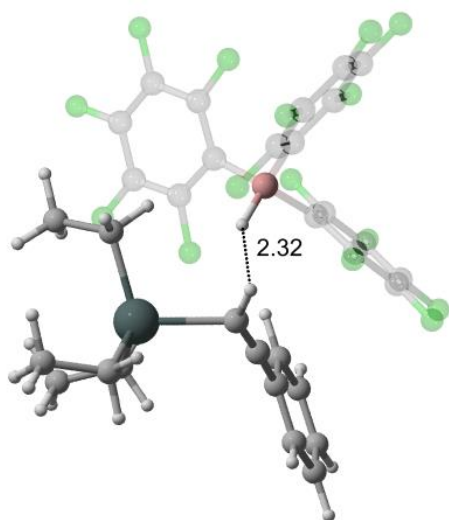
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				F	-1.77892000	1.14912500	5.85731900
				F	-2.02206600	-0.26322100	3.59980900
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				F	0.93429900	2.76414700	1.41642000
				F	-3.44444500	1.04634400	1.28404600
				F	-4.91932000	2.66759800	-0.28420800

F	-3.79520800	3.84794400	-2.48739900	H	3.61444100	1.03232700	4.70108800
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F	0.32641400	1.80837800	-1.52088600	C	2.87280100	-2.29082400	-0.83268500
F	-2.81671400	-1.13982500	-0.58175600	Sn	1.64738100	-1.91741700	-2.71241700
F	-3.32451000	-3.73749800	-0.33091100	C	2.01879000	0.11186400	-3.31457200
F	0.64392900	-1.53035700	2.67104100	H	2.74565100	0.04233900	-4.13375200
H	3.57586300	1.65150900	1.89038900	H	1.08499000	0.48836300	-3.74318900
C	1.00770300	-1.53002200	-5.27457800	C	2.76839800	-3.27690600	-3.96075900
C	1.15164900	-1.13076200	-6.59686100	H	2.41306900	-3.13442200	-4.99048200
C	1.01358300	0.22233300	-6.93633900	H	3.82083800	-2.96456900	-3.95864900
C	0.73000300	1.18303500	-5.95759100	C	-0.28092300	-2.77887100	-2.36517200
C	0.58860300	0.80184700	-4.62873400	H	-0.11928200	-3.73680600	-1.85794800
C	0.73087500	-0.56274900	-4.27928400	H	-0.84002000	-2.13778100	-1.68620400
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H	1.36675500	-1.86605500	-7.36590900	H	3.48481600	0.71264700	-1.80683700
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				C	-0.51740100	1.05839900	3.13603700
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				C	-0.03020200	1.69690300	4.27624300
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				C	-1.07469900	1.73037300	-0.60538100
				C	-1.42044500	3.05346800	-0.32246500
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				C	-3.06381900	-0.28207000	0.73641600
				C	-1.37429900	-1.90078400	0.79313900
				C	-4.04209600	-1.26443500	0.86743500
				C	-2.31064000	-2.92179900	0.92646200
C	4.18052500	0.89343700	2.62538500	C			
C	3.96969900	0.24469100	1.42173700	C			
C	3.00004400	-0.79342200	1.34381200	C			
C	2.23053000	-1.13602900	2.48945500	C			
C	2.47128100	-0.48872200	3.69131200	C			
C	3.43954400	0.52072400	3.75903000	C			
H	4.90559200	1.69746700	2.69230900	C			
H	4.53122000	0.51349900	0.53374000	C			
H	1.47429200	-1.90621400	2.40415300	C			
H	1.89480900	-0.75015900	4.57236500	C			



3'

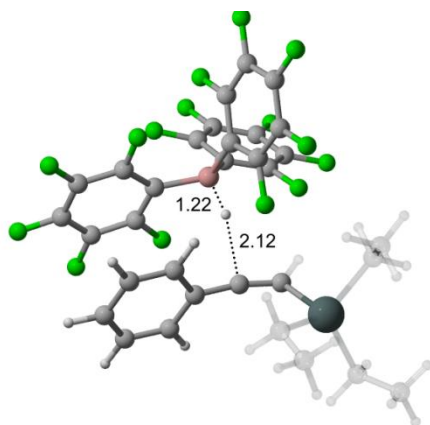
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F	-0.06860800	-2.30240300	0.77857700	H	1.13718300	-2.06276200	-4.90912800
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F	2.59927500	3.69941900	2.78201300	C	0.30852800	2.60351100	-3.54538400
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3''

C	5.12593000	-2.97681800	0.90576300	C	0.00101500	-1.84787500	1.87466000
C	4.09220400	-2.95230900	-0.02006400	C	0.24274900	0.24350000	2.90651900
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C	4.21431300	-0.99642000	2.00037600	C	1.25784200	-1.69608200	3.91204500
C	5.18460100	-2.00240300	1.91303100	C	-0.96528300	1.75327800	0.38324600
H	5.88379000	-3.75211600	0.85437500	C	-2.02277000	2.66262100	0.43114700
H	4.02121600	-3.70187000	-0.80171700	C	0.26885300	2.33986800	0.10512400
H	2.39824000	-0.20278300	1.14316900	C	-1.87127500	4.03525000	0.22218200
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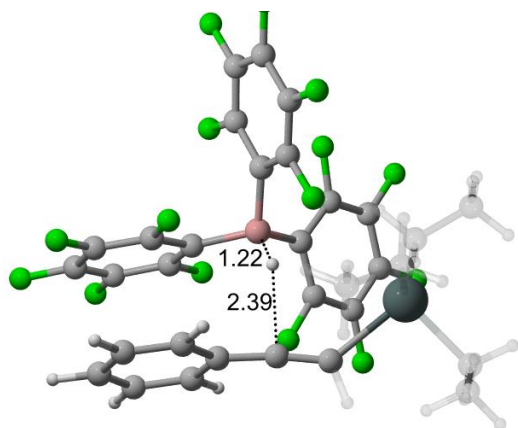
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F	1.00473700	-3.78779900	2.82841800	H	-8.88275500	-1.98182900	-4.84862100
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F	0.03328000	1.57610600	3.01131800	H	-8.70212800	-3.55511800	-9.38186700
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F	-4.57665500	-2.33576800	-2.06732600	H	-11.78180100	0.43724200	-7.30576500
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H	-0.40522000	-0.27771000	-0.42551700	H	-10.27483000	-0.30120100	-7.86041300



TS2

C	-8.58086400	-6.21556600	-1.65886600	C	-7.55426500	-2.12636200	-6.57207300
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C	-11.59979000	-4.39615100	-5.01926800	C	-12.26093300	-3.86222000	-0.44979100
Sn	-10.40351000	-3.34404400	-6.59251800	C	-11.94975200	-5.22283500	-0.33836900
C	-10.08506600	-4.76590100	-8.17666400	C	-11.66531600	-3.05699700	0.52285100
H	-9.33075100	-5.48910100	-7.84421800	C	-11.12741600	-5.75874800	0.64268100
H	-11.01676500	-5.32596300	-8.31963100	C	-10.83296000	-3.54876400	1.52752700
				C	-10.55589900	-4.90951200	1.58634400
				C	-13.28505200	-1.75881700	-1.91630300
				C	-14.21565500	-1.01959200	-1.18104500
				C	-12.56972600	-1.01074100	-2.84628900
				C	-14.43307700	0.34435000	-1.35061700
				C	-12.74687300	0.35447400	-3.05584000
				C	-13.69091100	1.04095700	-2.30189100
				F	-13.88209500	2.35696800	-2.48590700
				F	-12.01480300	1.01079700	-3.98054600
				F	-11.60884300	-1.59806900	-3.62481700
				F	-14.94951900	-1.63472800	-0.22863800
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				F	-12.44706800	-6.09563400	-1.24945200

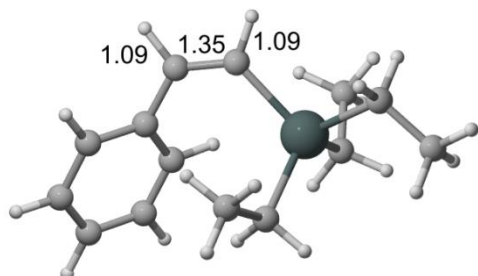
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F	-9.73158500	-5.39835000	2.52881600	C	-8.80211500	-1.88607300	-8.09603600
F	-10.26668900	-2.71655200	2.42142900	H	-8.00503900	-2.53481400	-7.71261000
F	-11.84999200	-1.71583900	0.52163100	H	-8.34155400	-1.17948500	-8.79798700
F	-14.87620600	-4.60998200	0.42666600	H	-9.19559100	-1.30527900	-7.25573300
F	-17.26920200	-5.73919400	0.00885000	C	-11.02603700	-7.17965700	-7.05167800
F	-18.34115800	-5.84305600	-2.50686000	H	-10.74994100	-8.20975600	-7.31060400
F	-16.94668800	-4.78223600	-4.61827600	H	-10.69314800	-7.00340900	-6.02073400
F	-14.54579600	-3.64410900	-4.22647600	H	-12.12135600	-7.12813700	-7.04707900
H	-12.47682900	-3.78713600	-2.67442000	C	-13.67136600	-4.19348300	-8.78146800



TS2'

C	-8.20031900	-0.66059700	-2.52002300	C	-14.35954500	0.24074300	-4.84525300
C	-8.58923200	-1.35832600	-3.65127500	C	-12.76056100	-0.34039300	-6.45515500
C	-9.36709500	-2.54057400	-3.51607500	C	-14.77459700	1.32560900	-5.61022700
C	-9.75956900	-2.98854900	-2.22498700	C	-13.14062400	0.72798400	-7.26335100
C	-9.34165300	-2.28819700	-1.10366100	C	-14.16140000	1.56970500	-6.83756800
C	-8.57165200	-1.12769900	-1.25005900	C	-13.82938000	-3.17559200	-4.28748300
H	-7.62502000	0.25419100	-2.61521400	C	-15.13008200	-3.24203900	-4.79357100
H	-8.32107400	-1.01368600	-4.64411700	C	-13.33333000	-4.41131300	-3.86757700
H	-10.36753200	-3.87833500	-2.13507000	C	-15.86977100	-4.42193300	-4.88660400
H	-9.63130600	-2.62816900	-0.11477300	C	-14.02388500	-5.61430400	-3.94070700
H	-8.26978600	-0.57055900	-0.36781100	C	-15.31455000	-5.62230300	-4.46048700
C	-9.62999900	-3.30742200	-4.64324400	F	-16.00648600	-6.76902500	-4.55146600
C	-9.68707100	-4.05846100	-5.66126600	F	-13.45787800	-6.76398800	-3.52440400
Sn	-10.92060400	-4.12994800	-7.53660200	F	-12.07816400	-4.49012300	-3.34773700
C	-9.91455500	-2.68936500	-8.78562300	F	-15.75345000	-2.14155400	-5.27129700
H	-9.51130200	-3.24750200	-9.64017100	F	-17.11137400	-4.41116000	-5.40288400
H	-10.68195000	-2.01148500	-9.17372600	F	-14.99050900	0.05377800	-3.66387200
C	-10.41701800	-6.16551300	-8.03415800	F	-15.75970600	2.13648800	-5.18717400
H	-10.76969000	-6.36473400	-9.05460500	F	-14.54811100	2.60751700	-7.59656000
H	-9.32330500	-6.26101800	-8.06617500	F	-12.52456400	0.95549500	-8.44106600
C	-13.04872800	-3.99598400	-7.38862400	F	-11.72249000	-1.09145300	-6.92710100
H	-13.39679500	-4.76859200	-6.69782400	F	-13.79483100	-2.75723800	-1.48783500

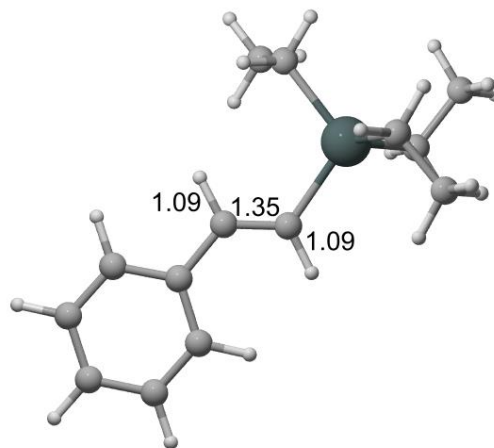
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F	-11.38665600	0.54795500	0.82387800
F	-10.43705900	1.53764400	-1.54530000
F	-11.09223100	0.37049600	-3.86327700
H	-11.77909500	-2.25822900	-4.73578400



P1

C	-0.00767200	1.10035400	0.07228200
H	-1.07334600	1.29944500	0.21777500
C	0.82848100	2.12086900	-0.19868600
C	0.38779500	-0.31280400	0.24111100
C	-0.15804000	-1.08040500	1.28471500
C	1.31453600	-0.92302300	-0.62040600
C	0.24949300	-2.39819400	1.49254000
H	-0.88961300	-0.62765400	1.95000000
C	1.71957300	-2.24333600	-0.41885100
H	1.69341300	-0.36608700	-1.47141200
C	1.19644900	-2.98316500	0.64499700
H	-0.17076600	-2.96989500	2.31577700
H	2.43530900	-2.69738300	-1.09930600
H	1.51138400	-4.01082500	0.80412200
Sn	2.97481800	2.08586500	-0.21215300
C	3.57427600	4.12983200	0.15325500
C	5.09713200	4.30913100	0.26077000
H	3.08553300	4.47097200	1.07544500
H	3.17399800	4.75718400	-0.65458300
H	5.37569800	5.35577200	0.44449600
H	5.51581400	3.71369100	1.08216900
H	5.60704600	3.99600400	-0.65950700
C	3.75990900	1.47428700	-2.13350800
C	2.88809500	1.91571300	-3.31966600
H	3.88053400	0.38335400	-2.12961300
H	4.77070900	1.89234500	-2.22982400
H	3.30794400	1.58758600	-4.28031500
H	1.87207100	1.50802100	-3.24741600
H	2.79216200	3.00821500	-3.36351900
C	3.70218100	0.82546600	1.38079600

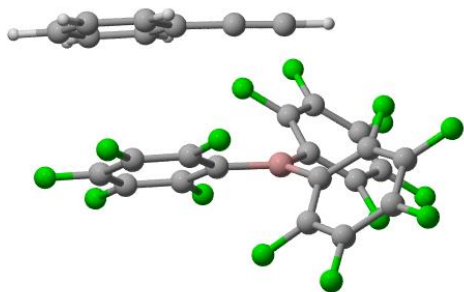
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H	4.77519400	1.02592100	1.50235500
H	3.61062500	-0.21873800	1.06206200
H	3.35798100	0.39203300	3.50247600
H	3.05435900	2.07785000	3.06193100
H	1.89398400	0.82228600	2.60903200
H	0.36242400	3.10425600	-0.29601500



P2

C	0.12840000	0.95553600	-0.36377400
H	-0.88085500	1.00722100	-0.77865600
C	0.87009900	2.08013200	-0.31590100
C	0.50288200	-0.39847900	0.08458300
C	-0.42501700	-1.44395900	-0.06772400
C	1.75035800	-0.70086900	0.66169100
C	-0.12361000	-2.74502900	0.33845100
H	-1.39466100	-1.22860900	-0.51155800
C	2.05433200	-1.99785300	1.06818700
H	2.48776400	0.08529200	0.79369600
C	1.11926800	-3.02804500	0.90897500
H	-0.85824900	-3.53550400	0.20939500
H	3.02391800	-2.20898900	1.51178800
H	1.35949600	-4.03879100	1.22726200
Sn	0.16272400	3.96690600	-1.01505800
C	1.57597200	4.80671000	-2.41585900
C	1.15600200	6.19405600	-2.92788900
H	1.68888300	4.10650200	-3.25320600
H	2.55797900	4.86164900	-1.92815600
H	1.88471200	6.60642800	-3.63893800
H	0.18674600	6.15808400	-3.44203200
H	1.06050900	6.91565200	-2.10641500
C	-0.02179500	5.33275200	0.64886600
C	1.32274100	5.62157300	1.33604700

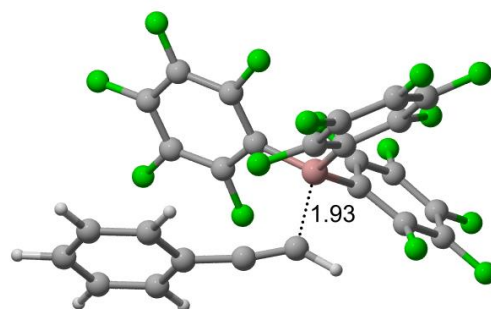
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H	-0.47039700	6.26565500	0.28265700
H	1.21068000	6.31984800	2.17665500
H	1.77536600	4.70461700	1.73438500
H	2.04498200	6.06610500	0.63938000
C	-1.72494300	3.63429600	-2.00740900
C	-1.57959300	2.91269700	-3.35768900
H	-2.21574400	4.60624600	-2.14698200
H	-2.37597500	3.06053600	-1.33472500
H	-2.55318100	2.74958500	-3.83963800
H	-0.96311100	3.49065200	-4.05746300
H	-1.10290000	1.93134800	-3.24300800
H	1.87871000	2.01298000	0.09771500



4

C	-6.46109500	-7.57880700	-4.95325600
C	-7.15488100	-6.93397600	-5.97506300
C	-7.71947100	-5.66235000	-5.75560600
C	-7.55905300	-5.04507800	-4.49959600
C	-6.86901100	-5.70087300	-3.48197900
C	-6.32262900	-6.96933400	-3.70254900
H	-6.04244400	-8.56546300	-5.12780900
H	-7.28400300	-7.41093300	-6.94134300
H	-7.98275300	-4.06234900	-4.33205100
H	-6.75912600	-5.22199500	-2.51291800
H	-5.79389700	-7.48075600	-2.90338400
C	-8.46563500	-5.02488500	-6.79292800
C	-9.11883800	-4.50601700	-7.67222800
H	-9.67741400	-4.03919700	-8.45208600
B	-11.97410100	-5.22209300	-5.86815500
C	-12.61778200	-5.96853900	-7.09266500
C	-13.25476300	-7.20908100	-6.95878600
C	-12.62415400	-5.43002500	-8.38484900
C	-13.84667600	-7.87977300	-8.02248400
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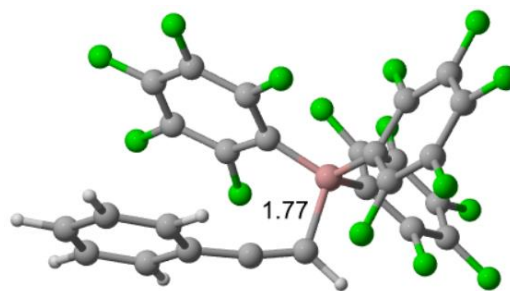
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C	-11.30119600	-2.77670300	-5.22273800
C	-13.47565600	-3.11643200	-6.09559000
C	-11.52787400	-1.40841600	-5.13727000
C	-13.74785500	-1.75628800	-6.00417100
C	-12.76192100	-0.89432400	-5.52938500
C	-11.16560900	-6.03244900	-4.80655900
C	-10.47762300	-7.21630100	-5.12820900
C	-11.10723700	-5.66537700	-3.45122000
C	-9.79759000	-7.98400800	-4.19226400
C	-10.41990900	-6.39784900	-2.49173100
C	-9.75785700	-7.56441600	-2.86592500
F	-9.09944600	-8.28167700	-1.95423200
F	-10.38951100	-5.99665300	-1.21300900
F	-11.76543300	-4.57691600	-3.00988300
F	-10.43823200	-7.65905100	-6.39679800
F	-9.18180600	-9.11718200	-4.55173700
F	-10.09877500	-3.20877600	-4.80954900
F	-10.57908600	-0.58438400	-4.67304600
F	-13.00134600	0.41513700	-5.44165100
F	-14.94175100	-1.26905500	-6.36650400
F	-14.47740100	-3.89606600	-6.54815000
F	-12.05995500	-4.22565300	-8.62254800
F	-13.14212500	-5.52723300	-10.69963400
F	-14.35619700	-7.94679900	-10.33081100
F	-14.45283700	-9.05992500	-7.83911300
F	-13.33900200	-7.79741400	-5.74902300



TS3

C	-6.10419000	-7.39399400	-5.21810800
C	-7.05273100	-6.87240100	-6.08682100
C	-7.61276500	-5.59599700	-5.83143700
C	-7.19178200	-4.85038300	-4.70261600
C	-6.25024300	-5.39170500	-3.83645600
C	-5.71067200	-6.65915300	-4.09170700
H	-5.68374000	-8.37764700	-5.40123600

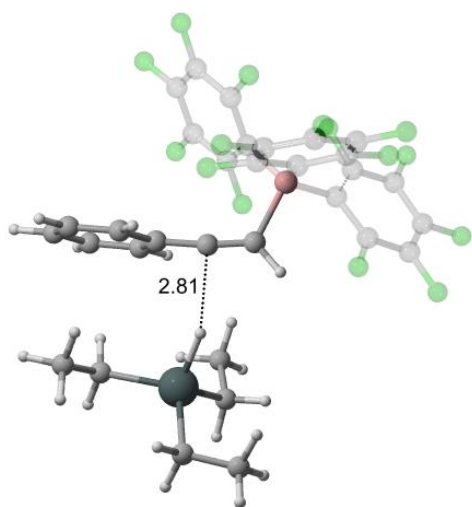
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H	-5.93762400	-4.83372500	-2.95929200
H	-4.98067100	-7.07945900	-3.40567700
C	-8.63069600	-5.10336600	-6.65669000
C	-9.67106500	-4.74799800	-7.24303200
H	-9.93643100	-4.22396400	-8.14545200
B	-11.28116300	-5.11813000	-6.24744300
C	-12.15117900	-5.93067200	-7.34650000
C	-12.84659800	-7.11399400	-7.06452900
C	-12.32126500	-5.47512800	-8.66086300
C	-13.60265400	-7.81031600	-8.00512200
C	-13.05652600	-6.13961100	-9.63419500
C	-13.70222500	-7.32743900	-9.30489100
C	-11.77051900	-3.59757300	-5.97591700
C	-10.95109200	-2.64450900	-5.35794800
C	-13.04123800	-3.11904100	-6.31982900
C	-11.31999200	-1.32524300	-5.12952200
C	-13.45714000	-1.80608200	-6.10240700
C	-12.58828100	-0.89688300	-5.51067900
C	-10.83800200	-5.97174200	-4.94433400
C	-10.18133100	-7.20097000	-5.08159100
C	-11.02716700	-5.57126100	-3.61887900
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C	-10.56054000	-6.29568600	-2.52055300
C	-9.87990500	-7.48985000	-2.72064400
F	-9.41084900	-8.19038500	-1.67935200
F	-10.76207300	-5.84415800	-1.27246700
F	-11.70361900	-4.44214800	-3.31749500
F	-9.97907200	-7.71864200	-6.31756800
F	-9.04843100	-9.11019300	-4.23622300
F	-9.72423900	-2.99639300	-4.90311700
F	-10.47435200	-0.47021800	-4.53158900
F	-12.96871900	0.36798300	-5.29765100
F	-14.69031000	-1.41535400	-6.45721900
F	-13.96992200	-3.93273700	-6.86659300
F	-11.78158200	-4.28920200	-9.04836300
F	-13.16440100	-5.63881100	-10.87462200
F	-14.42074000	-7.98531800	-10.22163800
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5

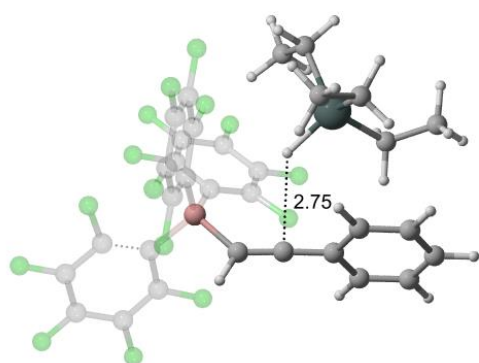
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C	2.28677500	1.30230000	2.83213300
C	3.16195200	0.98908800	3.86289300
C	4.04996500	-0.08615700	3.71911900
H	4.75872800	-1.69351200	2.45981300
H	3.16520600	-1.16918900	0.61323600
H	1.58012000	2.12126700	2.91933100
H	3.15342200	1.56932800	4.78005200
H	4.72743900	-0.33106800	4.53229400
C	1.33186400	0.76166800	0.66877400
C	0.33279000	0.88464600	-0.08375600
H	0.20767800	1.43956200	-1.00368700
B	-1.13331900	0.07972300	0.50744300
C	-1.68436700	-0.77293800	-0.77197700
C	-2.13179800	-2.09926900	-0.72256500
C	-1.86075700	-0.15924600	-2.01814700
C	-2.66305800	-2.77457800	-1.81897600
C	-2.38041000	-0.79487800	-3.14093600
C	-2.78244700	-2.12263200	-3.04196800
C	-2.22378000	1.25059500	0.83460300
C	-2.02977000	2.63033600	0.84015800
C	-3.53117400	0.84877000	1.13014700
C	-3.04265400	3.55103500	1.10546500
C	-4.57236700	1.72826000	1.40179900
C	-4.32598800	3.09871000	1.38725000
C	-0.66713400	-0.79344400	1.80723100
C	0.19364100	-1.88695200	1.65863100
C	-0.92249600	-0.44620300	3.13558700
C	0.74905300	-2.59557200	2.71524900
C	-0.38684500	-1.12893800	4.22957100
C	0.45761400	-2.21114600	4.02060200
F	1.00335400	-2.86187000	5.05801300
F	-0.65931900	-0.72836000	5.48248400

