Supporting Information

for

Expanding the Scope of Bis(catecholato)germane Catalysis: Hydrosilylation, Hydroboration, Friedel-Crafts Alkylation and Oligomerization

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General Experimental

All reactions were conducted under a nitrogen atmosphere using an MBraun Labmaster 130 glovebox. Solvents and reagents were purified by standard methods. NMR data were obtained on a 600 MHz INOVA, 400 MHz INOVA or a 400 MHz Bruker Avance III NMR spectrometer. The standards used were as follows: residual $CHCl_3$ (7.26 ppm), $CHDCl_2$ (5.32 ppm), toluene-d_8 (2.09 ppm) for ^1H NMR spectra; $CDCl_3$ (77.16 ppm) for ^{13}C NMR spectra; J values are reported in Hertz.

General Catalytic Procedures

A mixture containing the substrates (0.2 mmol of substrate at 1 eq.), catalyst (0.010 mmol for 5 mol%), mesitylene (0.022 mmol) as an internal standard, and, when specified, an additive (0.2 mmol for additives at 1 eq.), in 0.5 mL deuterated solvent (CD_2Cl_2, tol-d_8) were allowed to react for 24 hours in NMR tubes sealed with Parafilm® and electrical tape. Control experiments without catalyst were performed in parallel. Conversion of substrates to products was determined by integration against mesitylene (C_9H_{12}) as an internal standard. Isolation of the Friedel-Crafts alkylation products was performed using preparative TLC (silica gel plates; 80:20 dichloromethane:hexanes).

Test for Hidden Boron Catalysis

A mixture containing HBpin (0.2 mmol) and $Ge(cat^{Cl})_2(ACN)_2$ (0.02 mmol for 10 mol%) in 0.5 mL tol-d_8, and an additional reaction mixture containing HBpin, phenylacetylene and TMEDA (0.2 mmol) with $Ge(cat^{Cl})_2(ACN)_2$ (0.02 mmol for 10 mol%) in 0.5 mL tol-d_8, were allowed to react for 24 hours in NMR tubes sealed with Parafilm® and electrical tape. Both mixtures were analyzed using ^{11}B NMR spectroscopy. No signal was observed which could reasonably be assigned to either BH_3 or BH_3-TMEDA.

Hammett Plot

A solution of styrene (0.1 mmol), substituted styrene (0.1 mmol), and mesitylene (0.022 mmol) dissolved in 0.5 mL of toluene-d_8 was added to solid $Ge(cat^{Cl})_2(ACN)_2$ (0.01 mmol) and the reaction was transferred to an NMR tube. The NMR tube was sealed with Parafilm® and electrical tape and heated to 100 °C for 30 minutes and then ^1H NMR spectra were recorded at room temperature. The experiments were run in duplicate to ±5% conversion. The integrations of

the signals assigned to one of the vinylic hydrogens of the styrene and the styrene derivatives were measured and converted to k_X/k_H values which were plotted against the Hammett parameter for each substituent.

Visual Kinetic Analysis

For each experiment, a suspension of $Ge(cat^{Cl})_2(ACN)_2$ (0.01 mmol) in 0.5 mL of CD_2Cl_2 was transferred to an NMR tube with a Teflon cap. After lock and shimming, 0.25 mL of a solution containing α-methylstyrene was added and a ${}^1H$ NMR spectrum was taken every 1-2 minutes for 30 minutes. The total concentration of products formed (**3,4,5,6**) was monitored.
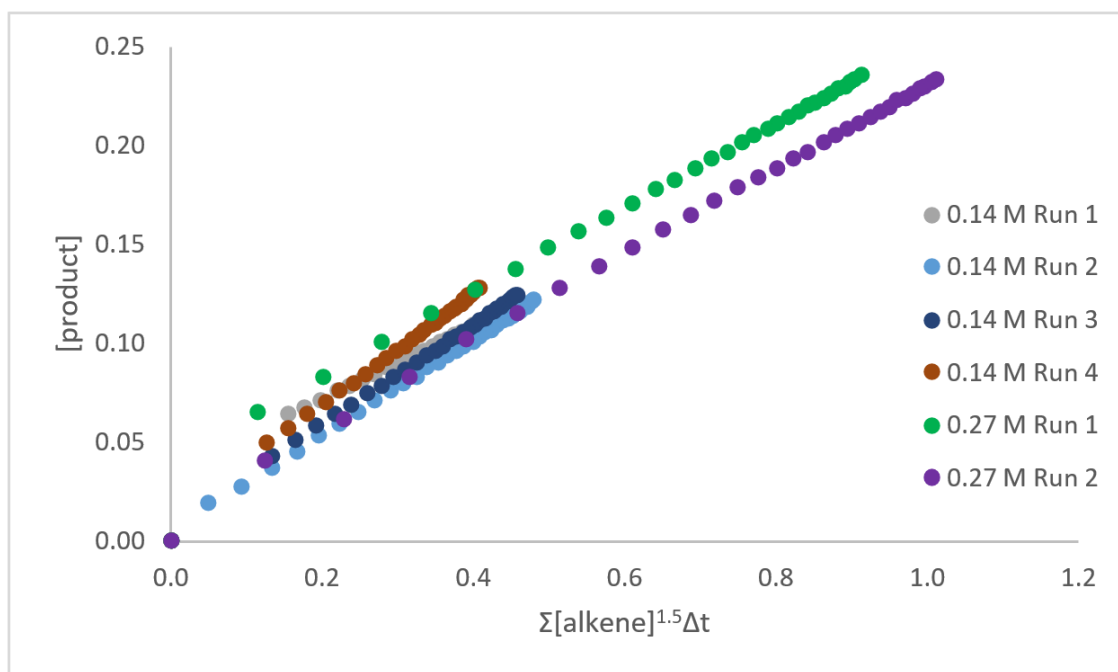

Figure S1: VTNA plot of 6 different runs at a reactant order of 1.5 for α-methylstyrene.
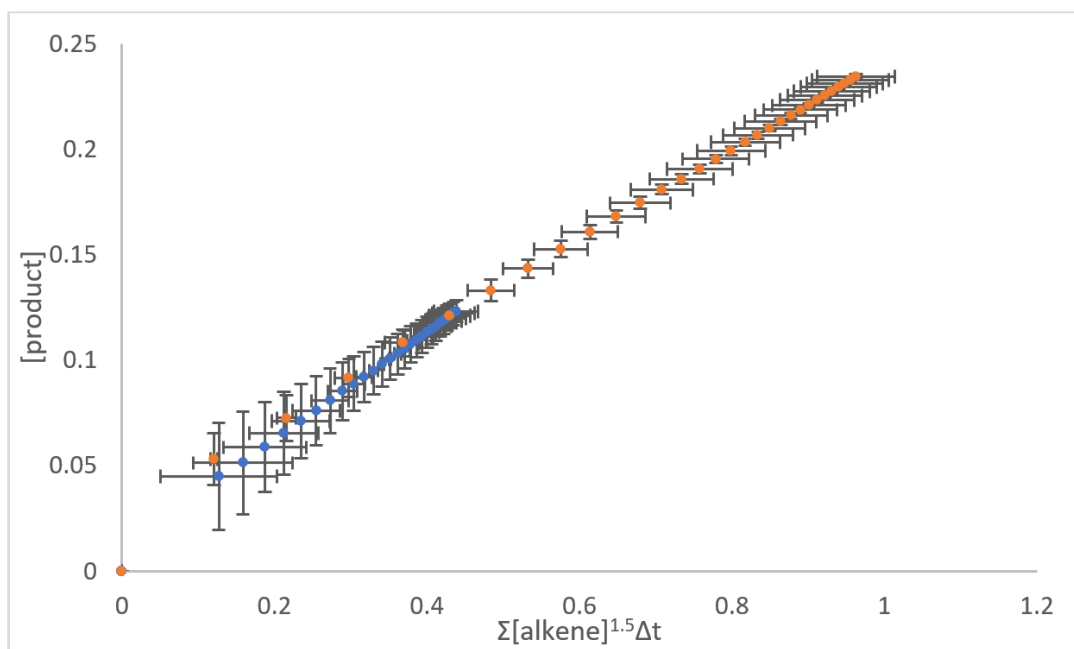
Figure S2: VTNA plot of two averaged runs at 0.14M and 0.27M at reactant order of 1.5 for α-methylstyrene showing error bars.
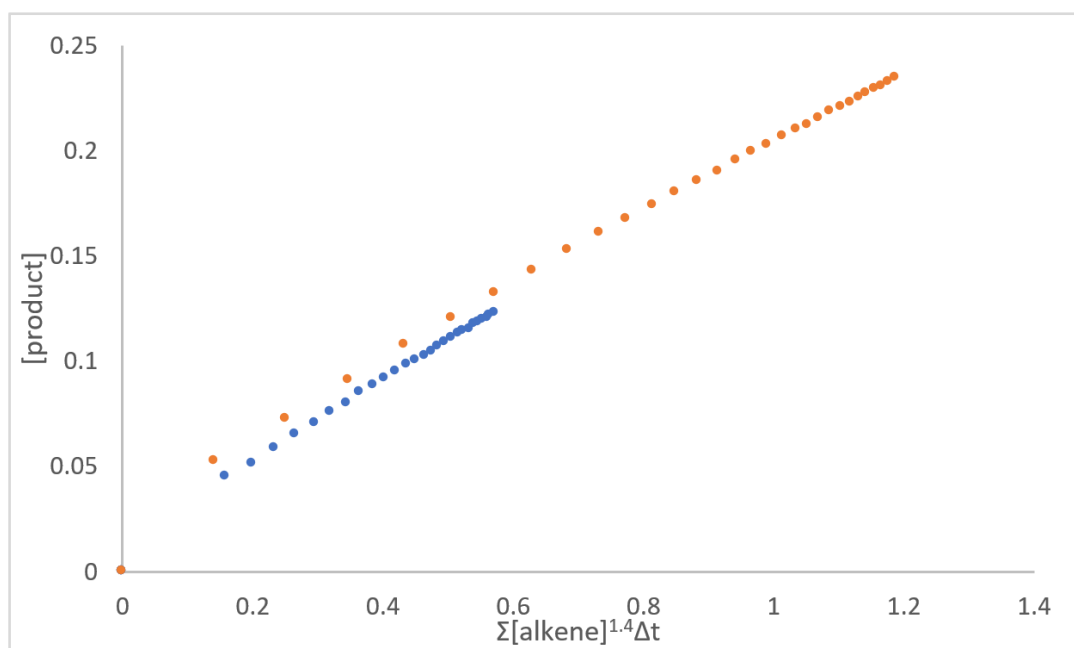
Figure S3: VTNA plot of two averaged runs at 0.14M and 0.27M at reactant order of 1.4 for α-methylstyrene.
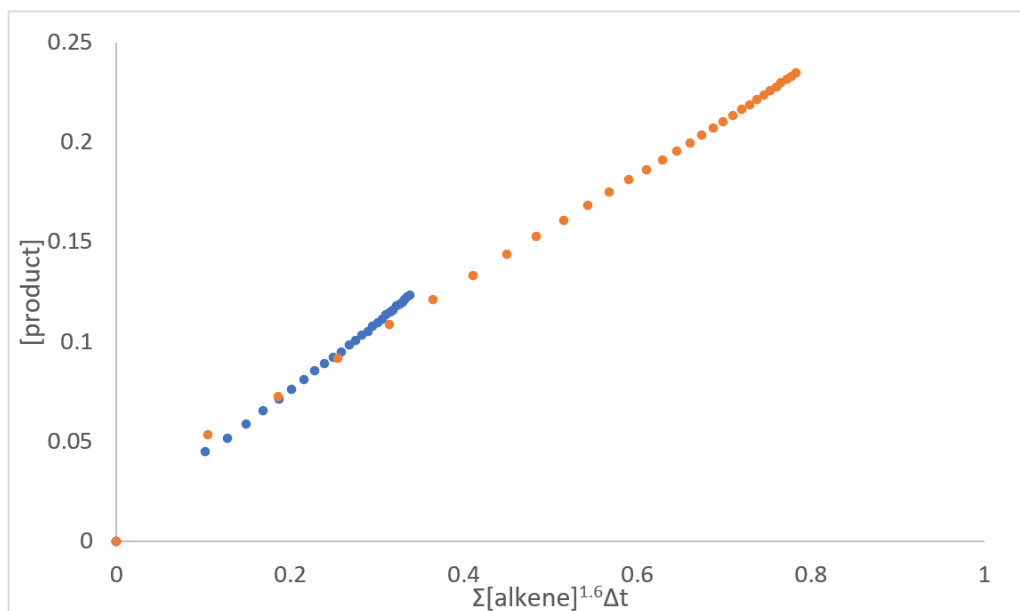
Figure S4: VTNA plot of two averaged runs at 0.14M and 0.27M at reactant order of 1.6 for α-methylstyrene.