F	-1.69138100	0.62102800	3.44886900	C	-3.32921800	-0.39469400	-0.21095500
F	0.58864600	-2.26830000	0.41940000	C	-4.48186000	-2.77362500	0.51382100
F	1.60059100	-3.61193400	2.49121200	C	-4.04125800	-1.11754200	-1.15973700
F	-0.80708100	3.16705200	0.59008400	C	-4.62228300	-2.32799900	-0.79511600
F	-2.78566000	4.86998500	1.09163600	C	-2.87469700	1.54041000	2.51143800
F	-5.31208900	3.96857900	1.64430500	C	-2.12827100	2.50736000	3.19609700
F	-5.80258700	1.27263900	1.68558400	C	-4.15771100	1.96521000	2.14827500
F	-3.82183100	-0.47064300	1.19436700	C	-2.57513100	3.79241300	3.47358600
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F	-2.50516800	-0.13917800	-4.30611700	C	-3.85309800	4.16926100	3.07153900
F	-3.28980400	-2.75903600	-4.10476500	C	-1.76510500	-0.78462200	3.47483800
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				F	-0.25874500	-3.01206300	6.69896400
				F	-1.88107100	-0.85168300	7.14652700
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				F	-0.67780900	-2.36859300	2.06226700
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				F	-0.89538900	2.20017700	3.67235000
				F	-1.79396900	4.66386100	4.13477300
				F	-4.30961700	5.40136800	3.32879200
				F	-5.89330500	3.58394300	2.03355200
				F	-5.02353500	1.13173100	1.53168300
				F	-2.85168100	0.80731300	-0.63435800
				F	-4.18735100	-0.65253900	-2.41104200
				F	-5.31725000	-3.04386100	-1.68772000
				F	-5.05439000	-3.92807600	0.88892000
				F	-3.71085700	-2.51841600	2.68273400
				C	4.36586900	1.26334900	0.34935300
				H	4.04623300	0.48348000	1.04926900
				H	5.16154600	0.81847900	-0.26288400
				C	4.90496300	2.48075300	1.11689200
				H	5.72681900	2.20438600	1.79164300
				H	5.28814600	3.25043000	0.43585600
				H	4.12536800	2.94814400	1.73100800
				C	2.04926900	-0.00876100	-2.03607000
				H	2.80272500	-0.20303900	-2.81115400
				H	1.12536700	0.24838200	-2.56963200
				C	3.24972900	3.29801400	-2.33750700
				H	3.57418500	4.17459300	-1.76251200
				H	4.12827900	2.95794100	-2.90184900
C	3.26953600	-1.26898600	3.28053300	F	-4.18735100	-0.65253900	-2.41104200
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C	1.49217700	0.20633700	2.53893700	F	-5.05439000	-3.92807600	0.88892000
C	2.03039900	1.25847900	3.32293800	F	-3.71085700	-2.51841600	2.68273400
C	3.17932700	1.03829300	4.06898900	C	4.36586900	1.26334900	0.34935300
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H	1.70640600	-1.85577000	1.91473700	C	4.90496300	2.48075300	1.11689200
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H	3.59953700	1.83961400	4.66829700	H	5.28814600	3.25043000	0.43585600
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C	0.33158200	0.41363600	1.79728300	C	2.04926900	-0.00876100	-2.03607000
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H	-1.02697900	0.91377300	0.26697100	H	1.12536700	0.24838200	-2.56963200
B	-2.25395200	0.07199800	2.17660300	C	3.24972900	3.29801400	-2.33750700
C	-3.12317700	-0.80634700	1.11175100	H	3.57418500	4.17459300	-1.76251200
C	-3.75159700	-2.01667600	1.42858100	H	4.12827900	2.95794100	-2.90184900



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C	1.83575400	-1.26895400	-1.18270700
H	1.03245800	-1.12936600	-0.45085300
H	1.56052900	-2.13313200	-1.80162300
H	2.74316800	-1.54130300	-0.62887100
C	2.11326800	3.68152600	-3.29961900
H	1.79227100	2.82692700	-3.90817700
H	1.23155600	4.04589000	-2.75783800
H	2.42073000	4.47618100	-3.99228000
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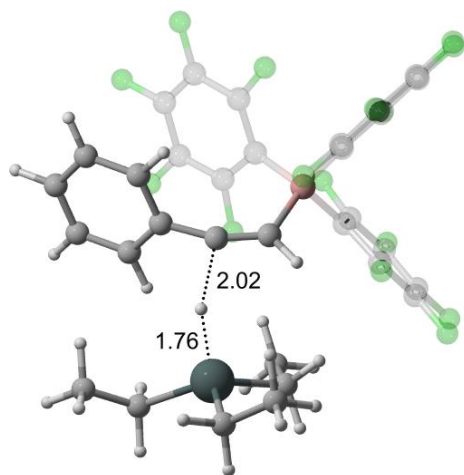


6'

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C	4.36988500	0.60777600	-0.46967300
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C	5.89427000	-1.02283800	0.44835100
H	5.20439200	-3.06914200	0.53106900
H	2.98039000	-2.53185300	-0.46115600
H	4.11014900	1.62490600	-0.74144700
H	6.33188100	1.08471900	0.26368500
H	6.85690500	-1.25569800	0.89470200
C	2.18339900	-0.12925600	-1.24692700
C	1.08570200	0.13673400	-1.81338800
H	1.04090500	-0.00087100	-2.89579000
B	-0.49545000	0.52710000	-1.24391400
C	-1.13375700	1.45485200	-2.43393700
C	-2.36779500	1.25693100	-3.05655400
C	-0.45112700	2.60308200	-2.84351100
C	-2.88380200	2.12103100	-4.02170900
C	-0.92493200	3.49148200	-3.80286100
C	-2.15781100	3.24554000	-4.40034800
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C	-2.04576300	2.65047000	1.66103200
C	-0.95985700	3.10179800	2.40596300
C	-1.13216800	-0.97484400	-1.12359200
C	-1.13093300	-1.82946200	-2.23311700
C	-1.62623700	-1.56417000	0.04345100
C	-1.55583200	-3.15183500	-2.20985300
C	-2.06408400	-2.88540500	0.11472200
C	-2.02544500	-3.69129000	-1.01566300
F	-2.42852700	-4.96746100	-0.95733300
F	-2.50290700	-3.39232000	1.28069400
F	-1.71188400	-0.87616400	1.20265500
F	-0.68797900	-1.37175000	-3.43322500
F	-1.51359500	-3.90983400	-3.31792200
F	1.78664800	1.62462100	0.60763700
F	1.38506800	3.13791600	2.72890200
F	-1.14641000	3.87041500	3.48766700
F	-3.29263900	2.98829200	2.02530300
F	-2.91975400	1.41779600	-0.10905900
F	0.75147700	2.89915500	-2.28569100
F	-0.21169100	4.57545600	-4.15382000
F	-2.63942300	4.08363300	-5.32883200
F	-4.07627200	1.87811200	-4.58889300
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H	3.07372000	-3.73018700	1.91728100
H	2.02608600	-4.18764600	3.24525500
C	1.09885100	-4.41118500	1.29157500
H	1.40304800	-5.45382700	1.12900500
H	0.06724500	-4.42976200	1.66220600
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C	3.17661100	-0.42003300	3.17733400
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H	3.64763700	-0.01447200	2.27582700
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H	0.28121700	-1.89900700	4.96355600
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H	3.76789900	-1.57473300	4.94787500
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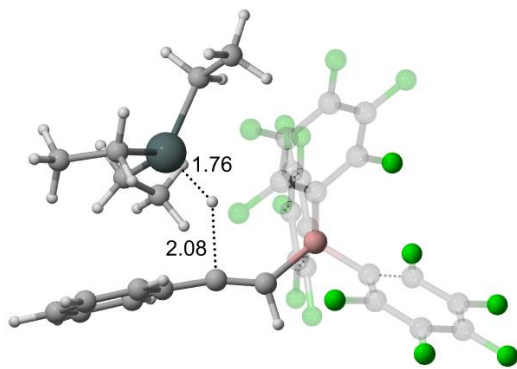
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H	0.95646200	-1.06078900	1.02772800



TS4

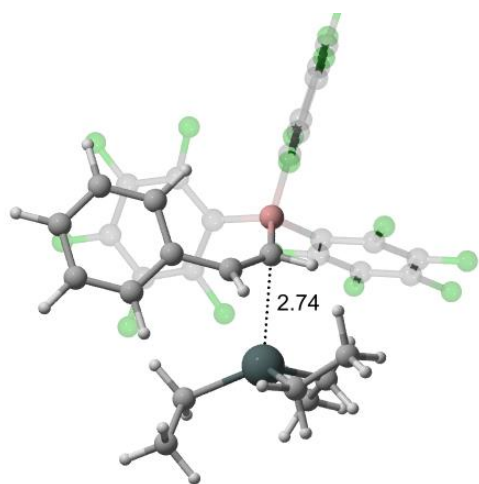
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C	1.64804000	1.15963200	4.25586000
C	2.43141300	0.75715600	5.33194800
C	3.21969200	-0.39479700	5.22707700
H	3.83759100	-2.05250600	3.98459100
H	2.40394700	-1.37003200	2.06912700
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H	3.82670500	-0.70795800	6.07169600
C	0.71363800	0.71484500	2.06438100
C	-0.39834600	0.89654500	1.47300100
H	-0.51883900	1.41161900	0.53109400
B	-1.85605000	0.28592900	2.14809300
C	-2.48401500	-0.65606800	0.95602500
C	-2.98034000	-1.95428400	1.12098600
C	-2.62287500	-0.15950800	-0.34473100
C	-3.50325700	-2.71927900	0.08036300
C	-3.13279900	-0.88578000	-1.41538700
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C	-1.67532200	0.00102600	4.81648200
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C	2.07300600	3.51925800	-2.19914100
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TS4'

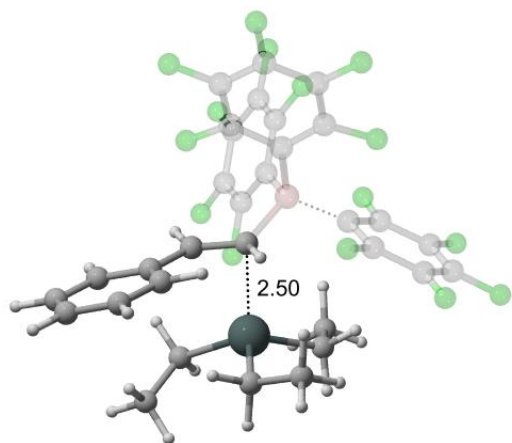
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H	2.08351600	0.65524400	1.36939100	F	-5.47660000	2.36508100	3.29856500
H	4.41601000	-0.04937300	1.91767300	F	-4.94413100	0.71623200	1.25915400
H	5.07646000	-2.42600500	1.65037700	F	-1.26301900	2.33137900	-0.81594500
C	0.17592300	-0.91420000	0.41963200	F	-2.22600000	3.91306600	-2.76451500
C	-0.81519700	-0.37010900	-0.16742300	F	-4.57270600	3.27110700	-4.03059700
H	-0.57762200	-0.12906900	-1.21055400	F	-5.92611100	1.01063600	-3.29811600
B	-2.42435900	-0.07929400	0.23218200	F	-4.99452200	-0.57516800	-1.37235600
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C	-2.42427400	1.95959000	-1.41876100	H	0.14585400	-4.67241000	4.31159100
C	-4.77350400	1.32812400	-2.68637600	C	-0.84370100	-4.85308700	2.38289900
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C	-3.29179500	-3.79803200	-0.73795200	H	3.21736400	-1.14757300	5.32801500
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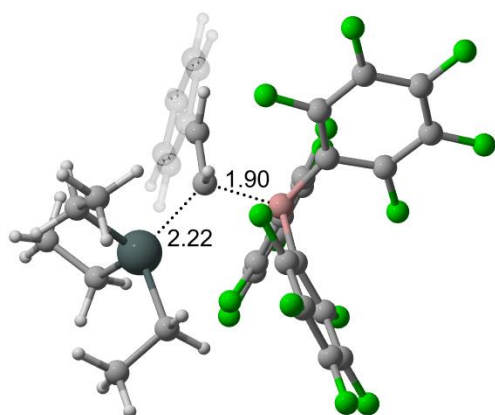
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C	2.94517800	0.94801800	4.69811500
H	4.54365400	0.20907000	3.44692300
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H	-1.11978900	0.86229300	-0.03204200
B	-1.96817800	0.07483000	1.97890100
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C	-4.85514100	2.20891400	3.62220700
C	-4.50892300	3.53069300	3.35104300
C	-1.33891700	-0.79448900	3.23220800
C	-0.60028800	-1.94296000	2.96744000
C	-1.36577100	-0.46660700	4.58968300
C	0.07911300	-2.70747500	3.90318000

C	-0.71037800	-1.19910200	5.57962900
C	0.02606000	-2.32636800	5.23990600
F	0.67825100	-3.02859000	6.17647700
F	-0.74864400	-0.79326000	6.85943900
F	-1.98021400	0.65376900	5.03395400
F	-0.53063400	-2.40169300	1.67765100
F	0.77258600	-3.79977700	3.53380400
F	-1.40675800	3.08253800	1.56530300
F	-2.98546800	5.06027500	2.38179000
F	-5.29801700	4.53630300	3.75606300
F	-5.98281100	1.93992300	4.30091400
F	-4.39867800	-0.07322600	3.51016800
F	-3.26960800	1.07388800	-0.42655500
F	-5.03898300	-0.16165100	-1.98357000
F	-5.87623000	-2.70973300	-1.39991100
F	-4.89635400	-3.96309500	0.82783300
F	-3.16766900	-2.75796800	2.42252000
C	2.13664600	-2.41493400	0.47262700
H	2.19855700	-2.06603900	1.50707700
H	1.77969000	-3.44949000	0.51883300
C	3.50113500	-2.32697200	-0.22513900
H	4.25016400	-2.92105800	0.31316400
H	3.46519900	-2.70590800	-1.25369400
H	3.87569000	-1.29741900	-0.27296200
C	-1.05580500	-2.35502100	-1.38607800
H	-0.86781000	-2.27422200	-2.46597900
H	-1.97064000	-1.79474000	-1.18924200
C	1.36548000	0.04235100	-2.03634400
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C	-1.20733100	-3.82325100	-0.96918200
H	-1.44997200	-3.92149000	0.09130000
H	-2.01782800	-4.29494000	-1.53885900
H	-0.29587200	-4.40319600	-1.15867200
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H	-0.57182600	0.58139100	-2.91841100
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7'

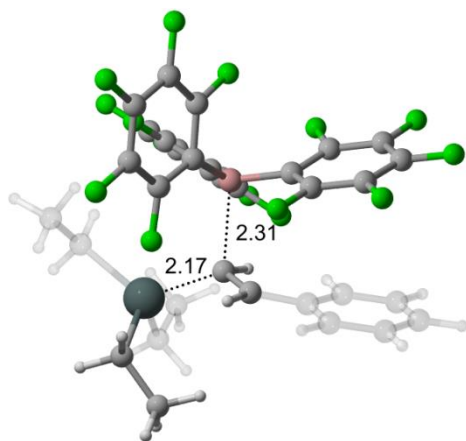
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C	3.74683800	-1.08523500	2.10581900	F	-2.56084700	-2.93735100	0.29172800
H	3.44850700	-3.07007700	2.90160200	F	-3.98743700	-4.82292700	1.47892200
H	1.01626400	-3.08896200	2.41674500	F	-1.61537200	-0.17170700	3.41494900
H	1.30916300	0.89252600	0.79715000	F	-1.20432700	1.75786200	5.19580600
H	3.72869200	0.91027600	1.27975800	F	-2.08323500	4.31382500	4.71518600
H	4.81124200	-1.07076900	2.32204800	F	-3.40142700	4.85867800	2.37932700
C	-0.43933300	-1.18217000	1.27341000	F	-3.83328300	2.96750900	0.58307800
C	-1.19540800	-0.30966600	0.51800900	F	-1.67352800	2.11491800	-1.00338000
H	-0.63038400	0.52749500	0.10574400	F	-2.51676200	2.83799900	-3.42307400
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C	-3.44498900	0.54404100	-0.69203000	F	-6.21061800	-0.09193600	-3.03059200
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C	-5.08664600	0.44482900	-2.52803500	H	-2.51470200	-0.79873900	-2.98270200
C	-3.21254500	1.91902900	-2.73192200	H	-1.56949800	-2.04942000	-3.76458100
C	-4.37738100	1.37898900	-3.27108600	C	-3.29219700	-2.81635700	-2.68509700
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C	-2.93446900	3.62084900	2.61179500	H	1.49530900	-1.32761400	-2.93098200
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TS5

C	2.41506600	1.84513800	4.67219300
C	1.57440600	2.04582000	3.58369000
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C	2.50292600	-0.52808900	4.15931200
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H	2.70770900	2.68342900	5.29667200
H	1.20080600	3.04106500	3.35841500
H	1.35651200	-1.16623900	2.47055700
H	2.87258600	-1.52491400	4.38031200
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C	0.19810400	1.22357600	1.74248400
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H	-1.15907300	0.96123500	0.27632200
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C	-3.22562200	-0.84039000	1.35490700
C	-3.91951400	-1.94984000	1.85791700
C	-3.70602500	-0.39292700	0.11808400
C	-4.94955300	-2.59440700	1.17398100
C	-4.72908400	-1.00308500	-0.59825700
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C	-4.64376600	3.60567400	3.24217700
C	-1.44500800	-0.70492300	3.47200400
C	-1.00152500	-2.02831400	3.40910200
C	-1.16137100	-0.07382700	4.68804800
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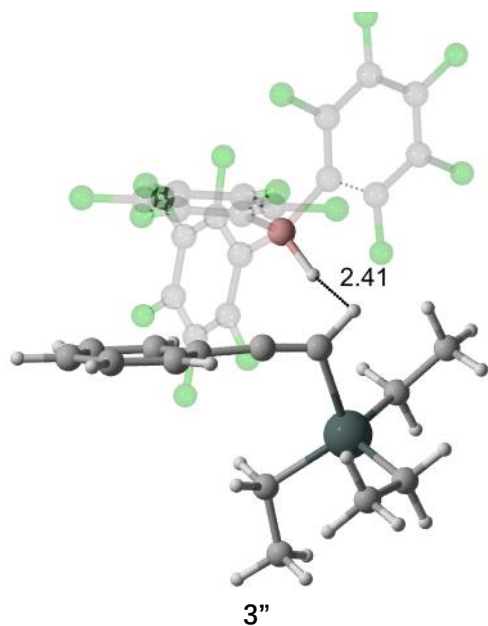
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F	-1.44685900	1.23455000	4.87381500
F	-1.13425300	-2.72628200	2.25109100
F	0.02525600	-3.97583200	4.30382200
F	-1.93573800	2.94863400	0.96238000
F	-3.50898000	4.93858000	1.65302700
F	-5.44152200	4.63030800	3.57169600
F	-5.73572000	2.19216800	4.79585500
F	-4.15267400	0.14672200	4.13090800
F	-3.16309900	0.70250300	-0.47079000
F	-5.10191300	-0.52734500	-1.79802500
F	-6.33870900	-2.73723200	-0.74220700
F	-5.56064100	-3.65983200	1.71504600
F	-3.64511400	-2.45973100	3.07603100
C	1.61033700	-2.67387200	0.56726700
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H	1.47841400	-3.58276000	-0.03500400
C	3.04352500	-2.14716100	0.39597400
H	3.78315400	-2.89481800	0.71150100
H	3.25662500	-1.89955400	-0.65026900
H	3.22601500	-1.24081900	0.98490300
C	-1.52000600	-2.51754100	-1.03112000
H	-2.18910200	-1.84145100	-1.57195700
H	-2.11053500	-2.99040700	-0.24190800
C	0.93792900	-0.18433300	-1.77917200
H	1.66440200	0.51339100	-1.34249200
H	1.51415400	-0.87093400	-2.41379600
C	-0.95651300	-3.57437900	-1.99617200
H	-0.32298000	-4.30469200	-1.47886000
H	-1.76552900	-4.13535200	-2.48156000
H	-0.35423400	-3.12166500	-2.79447100
C	-0.09971900	0.57266400	-2.62241200
H	-0.82128200	-0.11213400	-3.08446800
H	-0.67485000	1.28666700	-2.02101400
H	0.37524500	1.14049000	-3.4333100
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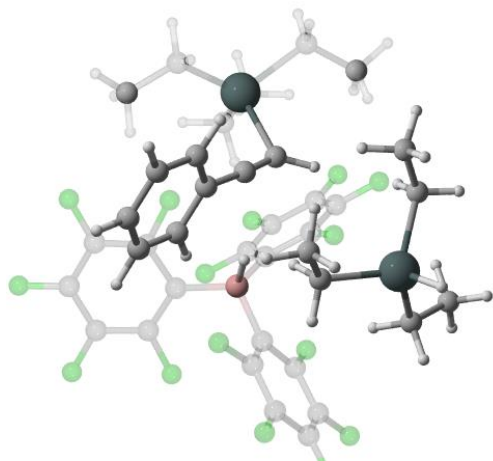
TS5'

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C	1.85116500	1.58288800	2.53913300
C	2.39896300	0.92044200	3.64529300
H	2.59560900	-0.96400200	4.67998900
H	1.19404500	-2.20346100	3.05319700
H	0.64857900	1.41323100	0.77551800
H	2.02595600	2.64600400	2.40081400
H	2.99483600	1.47147400	4.36737400
C	-0.05830600	-1.24929600	0.91575500
C	-0.76458600	-0.76679000	-0.15670300
H	-0.49921100	0.24991200	-0.42630100
B	-2.75232100	-0.01861000	0.76140800
C	-3.16461500	0.75903700	-0.57641700
C	-4.32568100	0.45952600	-1.30748900
C	-2.41812800	1.81828300	-1.11926200
C	-4.72030900	1.14593200	-2.45486900
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C	-3.93768700	2.18504800	-2.94099100
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C	-2.32262000	2.18373800	2.21213100
C	-1.30128100	0.73124600	4.32478900
C	-1.87497900	2.84575500	3.35272000
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C	-4.87494400	-0.87289900	1.86012400
C	-4.36216000	-3.56056000	1.67357400
C	-5.79505800	-1.77291700	2.38141500

C	-5.53556700	-3.13833500	2.28612200
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F	-6.92443100	-1.34412500	2.96365300
F	-5.18147500	0.44222900	1.95709500
F	-2.35158300	-3.13049400	0.59671400
F	-4.09135800	-4.87179600	1.57325200
F	-1.69094900	-1.23926100	3.16743000
F	-0.82562800	0.00812500	5.34986000
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F	-1.97439200	4.18049000	3.44754300
F	-2.91231600	2.96718200	1.28883800
F	-1.25681100	2.20796500	-0.54321600
F	-1.99252300	3.51218500	-2.72102000
F	-4.29134000	2.84360900	-4.04829600
F	-5.84313600	0.79712600	-3.09934500
F	-5.15232500	-0.53833900	-0.93750800
C	-2.96007100	-2.34603600	-2.81990900
H	-3.45915900	-1.38199600	-2.95736500
H	-2.67600200	-2.67442600	-3.83054200
C	-3.91823300	-3.36926400	-2.19566100
H	-4.76172600	-3.57708400	-2.86674300
H	-3.41954000	-4.32293000	-1.98665700
H	-4.34009000	-3.00369300	-1.25656800
C	0.16176700	-0.99657000	-3.34918900
H	0.19467800	-1.63084200	-4.24584100
H	1.19210100	-0.94227100	-2.97503100
C	-0.07769800	-3.92620500	-1.44915500
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C	-0.34216200	0.40780700	-3.71483500
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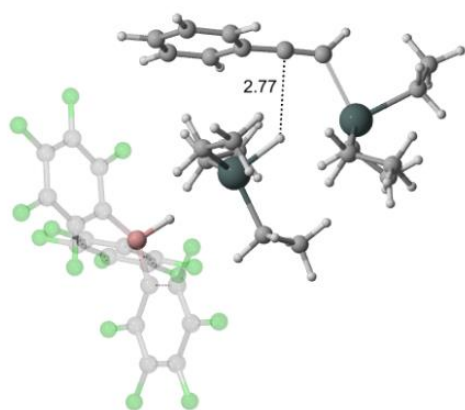
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H	-8.06100800	-5.52483700	-0.69978500	C	-15.83790900	-1.19297900	-3.32205100
C	-10.13045000	-2.49235100	-4.47134400	C	-16.98777500	-1.06331200	-5.82307500
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				F	-12.93822800	-7.43983800	-6.00984500
				F	-12.31894200	-4.86518300	-5.66800100
				F	-15.34369200	-1.22345400	-2.05972700
				F	-17.50869900	0.29205800	-2.49736500
				F	-18.63981900	0.42235300	-4.98731300
				F	-17.53976800	-1.00975100	-7.05105200
				F	-15.36300500	-2.53322300	-6.63615700
				H	-13.19707800	-2.57211400	-5.14613400



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C	-1.45451900	0.39177500	-2.38453500	H	0.88384000	3.69698800	-0.79610400
C	-0.59576700	-0.50069200	-2.53906000	C	-0.05742400	3.63636200	-2.74415600
C	-2.49927900	1.29531800	-2.19376300	H	-1.05341800	3.91932700	-2.37577400
C	-3.23710400	1.77561800	-3.30448100	H	0.41384700	4.54437700	-3.13912700
C	-2.78445000	1.75957500	-0.88642100	H	-0.20534300	2.95771700	-3.59339600
C	-4.26338600	2.68488700	-3.09889300	C	2.82450700	0.82605200	-3.64306200
H	-2.98887700	1.42515100	-4.30115900	H	2.60030000	-0.10595500	-3.11021200
C	-3.80322400	2.68431400	-0.70185900	H	3.86240700	0.72155200	-3.98502300
H	-2.18188200	1.41247600	-0.05795200	C	3.96619800	1.94988300	-0.47566000
C	-4.54417800	3.13732300	-1.80010200	H	4.41665000	2.86937900	-0.08184900
H	-4.84054700	3.05442600	-3.94058900	H	3.25922900	1.59948100	0.28244900
H	-4.01628200	3.05530500	0.29545800	C	1.89715700	1.00799700	-4.85481100
H	-5.34306000	3.85750900	-1.64724000	H	2.12587100	1.93158000	-5.40046900
C	-0.37640700	-3.16295200	-4.49644200	H	1.98895700	0.17849100	-5.57065200
H	-0.72232800	-2.63017400	-5.39014500	H	0.84261200	1.06605100	-4.55815000
H	-0.61028100	-4.22471800	-4.65409500	C	5.04591300	0.88462500	-0.72099200
C	1.13402900	-2.97243200	-4.29638900	H	4.61019800	-0.05212100	-1.08759400
H	1.50162300	-3.47183400	-3.39373900	H	5.78531000	1.21514400	-1.46175200
H	1.69525900	-3.38200200	-5.14552000	H	5.59170400	0.65150300	0.20287200
H	1.40485900	-1.91437700	-4.21878700	C	-1.27564100	-3.69960500	-1.05568500
C	-4.58540900	-1.81937300	-2.21252500	H	-0.69534200	-3.08947200	-0.36258600
H	-5.60752900	-1.66800500	-2.58177100	H	-2.25610000	-3.84332200	-0.58882900
H	-4.61472400	-2.64352400	-1.49207400	C	-0.58493400	-5.04326000	-1.33087800
H	-4.29716500	-0.92381700	-1.65625200	H	-0.44391900	-5.59793500	-0.39515900
C	-3.62492500	-2.10714500	-3.37655200	H	-1.17077700	-5.68323700	-2.00230000
H	-3.97234200	-2.97396600	-3.95495700	H	0.40552000	-4.91237400	-1.77958400
H	-3.60242800	-1.26650200	-4.08190300	B	-0.07930400	0.00621000	1.35887300
H	0.48443500	-0.53514900	-2.57932400	C	0.84269700	1.18545500	1.99982100
H	3.48621700	3.82208100	-3.04193800	C	0.43528500	2.51361100	1.87340800
C	0.79501900	2.99949000	-1.63767400	C	2.07259000	1.02008500	2.63536600
H	0.31182300	2.10674400	-1.22479400	C	1.18191900	3.60508600	2.30040700
				C	2.85794200	2.08037600	3.08594000
				C	2.41393300	3.38584400	2.91043100
				C	-1.49816600	-0.21299700	2.13860000
				C	-1.76783500	0.13810300	3.46267400
				C	-2.58076700	-0.77906100	1.46914300
				C	-3.01009300	-0.03928200	4.07067700
				C	-3.83795100	-0.98116200	2.02710300
				C	-4.05770900	-0.60211100	3.34711600
				C	0.72699900	-1.39611000	1.13501300
				C	0.60750200	-2.54585800	1.91731800
				C	1.59764900	-1.53093000	0.05575300
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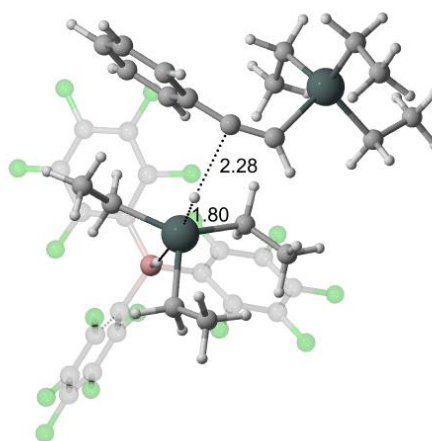
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F	1.82417400	-0.46909500	-0.76917600	C	3.38968900	1.06790400	-5.27425700
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F	1.08963300	-4.82560500	2.41552300	H	3.60401800	2.11625200	-5.03138300
F	-0.79721600	0.66266200	4.24245100	H	4.31620500	0.50386300	-5.11228200
F	-3.20937500	0.32282600	5.34960300	C	2.12192700	-3.33481500	-7.36123300
F	-5.26263600	-0.77871100	3.91404600	H	2.49666700	-3.47811000	-8.38295200
F	-4.83714500	-1.53125500	1.30530700	H	2.61565700	-4.07910900	-6.72572600
F	-2.43784700	-1.18109200	0.16965900	H	1.05380100	-3.59116800	-7.38538200
F	2.57825400	-0.21952100	2.84821300	C	2.37004200	-1.90525400	-6.86576500
F	4.04777400	1.85499800	3.67132600	H	3.44531300	-1.68060000	-6.89272600
F	3.16237200	4.42265500	3.32237700	H	1.89295900	-1.17316500	-7.52986300
F	0.73300000	4.86381400	2.12711300	H	-0.45698900	-2.57931300	-6.29515500
F	-0.77193200	2.79511600	1.30947900	H	0.49634300	-0.96851100	-2.76233600
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Sn	2.80250100	2.45733900	-2.21471400	H	-2.01223500	0.94417000	-1.53278700
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C	-1.39584800	-1.46029300	-4.73040300	H	-0.56099400	-4.36660800	-0.34765800
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C	-2.86754700	-1.61350300	-2.79874000	H	3.44780600	-1.14409600	-1.90797400
C	-3.98416300	0.87167400	-3.50492400	H	4.35247100	-0.67641200	-0.46658400
H	-2.56960600	0.89208700	-5.13359800	C	2.37688100	-3.20239500	-3.66265200
C	-3.88917700	-1.07328700	-2.03273800	H	2.12800200	-3.02859900	-2.61588800
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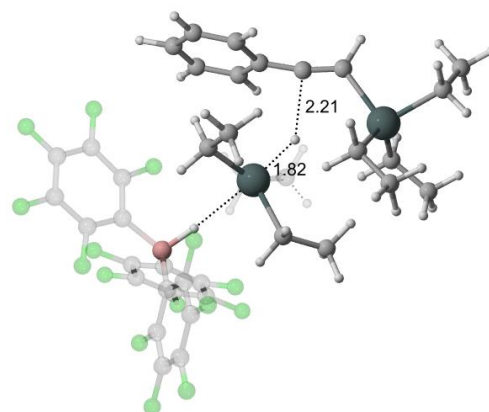
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C	-1.74789400	1.53225900	2.30813800
C	-2.02947100	2.78642900	2.85122500
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C	-3.24235800	3.45380800	2.67237200
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C	-0.41855700	-0.63530600	3.30966400
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C	-0.46430300	-3.11526900	4.72303600
F	-0.49246800	-4.28710900	5.38125300
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F	1.61959200	-1.38837100	2.33066100
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F	-3.44768900	4.66705100	3.21550200
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F	-4.99916200	0.99846500	0.65043500
F	-2.65784600	-0.25311700	1.01585600
F	1.09053200	0.89754600	5.09710900
F	3.22615800	2.41758600	5.62168100
F	4.25268100	4.09147000	3.71310800
F	3.07249400	4.20360300	1.23804600
F	0.93110600	2.69094700	0.68826000
H	-0.08781900	0.35361500	1.28922000
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TS6

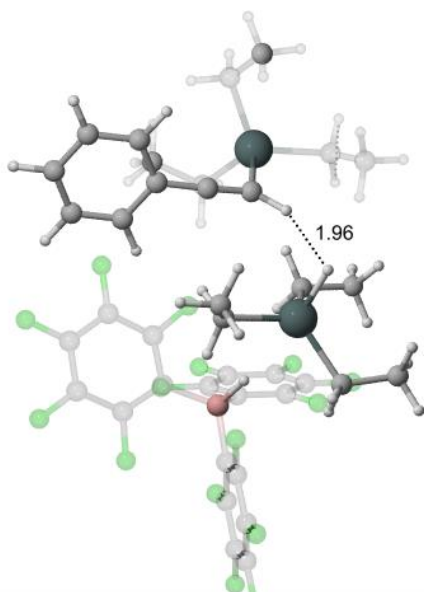
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H	1.42280400	0.87626200	4.73978200
C	0.22894900	0.36238900	2.95992700
H	-0.45506400	-0.43353200	2.63947500
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C	2.54724400	5.79937200	5.67058400

H	1.73017600	5.13860400	5.96936700	C	6.51801000	0.81391200	7.70962100
H	2.99316000	6.17070200	6.59702400	C	5.87725100	-0.30371100	8.23554900
C	2.02669500	6.96166700	4.81465800	F	6.44264100	-1.52072600	8.13980100
H	1.25545800	7.53469400	5.34744200	F	7.70883800	0.67570100	7.09273200
H	2.82952700	7.66432200	4.55808200	F	6.57384100	3.10391700	7.26395200
H	1.58786800	6.61613200	3.87156200	F	2.87925600	1.19149900	9.57957700
C	4.32987600	2.53662800	4.79445100	F	4.02053200	-1.22017100	9.38011800
H	3.44131500	2.06785400	4.35988000	F	2.41170700	5.39001600	10.45041400
H	4.34061700	2.24989200	5.84429500	F	-0.23946400	5.52788900	10.54314100
C	6.02109900	5.67341300	4.77302100	F	-1.78785700	4.08951900	8.79037300
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H	6.56750100	5.21651500	5.60510800	F	2.09060400	2.34871100	6.79004700
C	5.60667100	2.03985200	4.10200300	F	4.76342500	3.17894300	11.19783600
H	6.50112300	2.45253300	4.58001400	F	6.30517000	4.69503400	12.80368300
H	5.69430600	0.94571600	4.15163900	F	7.26521200	7.10362700	11.92248600
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C	6.83986500	5.60638900	3.47564700	F	5.13414200	6.46471200	7.77664300
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H	4.07927100	-2.85413900	2.43292800				
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C	1.56602600	3.14247700	7.76672600	C	1.21462000	2.60189600	4.32754900
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C	4.07301200	1.12309800	8.94409800	C	-0.50434800	4.26678800	4.64750400
C	5.90441800	2.05781600	7.81457200	H	-0.44209200	5.99302200	3.35110700
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TS6'

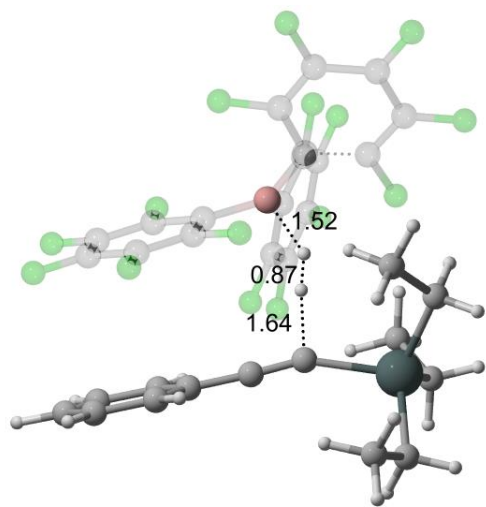
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C	6.19287000	0.93620800	-0.51994100	C	2.36790100	5.78363300	9.33336600
H	6.54507000	0.76576100	-1.54524200	C	2.09193000	7.04033700	9.87360000
H	6.60183000	0.13171300	0.10296600	C	1.30863900	5.22681300	8.61585300
H	5.10182100	0.81241800	-0.53339000	C	0.87846300	7.70801300	9.70001900
C	6.60812600	2.32194400	-0.00273400	C	0.08466500	5.84995300	8.41521300
H	7.70131200	2.42162000	-0.02474300	C	-0.13495400	7.11108100	8.95894900
H	6.21878800	3.11378500	-0.65542800	C	3.73190400	3.62191200	10.31110800
H	3.44917500	2.14638100	0.77993700	C	2.73643000	3.26993000	11.22184600
H	4.28696500	3.33114800	4.26343400	C	4.73887500	2.66660100	10.16213400
C	3.01711300	5.60437000	5.70718500	C	2.72110500	2.06283500	11.91974300
H	1.99430600	5.27320000	5.51322000	C	4.77017800	1.45041200	10.83489500
H	2.99570300	6.15677700	6.64750600	C	3.74416300	1.14170400	11.72294700
C	3.53313800	6.50403900	4.57764300	F	3.74343600	-0.03009100	12.38107900
H	2.85052200	7.34454700	4.38972300	F	5.76810200	0.56861900	10.62858700
H	4.50992500	6.93381600	4.82826500	F	5.77190600	2.90639300	9.30952700
H	3.65021700	5.95887200	3.63196400	F	1.71524600	4.11836100	11.49121000
C	3.48906700	2.05293300	6.87220300	F	1.72711100	1.77817000	12.78118700
H	2.39793500	2.08342000	6.80792200	F	3.01206000	7.68691900	10.62432300
H	3.72032400	2.08891700	7.93849700	F	0.67795400	8.92306500	10.24049100
C	6.32685400	4.32874300	6.42239400	F	-1.30958000	7.73789300	8.77111600
H	6.57544500	5.26304600	5.90462200	F	-0.89015800	5.25089300	7.69060700
H	6.36660300	4.54985400	7.49184500	F	1.44715900	3.99412400	8.05655100
C	4.04233600	0.76798400	6.24545100	F	5.23917400	5.17596900	12.08033200
H	5.12713100	0.68723800	6.38246900	F	7.37366500	6.70749000	12.57515600
H	3.59528500	-0.12488500	6.70302900	F	8.37506600	8.37334400	10.64672700
H	3.84969900	0.71584700	5.16548600	F	7.17001900	8.46678900	8.18301100
C	7.33876400	3.23092300	6.07708900	F	5.02871200	6.94367000	7.66363200
H	7.11839200	2.29541500	6.60426500	H	4.01708300	4.61349700	8.28609400
H	7.35184100	3.01035900	5.00440700	Sn	4.26126800	3.87363800	6.00342000
H	8.35785300	3.52746800	6.35935900	Sn	5.96278100	2.71477600	2.01791800
C	6.43626700	1.00428500	3.22630800				
H	6.09522900	1.17845400	4.24787200				
H	5.84320800	0.17016500	2.83149900				
C	7.93506900	0.66314200	3.19264700				
H	8.14011400	-0.24510400	3.77293600				
H	8.29377600	0.48519700	2.17143800				



8''

C	-0.66990200	-1.94691800	3.78170800	H	-0.36230400	-3.85846800	0.41669900
C	0.09979900	-2.63693200	3.08630600	C	-1.85616500	-1.18874000	0.60113300
C	-1.40068800	-1.08462800	4.60665500	H	-1.28992300	-0.63765000	1.35892900
C	-1.77001600	0.19294200	4.12017300	H	-2.27061600	-0.44019000	-0.07622500
C	-1.76031900	-1.48086500	5.91894100	C	-2.98213200	-2.01198600	1.23866200
C	-2.47444400	1.06392300	4.94011400	H	-3.65021900	-1.38544400	1.84698400
H	-1.49597300	0.47705700	3.11299900	H	-3.60295400	-2.48998300	0.47165400
C	-2.46709400	-0.60029000	6.72583900	H	-2.60340300	-2.81394000	1.88557100
H	-1.47510600	-2.46512400	6.27639900	C	1.61772300	-1.65540300	-0.27856900
C	-2.82081200	0.66720600	6.23781500	H	1.82605800	-1.64881300	0.80045600
H	-2.74638700	2.04805300	4.57218200	H	1.66503100	-0.61180900	-0.59547100
H	-2.74622200	-0.89182400	7.73345500	C	-0.98619700	-2.92240500	-2.50811300
H	-3.37167600	1.35119700	6.87708800	H	-2.06541300	-3.11543900	-2.49428500
C	2.39579700	0.07122400	3.27756300	H	-0.83181600	-2.05158200	-3.15101200
H	1.72800400	0.29541600	2.44146800	C	2.66984200	-2.49268700	-1.01824500
H	3.41316300	0.25918000	2.91164900	H	2.52192200	-2.43993800	-2.10120800
C	2.07656700	0.95823000	4.49109800	H	3.68887100	-2.13171900	-0.81870000
H	2.75483700	0.76763300	5.33142800	H	2.63340100	-3.55201800	-0.73364500
H	2.16680400	2.01686400	4.22285700	C	-0.22154400	-4.14039000	-3.04601800
H	1.05241000	0.80603400	4.84892100	H	0.85374600	-3.94145300	-3.12052000
C	2.63430300	-4.71975900	2.14519700	H	-0.35076600	-5.02093600	-2.40414600
H	3.31090600	-5.41449100	1.63277500	H	-0.57054200	-4.41289900	-4.05105900
H	2.22188200	-5.24512600	3.01473800	C	2.18207200	-2.47179000	5.79790100
H	1.81076300	-4.50982700	1.45557100	H	3.16177700	-2.21994500	6.22475700
C	3.38404500	-3.44129900	2.54200000	H	1.46482100	-1.78116700	6.25893600
H	4.25600700	-3.68281700	3.16467800	C	1.81743100	-3.93116300	6.11127700
H	3.75535600	-2.92011700	1.65428800	H	1.78268300	-4.10903700	7.19342300
H	0.04305900	-3.34778200	2.26007600	H	0.83614100	-4.20091200	5.70243700
				H	2.54860600	-4.63163700	5.69086200
				B	-0.51210300	1.21942500	-2.00075800
				C	-1.45027000	1.23724300	-3.33085000
				C	-2.56729100	0.40795200	-3.42948700
				C	-1.21752600	2.02722200	-4.45660600
				C	-3.38550000	0.33134100	-4.55135000
				C	-2.00632600	1.98753200	-5.60493600
				C	-3.09859000	1.12792400	-5.65556100
				C	-1.09353400	2.10015900	-0.74916100
				C	-2.23439800	2.90482500	-0.75314800
				C	-0.46461300	2.02055600	0.49398900
				C	-2.72906500	3.55908700	0.37884400
				C	-0.89948200	2.67192600	1.63895300
				C	-2.05810400	3.43928400	1.58867500
				C	1.05139100	1.52965800	-2.34836400
				C	1.76257600	2.68113300	-2.01412400

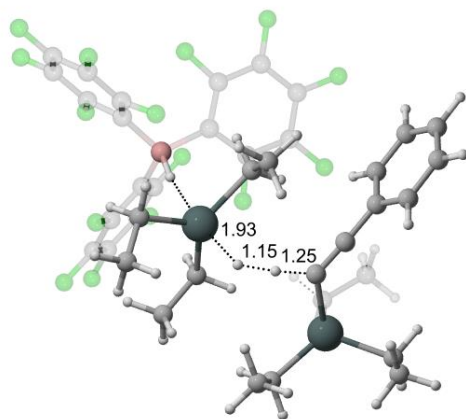
C	1.80409100	0.56243700	-3.01560600	C	-3.30780500	-1.22034400	1.76501400
C	3.11823700	2.85810300	-2.28332500	H	-2.08764300	-0.59121300	0.09923900
C	3.15759400	0.69130200	-3.31003300	C	-3.31991400	-1.81210500	3.03236100
C	3.82551400	1.85218200	-2.93348800	H	-2.13025600	-2.68340400	4.60916700
F	5.13606700	2.00050100	-3.19712600	H	-4.23554300	-0.88120000	1.31349800
F	3.82752600	-0.29326100	-3.94165500	H	-4.25793300	-1.93075400	3.56662800
F	1.21311800	-0.59461600	-3.41357900	Sn	3.18106500	-1.57193900	-0.67612300
F	1.14200400	3.71726700	-1.39762100	C	3.42614600	-3.67281600	-0.27764800
F	3.75249200	3.99000100	-1.92122600	C	3.51648400	-3.99417200	1.22246000
F	-2.94461800	3.09899600	-1.88569900	H	4.32760900	-4.01725000	-0.80104000
F	-3.84861900	4.30109200	0.31151600	H	2.57881100	-4.19958100	-0.73377800
F	-2.51828500	4.04682300	2.70226900	H	3.61739500	-5.07356800	1.39569000
F	-0.22161900	2.55657000	2.80866000	H	4.38110000	-3.50698200	1.68951200
F	0.65608700	1.26084000	0.63633700	H	2.62096100	-3.65707300	1.75783900
F	-0.19198000	2.91253900	-4.47138700	C	4.76769300	-0.38469400	0.16295400
F	-1.72702400	2.77208500	-6.66247300	C	4.60442500	-0.04614200	1.65309900
F	-3.87135600	1.07159900	-6.75392500	H	4.84865200	0.53120000	-0.43177900
F	-4.44830300	-0.49683200	-4.58009300	H	5.70000200	-0.94135200	-0.00038800
F	-2.92916800	-0.36958200	-2.37400100	H	5.44672200	0.55863500	2.01425300
H	-0.52176000	0.07328500	-1.59629800	H	3.68835400	0.51940800	1.84395900
Sn	-0.41634300	-2.34286200	-0.52030600	H	4.55926600	-0.94854100	2.27413500
Sn	2.25027000	-2.02224900	3.69816100	C	2.77078200	-1.07674600	-2.73055100



TS2''

C	0.33634800	-1.29560600	0.98474300	C	-0.36904900	2.40033500	-1.38289700
H	1.57482400	1.41655600	0.35836300	C	0.79219000	4.44190700	-1.18761900
C	1.39941000	-1.07795700	0.39724900	C	-0.82382600	2.74314200	-2.64842000
C	-0.89638700	-1.47436500	1.66826600	C	0.34959300	4.83237900	-2.45007600
C	-0.91593300	-2.06721800	2.94784200	C	-0.45831600	3.97394700	-3.18920900
C	-2.10701000	-1.05475100	1.07910700	C	-0.04078800	2.25166900	1.92020800
C	-2.12341300	-2.23677300	3.61945500	C	0.37804900	1.46332400	2.99841700
H	0.01909400	-2.37518500	3.40469400	C	-1.40844500	2.54266000	1.90126300

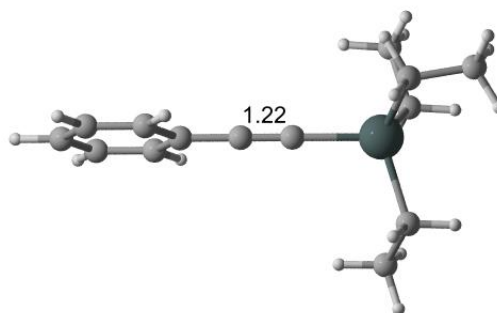
C	-0.47440900	0.99350900	3.98822200	H	-1.47135300	5.30305200	4.77286500
C	-2.29890000	2.08120200	2.86650400	C	5.87962800	4.50924700	1.91737600
C	-1.82906300	1.30253800	3.91898300	H	5.44825200	4.79830500	0.95325000
B	0.99695900	2.74092100	0.81721500	H	6.96316800	4.66112900	1.83281800
F	-0.75904300	1.19822300	-0.90090000	C	5.29447500	5.36961100	3.04739400
F	-1.60425100	1.90614300	-3.35038900	H	5.76166400	5.14696600	4.01415900
F	-0.88508900	4.32793700	-4.40677200	H	5.44234400	6.43684500	2.84382800
F	0.69496300	6.02483300	-2.95768600	H	4.21521800	5.21381900	3.15922900
F	1.55905200	5.33139500	-0.52263900	C	5.72259600	-0.24275500	0.59859800
F	3.46046900	2.59732200	-0.68720600	H	6.30245800	-0.92175700	-0.03934300
F	5.86628200	3.49090500	0.11563400	H	5.44934200	-0.79734600	1.50387100
F	6.12683100	4.76524800	2.52500900	H	4.79591800	-0.00563900	0.06603400
F	3.93371000	5.12209700	4.11679900	C	6.53020100	1.02408400	0.92377900
F	1.53046800	4.21818500	3.34355200	H	7.46894400	0.76133400	1.42914600
F	1.67869500	1.11577100	3.10987000	H	6.80787300	1.54976400	0.00464700
F	-1.93635700	3.31390100	0.92757300	H	3.20514600	1.77827800	0.49954800
F	-3.60573600	2.37724400	2.79082500	H	2.99660600	1.45186100	-0.57831600
F	-2.67253400	0.85734900	4.85657500	C	1.29138000	3.78299400	-0.72485900
F	-0.00880300	0.24016900	4.99705500	H	1.77135900	4.27872400	0.12195300



TS6''

C	2.46624200	2.79259200	2.30134400	H	6.85038300	2.42087800	-2.45326100
C	3.37669500	2.24547900	1.64647500	H	5.61845000	1.18631100	-2.15513800
C	1.43512000	3.45522600	2.98938100	C	2.73858000	0.23052900	-3.63455500
C	1.25652900	4.84655400	2.80117700	H	3.82677000	0.25604400	-3.75802400
C	0.55839800	2.74139100	3.83890200	H	2.52358500	-0.34597000	-2.72687100
C	0.21511400	5.50389000	3.44494200	H	2.32744700	-0.32889600	-4.48519600
H	1.93865800	5.39194100	2.16083300	C	5.48892300	1.83344700	4.27530900
C	-0.48117000	3.41059900	4.47393600	H	6.50902200	1.93768500	4.66748400
H	0.70184300	1.67422700	3.97500800	H	4.87528500	2.56867300	4.81071500
C	-0.65459400	4.78724800	4.27608900	C	4.96136900	0.41059600	4.51715000
H	0.07921600	6.57068900	3.29488800	H	4.93557200	0.17174600	5.58805100
H	-1.16089900	2.86457500	5.12095600	H	3.94353600	0.28745600	4.12807500

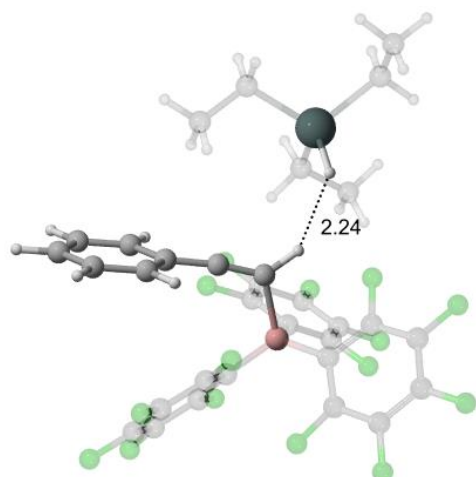
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B	2.64345900	5.83969200	-3.55773900
C	1.63238900	5.76266500	-4.82592100
C	0.53214300	4.90715600	-4.82677000
C	1.78524600	6.51087700	-5.99357600
C	-0.34603400	4.76662200	-5.89570700
C	0.93320400	6.40809400	-7.09125400
C	-0.14019200	5.52400800	-7.04472500
C	2.11675100	6.75106800	-2.31102800
C	0.96704100	7.54357900	-2.30432000
C	2.77642100	6.69935900	-1.08197200
C	0.48617400	8.20207600	-1.16972100
C	2.34440200	7.34141300	0.06862000
C	1.17489000	8.09260000	0.03189400
C	4.17819700	6.11793800	-4.00952900
C	4.91410400	7.27421400	-3.75542500
C	4.87204200	5.13011100	-4.70888600
C	6.24400800	7.43840900	-4.13842700
C	6.19748600	5.24517200	-5.11288100
C	6.89406500	6.41382400	-4.81929700
F	8.17714400	6.55125400	-5.19132700
F	6.81264900	4.24262300	-5.76789700
F	4.24583200	3.96344500	-5.01807400
F	4.34495400	8.32346600	-3.11682600
F	6.90608100	8.57519400	-3.85823100
F	0.23337400	7.71361900	-3.42547700
F	-0.64012200	8.93301500	-1.22567600
F	0.72115800	8.69642000	1.14573200
F	3.02557400	7.21426400	1.23174100
F	3.90443200	5.95072200	-0.95224800
F	2.78722900	7.41471600	-6.09898600
F	1.13366200	7.15412500	-8.19171500
F	-0.97126800	5.40720200	-8.09263600
F	-1.38690100	3.91515900	-5.82967500
F	0.25255800	4.16442800	-3.72133900
H	2.66711600	4.68506900	-3.10141500
Sn	2.81617300	2.83153200	-1.91219700
Sn	5.50591200	2.41233600	2.20455400