Hydrosilylation of Aldehydes
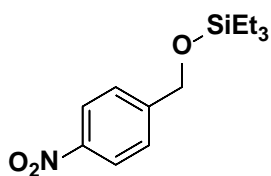
^{1}H NMR (600 MHz, CD$_2$Cl$_2$) 8.17 (d, J = 8.7 Hz, 2H), 7.52 (d, J = 8.7 Hz, 2H), 4.73 (s, 2H), 0.95 (t, J = 7.9 Hz, 9H), 0.54 (q, J = 7.9 Hz, 6H).[1]
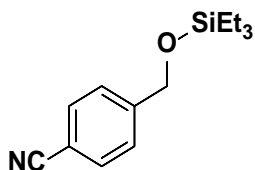
^{1}H NMR (600 MHz, CD$_2$Cl$_2$) δ 7.67 (d, J = 8.3 Hz, 2H), 7.50 (d, J = 8.0 Hz, 2H), 4.66 (s, 2H), 0.95 (t, J = 8.0 Hz, 9H), 0.55 (q, J = 8.0 Hz, 6H).[1]
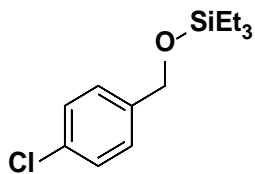
^{1}H NMR (600 MHz, CD$_2$Cl$_2$) δ 7.50 (d, J = 8.4 Hz, 2H), 7.25 (d, J = 8.4 Hz, 2H), 4.50 (s, 2H), 0.96 (t, J = 7.9 Hz, 9H), 0.56 (q, J = 8.0 Hz, 6H).[1]
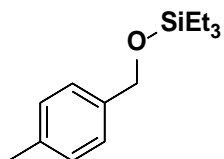
^{1}H NMR (400 MHz, CD$_2$Cl$_2$) δ 7.26 (d, J = 7.8 Hz, 2H), 7.18 (d, J = 7.7 Hz, 2H), 4.51 (s, 2H), 2.36 (s, 3H), 0.98 (t, J = 7.9 Hz, 9H), 0.57 (q, J = 7.9 Hz, 6H).[2]
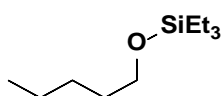
^{1}H NMR (600 MHz, CD$_2$Cl$_2$) δ 3.39 (t, J = 6.8 Hz, 2H), 1.55 (t, J = 7.1 Hz, 2H), 1.40 – 1.28 (m, 4H), 0.96 (t, J = 7.9 Hz, 9H), 0.91 (t, J = 7.0 Hz, 3H), 0.55 (q, J = 7.9 Hz, 6H).[3]
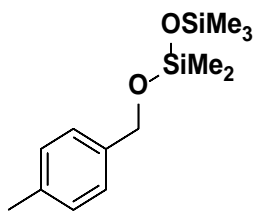
^{1}H NMR (600 MHz CD$_2$Cl$_2$) δ 7.27 (d, J = 7.5 Hz, 2H), 7.19 (d, J = 7.7 Hz, 2H), 4.52 (s, 2H), 2.37 (s, 3H), 0.14 (d, J = 3.4 Hz, 9H), 0.12 – 0.10 (m, 6H).[4]
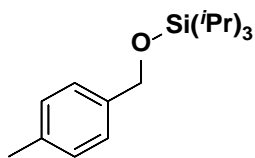
H NMR (600 MHz, CD$_2$Cl$_2$) δ 7.29 (d, J = 8.0 Hz, 2H), 7.22 (d, J = 7.6 Hz, 2H), 4.84 (s, 2H), 2.37 (s, 3H), 1.1-1.2 (m).
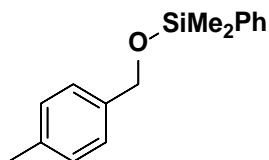
^{1}H NMR (600 MHz, CD$_2$Cl$_2$) δ 7.67-7.40 (5H), 7.31 (d, J = 7.6 Hz, 2H), 7.18 (d, J = 8.0 Hz, 2H), 4.55 (s, 2H), 2.40 (s, 3H), 0.68 (s, 3H).[3]

Oligomerization of Alkenes
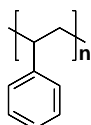
^{1}H NMR (400 MHz, CD$_2$Cl$_2$): δ 7.20-7.00 (br s, 3H), 6.65-6.45 (br s, 2H), 1.84 (br s, 1H), 1.47 (br s, 2H).[5]

3
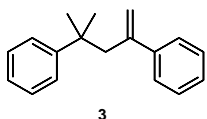
^{1}H NMR (400 MHz, Toluene-d_8): δ 7.00-7.30 (m, 10H), 5.10 (s, 1H), 4.74 (s, 1H), 2.71 (s, 2H), 1.15 (s, 6H).[6]

4
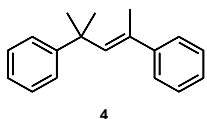
^{1}H NMR (400 MHz, Toluene-d_8): δ 7.00-7.30 (m, 10H), 6.09 (s, 1H), 1.53 (s, 3H).[7]

5
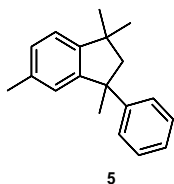
^{1}H NMR (400 MHz, Toluene-d_8): δ 7.00-7.30 (m, 9H), 2.33 (d, 1H), 2.05 (d, 1H), 1.58 (s, 3H), 1.24 (s, 3H), 1.00 (s, 3H).[6]

6
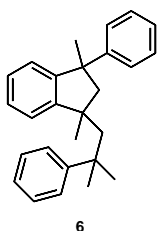
^{1}H NMR (600 MHz, Toluene-d_8): δ 7.20 – 7.50 (m, 15 H), 2.59 (d, J = 15 Hz, 1 H), 2.20 (d, J = 14 Hz, 1H), 1.90 (d, J = 15 Hz, 1H), 1.72 (d, J = 14 Hz, 1H), 1.60 (s, 3H), 1.28 (s, 3H), 1.15 (s, 3H), 0.96 (s, 3H).[8]

Hydroboration of Alkynes
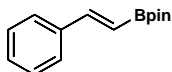
^{1}H NMR (400 MHz, Toluene-d_8): δ 7.60 (d, J = 18.5 Hz, 1 H), 7.27 (d, 2 H), 7.09 – 7.01 (m, 3 H), 6.32 (d, J = 18.5 Hz, 1 H), 1.12 (s, 12 H). ^{11}B NMR (128 MHz, Toluene-d_8): 30.79 (d).[9]
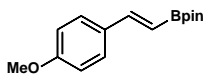
^{1}H NMR (400 MHz, Toluene-d_8): δ 7.60 (d, J = 18.2 Hz, 1 H), 7.23 (d, 2 H), 6.60 (m, 2 H), 6.20 (d, J = 18.3 Hz, 1 H), 3.28 (s, 3H), 1.14 (s, 12 H).[10]
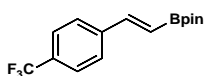
^{1}H NMR (400 MHz, Toluene-d_8): δ 7.46 (d, J = 18.4 Hz, 1 H), 7.20 (d, J = 8.1 Hz, 2 H), 7.03 (d, J = 8.1 Hz, 2 H), 6.28 (d, J = 18.4 Hz, 1 H), 1.12 (s, 12 H) ^{11}B NMR (128 MHz, Toluene-d_8): 30.05 (d).[10]
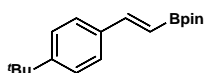
^{1}H NMR (400 MHz, Toluene-d_8): δ 7.65 (d, J = 18.5 Hz, 1 H), 7.29 (d, 2 H), 6.60 (d, 2 H), 6.20 (d, J = 18.5 Hz, 1 H), 1.20 (s, 9 H), 1.14 (s, 12 H).[10]
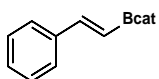
¹H NMR (400 MHz, Toluene-d_8): δ 7.72 (d, J = 18.5 Hz, 1 H), 7.27 – 7.24 (m, 2 H), 7.07 – 7.04 (m, 4 H), 6.84 – 6.81 (m, 2H), 6.38 (d, J = 18.5 Hz, 1 H). ¹¹B NMR (128 MHz, Toluene-d_8): 31.91 (d).[11]
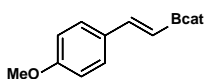
¹H NMR (400 MHz, Toluene-d_8): δ 7.75 (d, J = 18.5 Hz, 1 H), 7.23 (d, 2 H), 7.08 – 7.06 (d, 2 H), 6.85 - 6.82 (m, 2 H), 6.63 (m, 2H), 6.28 (d, J = 18.5 Hz, 1 H). ¹¹B NMR (128 MHz, Toluene-d_8): 32.16 (d).[12]
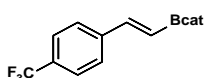
¹H NMR (400 MHz, Toluene-d_8): δ 7.52 (d, J = 18.8 Hz, 1 H), 7.25 (m, 2 H), 7.07 - 7.02 (m, 4 H), 6.84 (d, 2 H), 6.28 (d, J = 18.8 Hz, 1 H). ¹¹B NMR (128 MHz, Toluene-d_8): 31.93 (d).[13]