P3

C	-0.72166800	1.13419800	-0.02068000
C	-2.14911100	1.15838800	-0.05987500
C	-2.82829400	1.32762200	-1.28289200
C	-2.90069900	1.01373300	1.12325100
C	-4.22162700	1.35082900	-1.31770200
H	-2.25143000	1.43948900	-2.19582000
C	-4.29381800	1.03786700	1.08020300
H	-2.37971800	0.88345000	2.06679300
C	-4.95932400	1.20626000	-0.13831600
H	-4.73344500	1.48205100	-2.26729300
H	-4.86196700	0.92513100	1.99965600
H	-6.04527900	1.22469600	-0.16861000
C	0.50132200	1.11342800	0.01220600
Sn	2.59522800	1.07868800	0.04613800
C	3.19664900	-0.95164400	-0.34823900
H	2.85303300	-1.57123100	0.48979100
H	4.29355700	-0.99681300	-0.34016000
C	3.25448700	1.78040200	1.97253600
H	2.71972600	2.71354800	2.18881700
H	2.93330900	1.05732200	2.73259700
C	3.25760300	2.43073900	-1.49374900
H	4.35222900	2.37504300	-1.55756500
H	2.87116000	2.06642200	-2.45377000
C	2.80389100	3.87848500	-1.24749100
H	3.13693900	4.55000400	-2.05029600
H	1.71099500	3.94995100	-1.19052100
H	3.20643300	4.27293200	-0.30579100
C	2.64366900	-1.49262900	-1.67653200
H	3.00445000	-0.90771500	-2.53204100
H	2.94482200	-2.53533200	-1.84486600
H	1.54778200	-1.45869500	-1.69549800
C	4.77419600	2.00092100	2.04374500
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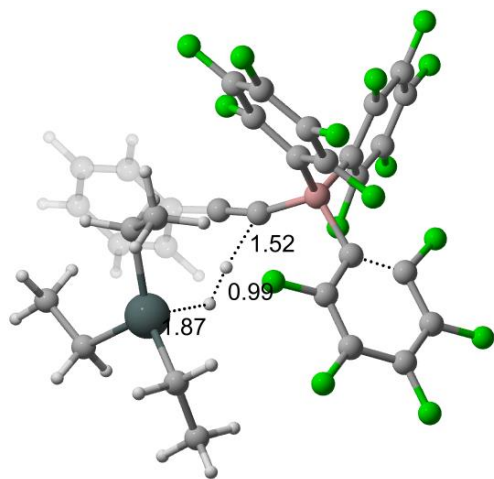
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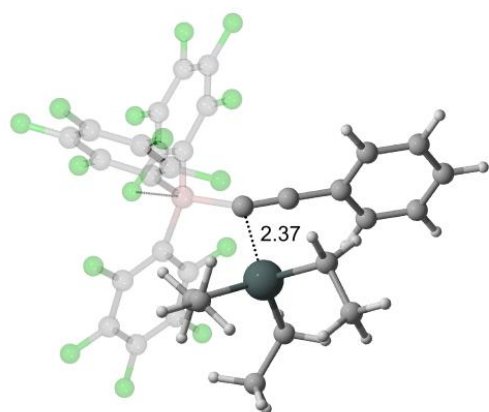
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 C 2. 08190000 -0. 20535200 2. 56427200
 C 3. 21903800 -0. 79517600 3. 09798400
 C 3. 43083100 -2. 17220800 2. 94262000
 H 2. 68429500 -4. 03669800 2. 14357500
 H 0. 63264300 -2. 99496200 1. 18510300
 H 1. 89143400 0. 85480100 2. 67958500
 H 3. 94074800 -0. 19129700 3. 63905200
 H 4. 32045400 -2. 62808800 3. 36830300
 C -0. 01944400 -0. 43187300 1. 34883800
 C -1. 13467900 0. 03690000 1. 01908100
 H -1. 45625500 0. 46357400 0. 07793200
 B -2. 42451900 0. 08560500 2. 28458400
 C -3. 71897700 -0. 51498800 1. 49929500
 C -4. 56943800 -1. 49856200 2. 01829500
 C -4. 09893200 -0. 05170400 0. 23339700
 C -5. 67113200 -2. 00863200 1. 33333000
 C -5. 18218300 -0. 53318100 -0. 49006600
 C -5. 97777100 -1. 53103200 0. 06453300
 C -2. 51212700 1. 68041000 2. 60439100
 C -1. 38898400 2. 41338100 3. 00368800
 C -3. 68717400 2. 43792300 2. 53496400
 C -1. 39585200 3. 77344500 3. 28101900
 C -3. 74422100 3. 80303200 2. 81285400
 C -2. 58893600 4. 48125600 3. 18080500
 C -1. 92188600 -0. 83437100 3. 53317100
 C -1. 55653400 -2. 16982800 3. 33038100
 C -1. 79350500 -0. 40460100 4. 85572900

C -1. 04805300 -3. 00259900 4. 31748400
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 F -0. 41075000 -3. 29373800 6. 58307600
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 F -2. 17072800 0. 83813700 5. 22883800
 F -1. 70190600 -2. 72767000 2. 10114300
 F -0. 68765900 -4. 26723200 4. 03297200
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 F -4. 87056200 1. 86846700 2. 21869300
 F -3. 41306800 0. 96645300 -0. 35081100
 F -5. 47670800 -0. 03445100 -1. 70136100
 F -7. 03066600 -2. 01185100 -0. 60781000
 F -6. 44163400 -2. 95478200 1. 89228100
 F -4. 38546000 -1. 99907900 3. 25971600
 C -0. 29691600 3. 49780000 -0. 40014200
 H -0. 13959200 2. 88771800 0. 49718700
 H 0. 47059300 4. 28304800 -0. 37298400
 C -1. 69966100 4. 12562100 -0. 38378700
 H -1. 83252500 4. 79086100 0. 47817400
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 C 2. 16976700 1. 69569400 -2. 16756700
 H 2. 77865800 2. 60778700 -2. 22161800
 H 2. 36550900 1. 13891400 -3. 09253800
 C -0. 43816700 3. 34151000 -3. 94533600
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 H 3. 64062700 0. 58862300 -0. 96530500
 H 2. 39552900 1. 39803200 -0. 00789800
 C -0. 16023600 2. 54329600 -5. 22945800
 H 0. 90313800 2. 29107800 -5. 32767500
 H -0. 72300200 1. 60170600 -5. 24808800
 H -0. 44396200 3. 10963000 -6. 12651800
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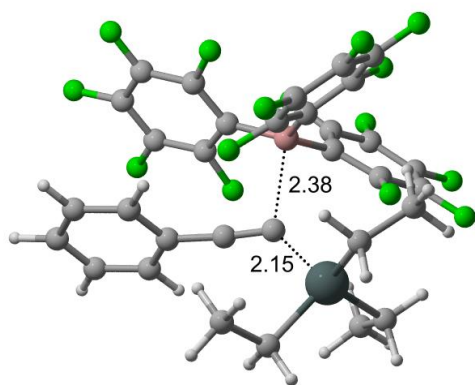
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C	2.53772900	0.40525600	2.46746200	F	-3.55273600	-1.12126700	7.25925900
C	3.91345300	0.19877100	2.41240000	F	-3.53128300	0.64741400	5.27776600
C	4.43080700	-0.89828400	1.71408400	F	-1.71206200	-2.67281200	2.37780800
H	3.97841100	-2.65171800	0.53808700	F	-1.72855300	-4.42235300	4.40074400
H	1.51231300	-2.32165500	0.67408300	F	-0.41382800	1.69747400	3.98245900
H	2.11855700	1.24949700	3.00533000	F	-0.52987500	4.26168800	4.66500400
H	4.58373900	0.89427300	2.90859700	F	-2.78040500	5.74565000	4.16196800
H	5.50521000	-1.05212000	1.66922200	F	-4.92143900	4.56000400	2.92867700
C	0.26610300	-0.30671500	1.92023100	F	-4.83264000	2.00552900	2.20677300
C	-0.94057300	-0.04736300	1.92205100	F	-2.64508900	1.67642800	0.01426300
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C	-4.44852500	-1.20661000	1.21224800	F	-4.63156100	-2.02503400	2.26957400
C	-3.48094200	0.59597800	0.08074200	C	0.35708900	3.29990600	0.46140300
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C	-5.22241300	-0.64072600	-1.00117600	C	-0.75782900	4.34926700	0.58858800
C	-2.58187800	1.72144900	2.96535500	H	-0.59014200	4.98531000	1.46585500
C	-1.54413500	2.36955500	3.64125900	H	-0.80453100	5.00687000	-0.28761000
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C	-2.56242500	-0.90031700	3.72691800	C	-1.22599300	2.51178500	-2.78533600
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				H	3.43513300	2.49994800	-0.83359700
				C	-1.44713300	1.36757500	-3.78692400
				H	-0.51693000	1.07942200	-4.29203300
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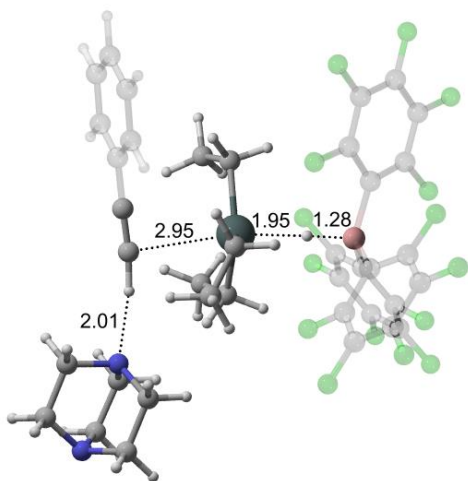
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H	-0.53605100	0.44625700	-4.99771900	C	-3.13654500	0.11376700	0.91242900
C	0.89594200	-0.35196100	-6.40898600	C	-4.15467200	1.00771600	1.22208500
H	0.43191200	0.11445700	-7.27274600	C	-4.20049900	2.24015800	0.57384200
C	2.04031100	-1.14283500	-6.56773900	C	-3.22782000	2.54153500	-0.37121200
H	2.46345600	-1.28565600	-7.55800800	C	-2.23028300	1.60896200	-0.64900200
C	2.64027100	-1.75567000	-5.46128800	C	-0.00775900	-1.18243000	0.87696500
H	3.52353500	-2.37336500	-5.59283200	C	0.02983700	-0.60281700	2.14682800
C	2.09951700	-1.58062400	-4.19078600	C	0.96309500	-0.94364900	3.12719200
H	2.54389400	-2.05706200	-3.32273000	C	1.92529800	-1.90865300	2.85807400
B	-1.03812000	-0.80707200	-0.35331800	C	1.93345200	-2.51939400	1.60773600
F	-1.46661900	-3.55387900	0.94620700	C	0.98379900	-2.14840500	0.66441300
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F	-5.08654500	0.70159100	2.13803500	C	0.93523200	2.27027800	0.57204600
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F	1.04893700	-2.79784500	-0.52395300	H	3.38273600	0.10020300	1.35808200
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				H	3.23058700	3.97882600	-3.67107200
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TS5''

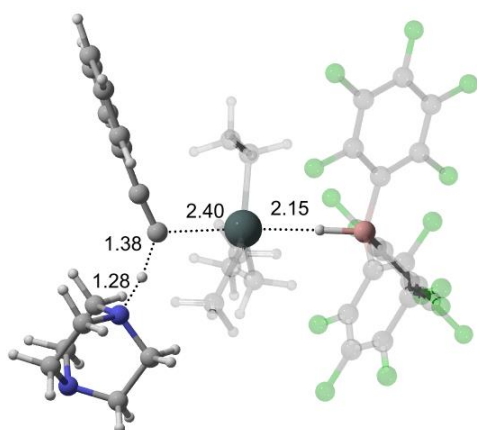
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C	0.46974000	-0.71107000	2.11298200	F	-2.50335400	-1.83439600	2.07913100
C	1.12160800	-0.18853000	3.25108900	F	-1.62884400	-3.47585800	3.98634500
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H	1.47710100	-3.95958800	2.36334700	F	-2.62233000	6.78784000	3.06529600
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H	1.00743500	0.86190800	3.49110200	F	-5.16573900	2.92486300	2.29823500
H	2.36067500	-0.63035500	4.94992500	F	-3.63818100	2.15663000	-0.27980000
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C	-0.36673000	0.12465700	1.33432600	F	-7.20209600	-0.77522400	-1.09909000
C	-1.14610500	0.87720000	0.73610500	F	-6.86877800	-1.88259400	1.38002500
B	-2.90801400	1.05282700	2.32665600	F	-4.95001800	-1.03019000	3.00116500
C	-4.09594700	0.53097500	1.39887700	C	1.32877800	1.61350100	-1.33399900
C	-5.00511400	-0.46698500	1.77736800	H	1.43241100	0.52776400	-1.45725900
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C	-2.80204900	2.63298900	2.53047300	H	1.95162200	1.66368200	0.76464800
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F	0.39103300	-1.08601400	2.08053800	H	-3.14074600	-1.58431500	3.36874700
F	1.18189000	-0.52546800	4.58720300	C	-4.04460400	1.30574700	0.41293200
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				C	-2.76260900	5.70082900	-1.31657800
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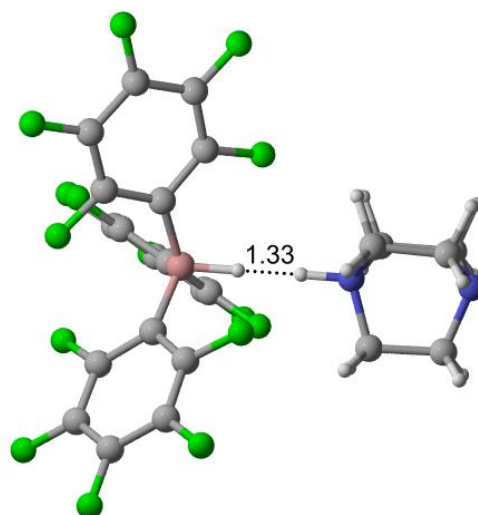
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H	-2.55296600	-1.98795600	-1.83464100	C	4.09928000	0.97936000	-3.35418000
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H	-1.00337300	2.94598800	1.10241400	C	3.71887100	2.31713900	-3.37208400
H	0.30849600	1.87922600	1.55821700	F	3.65385400	-5.19636900	0.35845500
C	-1.49024700	1.60526300	2.75323300	F	3.90488900	-2.61341900	1.00543000
H	-1.26925300	0.58977600	3.09638100	F	1.82191200	-5.99657800	-1.51045200
H	-1.16998400	2.29423100	3.54573100	F	0.22690200	-4.12516200	-2.72968900
H	-2.57688200	1.69711900	2.65646400	F	0.46062800	-1.52773600	-2.09352400
C	-1.25527100	1.43194000	-2.20056500	F	0.98290300	-1.15895700	2.36106900
H	-0.24301200	1.28539700	-2.59000100	F	1.82219100	-0.60699000	4.84933700
H	-1.40457100	2.51206700	-2.10576100	F	4.15126600	0.79142300	5.24465300
C	-2.28311000	0.81126000	-3.15555900	F	5.61215500	1.61678200	3.08209300
H	-2.29344600	1.35207000	-4.11053600	F	4.79560200	1.07744800	0.59632700
H	-2.04525300	-0.23426500	-3.37095100	F	1.66849400	2.46587900	-0.40199000
H	-3.29915600	0.84326300	-2.74919200	F	2.51517600	4.09289800	-2.36240800



TS7

B	2.21327000	-0.36157100	-0.11991000	H	-5.10287400	-2.88237700	4.17273300
C	2.16984800	-1.94293600	-0.49015100	H	-4.63435700	-1.58621900	5.27796400
C	1.27128100	-2.40989800	-1.44908700	N	-4.67477600	-0.19200900	2.41641900
C	2.96346400	-2.93366300	0.08821600	C	-5.83487100	-0.77528900	1.68920200
C	1.13202700	-3.74567300	-1.80706500	H	-5.44177500	-1.50233600	0.97392700
C	2.86430100	-4.28571100	-0.23743800	H	-6.30334100	0.03567300	1.12413500
C	1.93740000	-4.69777300	-1.18949100	C	-5.14536700	0.88451300	3.33095500
C	2.82647500	-0.04235300	1.35142200	H	-5.55883000	1.68313200	2.70824500
C	4.00856200	0.65192200	1.61016900	H	-4.26559300	1.28041200	3.84477500
C	2.13961300	-0.45341900	2.49370400	C	-3.98759900	-1.25498300	3.19767300
C	4.46657800	0.93852700	2.89632000	H	-3.09133600	-0.81641800	3.64340700
C	2.55111200	-0.19136300	3.79416200	H	-3.67520300	-2.02799300	2.49271600
C	3.73031300	0.51871700	3.99907000	C	-3.33046100	1.16545800	0.59106400
C	2.79933700	0.57720700	-1.30849700	C	-3.60364200	2.19759100	-0.03495600
				C	-3.80424100	3.38616800	-0.79023300

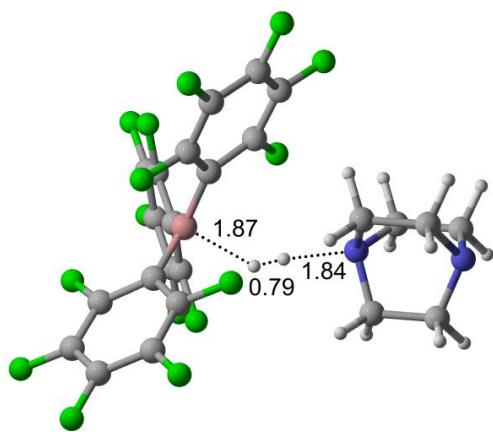
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H	-4.90217100	2.40741900	-2.37070700
C	-4.65954500	4.51590900	-2.76212700
H	-5.19401900	4.48245100	-3.70708500
C	-4.12228500	5.72349500	-2.30284500
H	-4.24085800	6.62821900	-2.89224700
C	-3.42808000	5.76759400	-1.08888200
H	-3.00611200	6.70412000	-0.73619900
C	-3.27016800	4.60905900	-0.33260200
H	-2.72752700	4.63031400	0.60748800
H	-3.92409600	0.37219900	1.54902900
Sn	-1.04997500	0.53342500	0.19004500
C	-1.44355000	-1.54736500	0.56834200
H	-1.69217400	-1.61872400	1.63240200
H	-0.50002300	-2.08316100	0.44504500
C	-2.53716500	-2.16833000	-0.30745200
H	-2.77402800	-3.19235200	0.01400500
H	-3.46652800	-1.58557700	-0.28427800
H	-2.22022500	-2.22573400	-1.35360700
C	-0.39448000	1.78718000	1.81070100
H	-0.64843900	2.81396100	1.52068400
H	0.69570500	1.73310800	1.85011300
C	-1.00738000	1.44372400	3.17237400
H	-0.75948200	0.42213900	3.48233600
H	-0.63751000	2.11735700	3.95677700
H	-2.09960000	1.53878100	3.14926800
C	-0.96880600	1.27459100	-1.82368900
H	0.05199600	1.12917200	-2.18494500
H	-1.13573400	2.35641400	-1.75883400
C	-1.97029800	0.62511100	-2.78742400
H	-1.94557500	1.12189700	-3.76648000
H	-1.73590600	-0.43134300	-2.95144200
H	-2.99855100	0.68541100	-2.41419200



10

B	-0.22626900	-0.11696800	0.49322400
F	1.34660000	2.30058900	0.14530000
F	2.19718800	3.96051100	2.06976300
F	1.56105800	3.48705100	4.69765500
F	0.05518300	1.29816600	5.34938100
F	-0.80971200	-0.37774300	3.44315000
F	-2.61542800	-1.78551700	1.28492000
F	-2.55120100	-4.39733800	1.88708700
F	-0.18635600	-5.77235700	1.86281800
F	2.13524400	-4.46366500	1.20551300
F	2.09877100	-1.85379000	0.59794400
F	-2.64318800	1.33080800	1.57319000
F	-4.72816500	2.17329100	0.11256300
F	-4.81750400	1.70668000	-2.58149700
F	-2.74759400	0.37370000	-3.79520200
F	-0.65147500	-0.47753900	-2.35922800
C	0.22925100	0.87019000	1.70351400
C	0.99312700	2.00423000	1.43603700
C	1.45035600	2.89024600	2.40559100
C	1.13273700	2.65180400	3.73895700
C	0.36832000	1.53466800	4.06501400
C	-0.06360100	0.67745400	3.05456900
C	-0.26809900	-1.69051800	0.90396100
C	-1.41744000	-2.40555700	1.24450700
C	-1.41245900	-3.76146700	1.56688800
C	-0.21145100	-4.46576400	1.55890300
C	0.96362300	-3.79825900	1.22834400
C	0.90353300	-2.44445200	0.91586800
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C	-2.62013300	1.07636700	0.24809400

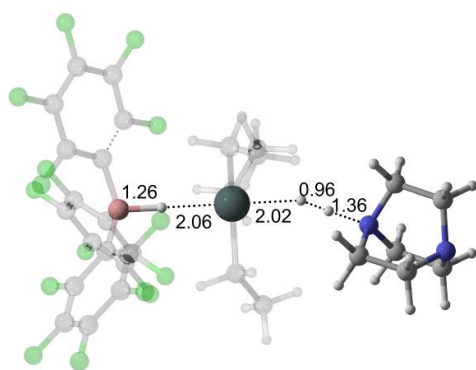
C	-3.71833900	1.52077700	-0.48582500	F	0.60179800	-0.13523000	3.21592000
C	-3.77050600	1.28372100	-1.85686600	F	-2.97493300	-1.85288200	1.53976000
C	-2.72100800	0.60496200	-2.46788500	F	-2.75052800	-4.36562300	2.42837200
C	-1.64915500	0.18170000	-1.68928500	F	-0.30910400	-5.58985600	2.52045700
N	2.45218100	0.11751500	-1.89595700	F	1.92479900	-4.23503300	1.71201000
N	4.33538600	0.26572700	-3.56760900	F	1.72982100	-1.70752900	0.84156100
C	2.56959500	-1.20422800	-2.60422200	F	-2.36528000	2.19887900	1.17656500
H	1.59823800	-1.40818500	-3.05766600	F	-4.63115200	2.88199600	-0.08439700
H	2.76122000	-1.95606000	-1.83698600	F	-5.61289500	1.32354500	-2.10241000
C	3.72312400	-1.06711700	-3.64040100	F	-4.28883600	-0.95114700	-2.83682000
H	4.49817600	-1.81580000	-3.45424000	F	-2.02565500	-1.66635600	-1.57349000
H	3.34937900	-1.22007400	-4.65670600	C	0.22627600	0.93341100	1.11703100
C	3.32712900	1.28750200	-3.87743800	C	0.53770200	2.05709200	0.34105400
H	2.97971700	1.13269100	-4.90273200	C	1.42240100	3.04654200	0.74957800
H	3.80609700	2.26962100	-3.83274100	C	2.02789200	2.94589700	2.00023900
C	2.13558700	1.21120700	-2.87859000	C	1.73510300	1.85885500	2.81892800
H	1.99266300	2.12541700	-2.30018000	C	0.85230700	0.88122500	2.36728000
H	1.18840300	0.94545000	-3.35072100	C	-0.63286400	-1.66548100	1.12099100
C	3.72476800	0.42996800	-1.15764100	C	-1.74408600	-2.40324300	1.54724700
H	3.86145600	-0.35726300	-0.41448800	C	-1.65530500	-3.70900800	2.02253000
H	3.56291700	1.37582100	-0.63824500	C	-0.41327000	-4.33494300	2.07441700
C	4.86448100	0.49068600	-2.21621900	C	0.72307100	-3.64098100	1.66326000
H	5.35772400	1.46645800	-2.19454100	C	0.59326700	-2.33405700	1.21267900
H	5.62259700	-0.27041500	-2.01143000	C	-2.07943900	0.24438100	-0.15799200
H	1.66768900	0.05435500	-1.19929800	C	-2.79569500	1.39759800	0.17978100
H	0.67362600	-0.04002200	-0.31362300	C	-3.97774600	1.77096100	-0.45233000
				C	-4.48295500	0.97719500	-1.47867900
				C	-3.80577900	-0.18280400	-1.85001600
				C	-2.63765600	-0.52951000	-1.18220800
				N	2.56412200	0.08720300	-1.77784100
				N	4.83525600	0.30049200	-2.94895400
				C	2.91079900	-1.19063000	-2.43343600
				H	2.11203800	-1.43021100	-3.14449000
				H	2.91746000	-1.96986800	-1.66422500
				C	4.29744600	-1.05540500	-3.14010200
				H	5.02142800	-1.77023800	-2.73390300
				H	4.21561400	-1.24196300	-4.21657800
				C	3.88592000	1.27428100	-3.51043200
				H	3.79606400	1.08176200	-4.58521600
				H	4.31103000	2.27637600	-3.38738900
				C	2.50157100	1.15663500	-2.79391900
				H	2.22467300	2.08781500	-2.29087100
				H	1.69717100	0.90806100	-3.49506700
				C	3.60633300	0.41741800	-0.78514200



TS8

B	-0.75429700	-0.18364500	0.58653800				
F	-0.01214400	2.20801400	-0.88034200				
F	1.70970300	4.08522000	-0.05112400				
F	2.88307000	3.88749500	2.41009800				
F	2.30513500	1.76206200	4.02794800				

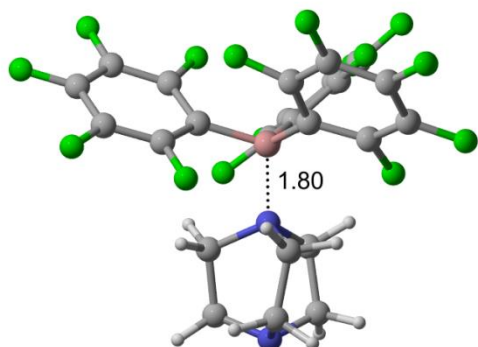
H	3.61763200	-0.37404000	-0.03082000	C	-1.51817700	1.70651200	1.12737300
H	3.31928400	1.34920500	-0.28871000	H	-1.51857000	2.64002100	0.55258000
C	4.98639900	0.55510900	-1.50804200	H	-0.09847000	0.43967200	-1.12607300
H	5.40223600	1.56065900	-1.38080700	H	0.83899900	0.22397400	-1.08552000
H	5.71554500	-0.15863900	-1.10918100	B	-4.81826900	-0.46642300	1.19650000
H	0.86568000	-0.31340900	-1.19934700	C	-5.16501500	0.93725100	1.93052400
H	0.12695600	-0.54272200	-1.01908300	C	-4.97027500	2.14486200	1.26076700



TS9

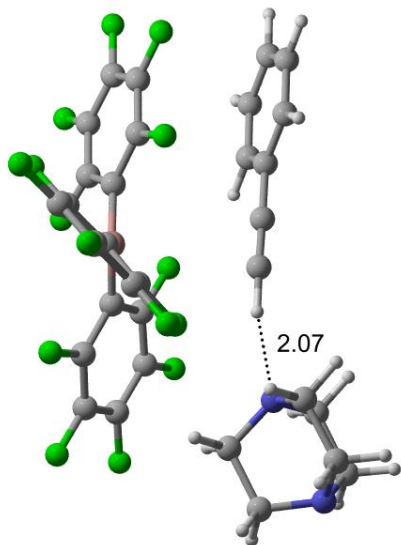
N	2.16817100	-0.04611300	-1.05574300	C	-5.37188400	-1.70271100	-1.04185000
N	4.66583300	-0.52164900	-1.01081900	C	-7.90173400	-0.67524300	-1.30217700
C	2.56253700	-0.69599600	-2.33156300	C	-6.13253500	-2.05883100	-2.14876700
H	2.29366500	-0.01531000	-3.14512400	C	-7.41519800	-1.53509200	-2.28184700
H	1.96370700	-1.60461700	-2.43986400	F	-6.40279700	2.36164300	5.08260900
C	4.09419800	-0.99354600	-2.27948000	F	-5.93102100	-0.02677300	3.97487400
H	4.28682100	-2.06735200	-2.36535400	F	-5.94709400	4.66571600	3.67952300
H	4.61819000	-0.49523200	-3.10095100	F	-4.99106900	4.52082800	1.11202100
C	4.43509900	0.92387100	-0.88480400	F	-4.50546900	2.13270300	-0.01837700
H	4.94383400	1.42725600	-1.71278400	F	-2.51797200	-0.64425100	2.93620700
H	4.89600200	1.26731100	0.04639100	F	-1.89325000	-2.65781800	4.59819700
C	2.90549400	1.23369900	-0.89687700	F	-3.55992100	-4.82528900	4.83241400
H	2.56579400	1.69743200	0.03344500	F	-5.86291000	-4.92234500	3.35799500
H	2.61444900	1.88713000	-1.72505400	F	-6.50516200	-2.92763100	1.69713400
C	2.47092000	-0.94943700	0.08494300	F	-4.12975100	-2.25458800	-0.96091100
H	1.88967100	-1.86420400	-0.05624300	F	-5.64398500	-2.89203000	-3.08618100
H	2.11605400	-0.46175300	0.99714900	F	-8.17292400	-1.85771000	-3.34110100
C	4.00866400	-1.21595300	0.10580800	F	-9.14206400	-0.17165100	-1.41688600
H	4.45507700	-0.86316800	1.04052700	F	-7.65211700	0.47349000	0.70884700
H	4.22063000	-2.28604900	0.01970800	H	-3.70894200	-0.25698200	0.64668000
Sn	-1.88912200	0.10108200	-0.25195600	H	-3.92539100	0.41343900	-1.96957600
C	-2.84668000	0.47941400	-2.13515100	H	-2.37273800	1.74810500	1.80743300
H	-2.57305100	-0.34000600	-2.81040500	H	-2.06889300	-2.37765000	0.77891800
C	-1.24846300	-1.89087200	0.24568800	C	-2.47524500	1.84092300	-2.73670000
H	-0.41828100	-1.80189600	0.95727200	H	-1.39340000	1.93490600	-2.89433800