Friedel-Crafts Alkylation
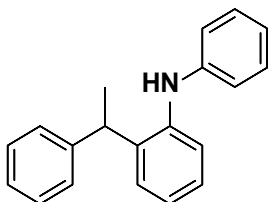
¹H NMR (400 MHz, Toluene-d_8) δ 7.16 – 7.11 (m, 2H), 7.10 – 7.03 (m, 4H), 6.83 – 6.78 (m, 8H), 4.94 (s, 1H), 3.92 (q, J = 7.2 Hz, 1H), 1.50 (d, J = 7.2 Hz, 3H).[14]
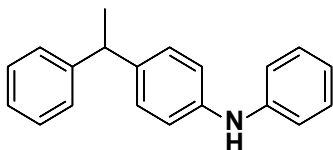
¹H NMR (400 MHz, Toluene-d_8) δ 7.33 – 6.85 (m, 13H), 6.67 – 6.57 (m, 2H), 5.02 (s, 1H), 4.05 (q, J = 7.1 Hz, 1H), 1.42 (d, J = 7.2 Hz, 3H).[14]
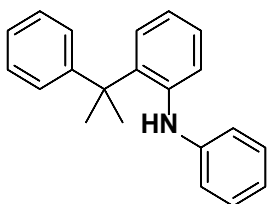
¹H NMR (400 MHz, Toluene-d_8) δ 7.23 – 7.20 (m, 2H), 7.16 – 7.12 (m, 2H), 7.08 – 7.04 (5H), 6.82 – 6.75 (2H), 1.57 (s, 6H).[15]
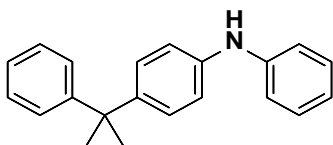
¹H NMR (400 MHz, Toluene-d_8) δ 7.24 – 7.19 (m, 1H), 7.14 (dd, J = 8.5, 6.8 Hz, 1H), 7.09 – 7.03 (m, 5H), 6.83 – 6.74 (m, 7H), 1.56 (s, 6H).[15]
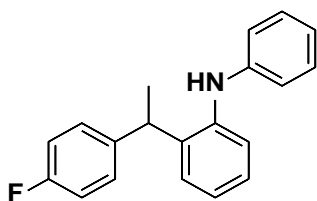
^{1}H NMR (400 MHz, Toluene-d_8) δ 7.15-6.70 (18 H), 4.02 (q, J = 7.2 Hz, 1H), 1.44 (d, J = 7.2 Hz, 3H).[15]
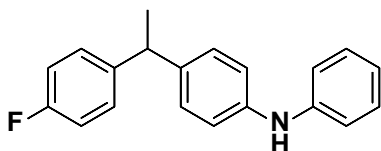
^{1}H NMR (400 MHz, Toluene-d_8) δ 7.15-6.70 (18 H), 4.83 (q, J = 7.2 Hz, 1H), 1.44 (d, J = 7.2 Hz, 3H).[15]
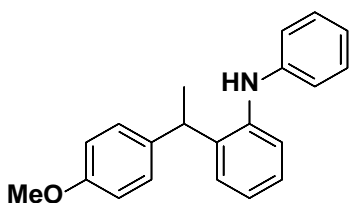
^{1}H NMR (400 MHz, Toluene-d_8) δ 7.13-6.67 (18 H), 3.94 (q, J = 7.3 Hz, 1H), 1.56 (d, J = 7.3 Hz, 3H).[15]
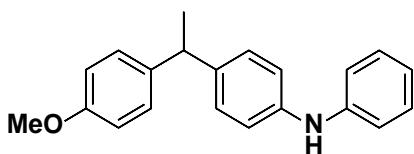
^{1}H NMR (400 MHz, Toluene-d_8) δ 7.13-6.67 (18 H), 4.09 (m, 1H), 1.55 (d, J = 7.2 Hz, 3H).[15]
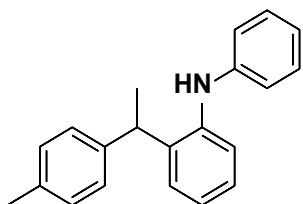
^{1}H NMR (400 MHz, Toluene-d_8) δ 7.32-7.24 (2 H), 7.07-7.05 (m, 2H), 6.95-6.93 (3H), 6.90-6.84 (m, 4H), 6.75-6.64 (3H), 4.05 (q, J = 6.8 Hz, 1H), 2.09 (s, 3H), 1.44 (d, J = 6.8 Hz, 3H).[15]
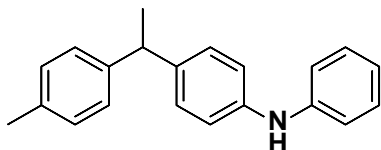
^{1}H NMR (400 MHz, Toluene-d_8) δ 7.32-6.68 (13 H), 3.93 (q, J = 7.2 Hz, 1H), 2.14 (s, 3H), 1.53 (d, J = 6.8 Hz, 3H).[15]
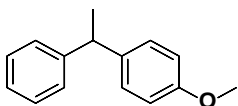
^{1}H NMR (400 MHz, Toluene-d_8) δ 7.27-6.69 (9 H), 3.36 (q, J = 7.3 Hz, 1H), 1.52 (d, J = 7.3 Hz, 3H).[16]
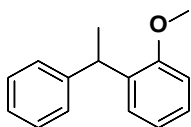
^{1}H NMR (400 MHz, Toluene-d_8) δ 7.27-6.69 (9 H), 3.95 (q, J = 7.3 Hz, 1H), 1.57 (d, J = 7.2 Hz, 3H).[16]

Computational Details

All calculations have been performed with ORCA 4.1.2 and ORCA 4.2. Geometry optimizations were performed with PBEh-3c/def2-mSVP as implemented in ORCA, using grid5 settings. All calculated geometries have been confirmed as energetic minima on the potential energy surface by analytical calculation of harmonic frequencies at the PBEh-3c level. In case of negative frequencies >10 cm^{-1}, the geometries were reoptimized with grid6, TightOPT and VeryTightSCF settings. For the fluoride ion affinities, the optimized geometries were than used to calculate the single point energies at B3LYP D3(BJ)/def2-TZVPP level of theory using the RIJCOSX approximation and def2/J as the auxiliary basis set. For the reaction coordinate calculations, the optimized geometries were used to calculate the thermodynamic values at BP86 D3(BJ)/def2-SVP level of theory using the RIJCOSX approximation and def2/J as the auxiliary basis set.

Calculated energetics of ligand dissociation and substrate activation with Ge(cat^{Br})$_2$.