H	-2.96303800	1.98729600	-3.70921600	C	-0.92906600	-2.39605700	0.38680200
H	-2.79150800	2.66486500	-2.08721400	C	-1.02278700	-3.72818600	0.79643100
C	-0.21691800	1.55226600	1.92340900	C	0.09887200	-4.38793500	1.27742000
H	-0.07381200	2.39216500	2.61579400	C	1.29729300	-3.68600800	1.35881500
H	-0.21657100	0.63435000	2.52224100	C	1.33573000	-2.36272000	0.94430400
H	0.65911200	1.52543200	1.26342000	C	-0.99583300	0.46442200	-0.78197900
C	-0.84969000	-2.72450900	-0.97870100	C	-1.85384500	1.44705200	-0.26908400
H	-0.46436500	-3.70991700	-0.68379300	C	-3.03157000	1.86268800	-0.89462100
H	-1.70738100	-2.89518700	-1.63754500	C	-3.42608600	1.28053400	-2.09052700
H	-0.07287900	-2.23365100	-1.57926600	C	-2.63599100	0.26974200	-2.62867200



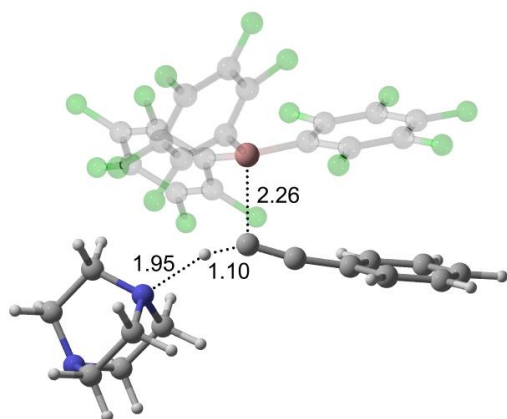
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B	0.38134200	-0.06498400	-0.04124900	H	2.40825700	1.29589600	-4.29581100
F	0.98930800	2.84022600	-0.13595500	C	3.09248100	2.22858100	-2.96168700
F	1.66082300	4.41990400	1.87435300	H	1.37863100	0.96568500	-2.40870200
F	1.74056200	3.45926700	4.44652600	H	0.91994600	1.86957600	-2.02180300
F	1.11177400	0.83253000	4.90471300	H	0.65254900	0.44099600	-3.02220300
F	0.45545100	-0.77324300	2.94433000	C	3.00193800	0.59454200	-0.64157200
F	-2.10644900	-1.86174400	-0.00457200	H	3.17451000	0.10751500	0.31245100
F	-2.19752900	-4.37226700	0.73112800	H	2.84661400	1.65517400	-0.46856300
F	0.02853300	-5.66499300	1.66855700	C	4.17386000	0.38094100	-1.63182100
F	2.39496200	-4.28243600	1.85115800	H	4.84788800	1.24292600	-1.59154200
F	2.53242000	-1.74180300	1.13470100	H	4.75939000	-0.50707000	-1.37335600
F	-1.62051700	2.05593800	0.91400000				
F	-3.78738600	2.82160600	-0.33933900				
F	-4.54774100	1.67019500	-2.70605400				
F	-3.00480300	-0.33937000	-3.76707800				
F	-0.81600800	-1.15644800	-2.53074000				
C	0.78694500	0.89485400	1.23928200				
C	1.06827700	2.25934600	1.09293500				
C	1.39570700	3.12749900	2.12418900				
C	1.42814600	2.64828300	3.42990100				
C	1.11400100	1.31557500	3.65339900				
C	0.79601000	0.48184200	2.57873300				
C	0.25707300	-1.64934500	0.40578800				



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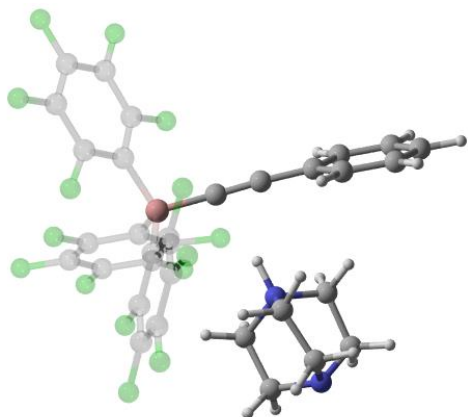
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C	-1.21519700	-1.28975300	-0.63352500	H	5.56787400	-0.84152300	-2.65667600
C	-2.62291800	-1.52033800	-0.56893200	C	5.51530800	-1.25078600	-0.04973600
C	-3.44631400	-1.24310500	-1.67701600	H	6.18113200	-0.44610800	-0.38147600
H	-2.99699900	-0.85542300	-2.58572000	H	5.97329900	-1.71873800	0.82908700
C	-4.82247800	-1.44475100	-1.59758200	B	-0.59280200	1.74478500	1.12778600
H	-5.44944900	-1.21362900	-2.45375800	F	-1.99834500	1.20427900	3.64975700
C	-5.39829500	-1.92095900	-0.41621600	F	-4.63635000	0.81516600	3.88364500
H	-6.47330800	-2.06348200	-0.35297800	F	-6.25355000	0.98765100	1.69451800
C	-4.58641100	-2.20858900	0.68530400	F	-5.18599500	1.54756300	-0.75404300
H	-5.02892800	-2.58234400	1.60472000	F	-2.54392300	1.81759700	-1.04314800
C	-3.20850600	-2.01590400	0.61287900	F	-1.83571200	4.32709300	0.59411100
H	-2.57606600	-2.23837200	1.46435500	F	-1.03543700	6.08159600	-1.26968900
H	1.05993800	-0.98384200	-0.63887800	F	1.11741900	5.52216100	-2.85554800
N	3.09637300	-1.34171500	-0.61859100	F	2.48377000	3.17649400	-2.52384400
C	3.46114500	-1.05411300	-2.01991800	F	1.73098300	1.43379200	-0.63752200
H	3.42330600	0.03113900	-2.16025600	F	1.93230900	2.95748500	1.97686100
H	2.69451400	-1.49902200	-2.66539700	F	3.81201600	1.75472600	3.43646300
C	3.12663800	-2.80111800	-0.40329900	F	3.43305800	-0.78703000	4.35691200
H	2.37535400	-3.25389600	-1.06062100	F	1.10652900	-2.10415900	3.80688900
H	2.81919200	-2.99655700	0.63086100	F	-0.81068000	-0.91919600	2.38986000
C	4.08522300	-0.70926300	0.27323200	C	-2.12850700	1.49976800	1.28600900
H	3.79812000	-0.93817500	1.30516000	C	-2.73743700	1.24408100	2.52429600
H	4.02059900	0.37573100	0.14039900	C	-4.10611700	1.06393100	2.67710500
N	5.44648700	-2.25664900	-1.12203500	C	-4.93564000	1.15276100	1.56231000
C	4.55990700	-3.35121700	-0.69396000	C	-4.38673100	1.42838100	0.31379100
H	4.99869400	-3.81424400	0.19719500	C	-3.01212600	1.58264100	0.19602600
H	4.54532600	-4.10736200	-1.48710500	C	-0.11010600	2.77880800	0.04346600
C	4.88050000	-1.62920400	-2.32790900	C	-0.77114900	3.99621800	-0.16487900
				C	-0.37378200	4.92596300	-1.11860400
				C	0.72517600	4.64557500	-1.92723500
				C	1.41805700	3.45005300	-1.75537700
				C	1.00256400	2.55759200	-0.77543600
				C	0.46988900	1.06791900	2.06255300
				C	1.68106200	1.70032400	2.39100200
				C	2.67200900	1.10514000	3.16132200
				C	2.48148900	-0.18935100	3.63515100
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TS10

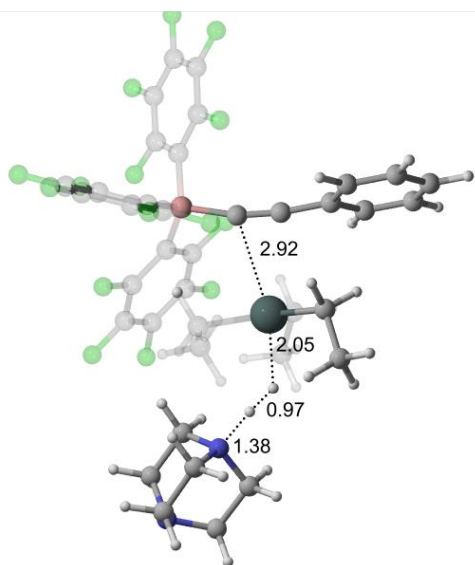
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C	-2.35190000	-1.76463800	-1.21993400
C	-3.15857100	-1.56962500	-2.36086000
H	-2.74605700	-1.04803400	-3.21791500
C	-4.47801900	-2.01009200	-2.36017700
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C	-5.00608000	-2.64228200	-1.22849800
H	-6.04258200	-2.96730000	-1.22599300
C	-4.20790100	-2.85241700	-0.09808200
H	-4.62226000	-3.34315000	0.77770500
C	-2.88391800	-2.42551900	-0.09052200
H	-2.25664800	-2.56859200	0.78147900
N	2.87712900	-1.59681700	-0.82101400
C	3.27516900	-1.72309600	-2.23657500
H	3.46722500	-0.71614200	-2.62185400
H	2.42303400	-2.13500700	-2.79017700
C	2.57857600	-2.93720500	-0.28136200
H	1.72819300	-3.34365100	-0.84085600
H	2.26069800	-2.82134600	0.76006500
C	3.99208500	-1.00518700	-0.05794200
H	3.66985000	-0.90129100	0.98226900
H	4.17723200	-0.00094900	-0.45119900
N	4.95165200	-3.09602800	-1.01240400
C	3.84399900	-3.84596500	-0.39912100
H	4.17328600	-4.19766800	0.58493700
H	3.64629200	-4.72875600	-1.01757100
C	4.53631000	-2.63939800	-2.34828400
H	4.33498200	-3.52398100	-2.96305300
H	5.37775200	-2.10452700	-2.80267500
C	5.25358600	-1.92121200	-0.17846700
H	6.09257400	-1.38522600	-0.63601700

H	5.58369200	-2.27628900	0.80421500
B	-0.39734100	1.05184600	0.39795700
F	-1.68442500	0.50895900	3.05901500
F	-4.28706600	0.16091000	3.45520900
F	-6.06470000	0.42217900	1.39257200
F	-5.14903300	1.05317400	-1.10869900
F	-2.53514700	1.34784700	-1.55529200
F	-1.83865500	3.61607100	0.11651500
F	-1.14933400	5.63495900	-1.46036700
F	1.12139800	5.50928400	-2.98357500
F	2.71144800	3.28127500	-2.85137100
F	2.06912300	1.25816900	-1.25674900
F	1.81334400	2.68700300	1.50612600
F	3.59513900	1.88815500	3.30106600
F	3.48699600	-0.63650000	4.35354200
F	1.51037600	-2.34993900	3.54992500
F	-0.31432700	-1.57469400	1.77989100
C	-1.95374100	0.89500300	0.71157400
C	-2.48316200	0.61149000	1.97562100
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C	-4.75384900	0.58660500	1.17734000
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C	0.02385400	2.26861300	-0.55319400
C	-0.72671100	3.45072400	-0.63116400
C	-0.38065300	4.53596600	-1.43169100
C	0.77455400	4.47969800	-2.20358300
C	1.57472500	3.34350800	-2.13835000
C	1.19834200	2.28909800	-1.31547500
C	0.66956100	0.58262200	1.49452800
C	1.69564300	1.41969400	1.95375500
C	2.63591800	1.03646500	2.90866400
C	2.58271500	-0.24217300	3.44974100
C	1.57613700	-1.11043600	3.03619700
C	0.64932600	-0.68473800	2.09385100
H	1.13831900	-0.73391700	-0.94370500



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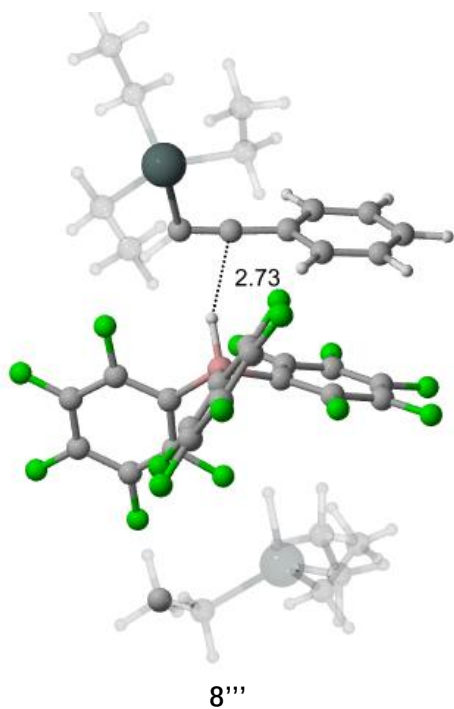
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C	0.38086200	4.03798800	-1.17881000	C	0.71125300	-1.08827400	1.58514200
C	0.68337700	4.94137900	-0.13915100	C	-0.50744500	-1.03452600	-1.34115000
H	0.48067600	4.64988000	0.88770700	C	-1.02314300	-2.32852800	-1.20636800
C	1.21583500	6.19785800	-0.42822300	C	-0.78921900	-3.36060900	-2.10806900
H	1.43944100	6.88696000	0.38168100	C	0.01212200	-3.12482800	-3.22290100
C	1.45075400	6.57539300	-1.75470700	C	0.55746800	-1.86022600	-3.40111600
H	1.86266500	7.55554000	-1.97763200	C	0.28591800	-0.85753600	-2.47143300
C	1.13664000	5.69251500	-2.79416900	C	-2.56962800	0.15116100	-0.20073300
H	1.30157700	5.98800200	-3.82676400	C	-3.38275500	-0.26011000	0.85516900
C	0.60513100	4.43462900	-2.51313300	C	-4.77534900	-0.21951500	0.81427800
H	0.35626900	3.74473300	-3.31400900	C	-5.41654400	0.23818700	-0.33140900
B	-0.92241400	0.12124700	-0.24150200	C	-4.65061200	0.64131100	-1.42082200
F	-1.36690600	1.80584700	2.07094900	C	-3.26299200	0.58611000	-1.33367200
F	-0.14340400	1.71538500	4.44272800	N	5.13344800	1.38925700	0.03831800
F	1.69979900	-0.23861600	4.98280700	C	4.93581300	2.23102300	-1.14911300
F	2.28102600	-2.10617700	3.05937600	H	5.46698600	1.77014200	-1.98687600
F	1.09600400	-2.04447700	0.69659600	H	5.38631500	3.21080200	-0.96724600
F	-1.77239600	-2.63611400	-0.12603500	C	4.35446100	1.93456700	1.15807700
F	-1.31144000	-4.58162500	-1.91095100	H	4.66057700	2.97286900	1.31547900
F	0.26081100	-4.10478200	-4.10408700	H	4.59757100	1.37383800	2.06478300
F	1.35239900	-1.61198400	-4.46138800	C	4.67564600	0.02258300	-0.24947000
F	0.89300200	0.33932700	-2.73350800	H	4.74953400	-0.56489900	0.66998600
F	-2.84541000	-0.74859800	1.99759100	H	5.34524300	-0.42813100	-0.98734100
F	-5.50437800	-0.62514200	1.86904200	N	2.68162300	1.42644000	-0.57845400
F	-6.75672700	0.28382400	-0.38885600	C	2.83262000	1.84507300	0.86119600
F	-5.25570300	1.07367500	-2.54206000	H	2.32163800	1.09242700	1.46096200
F	-2.57755400	0.96693900	-2.43875600	H	2.30704900	2.79460800	0.97145300
C	-0.22522100	-0.11345600	1.24440600	C	3.42157800	2.38724400	-1.47137400
C	-0.47709900	0.81206900	2.26752200	H	3.03476600	3.38380400	-1.25539100
C	0.14086300	0.78778400	3.51293200	H	3.16355500	2.13128800	-2.50070000
				C	3.21572500	0.03261700	-0.78157900
				H	3.14991800	-0.17190700	-1.85058900
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TS11

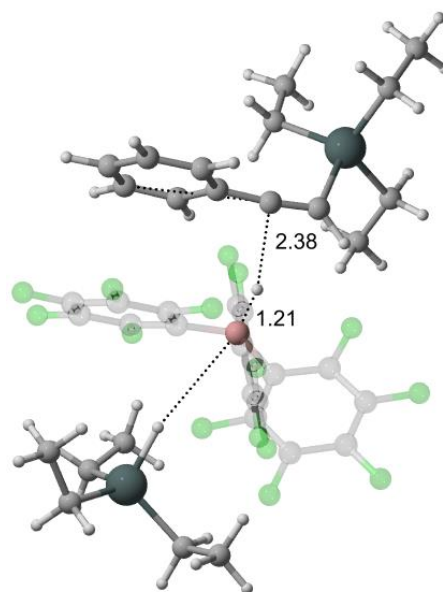
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C	-1.37381000	-0.93163300	-2.53635000	H	3.54484500	1.94889900	5.96841500
C	-1.92037000	-0.12997500	-3.55727200	H	3.50664700	3.66251400	5.53670100
H	-2.83089900	0.42590200	-3.35701500	B	-3.75741800	-1.43894600	0.89564900
C	-1.29613000	-0.05885600	-4.80065300	F	-4.24471000	-4.12729600	2.32237100
H	-1.72557100	0.56010700	-5.58344500	F	-5.55287200	-6.20042800	1.29470100
C	-0.12256600	-0.78137700	-5.04209600	F	-6.63346700	-6.07406900	-1.21779700
H	0.36298100	-0.72207800	-6.01216700	F	-6.36683600	-3.77467300	-2.68678700
C	0.41830500	-1.58926200	-4.03663600	F	-5.05742800	-1.66958500	-1.68299500
H	1.32120500	-2.16323200	-4.22585400	F	-6.00322900	-1.70549000	2.66786300
C	-0.20240800	-1.66880100	-2.79066100	F	-8.09681600	-0.04846000	2.94695800
H	0.20459300	-2.30401500	-2.01070600	F	-8.21380500	2.28304000	1.51068600
N	1.17689900	2.21858400	3.82532900	F	-6.18056800	2.90498900	-0.21809200
C	0.65471400	1.17455700	4.74730100	F	-4.10400900	1.28428700	-0.52141800
H	1.13867000	0.23035300	4.49048600	F	-3.88102800	-0.05169000	3.68040400
H	-0.41586500	1.06913000	4.56457300	F	-2.18942600	-0.47875200	5.66946900
C	0.52380100	3.51888400	4.12843500	F	-0.20776300	-2.35178000	5.46052800
H	-0.55117400	3.38793900	3.98317300	F	0.00875300	-3.83197200	3.15743200
H	0.87801700	4.24735100	3.39221200	F	-1.66956200	-3.41702700	1.12244000
C	2.64749100	2.34265700	3.99587100	C	-4.53095600	-2.79766400	0.35189100
H	2.99751900	3.10107700	3.28841300	C	-4.72084800	-3.98322200	1.06364200
H	3.09318400	1.38467300	3.71232400	C	-5.41186400	-5.08359100	0.55840500
N	1.69476800	2.88241600	6.23061800	C	-5.96536300	-5.02391200	-0.71507600
C	0.87861400	3.92422100	5.59311700	C	-5.82403300	-3.85649300	-1.45831800
H	1.44034600	4.86345300	5.61600100	C	-5.12524400	-2.78331700	-0.91435600
H	-0.02915700	4.06463900	6.18770800	C	-4.94357000	-0.31114500	1.06437000
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H	0.09955500	-1.89131200	0.58693700	C	2.29124800	-2.11824000	-2.21130100
H	-1.25515700	2.15597500	-1.67246200	C	1.38918800	-1.99539900	-3.06957900
C	1.64543600	-1.08147900	1.88583600	Sn	2.05056000	-0.44326600	-4.61226600
H	2.26011000	-1.98995400	1.86448300	C	2.71574900	-1.67484500	-6.24644500
H	2.32277800	-0.22166600	1.94099200	H	3.60587700	-2.22262500	-5.91424600
H	1.06354600	-1.11174500	2.81201200	H	1.93948600	-2.42423500	-6.44104600
C	-2.15887000	3.08005500	1.55291500	C	0.25259600	0.67874400	-4.95063300
H	-2.57948300	3.24510700	0.55574800	H	0.34056000	1.09800000	-5.96204100
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C	0.57315900	3.19192100	-1.09509800	H	3.15244200	1.14900400	-2.76060300
H	0.67366000	3.74185100	-2.04015500	H	4.39849500	0.05157600	-3.34854900
H	0.11036600	3.86998000	-0.36972800	C	3.01689700	-0.86408300	-7.51927100
H	1.58415700	2.96858500	-0.73473200	H	3.81531100	-0.13009700	-7.35794600



C	5.16827700	-3.15844900	-0.13300500	C	0.75118900	-0.77610300	1.06500500
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C	3.34002500	-2.07839100	-1.29479400	C	1.35348100	-0.04037800	2.08824000
C	3.49915500	-0.91903500	-0.49211700	C	1.93479200	-2.73315400	2.00211800
C	4.50473000	-0.88655000	0.46458200	C	2.20886300	-0.59548700	3.03993400
C	5.32518800	-2.00490500	0.65147500	C	2.50301700	-1.95253600	3.00222900
H	5.80657600	-4.01992400	0.03456600	C	-0.49176400	1.39029100	-0.12408000
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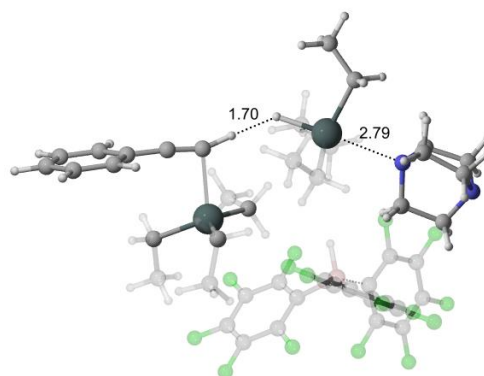
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C	-0.85076900	4.22732900	-0.19019300
F	-1.01818400	5.55961200	-0.21017600
F	1.44556900	4.46483900	-0.73907000
F	1.79070900	1.81383900	-0.68082500
F	-2.82940300	1.26849600	0.37435000
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F	0.62842000	-2.94923200	0.08848800
F	2.23781500	-4.04418800	1.91984200
F	3.34047700	-2.49742800	3.90213000
F	2.76287500	0.17607000	3.99436600
F	1.15739000	1.29295000	2.20622600
F	-1.81354500	-1.63568200	1.99249300
F	-4.02091800	-3.07205300	1.57519700
F	-5.03153300	-3.38489200	-0.95222400
F	-3.73511300	-2.21938000	-3.07515600
F	-1.52087300	-0.77754100	-2.69037300
H	0.45808700	-0.39278900	-1.15624300
C	-1.48149900	3.15329200	4.76874800
H	-2.19756000	3.57942300	5.48384400
H	-0.56170600	2.95148300	5.33332400
C	-1.19678800	4.15269100	3.63444200
H	-0.79708100	5.10294200	4.01505400
H	-0.46394700	3.74888800	2.92555700
H	-2.10448900	4.38920300	3.06470100
C	-1.92574500	-0.33656200	5.44193800
H	-2.07247300	0.05237100	6.45831400
H	-2.70677000	-1.09063600	5.28190000
C	-0.53656600	-0.98246300	5.31024000
H	0.26836900	-0.25205800	5.46322100
H	-0.38805200	-1.78701700	6.04412700
H	-0.39841400	-1.41671900	4.31389000
C	-4.34476900	1.44300800	3.53674500
H	-4.89616100	1.67754800	4.45747300
H	-4.46466500	2.30909100	2.87350900
C	-4.92432200	0.18389100	2.87187400
H	-4.42527400	-0.02524800	1.91995700
H	-4.80639600	-0.70517100	3.50359100
H	-5.99718700	0.29376300	2.66110700
Sn	-2.25125200	1.27085900	4.03343500
H	-1.35917600	0.91666800	2.61915700



TS6''

C	-8.79209000	-6.82574700	-1.87026400
C	-9.66772400	-6.49358500	-2.89158400
C	-10.10399500	-5.14936800	-3.02879500
C	-9.64589200	-4.15379400	-2.12597300
C	-8.73927200	-4.49919800	-1.13389600
C	-8.32588200	-5.82933500	-0.99815400
H	-8.47604700	-7.85513800	-1.73706100
H	-10.04767700	-7.24759600	-3.57304300
H	-10.01861500	-3.14357900	-2.22117800
H	-8.38227900	-3.74330200	-0.44236200
H	-7.64556800	-6.09876900	-0.19524400
C	-11.01634900	-4.81401600	-4.02431100
C	-11.72153900	-4.46841700	-5.00583000
Sn	-10.57870300	-3.21160100	-6.48847100
C	-10.01973800	-4.55231200	-8.07470900
H	-9.31481600	-5.28483400	-7.66332400
H	-10.91473000	-5.11035100	-8.37408200
C	-12.10832300	-1.77437700	-6.94826300
H	-11.71529100	-1.12294700	-7.73972800
H	-12.95790900	-2.31614600	-7.38101300
C	-8.94637200	-2.38471900	-5.36898000
H	-9.37879100	-1.92028000	-4.47593700
H	-8.30187000	-3.20169900	-5.02311300
C	-9.40494600	-3.82415100	-9.28312200
H	-8.48897800	-3.28507400	-9.01325500
H	-9.14126700	-4.53422300	-10.07694700
H	-10.10069200	-3.09642400	-9.71802700
C	-12.54333400	-0.95238300	-5.72484700