Complex	Enthalpy (hartree)	Enthalpy (kJ/mol)	Gibbs (hartree)	Gibbs (kJ/mol)
Ge(cat^{Br})$_2$(ACN)$_2$	-23692.90088	-62205711.27	-23692.99072	-62205947.13
Ge(cat^{Br})$_2$(ACN)	-23560.25869	-61857459.2	-23560.34328	-61857681.27
Ge(cat^{Br})$_2$(THF)$_2$	-23892.05995	-62728603.39	-23892.15298	-62728847.65
Ge(cat^{Br})$_2$(THF)	-23659.83407	-62118894.35	-23659.92072	-62119121.85
Ge(cat^{Br})$_2$	-23427.62475	-61509228.78	-23427.70542	-61509440.58
ACN	-132.6064582	-348158.2559	-132.6361785	-348236.2865
THF	-232.1676769	-609556.2356	-232.1991325	-609638.8223
Styrene	-309.302937	-812074.8612	-309.3421922	-812177.9256

Ge(cat^{Br})$_2$(Styrene)	-23736.96198	-62321393.68	-23737.0548	-62321637.37
Cis-Ge(cat^{Br})$_2$(Styrene)(ACN)	-23869.59659	-62669625.85	-23869.69422	-62669882.18
Trans-Ge(cat^{Br})$_2$(Styrene)(ACN)	-23869.60727	-62669653.89	-23869.70222	-62669903.19
Phenylacetylene	-308.0730972	-808845.9166	-308.1092989	-808940.9643
Trans-Ge(cat^{Br})$_2$(PhCCH)(ACN)	-23868.37636	-62666422.13	-23868.4692	-62666665.87
Para-tolualdehyde	-384.4930966	-1009486.625	-384.5336354	-1009593.06
Trans-Ge(cat^{Br})$_2$(*para*-tolualdehyde)(ACN)	-23812.15959	-62518825.01	-23812.24953	-62519061.14
HSiEt$_3$	-527.3560081	-1384573.199	-527.3986291	-1384685.101
SiEt$_3^+$	-526.494541	-1382311.417	-526.5342082	-1382415.564
ACN--SiEt$_3^+$	-659.1825821	-1730683.869	-659.2302814	-1730809.104
Ge(cat^{Br})$_2$H$^-$	-23428.35791	-61511153.7	-23428.43766	-61511363.07
Ge(cat^{Br})$_2$(ACN)H$^-$	-23560.9817	-61859357.45	-23561.06848	-61859585.28
Ge(cat^{Br})$_2$(H)(SiEt$_3$)	-23955.0062	-62893868.79	-23955.1002	-62894115.58
4-methylacetophenone	-423.7597565	-1112581.241	-423.7999731	-1112686.829
Trans-Ge(cat^{Br})$_2$(Me-Ph-(C=O)CH$_3$)(ACN)	-23984.07199	-62970181.02	-23984.1691	-62970435.96
HBpin	-411.3904697	-1080105.678	-411.4302557	-1080210.136
Trans-Ge(cat^{Br})$_2$(HBpin)(ACN)	-23971.69996	-62937698.25	-23971.79894	-62937958.12

NMR Spectra
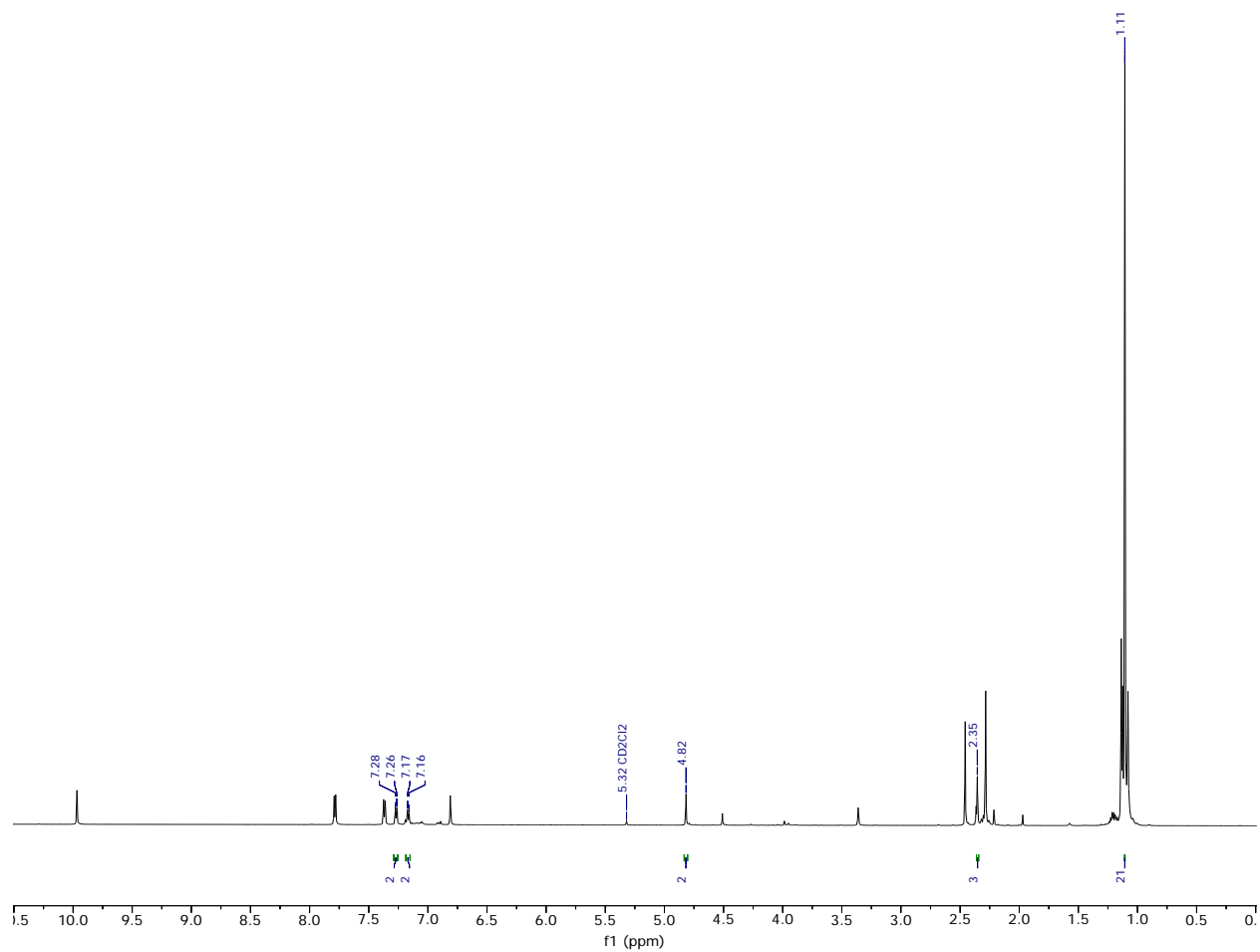
Figure S.5: ^{1}H NMR (Tol-d_8, 400 MHz) spectrum of the hydrosilylation of *para*-tolualdehyde with HSi(^{i}Pr)$_3$ (Scheme 1, Entry 10).
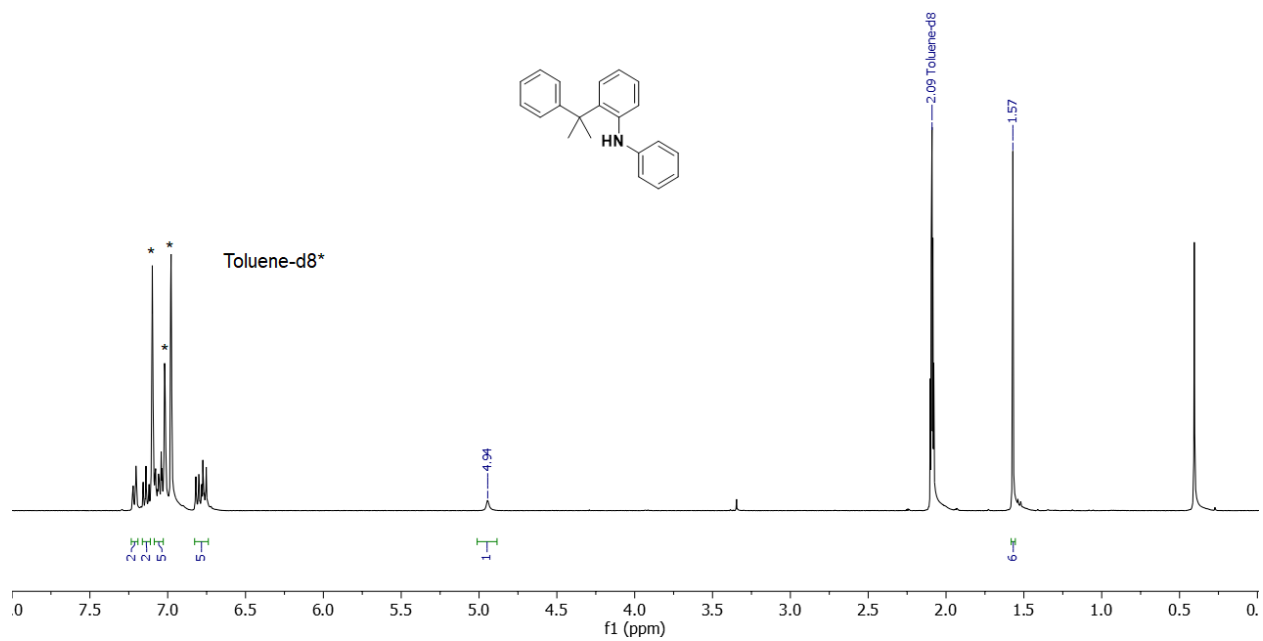
Figure S.6: ^{1}H NMR (Tol-d_8, 400 MHz) spectrum of the isolated *ortho* Friedel-Crafts alkylation product of HNPh$_2$ and α-methylstyrene (Table 6, Entries 5-8).