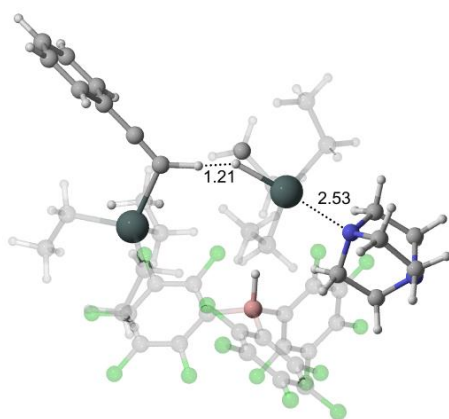
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H	-12.96924000	-1.58471000	-4.94028600	H	-13.03718700	-0.37137700	3.71831700
H	-11.70546000	-0.39961000	-5.28601800	C	-13.74950700	0.87551100	2.08382200
C	-8.13217400	-1.35224500	-6.16805800	H	-13.24098600	1.79219700	2.41369900
H	-7.66158400	-1.79608200	-7.05368800	H	-13.12603900	0.41565200	1.30800600
H	-8.75699700	-0.51719500	-6.50742200	H	-14.69029400	1.18088600	1.60862600
H	-7.33047400	-0.92474400	-5.55345600	C	-14.77560000	-3.49926000	4.07361800
H	-12.80131800	-4.41824600	-5.10841900	H	-14.79850600	-3.06250900	5.08074100
B	-13.24174300	-3.34012300	-1.71571000	H	-15.65884600	-4.14619200	3.99594500
C	-14.68020700	-4.08296900	-1.93007800	C	-13.49625100	-4.32978700	3.87818200
C	-15.26328500	-4.08427200	-3.19573200	H	-12.59385400	-3.71115400	3.96580000
C	-15.43400700	-4.73978600	-0.95678600	H	-13.41134200	-5.13372400	4.62266500
C	-16.48915400	-4.66675100	-3.49932400	H	-13.47646000	-4.79638200	2.88640400
C	-16.66527400	-5.34169000	-1.20635200	C	-17.05984400	-1.53410100	2.18305700
C	-17.20206800	-5.30444400	-2.48937500	H	-17.55926300	-1.25860900	3.12196000
C	-12.35408100	-3.94222000	-0.48694600	H	-17.11489600	-0.65328100	1.53112200
C	-12.14386500	-5.32480100	-0.42027300	C	-17.77635200	-2.72449100	1.52515600
C	-11.66241400	-3.21725600	0.48621800	H	-17.32704200	-2.97094800	0.55761700
C	-11.36469100	-5.95636700	0.53987600	H	-17.72635900	-3.62782200	2.14586800
C	-10.86371100	-3.80536500	1.46535600	H	-18.83928200	-2.51011200	1.34723400
C	-10.71386400	-5.18597100	1.49791200	Sn	-14.98051800	-1.91285700	2.61754100
C	-13.40386600	-1.71379200	-1.74335800	H	-14.18141200	-2.43244100	1.19812100
C	-14.54909100	-1.00779600	-1.36843300				
C	-12.37534200	-0.90116400	-2.21796700				
C	-14.66085100	0.38042200	-1.43072100				
C	-12.43586700	0.48358400	-2.30670800				
C	-13.59525200	1.13757000	-1.90265500				
F	-13.68309500	2.47567100	-1.97267500				
F	-11.39379100	1.19276900	-2.78766100				
F	-11.19944500	-1.46108700	-2.63579700				
F	-15.64445300	-1.65540300	-0.90995500				
F	-15.78954300	0.99515800	-1.03285700				
F	-12.70496100	-6.13225200	-1.35687700				
F	-11.19948900	-7.29419100	0.53264800	C	-0.97908000	2.03087700	5.23956500
F	-9.93299300	-5.76762100	2.42558000	C	-1.38192800	1.88829200	4.08466200
F	-10.22571400	-3.04645100	2.37760700	C	-0.40424300	2.14325700	6.53063100
F	-11.71334700	-1.86480400	0.51936800	C	0.49642300	3.19349200	6.80819800
F	-14.98902700	-4.82117500	0.31935100	C	-0.71450300	1.19592200	7.52854600
F	-17.34027500	-5.96082700	-0.22160500	C	1.08120000	3.28480700	8.06742300
F	-18.38645000	-5.88166500	-2.75164200	H	0.72423500	3.91981800	6.03443200
F	-16.98416100	-4.62805400	-4.75271700	C	-0.12547400	1.30046100	8.78461500
F	-14.62136300	-3.47638900	-4.24230000	H	-1.40900400	0.39276100	7.30430100
H	-12.58837900	-3.62033500	-2.69386500	C	0.77239400	2.34010400	9.05316700
C	-13.99185500	-0.09753500	3.25039900	H	1.77634900	4.09035200	8.28299600



16

H	-0.36173900	0.57206200	9.55414800	H	3.13076700	-1.25154600	4.06418700
H	1.23219000	2.41510900	10.03428400	Sn	-2.89090800	2.16175900	0.05842600
C	1.86706300	2.23167800	2.84118100	Sn	0.57271500	0.60745900	3.35378000
H	1.72629300	2.98853700	3.62325300	N	-2.09367600	2.00129800	-5.25923300
H	1.54262400	2.67069100	1.89764000	C	-3.41817100	1.44686900	-4.94688000
C	3.33812000	1.79038700	2.76586400	H	-3.50319300	0.45930800	-5.41265900
H	3.49805300	1.04605700	1.97973300	H	-4.17393000	2.09678600	-5.40292000
H	3.97912600	2.64839300	2.53034800	C	-2.03590500	3.38558300	-4.76872500
H	3.69043100	1.36599800	3.71387700	H	-2.70879500	4.00141600	-5.37657000
C	-1.35000800	-1.73345300	2.89125700	H	-1.01663400	3.75595100	-4.92479100
H	-1.96043300	-2.33673300	2.21100100	C	-1.07266200	1.20834700	-4.55355900
H	-0.62929800	-2.40956100	3.36338300	H	-0.08587600	1.54403200	-4.88565100
H	-2.01234100	-1.34546600	3.67469300	H	-1.18171500	0.16201800	-4.85527800
C	-0.65859000	-0.61200600	2.11037800	N	-2.51144400	2.06949100	-2.70733600
H	-0.01871600	-1.00565000	1.31947600	C	-2.43354500	3.44304700	-3.26146600
H	-1.38331600	0.04139100	1.62277500	H	-1.70596100	4.01250100	-2.67354200
H	-3.04684400	2.21146100	1.86440700	H	-3.41181100	3.91302500	-3.12197000
C	-4.43423700	3.58634900	-0.45123100	C	-3.60756600	1.34744900	-3.40322500
H	-3.94767500	4.52696500	-0.73959100	H	-4.56374700	1.77379300	-3.08001000
H	-4.95397800	3.22278900	-1.34509300	H	-3.57282100	0.30610400	-3.07855300
C	-5.43960200	3.83402900	0.68299500	C	-1.23578500	1.36765400	-3.01193300
H	-6.20614800	4.56562400	0.39227400	H	-1.24242200	0.40544100	-2.50046900
H	-5.95954100	2.91133100	0.96938500	H	-0.42193000	1.96201500	-2.59154000
H	-4.94355100	4.21260800	1.58424300	H	-2.05608500	2.00262500	3.22465600
C	-0.87187800	2.93981400	0.04705200	B	0.73018900	-1.56510800	-1.46553000
H	-0.56939800	3.21069000	-0.96644700	C	0.31279400	-2.58101600	-2.66730900
H	-0.19825000	2.13445200	0.35626800	C	-0.97854200	-2.66300500	-3.18205900
C	-3.38554700	0.07472500	-0.20000100	C	1.22514000	-3.46629400	-3.24240200
H	-3.96655400	-0.02037500	-1.12017900	C	-1.35232600	-3.54389400	-4.19498300
H	-2.47151700	-0.50638400	-0.36057000	C	0.90158200	-4.36790900	-4.25068900
C	-0.72145300	4.15647900	0.97147800	C	-0.40420000	-4.40623600	-4.73371800
H	-0.98868100	3.92080900	2.00918000	C	1.55585900	-0.24006900	-1.95646400
H	0.30896000	4.53710100	0.97395900	C	1.89480400	0.10267700	-3.26612900
H	-1.37097100	4.98335900	0.65748800	C	1.86000400	0.75150100	-1.02549500
C	-4.20058800	-0.48763700	0.97343900	C	2.46639200	1.32552500	-3.62467700
H	-3.68488500	-0.36967600	1.93271000	C	2.42650000	1.98134300	-1.32451400
H	-5.16790000	0.02133400	1.07111600	C	2.73088200	2.27891100	-2.64940900
H	-4.40415500	-1.55820900	0.83715500	C	1.46512000	-2.41792600	-0.27439300
C	1.32196700	-0.47098600	5.05214800	C	2.79289400	-2.31836800	0.14246100
H	1.83828400	0.22923000	5.71820700	C	0.70221200	-3.33801200	0.45084400
H	0.46795500	-0.87063000	5.61115900	C	3.32513100	-3.04332800	1.20828700
C	2.25944400	-1.61493100	4.62128900	C	1.19059600	-4.09084100	1.51493700
H	2.63818600	-2.16209300	5.49283900	C	2.51857900	-3.93884600	1.90116900
H	1.74492400	-2.34124500	3.98456500	F	3.01076600	-4.63750900	2.94061800

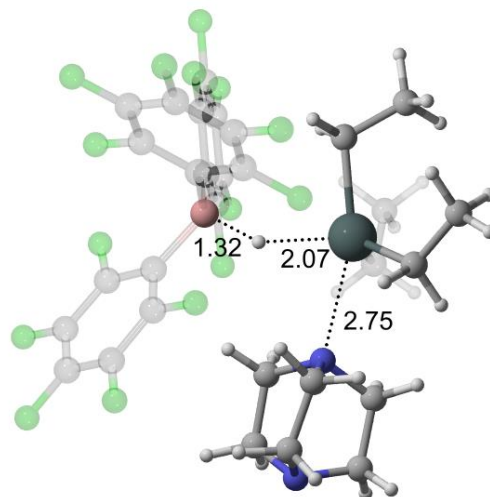
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F	-0.60438700	-3.51833700	0.14055700	H	9.13419400	3.55642600	-0.61239700
F	3.65531400	-1.48361800	-0.48459100	H	9.05731000	2.52888600	0.82450100
F	4.60911900	-2.87872800	1.58341700	C	4.50335800	-0.99318000	1.02749800
F	1.65519800	-0.74229400	-4.29484300	H	4.11460300	-1.86556500	0.49136200
F	2.74636700	1.59931600	-4.91185700	H	5.15550200	-1.36305100	1.82731400
F	3.26796500	3.46724100	-2.97544500	H	3.64656500	-0.49709300	1.49915800
F	2.67658300	2.89054800	-0.35679600	C	5.25291200	-0.05599900	0.07175800
F	1.58449800	0.52938900	0.29581200	H	6.14215100	-0.54445600	-0.33713300
F	2.51641100	-3.45050900	-2.83249300	H	4.64028300	0.21447300	-0.79141700
F	1.82875100	-5.19375100	-4.77003500	H	2.65516300	3.33786200	-0.45410100
F	-0.74328800	-5.26645800	-5.70890400	C	0.71655200	4.41677000	-2.43303700
F	-2.61944400	-3.56878100	-4.65541900	H	1.08001700	5.38101300	-2.81129500
F	-1.96588900	-1.85377900	-2.71229100	H	0.01876500	4.03246800	-3.18636900
H	-0.28925800	-1.12672900	-0.97466800	C	-0.00939200	4.61164000	-1.09383900



TS14

C	3.62013900	2.64837200	2.68130300	H	3.89832600	5.99727700	-2.12340600
C	3.94159700	2.71546600	1.48006700	C	1.57960300	0.60447100	-0.61824700
C	3.31881000	2.50387500	4.04947500	H	2.35419200	0.86170700	0.10965700
C	3.60728800	3.54418700	4.96194600	H	0.66581200	1.12869000	-0.31163000
C	2.73739200	1.30129900	4.51455800	H	1.39131000	-0.47339300	-0.52945800
C	3.31925100	3.37817000	6.31209800	C	6.70254000	1.19375100	2.99665500
H	4.05308500	4.46325900	4.59520000	H	7.03919700	2.10434800	3.50737500
C	2.45633300	1.14774600	5.86746500	H	5.88048400	0.78485100	3.59655100
H	2.52083200	0.50850100	3.80563700	C	7.84957300	0.17061300	2.90116300
C	2.74634600	2.18306700	6.76477300	H	8.21347200	-0.11404200	3.89656400
H	3.54046400	4.17579900	7.01471700	H	7.53293900	-0.75045400	2.39721600
H	2.01257300	0.22412300	6.22624400	H	8.70684500	0.56698900	2.34453400
H	2.52554200	2.05791300	7.82092600	Sn	2.40561800	3.06990700	-2.31692300
C	7.10202000	3.22834900	0.10103000	Sn	5.92375200	1.71584300	1.05983200
H	7.06652800	4.11843900	0.74110000	N	2.13035300	2.38794900	-7.37632300
H	6.63874900	3.49466000	-0.84989400	C	0.91007400	1.86328400	-6.75065300
C	8.55292100	2.76768000	-0.11962100	H	0.76687100	0.82756500	-7.07435000

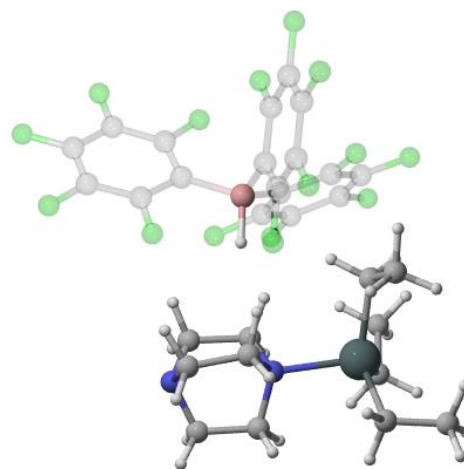
H	0.06008000	2.44933200	-7.11771500	F	8.02147000	3.91335900	-5.95362300
C	2.24876200	3.81628300	-7.05868300	F	7.72247400	3.46165800	-3.26501600
H	1.45045800	4.35963800	-7.57632000	F	6.56169500	1.20776300	-2.38948500
H	3.20476000	4.17308600	-7.45627300	F	6.86906900	-2.89629200	-5.54401300
C	3.29147200	1.67944200	-6.81460400	F	5.80431200	-4.62638600	-7.31512500
H	4.18610800	1.98506100	-7.36472800	F	3.11614000	-4.58461600	-7.83750200
H	3.15452100	0.60742100	-6.98097700	F	1.50996400	-2.78436000	-6.53249100
N	2.22673600	2.73056300	-4.81639500	F	2.53889400	-1.08757600	-4.74660400
C	2.16301100	4.04255000	-5.51860000	H	4.50941100	-0.39838500	-3.32648100



TS12

C	4.76383600	-1.91609400	-5.05242600	B	0.20442700	-0.08067100	0.27836800
C	3.40555100	-1.94592900	-5.35412100	C	-0.51829600	1.29662900	0.73940400
C	5.53142100	-2.85332000	-5.74581300	C	-0.61233200	2.47050900	0.00208300
C	2.83473000	-2.81822000	-6.27860900	C	-1.02147700	1.38693900	2.04007800
C	5.01062700	-3.75045300	-6.67224200	C	-1.18797000	3.64524800	0.48021400
C	3.64442600	-3.73118500	-6.94393400	C	-1.60325200	2.53371100	2.56708500
C	6.24074700	0.35275100	-4.58848200	C	-1.69243400	3.67700200	1.77506700
C	6.43516200	0.63205000	-5.94173900	C	1.51056800	-0.29314800	1.23206000
C	6.70559900	1.35647100	-3.73725000	C	1.77824100	-1.40067900	2.04291100
C	7.02320500	1.80641000	-6.41633700	C	2.46214500	0.72751600	1.32960100
C	7.30532900	2.53617100	-4.15538100	C	2.92240700	-1.51772600	2.83277200
C	7.46146600	2.77120300	-5.51818400	C	3.62047700	0.65309400	2.09402900
C	6.25702800	-1.78746100	-2.85754600	C	3.85857800	-0.48943000	2.85227400
C	7.63258300	-1.76004300	-2.63213000	C	-0.76658500	-1.37315300	0.10412000
C	5.55065500	-2.64564200	-2.01118500	C	-2.14232700	-1.41274200	0.34729200
C	8.26511700	-2.48943700	-1.62520400	C	-0.24576700	-2.56906900	-0.39418200
C	6.13814100	-3.40746900	-1.00638100	C	-2.93071600	-2.54339300	0.13224700
C	7.51167200	-3.31904900	-0.80173400	C	-0.98758800	-3.71785600	-0.63319200
F	8.10189800	-4.02786500	0.17802900	C	-2.35292500	-3.70669800	-0.36335900
F	5.39416100	-4.20208800	-0.20998600	F	-2.08148600	2.55186700	3.82082100
F	4.20272300	-2.74265600	-2.12533400	F	-0.95754800	0.30492400	2.84800000
F	8.44447500	-0.99304600	-3.39852800				
F	9.59684000	-2.40125500	-1.44122500				
F	6.02313200	-0.22974500	-6.90137600				
F	7.15397300	2.02160700	-7.73885800				

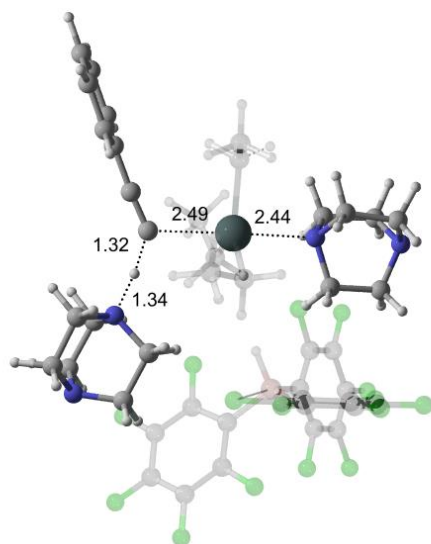
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F	-1.24713300	4.74335700	-0.29357200	C	-0.55018400	-2.59811700	-4.20138200
F	-0.10235200	2.53729400	-1.25960000	H	-1.22436300	-2.06746400	-4.88244300
F	2.28983400	1.87622100	0.62728700	H	-0.30287800	-3.55941700	-4.66940200
F	4.50734600	1.66373600	2.10049000	H	-1.11452300	-2.81903300	-3.29038700
F	4.96613900	-0.59035100	3.59812100	C	-1.76741300	0.12163200	-2.57519500
F	3.12525200	-2.61375500	3.57950500	H	-2.01005000	-0.89584800	-2.26087300
F	0.91668200	-2.43498700	2.11926700	H	-1.99978100	0.77237000	-1.72929900
F	1.07803000	-2.64404400	-0.68449800	C	-2.63493100	0.49378800	-3.79012000
F	-0.40541200	-4.82519900	-1.12385100	H	-2.34354500	-0.04326100	-4.70180300
F	-3.09826400	-4.79657400	-0.58722900	H	-3.68606000	0.24132600	-3.59775200
F	-4.24995000	-2.50914100	0.37743400	H	-2.59280900	1.56268500	-4.01190100
F	-2.81319200	-0.32064700	0.77057100				
H	0.70461400	0.11545200	-0.93034400				
N	3.08990200	-0.02550100	-2.60975800				
C	3.76205400	-0.39152500	-3.88683200				
H	3.40976700	0.28061500	-4.67468700				
H	3.45208300	-1.40608100	-4.14646600				
C	3.45935100	-1.06125800	-1.60615400				
H	2.99537300	-2.00160900	-1.90512800				
H	3.02318400	-0.77120300	-0.65339200				
C	3.63677400	1.29324600	-2.17893200				
H	3.04925400	1.65872900	-1.33869400				
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N	5.66266900	-0.13625800	-2.29051900				
C	5.00815200	-1.19822800	-1.51484200	B	0.12218400	-0.04558100	1.30028100
H	5.34433800	-1.12962000	-0.47475400	C	-0.78922100	1.23426600	1.74421900
H	5.34417000	-2.16425700	-1.90715600	C	-0.71440100	2.48138100	1.13120900
C	5.31184900	-0.30336700	-3.70730600	C	-1.66710400	1.17711800	2.82895000
H	5.79627400	-1.21056100	-4.08431800	C	-1.45966300	3.59007300	1.52808400
H	5.72502100	0.54695100	-4.26052500	C	-2.43049900	2.25319700	3.26826200
C	5.14542100	1.15814600	-1.82374400	C	-2.32724000	3.47575000	2.60760900
H	5.72752700	1.96114600	-2.28895800	C	1.16714100	-0.35357200	2.51931200
H	5.30636100	1.21919300	-0.74246200	C	1.04242500	-1.35488500	3.48341200
Sn	0.37132700	0.12327500	-2.97092400	C	2.29005600	0.46050900	2.67538200
C	0.97204100	1.92915300	-3.98961000	C	1.95912200	-1.54912000	4.51549700
H	1.46024500	2.56461700	-3.24730500	C	3.23291400	0.30753400	3.68711200
H	1.73646600	1.64804500	-4.72216800	C	3.06540600	-0.71195200	4.61921600
C	0.72513200	-1.79677100	-3.90541200	C	-0.71246800	-1.35904800	0.78558200
H	1.27301600	-1.59519600	-4.83376100	C	-2.07437100	-1.40217900	0.47880600
H	1.39362600	-2.38020100	-3.26715800	C	-0.03927100	-2.55393800	0.51051300
C	-0.15857100	2.71448700	-4.66662400	C	-2.72423600	-2.52843100	-0.02681700
H	-0.89785500	3.05789700	-3.93685600	C	-0.64125700	-3.70469100	0.01407600
H	0.24485100	3.60565100	-5.16514700	C	-2.00541900	-3.69458500	-0.25757100



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H	2.35377300	4.21243100	2.00102700	F	5.26241900	-0.32661000	1.07362000
H	1.13147500	5.02859400	2.98785800	F	5.27142900	-0.72057100	-2.16238300
C	0.41523500	3.00577300	4.43422300	F	7.21729400	0.99313800	-2.86889700
H	0.24857900	3.95899600	4.94617800	F	7.05835100	3.63486700	-2.16953200
H	0.57240400	2.23943700	5.19955500	F	4.88796800	4.53140700	-0.74737700
C	-3.71263800	-0.96099200	-2.22812200	F	2.93189900	2.84792600	-0.04912100
C	-4.31109200	0.06417700	-1.97319100	F	3.35269700	-2.97365300	-1.09982400
C	-4.99772400	1.27859200	-1.66763400	F	2.61426500	-4.42854500	-3.22090600
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H	-3.96668200	2.43022000	-3.17077800	F	0.59666400	-0.61759100	-5.17506500
C	-5.38982600	3.64124200	-2.08858900	F	1.35557700	0.87152500	-3.07318100
H	-5.16343500	4.54386200	-2.64936100	C	2.95881500	-0.83163600	0.69016500
C	-6.36238200	3.66595400	-1.08297900	C	1.85485900	-1.48207200	1.24100000
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C	-6.65492700	2.49832500	-0.37143800	C	3.02691100	-2.19353100	3.20507800
H	-7.41295700	2.51096600	0.40673200	C	4.16417800	-1.56772100	2.70488900
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C	-1.03191400	-2.98805500	-1.25698800	C	6.07739700	2.78432400	-1.82581200
H	-1.49281700	-2.31419900	-0.52636900	C	4.97590700	3.23412300	-1.10643100
H	-0.38193100	-2.38273000	-1.89599800	C	3.97411600	2.32984600	-0.76703200
C	-1.51585400	-4.42626600	-3.12286600	C	2.36912900	-0.97940600	-1.96674900
H	-0.88526300	-3.81146700	-3.77207900	C	2.66782300	-2.33699600	-2.07891100
H	-2.33135800	-4.82593400	-3.73668600	C	2.30234700	-3.11895800	-3.17243700
C	-3.00784000	-4.35082600	-1.24099600	C	1.59808300	-2.54238400	-4.22365900
H	-3.82264200	-4.73035300	-1.86894400	C	1.28086800	-1.18897000	-4.16559600
H	-3.44985100	-3.67914000	-0.49440700	C	1.67532200	-0.44775300	-3.05528500
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C	-0.69789500	-5.56665200	-2.43258800	Sn	-1.99810200	1.57969800	0.85155000
H	-1.07587200	-6.55561500	-2.71635400	C	-3.41537400	3.14432500	1.24038200
H	0.35935000	-5.52412100	-2.71013100	H	-2.84903600	4.07107300	1.40211200
C	-0.24474300	-4.14064000	-0.55756200	H	-3.97939700	3.29757500	0.31582800
H	0.81677800	-4.11498700	-0.81920700	C	-4.37782400	2.88722000	2.40903000
H	-0.31627500	-4.06752400	0.53271700	H	-5.06354900	3.73312400	2.54424200
C	-2.20511900	-5.51132500	-0.56943500	H	-4.99279800	1.99998000	2.22982800
H	-2.25488400	-5.45134500	0.52414100	H	-3.85256000	2.73652700	3.35973100
H	-2.59761100	-6.49087800	-0.86626500	C	-2.35817700	-0.28758200	1.85117000
B	2.76068600	-0.01256400	-0.71021700	H	-2.23058100	-0.11828700	2.92794600
F	0.66338000	-1.44744200	0.57884600	H	-1.55608500	-0.96744800	1.54740600
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F	3.05576200	-2.82093700	4.39271300	H	-3.88705500	-1.11485000	0.51493300
F	5.30342000	-1.59809400	3.41777800	H	-3.81992500	-1.88040700	2.10792000

H	-4.55171800	-0.28294400	1.92633900
C	-1.10206100	1.55274600	-1.08210100
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C	-1.04702000	2.90315700	-1.81007500
H	-0.38436300	3.61747700	-1.30971400
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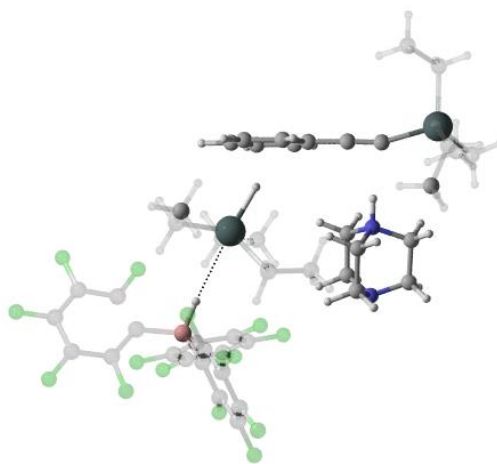


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C	1.12212200	1.62649800	1.87149000
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H	0.84931400	0.79009000	2.51789900
C	-0.55727100	2.91027600	3.05003000
H	-0.90533100	2.02668900	3.59240500
H	-1.41085800	3.57890000	2.91506800
N	1.76438700	3.79828200	2.89597400
C	2.26691900	2.47664300	2.49280700
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C	1.32770200	4.52355300	1.69746900
H	2.20215000	4.71677800	1.06891000
H	0.92012800	5.49064100	2.01172300
C	0.61756800	3.61844400	3.79239600
H	0.30456300	4.60044400	4.16320100
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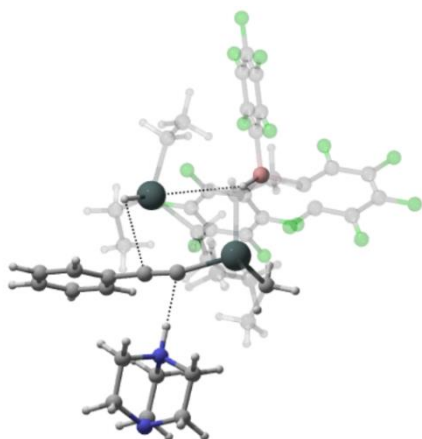
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H	-5.33295100	2.42772800	-2.51952900
C	-7.37042400	2.73628700	-1.87490500
H	-7.54961000	3.55242700	-2.56902200
C	-8.38580700	2.31657400	-1.00870300
H	-9.35463600	2.80753300	-1.02982900
C	-8.15479400	1.26426600	-0.11597100
H	-8.94319900	0.93775200	0.55621300
C	-6.91335600	0.63357500	-0.08411200
H	-6.72412900	-0.18160300	0.60760800
H	-2.77546400	-1.06086200	-1.33411000
N	-2.26320600	-2.17865800	-1.86880100
C	-1.08304100	-2.63084100	-1.08852800
H	-1.39334800	-2.73058000	-0.04699600
H	-0.32161500	-1.85112600	-1.14350200
C	-1.87509500	-1.99169200	-3.29046900
H	-1.07480600	-1.24754900	-3.32157700
H	-2.74180600	-1.58630500	-3.82222100
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H	-4.20382900	-2.80361000	-2.33679900
H	-3.64478100	-3.24754400	-0.71853500
N	-1.44242100	-4.39774100	-2.80446700
C	-1.41023000	-3.37207000	-3.85653600
H	-2.06213900	-3.69968800	-4.67284800
H	-0.39484600	-3.30453100	-4.25109900
C	-0.58208900	-3.98096200	-1.68624400
H	0.44046500	-3.88381200	-2.05193600
H	-0.58893700	-4.76938900	-0.92805200
C	-2.81998800	-4.54590500	-2.32212200
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H	-3.44225700	-4.90096300	-3.15008900
B	2.76333200	-0.77617400	-0.42712800
F	1.00612000	-2.71159500	0.81971900
F	0.72518500	-3.21764700	3.42510300
F	2.36007000	-1.99411200	5.26539700
F	4.28780700	-0.25129800	4.39309800
F	4.58220400	0.28119600	1.81057600
F	5.59230000	-1.47247700	-0.78217700
F	7.56464800	0.15536700	-1.60986500
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F	4.50312600	3.76445600	-1.81279700
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F	3.77601500	-3.64000800	-0.05577000	H	-0.78273300	2.42012400	-3.26833000
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F	2.82864900	-4.98223900	-4.46277400				
F	1.79953800	-2.50138000	-5.00945500				
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C	2.81048800	-1.19368800	1.15562900				
C	1.86116500	-2.07982200	1.66883900				
C	1.68764800	-2.36661800	3.01662400				
C	2.51133700	-1.74817800	3.95276400				
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C	3.76077800	1.59572400	-1.16122700	C	4.28712700	0.10664000	-1.21822300
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C	3.30034700	-4.30334700	-2.23537400	C	3.61882700	-2.19150100	-0.63410300
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C	2.29343400	-2.77312000	-3.78188600	C	2.86003600	-3.32975100	-0.89490100
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H	-2.74521900	3.69084800	1.17870400	H	2.93240000	-4.18941800	-0.23504200
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H	-1.20470900	0.01401500	2.82050100	H	3.77595100	4.73358500	-0.48870400
H	-0.75557500	-1.03413700	1.49579300	H	3.33298100	5.32670300	-2.08961900
C	-2.81219800	-1.26548200	2.16025700	H	3.24769400	3.59592100	-1.74572800
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H	-2.56827300	-2.08559100	2.84771500	H	8.38477100	0.90146200	-4.08167500
H	-3.61388600	-0.67467100	2.61756500	H	6.80879400	0.49609200	-3.38710700
C	-0.72096200	1.37269200	-1.35657600	H	7.05169200	2.05579000	-4.18398700
H	-0.75241500	0.37963200	-1.81150000	C	7.96473300	1.92206500	-2.19337600
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C	-1.32375600	2.40987200	-2.31353900	H	8.68933500	2.73077400	-2.35274300
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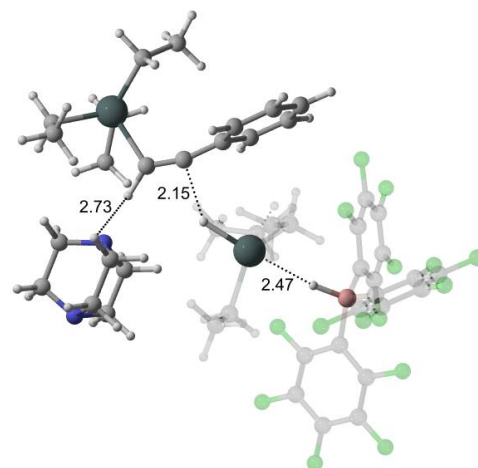
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H	7.72061100	3.81244600	0.97489700	H	1.96889600	3.92404800	3.21019200
C	7.15264800	1.88848300	1.81227100	C	0.44530500	2.39531000	1.70454300
H	7.38206100	2.13260900	2.85765700	H	0.15144800	3.44806300	1.71697300
H	6.31033200	1.18449700	1.81045600	H	-0.46037300	1.80042000	1.58184200
H	8.01593300	1.34549900	1.40971400	B	-4.96458300	-0.27523500	-1.03276000
C	-2.77070800	-0.77398400	-4.51638000	C	-5.89671400	-1.36849600	-1.80208400
H	-2.41096500	-1.77911500	-4.77140900	C	-5.32521000	-2.52205200	-2.34032800
H	-3.77413300	-0.89588500	-4.09936900	C	-7.26978600	-1.25278800	-2.01762100
C	-2.81666400	0.12156500	-5.76312800	C	-6.03134500	-3.48281100	-3.05597100
H	-3.45232400	-0.31418900	-6.54595400	C	-8.02184300	-2.18625000	-2.72909600
H	-3.22930900	1.10978500	-5.52796200	C	-7.39701100	-3.31035300	-3.25788300
H	-1.81936900	0.27200200	-6.19746200	C	-4.49822000	-0.74343700	0.46320700
C	-1.23324800	-1.40330700	-1.34304500	C	-5.02649100	-1.80374500	1.20160700
H	-0.91073100	-2.33757000	-1.81981400	C	-3.43156300	-0.09505800	1.08640500
H	-2.21356400	-1.60715200	-0.90914800	C	-4.52866300	-2.21242100	2.44055800
C	-2.07069600	2.04727500	-2.46303400	C	-2.90599600	-0.46095600	2.31740900
H	-2.28318100	2.53208600	-3.42464500	C	-3.45282800	-1.53807500	3.00466800
H	-3.01023200	2.02620900	-1.90838500	C	-5.58428600	1.23156100	-1.07927800
C	-0.23699400	-1.00962500	-0.24961800	C	-6.07812500	1.95747000	0.00329100
H	-0.57489500	-0.11524800	0.28351900	C	-5.61108700	1.91887900	-2.29443900
H	-0.11801500	-1.80628700	0.50002500	C	-6.54267700	3.26822000	-0.09239200
H	0.75534000	-0.81050500	-0.67108700	C	-6.06693600	3.22441100	-2.44236300
C	-1.02407400	2.85293700	-1.68605900	C	-6.53433800	3.91040100	-1.32552500
H	-0.03478200	2.81668200	-2.16364600	F	-6.97296900	5.17778500	-1.43804800
H	-1.30709200	3.91176600	-1.59849200	F	-6.05082600	3.83454500	-3.64440700
H	-0.92708000	2.46441200	-0.66685600	F	-5.17117300	1.30583900	-3.42282100
Sn	-1.52395300	0.01614300	-2.95296800	F	-6.14200000	1.39827600	1.23795000
Sn	6.32120600	2.71439200	-1.05789600	F	-6.99864900	3.92111600	0.99522800
N	2.71106000	1.57719000	1.16258800	F	-6.08730700	-2.50543100	0.74372700
C	3.30933000	2.58974800	2.09875900	F	-5.07691100	-3.25212400	3.09574500
H	3.54715500	3.47212800	1.50146000	F	-2.94514500	-1.91592500	4.19362300
H	4.23995300	2.16455800	2.48010900	F	-1.85790100	0.21493900	2.85652100
C	2.41644500	0.29452200	1.90127600	F	-2.83886000	0.97378200	0.48296000
H	3.37314700	-0.07953700	2.27463100	F	-7.95970900	-0.20277300	-1.50975000
H	2.02457900	-0.41099600	1.16856800	F	-9.34564300	-2.01491300	-2.90841100
C	1.44815700	2.12500900	0.54394800	F	-8.10359000	-4.22222400	-3.94981300
H	1.09605800	1.37921000	-0.16656500	F	-5.41248400	-4.57328500	-3.55298000
H	1.72853900	3.02508600	-0.00486600	F	-4.00112800	-2.76983500	-2.15549100
N	1.05337700	2.06017800	2.99802800	H	-3.93631800	-0.21445900	-1.67222700
C	1.39770600	0.63492700	3.02902000				
H	0.48245000	0.05479700	2.90473700				



17'

C	0.52183400	4.07533900	-1.83940700	H	-3.09624100	2.81962500	3.47118600
C	1.40935800	3.34959000	-2.27960700	H	-1.94994200	1.53968300	3.07914400
C	-0.45193800	4.92416600	-1.23504300	H	-1.66985600	3.17314100	2.48460400
C	-0.69545200	4.81812000	0.14939600	C	-3.17825900	-0.39692300	-1.15248000
C	-1.19152700	5.84581600	-2.00000800	H	-4.25706000	-0.19359800	-1.11884400
C	-1.66086800	5.62064800	0.75226700	H	-3.00116300	-1.25624300	-0.50111900
H	-0.15011200	4.07909100	0.72864100	C	-0.06268200	0.95202400	0.03791500
C	-2.15225900	6.64859000	-1.38711100	H	0.15292800	-0.00960200	-0.43785900
H	-1.02428100	5.90268900	-3.07153800	H	0.46431400	1.72139100	-0.53347700
C	-2.38801400	6.53893200	-0.01249700	C	-2.73785100	-0.71088400	-2.58937000
H	-1.86214400	5.51357600	1.81369700	H	-1.67705600	-0.98006500	-2.63141200
H	-2.73012600	7.34831800	-1.98404400	H	-3.29420200	-1.56158600	-3.00456500
H	-3.14782300	7.15544000	0.45890800	H	-2.89451100	0.14398400	-3.26041200
C	3.46207500	0.94246500	-1.01782400	C	0.45713000	0.92616200	1.48088900
H	4.39544500	0.43935500	-1.29899300	H	0.33858300	1.89724100	1.97764200
H	2.82874100	0.17858600	-0.56298700	H	-0.06520600	0.18094700	2.08571300
C	3.74255900	2.06010800	-0.00590600	H	1.52264400	0.66393900	1.51311400
H	2.82018100	2.58075400	0.27727300	C	1.02987700	0.23475600	-3.61818100
H	4.18745600	1.66023700	0.91389000	H	0.06909300	0.52535600	-3.18036000
H	4.44771300	2.80326100	-0.40583900	H	0.94938300	0.40901400	-4.69823600
C	3.34574100	3.35754900	-5.24297900	C	1.33935900	-1.24066400	-3.31592500
H	4.10615500	3.73668100	-5.93905300	H	0.55585100	-1.89185700	-3.71979200
H	2.54196100	2.92096800	-5.84777000	H	2.29211800	-1.55882300	-3.75807100
H	2.90834800	4.22026300	-4.72177700	H	1.38981000	-1.43398500	-2.24047900
C	3.92835900	2.33320900	-4.25712500	Sn	2.49148100	1.58681600	-2.82338400
H	4.33981500	1.47610300	-4.80467900	Sn	-2.17741300	1.30315700	-0.29521100
H	4.77339300	2.76467200	-3.70252400	N	4.50339600	7.71435900	-0.90641700
H	2.50777800	4.88313800	-1.77354600	C	3.40434100	8.14040700	-1.78031800
C	-3.25633800	2.09505800	1.41238000	H	3.83093900	8.61087300	-2.67045900
H	-3.78571600	2.98976700	1.05871600	H	2.81408300	8.89564200	-1.25444000
H	-4.02509600	1.35366100	1.65933500	C	3.95814100	7.11091500	0.31604100
C	-2.44915800	2.42472300	2.67614800	H	3.36129100	7.86345700	0.83826700
				H	4.79065300	6.83457700	0.96859700
				C	5.34226700	6.73727000	-1.60917800
				H	6.16752700	6.45099400	-0.95170100
				H	5.77132400	7.21754400	-2.49278300
				N	3.10650300	5.70746600	-1.52200500
				C	3.09111600	5.86342400	-0.02420500
				H	3.48018800	4.93461600	0.39576900
				H	2.04458000	5.96543400	0.27037000
				C	2.51121100	6.92692500	-2.17359700
				H	1.48341800	7.00739900	-1.81507200
				H	2.48837300	6.73296100	-3.24844800
				C	4.50825300	5.48632600	-2.01634400

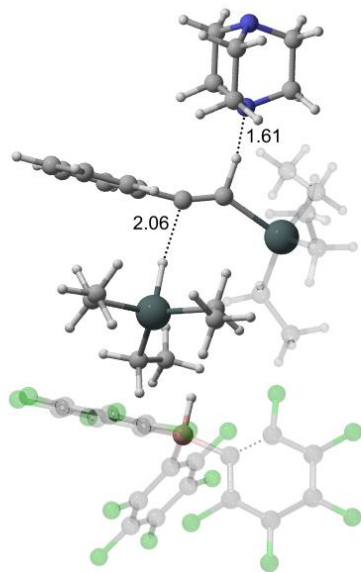
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H	4.86656700	4.56232900	-1.55993000
H	-2.23702900	2.53041000	-1.53510900
B	-0.64100900	-2.79264700	1.23281200
C	0.75379100	-3.62610800	1.06824900
C	1.91127100	-3.05397500	0.55186800
C	0.86560900	-4.98575600	1.36386100
C	3.09463600	-3.75305400	0.32910000
C	2.02365300	-5.73073500	1.16144500
C	3.15243300	-5.10715400	0.63537600
C	-0.99252000	-2.33984300	2.76331500
C	-0.24293700	-2.60522900	3.90993800
C	-2.10362500	-1.52438300	2.99380300
C	-0.56429900	-2.11742400	5.17809700
C	-2.47448800	-1.02476300	4.23568200
C	-1.69038500	-1.32188300	5.34639300
C	-1.83044000	-3.62427300	0.47709400
C	-2.93002800	-4.25077200	1.06173400
C	-1.78218800	-3.72721000	-0.91474700
C	-3.92658500	-4.89911300	0.33288200
C	-2.74646600	-4.36705900	-1.68536000
C	-3.83748200	-4.95542700	-1.05357200
F	-4.78922500	-5.57640800	-1.77513700
F	-2.64304200	-4.41696600	-3.03039300
F	-0.74287100	-3.17412400	-1.59412500
F	-3.08299500	-4.26170000	2.40733200
F	-4.97239300	-5.47750000	0.95525900
F	0.87648500	-3.36763600	3.85278100
F	0.20986200	-2.40710800	6.24275200
F	-2.01676300	-0.84181500	6.56102400
F	-3.57311100	-0.25429200	4.37715700
F	-2.90204900	-1.17261000	1.95040800
F	-0.18965100	-5.64240400	1.89759900
F	2.07218100	-7.04111800	1.46909900
F	4.28444300	-5.80559500	0.42773800
F	4.18094600	-3.13106100	-0.18450500
F	1.94352300	-1.73001100	0.23093400
H	-0.52628000	-1.76363300	0.61207900



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C	3.20198500	-1.89001800	3.72164800
C	3.90866700	-0.85936600	3.88216300
C	2.65707500	-3.10576700	3.25578900
C	3.08337100	-4.33461000	3.80588700
C	1.68741500	-3.09118600	2.22784400
C	2.54283300	-5.52371200	3.33144400
H	3.81577900	-4.33407000	4.60637300
C	1.14025600	-4.28476600	1.77434600
H	1.36856600	-2.14125900	1.81523700
C	1.56741400	-5.49883600	2.32624300
H	2.86012600	-6.47006400	3.75819200
H	0.36696400	-4.27211900	1.01334400
H	1.12656500	-6.42904400	1.98029900
C	4.68886900	0.79634100	1.04835800
H	4.00203600	0.23871500	0.40046000
H	5.48698900	1.18033300	0.40030500
C	3.95380300	1.95169400	1.74651700
H	4.62550100	2.52863100	2.39447300
H	3.52793500	2.64977700	1.01533200
H	3.12845600	1.58507100	2.36699700
C	5.15092100	-2.92780400	0.41025100
H	5.43287600	-3.91733200	0.02941100
H	4.08815100	-2.97244600	0.67099400
H	5.25918000	-2.21656300	-0.41710000
C	6.01807400	-2.53462600	1.61744000
H	5.90476200	-3.26696100	2.42620800
H	7.08124000	-2.53793700	1.34561000
H	3.80856000	-0.00155800	4.63018800
H	1.69003700	-1.53147300	5.20064500
C	7.08652100	0.22749600	3.70345500
H	6.79689400	1.25839300	3.93975900

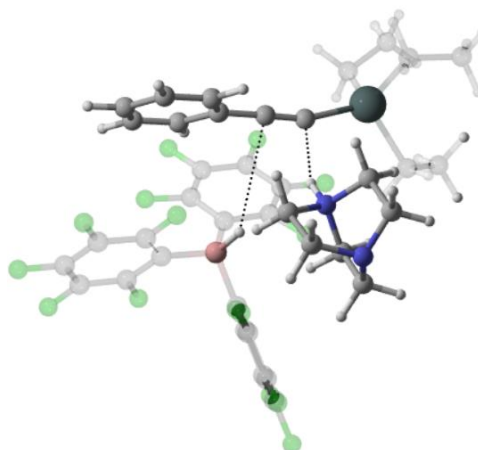
H	8.01473300	0.28980000	3.12133400	H	4.09658300	4.23645400	6.78746200
C	7.31002000	-0.58255900	4.98984500	C	1.91541700	2.75895300	6.85012500
H	8.07703900	-0.12009100	5.62395400	H	1.76268200	3.78522200	6.49982400
H	6.39215100	-0.65756600	5.58480300	H	1.00665600	2.44996000	7.37639600
H	7.64129300	-1.60525300	4.77274600	B	-3.68649400	-2.56955300	5.19769700
C	-0.71395700	-0.95254200	3.42535100	C	-3.96644900	-2.60918500	3.59000200
H	-0.66228500	-1.73861900	2.66659200	C	-3.06777900	-3.26824000	2.74998900
H	-1.77078300	-0.70162100	3.53084700	C	-5.01439200	-1.97895800	2.91838700
C	0.08059500	0.28394900	2.98627300	C	-3.15718700	-3.28758600	1.36506400
H	-0.24403100	0.63984300	1.99851500	C	-5.15215900	-1.97454200	1.52900500
H	-0.06066100	1.11617300	3.68605800	C	-4.21187000	-2.62871100	0.74166300
H	1.15958500	0.08980900	2.93024700	C	-3.76356100	-4.02663200	5.92244500
C	-0.02820600	-3.93870000	5.55497500	C	-4.37988500	-5.16951900	5.41463600
H	0.28602900	-4.35491900	4.59380500	C	-3.13918100	-4.20969300	7.15704500
H	-1.04468500	-4.29805600	5.72144200	C	-4.36392600	-6.40547200	6.05946000
C	-0.61528900	-0.62607400	7.04582200	C	-3.09668700	-5.41953300	7.84079600
H	-0.37723400	0.42261300	6.82517000	C	-3.71308600	-6.53466700	7.28176100
H	-1.70220200	-0.67867300	7.14529800	C	-4.53843200	-1.43153400	5.99458400
C	0.90652900	-4.40234500	6.67884000	C	-5.65671200	-1.68380700	6.79039400
H	0.53356700	-4.09934900	7.66321400	C	-4.16488200	-0.08892500	5.94002700
H	1.00067100	-5.49724000	6.69285100	C	-6.34030600	-0.69715300	7.49860800
H	1.91780400	-3.98804700	6.57015900	C	-4.81249400	0.93213900	6.62728500
C	0.05279200	-1.07649200	8.35222700	C	-5.91211300	0.62393300	7.42132600
H	1.14665400	-1.11760400	8.27246200	F	-6.55409000	1.59053300	8.10008500
H	-0.19046800	-0.39666200	9.18048400	F	-4.38782500	2.20870100	6.53408100
H	-0.28928000	-2.07438200	8.64388900	F	-3.11555000	0.29279900	5.16169500
Sn	-0.08748700	-1.80107900	5.31375500	F	-6.15605900	-2.93815000	6.89439800
Sn	5.55846800	-0.59977600	2.43385500	F	-7.41028700	-1.00593000	8.25429100
N	3.56589500	1.18803700	5.86533300	F	-5.05466800	-5.12509200	4.24093300
C	4.58124700	2.25719900	5.93180300	F	-4.97061400	-7.47632000	5.51326200
H	4.57229300	2.79120700	4.97489600	F	-3.68089500	-7.72006600	7.91595300
H	5.56348800	1.78609300	6.04726400	F	-2.45662400	-5.52720100	9.02245500
C	3.57126200	0.42821300	7.13581800	F	-2.51298800	-3.16140000	7.75546400
H	4.56291800	-0.02410000	7.25154500	F	-5.98285100	-1.32705300	3.60213900
H	2.84390700	-0.38129200	7.03814800	F	-6.18352700	-1.34023300	0.94189600
C	2.23027700	1.79354900	5.66417400	F	-4.31833400	-2.62793100	-0.59899900
H	1.50788400	0.97911000	5.59778100	F	-2.22425500	-3.92474000	0.61781900
H	2.23665700	2.31323400	4.70031500	F	-2.01447400	-3.94169000	3.28587100
N	3.02906400	2.76045100	7.81153800	H	-2.51599700	-2.23288700	5.30068000
C	3.22951200	1.39297600	8.31539600				
H	2.31390600	1.07844300	8.82561100				
H	4.03423400	1.41492000	9.05822300				
C	4.25063600	3.20781400	7.13062000				
H	5.06681300	3.21913400	7.86110400				



TS15'

C	2.76593700	1.85070600	1.62233700	C	0.11919500	-0.15877900	4.37500000
C	3.83552300	1.57425500	1.01380300	H	-0.19711000	0.83497800	4.03297800
C	1.83098400	2.56178400	2.42390800	H	-0.79937900	-0.74215600	4.50721400
C	2.10964000	2.74339200	3.79399200	C	0.86598600	-0.04913200	5.71163600
C	0.65293300	3.10333200	1.86964200	H	0.22622700	0.39280700	6.48735500
C	1.23007200	3.47016500	4.59164900	H	1.19084000	-1.02690800	6.07671300
H	3.00490700	2.29857300	4.21640700	H	1.76086700	0.57805400	5.62869000
C	-0.22027700	3.82449700	2.67567600	C	-0.21880900	-2.33766600	1.65722100
H	0.43234800	2.93194700	0.82097700	H	-1.18201200	-1.82866000	1.79901400
C	0.06671600	4.00991800	4.03527200	H	-0.28730500	-3.27798700	2.20516600
H	1.44011000	3.59729400	5.64910900	C	3.24781400	-1.54215600	3.11802700
H	-1.13151300	4.23570700	2.25203700	H	3.50895200	-2.38454200	2.47507900
H	-0.62555700	4.56380100	4.66249700	H	3.77973600	-0.66135200	2.74046800
C	6.30982000	-0.77524000	1.50159900	C	0.03305700	-2.59570500	0.16908300
H	7.19752600	-1.08235100	0.93405000	H	0.93983100	-3.18608600	0.01157900
H	5.92642000	-1.67162700	1.99832400	H	-0.79761200	-3.16524300	-0.26863400
C	6.68515600	0.29195100	2.53910900	H	0.12864700	-1.66420700	-0.40317100
H	5.81404000	0.60614800	3.12582600	C	3.70218300	-1.82812100	4.55302100
H	7.43493800	-0.08787600	3.24404200	H	3.55093200	-0.96483100	5.20966700
H	7.10717800	1.18773300	2.06528600	H	3.16695300	-2.67513200	4.98419300
C	4.81330900	1.76799000	-2.39651000	H	4.77116000	-2.07861500	4.57403300
H	5.31809000	2.25532700	-3.24107600	C	3.40486000	-1.59655600	-0.54644700
H	3.96306900	1.20955300	-2.80654100	H	2.52058300	-1.48172400	0.08248900
H	4.39771100	2.55858400	-1.75929700	H	3.08887600	-1.34380400	-1.56601900
C	5.76731600	0.85156000	-1.61520100	C	3.93898700	-3.03711000	-0.47884500
H	6.16446800	0.06984200	-2.27577400	H	3.17066000	-3.74889400	-0.80259700
H	6.63739400	1.41270300	-1.25295700	H	4.81289100	-3.18186600	-1.12641200
H	4.56457900	2.51891200	0.95013700	H	4.22577800	-3.32425500	0.53763000
				Sn	4.84186700	-0.13493800	0.06293200
				Sn	1.17288600	-1.09006700	2.73116500
				N	6.42993100	6.20452700	1.34557600
				C	5.11520900	6.33366100	0.70210000
				H	5.24935700	6.84711800	-0.25543700
				H	4.48393500	6.96708200	1.33357900
				C	6.26473900	5.54899200	2.65026500
				H	5.63553500	6.18702200	3.27921800
				H	7.24772800	5.47836500	3.12682600
				C	7.30347800	5.37979500	0.49965200
				H	8.28470700	5.31313200	0.98039900
				H	7.43693700	5.89126900	-0.45905800
				N	5.39451600	3.89252000	1.02411600
				C	5.62613600	4.13474900	2.46696700
				H	6.27319100	3.33636200	2.84174300
				H	4.66082500	4.05119000	2.97532700

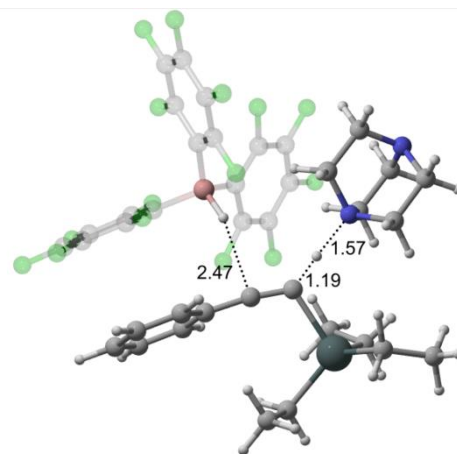
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H	4.29147700	4.70276400	-0.55932500
C	6.67900400	3.95970700	0.29570300
H	6.47903500	3.74847700	-0.75860300
H	7.32768000	3.16728400	0.68231700
H	1.48856900	0.23285700	1.55796300
B	1.44263600	-4.79119000	4.17835600
C	2.73285700	-5.77539100	4.38706800
C	3.96711000	-5.58831700	3.77011500
C	2.64071200	-6.94335400	5.14770700
C	5.04014300	-6.46882000	3.90109100
C	3.68058200	-7.85190300	5.31078200
C	4.89794700	-7.61116500	4.67857200
C	0.83616200	-4.14420300	5.55753200
C	1.52033000	-4.06434900	6.77378500
C	-0.40471500	-3.50065600	5.57500700
C	1.01557500	-3.44206400	7.91589600
C	-0.95411700	-2.87225100	6.68649000
C	-0.23665400	-2.84219300	7.87662900
C	0.37343900	-5.63956200	3.27271300
C	-0.77660600	-6.29215300	3.71855300
C	0.62196300	-5.78028200	1.90505200
C	-1.63539900	-7.00062600	2.87878500
C	-0.20454300	-6.47446100	1.02790500
C	-1.35060500	-7.09042200	1.52044200
F	-2.16800900	-7.76782800	0.69431000
F	0.08865500	-6.55382300	-0.28687100
F	1.73000800	-5.21439500	1.35753500
F	-1.12721600	-6.25537000	5.02363000
F	-2.73889100	-7.59853200	3.36627200
F	2.76413700	-4.58736200	6.90733900
F	1.73894900	-3.39942900	9.05142500
F	-0.73309000	-2.21697500	8.95955600
F	-2.15321900	-2.25956400	6.61185000
F	-1.15560300	-3.44315500	4.44322300
F	1.48272200	-7.22643600	5.78779000
F	3.52975400	-8.95518000	6.06760600
F	5.92076200	-8.47382400	4.81682400
F	6.21309700	-6.22338200	3.27869300
F	4.20262900	-4.50164600	2.98732300
H	1.78731000	-3.84568800	3.50363400



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C	-3.10671100	-1.15662100	0.33985000
C	-3.63440800	-1.40210600	-0.92490200
C	-3.84997200	-1.69250400	1.39324200
C	-4.78391800	-2.15664400	-1.15007900
C	-5.00429000	-2.44895800	1.22255300
C	-5.47335700	-2.68928500	-0.06724400
C	-0.48865100	-1.03894000	1.23701800
C	-0.39491700	-2.38428100	1.59425900
C	0.70825000	-0.33811900	1.38536400
C	0.77472900	-2.98587300	2.06387900
C	1.89254400	-0.88255900	1.85879400
C	1.93309100	-2.23045400	2.19805500
C	-2.22012100	1.07067700	1.45104500
C	-1.94842800	1.32047600	2.79794200
C	-2.95770300	2.07605500	0.82396900
C	-2.35253900	2.47641200	3.46616300
C	-3.37775300	3.24914300	1.44204900
C	-3.06983900	3.45376000	2.78327900
H	-1.37571400	0.13570200	-0.48032000
C	4.74404400	0.61888500	-3.47990300
H	5.06438200	-0.32327000	-3.94173700
H	3.94880600	1.01721100	-4.12401700
C	5.91799800	1.60920000	-3.40400400
H	6.74479400	1.21122200	-2.80355700
H	6.32114000	1.83722600	-4.39945600
H	5.61723300	2.56125100	-2.94871700
C	4.95830800	-1.37233500	-0.52687400
H	4.64513800	-1.37721800	0.52157200
H	4.63547500	-2.32851600	-0.95605500
C	6.48427100	-1.21892500	-0.63590600
H	6.83310900	-0.28353300	-0.18191300
H	7.00079600	-2.04001300	-0.12253700

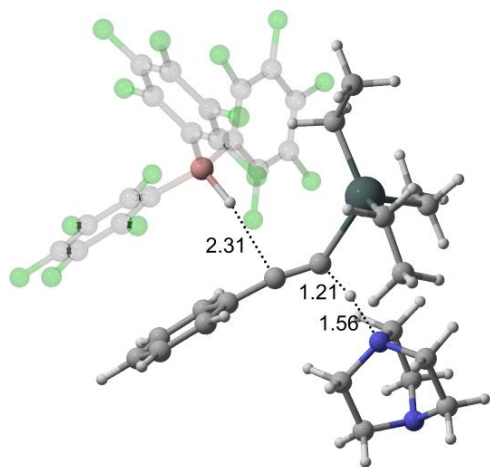
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C	1.14782300	-2.69369100	-3.89568300	F	-4.05713200	5.09090700	-1.67108900
H	1.02293000	-2.80890500	-4.98023800	F	-1.62490700	4.34912500	-2.69182700
H	2.20193300	-2.92684100	-3.69188700	F	-0.22816300	2.36235700	-1.57373700
C	-1.28592400	-0.21382100	-3.13738300	F	-2.16718100	-0.84911000	3.15825500
H	-1.82931900	-1.16340500	-3.21031300	F	-1.67759900	-0.30716700	5.72898100
H	-1.41707000	0.14359000	-2.11681400	F	-0.16431200	1.86432000	6.43732700
C	3.26935300	0.45858600	-4.94206100	F	0.85332000	3.49743100	4.48623100
H	3.51303300	-0.56163800	-5.26657700	F	0.37627700	2.97275800	1.89368900
H	3.72930700	1.14721800	-5.66315500	H	0.06917400	0.82259600	0.33595800
H	3.75825500	0.62293000	-3.97383600	N	3.27463500	-2.44138900	0.37094300
C	0.21798000	-3.66756700	-3.15472900	C	3.13573000	-2.86011300	1.81220800
H	0.44444600	-4.71604200	-3.39092700	H	2.10706500	-3.18999400	1.94805200
H	0.28592200	-3.55373200	-2.06701900	H	3.30078500	-1.96708100	2.41807700
H	-0.83183500	-3.49716100	-3.41864800	C	4.69034000	-2.00066300	0.09812100
C	-1.84659400	0.81134700	-4.13454900	H	4.91137600	-1.19826100	0.80286100
H	-1.33325200	1.77529100	-4.05346100	H	4.70203300	-1.58432500	-0.91051700
H	-1.75299500	0.47236500	-5.17405800	C	2.90512900	-3.57932300	-0.54400400
H	-2.91193700	0.99142500	-3.94330800	H	3.04979400	-3.21693700	-1.56307500
B	-1.04655400	0.75669500	0.78088700	H	1.84762200	-3.78477500	-0.38991600
C	-0.90078100	1.02613800	2.38776500	N	4.83569900	-4.38196200	0.80587600
C	-0.15527700	2.13109000	2.81122900	C	5.60136200	-3.24734700	0.27610100
C	-1.40470800	0.24085200	3.42401800	H	6.04163300	-3.54686400	-0.67937200
C	0.10291600	2.43016400	4.14547200	H	6.42100000	-3.02282300	0.96435300
C	-1.17319600	0.49956400	4.77500100	C	4.18080300	-3.98582100	2.05997200
C	-0.40825000	1.60150400	5.14048500	H	4.95335400	-3.65230600	2.75861100
C	-1.90525800	1.95025400	0.08355500	H	3.69455200	-4.86332300	2.49454100
C	-3.14352300	2.37620400	0.56494600	C	3.81783700	-4.78189400	-0.17421400
C	-1.43072600	2.66341900	-1.01609300	H	3.22556900	-5.59418600	0.25578200
C	-3.87689400	3.41633400	0.00347600	H	4.31959600	-5.16979200	-1.06513500
C	-2.13070300	3.70670000	-1.61862100	H	2.64297800	-1.65163900	0.15445600
C	-3.36538700	4.08669000	-1.10515700				
C	-1.55243300	-0.76093100	0.42150100				
C	-2.74055700	-1.14408400	-0.20491400				
C	-0.70233400	-1.83022400	0.69405700				
C	-3.05697600	-2.46297300	-0.53749900				
C	-0.97648400	-3.15811100	0.40305500				
C	-2.16858200	-3.48651000	-0.23061800				
F	-2.44292100	-4.76262100	-0.55101000				
F	-0.08394100	-4.13733800	0.71622300				
F	0.49898900	-1.60340600	1.31487300				
F	-3.66640400	-0.22663700	-0.55535400				
F	-4.20813300	-2.75422000	-1.16802800				
F	-3.69633000	1.74718400	1.62849200				



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C	3.29819900	-1.18863200	3.01379000	C	-2.14919000	3.10346800	1.44176700
C	2.58085400	-1.40332500	1.84387200	C	-0.53334500	3.28586800	-0.25143900
C	2.76230800	-0.53523100	0.74198700	C	-2.53222800	4.42810300	1.26433700
C	3.65851900	0.55340800	0.84113100	C	-0.88273100	4.61752900	-0.47058900
C	4.36322600	0.75980500	2.01953800	C	-1.89273600	5.19348700	0.29144900
C	4.18569800	-0.10982600	3.10240800	C	-1.84344100	-0.19883800	0.68748700
H	3.15375000	-1.84694300	3.86475600	C	-3.10709500	0.01037100	0.12874300
H	1.87640600	-2.22141100	1.76481900	C	-1.54964100	-1.54920600	0.90041100
H	3.76366000	1.23186800	0.00124700	C	-4.01461700	-1.01183500	-0.15602400
H	5.03106300	1.61024400	2.10931400	C	-2.41863700	-2.60265200	0.64454800
H	4.72616100	0.06832600	4.02739200	C	-3.67395100	-2.33212200	0.10761300
C	2.09345400	-0.78241300	-0.46957000	F	-4.52558500	-3.33130400	-0.17803300
C	1.63794900	-1.10788800	-1.58702600	F	-2.05537200	-3.87690300	0.89038500
Sn	2.76743100	-2.75815800	-2.53324500	F	-0.33530300	-1.89863700	1.39736100
C	1.24251200	-4.27170900	-2.63724400	F	-3.52637300	1.25263600	-0.21539300
H	0.55349200	-4.00469600	-3.44793500	F	-5.20710700	-0.73165800	-0.71567300
H	1.71901400	-5.21395900	-2.93667200	F	-2.80354900	2.39927900	2.39541200
C	3.38405500	-1.97343300	-4.44515400	F	-3.50926600	4.97737200	2.00872900
H	2.92778100	-0.98339800	-4.55732100	F	-2.24448200	6.47575700	0.09583100
H	4.46813200	-1.81305800	-4.40909300	F	-0.24919100	5.35240000	-1.40766600
C	4.38726800	-3.24238100	-1.20836900	F	0.48263800	2.80955500	-1.01939700
H	3.97080000	-3.34126600	-0.19875100	F	-1.68765600	-0.56004400	3.52819000
H	4.75978800	-4.23661400	-1.48688200	F	-0.46020100	-0.51524400	5.89451400
C	0.48792000	-4.43971900	-1.30911100	F	1.77216900	1.02527400	6.28670800
H	0.02456900	-3.50396900	-0.98245000	F	2.74435600	2.54087500	4.22294300
H	-0.30875000	-5.18854000	-1.39248200	F	1.57148900	2.46241600	1.81301500
H	1.15610000	-4.76487600	-0.50273800	N	-0.57424300	-0.51740100	-3.13632000
C	3.01067500	-2.88163200	-5.62787700	C	-1.60019200	-1.54481500	-2.84925000
H	3.33206500	-2.44297600	-6.58102200	H	-1.80962800	-1.51054500	-1.78093100
H	3.48130700	-3.86932900	-5.55043300	H	-1.16845100	-2.52464200	-3.07679500
H	1.92788800	-3.04333100	-5.69283800	C	-0.22341000	-0.56780000	-4.56996200
C	5.52996600	-2.21482500	-1.21974900	H	0.18091000	-1.56325000	-4.78630600
H	5.97608800	-2.11280100	-2.21634100	H	0.56811900	0.16712800	-4.75125700
H	5.18517700	-1.22310800	-0.90770400	C	-1.10208500	0.82908200	-2.80719400
H	6.33221000	-2.50940200	-0.53162800	H	-0.31372500	1.55497700	-3.01946200
H	0.68097900	-0.82052100	-2.24228900	H	-1.29394200	0.85811900	-1.73621000
B	-0.70110200	0.93692100	0.99991600	N	-2.66161200	-0.05490900	-4.53349700
C	-0.09431000	0.91189300	2.52246800	C	-1.50756300	-0.26735000	-5.41438200
C	1.02940400	1.69922500	2.79492800	H	-1.37080600	0.63087100	-6.02534200
C	-0.57129400	0.20009800	3.62362400	H	-1.73533700	-1.09943000	-6.08938900
C	1.65619600	1.76542400	4.03357300	C	-2.87001800	-1.25451000	-3.71082300
C	0.03639600	0.21671300	4.87938300	H	-3.09660700	-2.09523300	-4.37532000
C	1.16412400	1.00193100	5.08656200	H	-3.74425300	-1.08782400	-3.07504800
C	-1.15509100	2.47293600	0.69270500	C	-2.39051500	1.08913600	-3.64671300

H	-3.25706800	1.23293200	-2.99485900
H	-2.28515800	1.98703200	-4.26436400
H	0.22691700	0.66657900	0.26553800

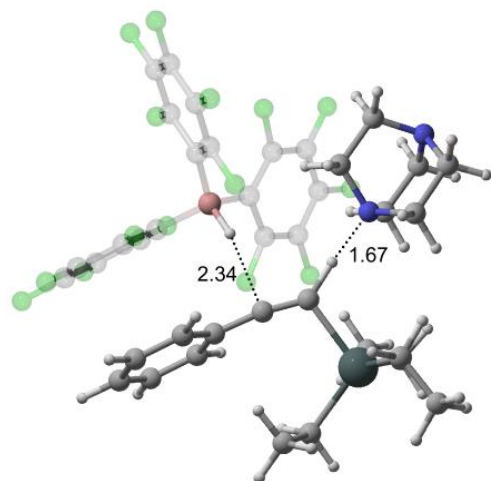


TS16'

C	-8.84970200	-0.16489600	-2.15654000
C	-9.17478000	-0.75974600	-3.36938500
C	-9.78287900	-2.03578700	-3.38652000
C	-10.07063100	-2.69364700	-2.16696800
C	-9.72096100	-2.09575600	-0.96290000
C	-9.11455100	-0.83412400	-0.95575000
H	-8.40769800	0.82618600	-2.14041700
H	-8.98967800	-0.24935600	-4.30884400
H	-10.56582000	-3.65549500	-2.18696700
H	-9.94401500	-2.59791500	-0.02669000
H	-8.86916900	-0.35942700	-0.01028000
C	-10.03032600	-2.66891200	-4.61875900
C	-10.04501900	-3.30055200	-5.70075300
Sn	-11.19444300	-3.35151600	-7.57181800
C	-10.08306500	-1.92676800	-8.73749100
H	-10.44252500	-1.99301400	-9.77243300
H	-10.35987000	-0.93083100	-8.37424000
C	-10.84375200	-5.39924200	-8.14730400
H	-11.16437300	-5.52307700	-9.18998500
H	-9.76477000	-5.59667000	-8.13518000
C	-13.30181700	-2.98703400	-7.55793000
H	-13.80756600	-3.95457900	-7.46700200
H	-13.56482000	-2.40940800	-6.67728300
C	-8.56174700	-2.12246600	-8.68398300
H	-8.26408300	-3.10703100	-9.06644000
H	-8.03823600	-1.36801800	-9.28552300
H	-8.18521500	-2.03926400	-7.65699100
C	-11.59353700	-6.38958000	-7.23986100

H	-11.38743300	-7.43270300	-7.51397600
H	-11.32345100	-6.26848100	-6.18435700
H	-12.67850100	-6.24940200	-7.30517100
C	-13.74543400	-2.24956500	-8.83134600
H	-13.27652400	-1.26214300	-8.90806100
H	-13.50349900	-2.80597800	-9.74634600
H	-14.83178900	-2.09591800	-8.82339300
B	-13.33386000	-1.73168200	-4.01108400
C	-13.14591300	-1.34028600	-2.43714100
C	-12.43992800	-0.17726300	-2.10964300
C	-13.57899900	-2.07397300	-1.33154000
C	-12.17820900	0.23856900	-0.81037200
C	-13.32355600	-1.70706800	-0.00984400
C	-12.61440600	-0.54190800	0.25502000
C	-13.91164000	-0.44442000	-4.83067800
C	-15.06564100	0.23914500	-4.44493000
C	-13.24795500	0.11331200	-5.92039500
C	-15.55347500	1.36588100	-5.09907500
C	-13.69783600	1.23291100	-6.61516300
C	-14.86553300	1.86438100	-6.20317600
C	-14.11818200	-3.14257800	-4.30706400
C	-15.36615400	-3.30083700	-4.91447100
C	-13.46152800	-4.35213000	-4.06532000
C	-15.91022200	-4.53625300	-5.26940900
C	-13.95571100	-5.60601500	-4.40155100
C	-15.19867000	-5.70266500	-5.01802400
F	-15.69721700	-6.90138400	-5.36565500
F	-13.24398700	-6.72304400	-4.14167900
F	-12.24791700	-4.35265500	-3.45079200
F	-16.12213000	-2.22971800	-5.24506200
F	-17.10892000	-4.60748500	-5.87659100
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F	-14.29580200	-3.21169400	-1.49056200
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H	-12.20837000	-1.91389600	-4.42622200
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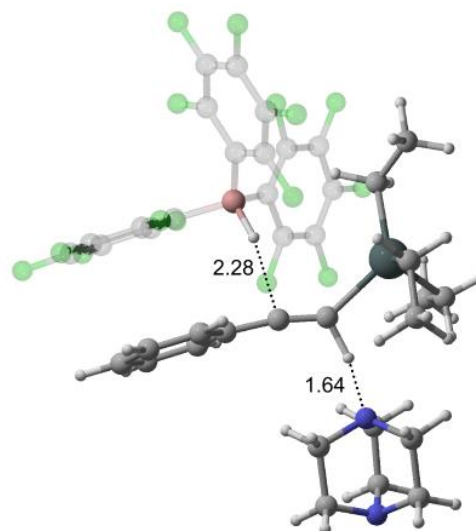
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H	-6.64190000	-4.04909200	-7.10568200	H	0.39085200	-3.89656500	-3.41368300
H	-7.53784100	-5.43279900	-7.74625600	H	1.57618000	-5.09840800	-2.92393400
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H	-8.88139300	-6.76671400	-6.26681800	H	2.37489200	-1.53000900	-4.96665200
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H	-7.06384900	-8.14419500	-5.64282000	H	5.03247000	-3.09197000	-4.61839100
H	-9.10694800	-4.04870500	-5.84643500	H	3.59270800	-3.72408400	-5.42901100



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C	3.18479200	-1.18070200	3.01250900	C	-2.09498800	3.24487100	1.40005300
C	2.43462300	-1.36238900	1.85779000	C	-0.49412500	3.23922800	-0.31761900
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C	4.27570900	0.75302800	2.01679100	C	-1.73345700	5.24953800	0.13136300
C	4.10144700	-0.12566400	3.09292600	C	-1.96755700	-0.11783000	0.75843300
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H	1.70768600	-2.16104000	1.78566600	C	-1.70722000	-1.47759900	0.95405300
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H	4.66827000	0.02659800	4.00670300	C	-3.86852600	-2.19393400	0.20118000
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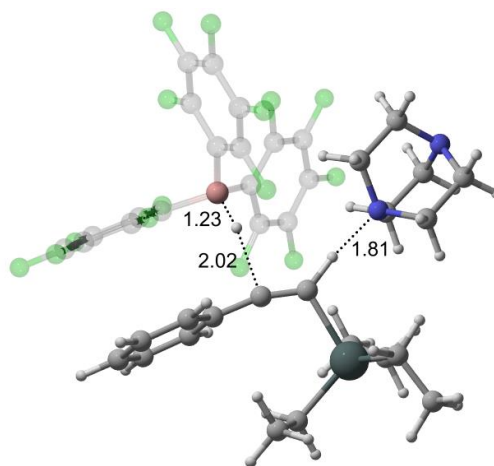
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F	-2.77379000	2.63459300	2.39965100
F	-3.33473700	5.22465200	1.87579300
F	-2.01304300	6.53729200	-0.13228400
F	-0.10582400	5.21812800	-1.59077200
F	0.48515700	2.66195600	-1.06432600
F	-1.79387500	-0.48650300	3.58891500
F	-0.55768100	-0.46047700	5.95015600
F	1.70073200	1.04328500	6.33409000
F	2.68984800	2.54290700	4.26616300
F	1.50624800	2.48632000	1.86269900
N	-0.84566400	-0.43616000	-3.12276700
C	-1.83241200	-1.48708200	-2.79349500
H	-2.02303800	-1.43537400	-1.72214600
H	-1.37558300	-2.45927700	-3.00634300
C	-0.54054000	-0.49624600	-4.56522800
H	-0.13048600	-1.48950400	-4.78395400
H	0.23514700	0.24669000	-4.78135700
C	-1.40687800	0.89668500	-2.79853400
H	-0.65425800	1.64474500	-3.05951900
H	-1.55640000	0.94367200	-1.72104200
N	-2.99112700	-0.05589600	-4.46369900
C	-1.85350400	-0.22572100	-5.37549000
H	-1.76002800	0.68284200	-5.97958700
H	-2.07403600	-1.05703500	-6.05413600
C	-3.12959400	-1.26089900	-3.63372900
H	-3.32789200	-2.11298800	-4.29309700
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H	-3.58560100	1.20166500	-2.90066700
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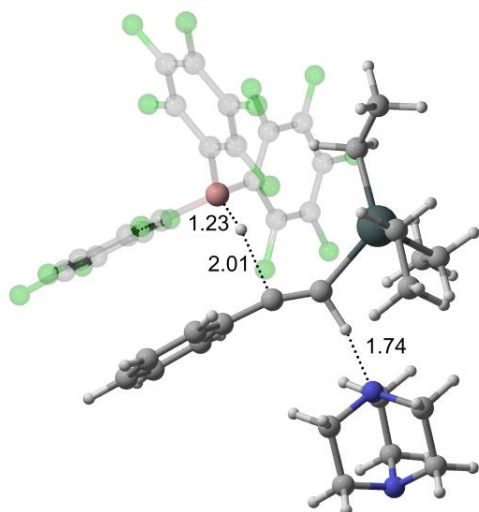
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C	2.28210200	0.22329600	3.83304000
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H	3.64426800	3.16982900	2.77633900
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C	1.99479200	-0.20528900	0.15729600
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H	-0.14558000	0.56582800	0.33135000	H	-8.10548100	-0.53878400	-2.47723200
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H	5.27464700	-0.87817200	-0.23192500	Sn	-10.52120900	-4.45629700	-7.09806300



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C	-11.95146900	-6.05044400	-7.30640900	F	-16.68809600	-0.55741700	-4.64516700
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H	-11.41600600	-6.94154300	-7.65827700	F	-15.65232100	0.81070800	-2.30544500
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H	-10.75744200	-3.19286000	-9.47550500	F	-14.70804500	4.41957400	-5.18653100
H	-9.28641400	-2.65571100	-8.67795800	F	-12.95344800	2.84471600	-6.58300700
C	-8.87016200	-4.93124600	-5.80783900	F	-12.52394000	0.30570900	-5.84987900
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H	-8.50808300	-5.92906700	-6.08698200	F	-13.66005300	-2.57190000	1.30792700
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H	-6.90256800	-4.18688200	-5.20768900	H	-14.02533400	-0.31639700	-7.82946100
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TS17'

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C	-9.70409800	-2.17688400	-3.37560500	H	-13.11778100	-1.15849600	-8.97543400
C	-9.92366900	-2.91011600	-2.18613900	H	-13.37209600	-2.66108600	-9.87525200
C	-9.46812300	-2.40778200	-0.97324200	H	-14.70640900	-1.93252100	-8.97536800
C	-8.81557500	-1.17029900	-0.92602100	B	-13.10439500	-1.83972300	-4.02850300
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H	-8.92103000	-0.35470700	-4.23129300	C	-12.17449700	-0.34286400	-2.09977300
H	-10.44644000	-3.85579200	-2.23394100	C	-13.32145900	-2.25209500	-1.36053900
H	-9.63838500	-2.96891000	-0.05958400	C	-11.88415000	0.02840100	-0.79332200
H	-8.48276800	-0.77216300	0.02813300	C	-13.04136700	-1.92710900	-0.03330000
C	-10.06795000	-2.70202800	-4.63388600	C	-12.31163200	-0.78015400	0.25461600
C	-10.03118800	-3.26085400	-5.76572800	C	-13.62637100	-0.52082300	-4.82962100
Sn	-11.16275700	-3.37589600	-7.63911800	C	-14.75825800	0.19114700	-4.42933100
C	-9.99801300	-2.04956400	-8.86824300	C	-12.95065700	0.03111100	-5.91382400
H	-10.35620400	-2.15195400	-9.90071000	C	-15.21373700	1.34097600	-5.06600700
H	-10.23461000	-1.02609600	-8.55641300	C	-13.36811900	1.17340200	-6.59122700
C	-10.82799300	-5.45366500	-8.10143800	C	-14.51460700	1.83416100	-6.16567200
H	-11.16757200	-5.63960000	-9.12873400	C	-13.91960100	-3.21932900	-4.36227600
H	-9.74674000	-5.63948400	-8.09673100	C	-15.17093200	-3.31938100	-4.97736100
C	-13.25672300	-2.92776300	-7.69046200	C	-13.32258100	-4.45847000	-4.11363600
H	-13.80082100	-3.87831500	-7.65424300	C	-15.77432700	-4.52828100	-5.32511400
H	-13.53618600	-2.37205300	-6.79968900	C	-13.88059000	-5.68864700	-4.43774500
C	-8.48552100	-2.30330000	-8.79850700	C	-15.12455300	-5.72697200	-5.05809100
H	-8.22814200	-3.31788700	-9.12687500	F	-15.68216100	-6.90047600	-5.39686300
H	-7.93075700	-1.60329100	-9.43689900	F	-13.23060600	-6.83631500	-4.16142100
H	-8.10619300	-2.18316500	-7.77635400	F	-12.11463200	-4.51492100	-3.49324800
C	-11.54669900	-6.39649500	-7.12243800	F	-15.87284300	-2.21482600	-5.31523600
H	-11.34627200	-7.45183500	-7.34958700	F	-16.97151500	-4.54322000	-5.93753400
H	-11.23957800	-6.22107500	-6.08499700	F	-15.47343600	-0.24036500	-3.36676600
				F	-16.31915800	1.97741700	-4.64191100
				F	-14.93878700	2.93764100	-6.80226300
				F	-12.67082600	1.64277100	-7.64572000
				F	-11.79069800	-0.52781100	-6.36890900
				F	-14.05544500	-3.37430000	-1.54065100
				F	-13.46509000	-2.71564200	0.97149500
				F	-12.01590100	-0.45908400	1.52569400
				F	-11.16858500	1.13919300	-0.53026700
				F	-11.69516900	0.47892600	-3.06724000
				H	-11.96076900	-2.05073900	-4.44011000
				N	-7.67072500	-4.90614900	-5.82859700
				C	-6.86479300	-4.21752300	-4.79763000
				H	-7.51651500	-4.01525300	-3.94216700
				H	-6.54514800	-3.25338400	-5.20776300

C	-6.82327500	-5.18485800	-7.00452200	H	-4.67585600	-5.66530600	-6.80069700
H	-6.46284900	-4.22799400	-7.39456100	C	-5.65067400	-5.11904000	-4.40302900
H	-7.45048200	-5.64505100	-7.77501100	H	-4.70027700	-4.62974600	-4.64151200
C	-8.18239600	-6.17956600	-5.27786600	H	-5.65241800	-5.33630600	-3.32971900
H	-8.77548900	-6.66662100	-6.05734100	C	-6.97834600	-7.06588800	-4.82378900
H	-8.85712400	-5.94161300	-4.44866500	H	-7.00993600	-7.25674900	-3.74595700
N	-5.70727000	-6.39337300	-5.13341600	H	-6.98813800	-8.03552800	-5.33263900
C	-5.64562700	-6.12255200	-6.57699100	H	-9.06407200	-3.86958700	-5.94105600
H	-5.69120300	-7.08045500	-7.10591300				