Figure S.7: ^{1}H NMR (CDCl$_3$, 400 MHz) spectrum of the isolated *ortho* Friedel-Crafts alkylation product of HNPh$_2$ and 4-methoxystyrene (Table 8, Entry 6).
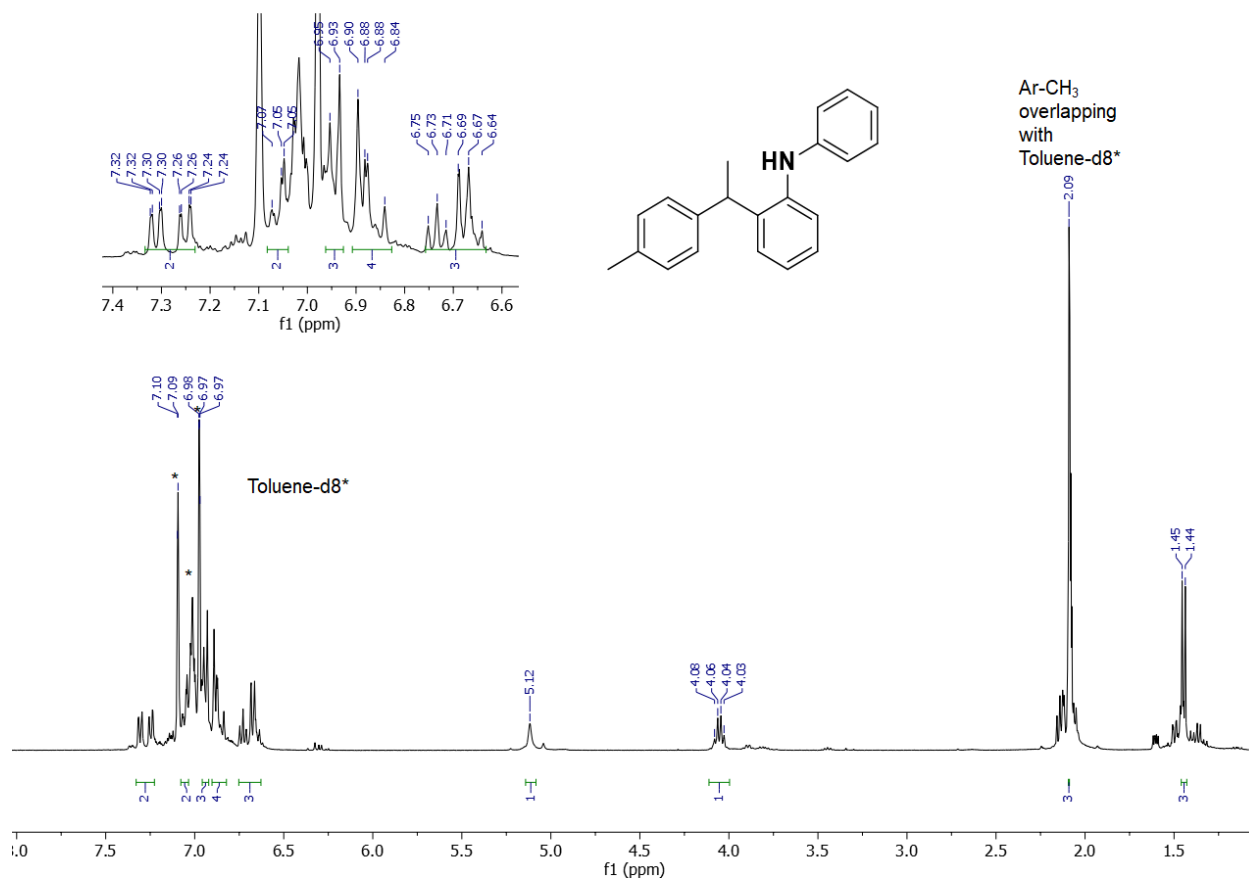
Figure S.8: ^{1}H NMR (Tol-d_8, 400 MHz) spectrum of the isolated *ortho* Friedel-Crafts alkylation product of HNPh$_2$ and 4-methylstyrene (Table 8, Entry 5).

Optimized Geometries

Ge(cat^{Br})$_2$(ACN)$_2$

Br	6.31150273503780	-0.53587316974055	1.63474070361356
Br	-6.42930051233438	2.28859126302645	1.67631340197940
Br	-3.60579223484346	1.63258283556596	-3.24453254153491
Br	3.44407791252394	0.06661078084264	-3.26755441084641
Br	6.29531766018062	-0.55178585788025	-1.66295071554108
Br	3.47578827799620	0.09692337291641	3.26114999580770
Br	-3.58050748216137	1.66704578732665	3.28413248553203
Br	-6.44221273176974	2.27029670023268	-1.62138588354555
Ge	-0.06692592356721	0.86448398366022	0.01068446112139

O	-1.33738215725605	1.15776216800694	1.28643318021577
O	-1.34684919017487	1.14579626114868	-1.25877806899504
O	1.20227160746859	0.57185549674446	-1.26702693181216
O	1.21445541762039	0.58266284967723	1.27810040655014
N	0.39892965455382	2.92859601003800	0.00372430396217
N	-0.53108034617178	-1.20048175647015	0.02107806596674
C	-0.78104720238023	-2.31406838775072	0.02236895839471
C	-1.09394666566559	-3.72386769249904	0.02537614472660
C	0.65455229238416	4.04077959175377	0.02030837271265
C	0.97967940934020	5.44756759456604	0.03829265586869
C	-2.51195805966487	1.41518117821872	0.71803968931698
C	-2.51711132504529	1.40841553425448	-0.68438522458824
C	2.38451494885086	0.32175749212255	0.70208272601235
C	2.37770216056843	0.31584170145225	-0.70036973106033
C	-3.68470241179963	1.66192656355043	-1.37846461710231
C	-4.86631570448186	1.92782107182589	-0.67337488441928
C	-4.86094636391168	1.93534382793130	0.71981499966422
C	-3.67391576438638	1.67668838733039	1.41846961800960
C	3.53936361676225	0.05609841444022	-1.40203604987513
C	4.72740077101182	-0.20145409675337	-0.70465994086429
C	4.73422249572154	-0.19486841233847	0.68850890071009
C	3.55294039651267	0.06909359029621	1.39492737313571
H	-0.94182035823955	-4.13201008264009	1.02260538013569
H	-2.13181140070209	-3.87067003720333	-0.26730043529123
H	-0.44683856539125	-4.24466188205608	-0.67791600276316
H	0.86182675015074	5.86551625329633	-0.95962400187025
H	0.31678361380833	5.96939349496134	0.72596046463189
H	2.00952977585491	5.58238892924578	0.36352439784130

Ge(cat^{Br})₂(ACN)

Br	6.29511738310464	-0.38475421316056	1.57307418194276
Br	-6.15919345643302	3.01439339699170	1.65030379288598
Br	-3.87437846212390	0.89064993351554	-3.13396528215532
Br	3.43184536816781	1.12747414339038	-3.12965544506298

Br	6.32343777330576	0.49794196193726	-1.60200247597609
Br	3.37887793380295	-0.61436325572981	3.16381022318387
Br	-3.24925416135689	2.46313997498051	3.17319059986748
Br	-6.47511397276012	2.21570755731963	-1.53133678828371
Ge	-0.18655540683728	0.43667143030626	0.01523101812990
O	-1.25559174923376	1.23195282482015	1.21189760381981
O	-1.48957012309002	0.65254956134392	-1.23406439798570
O	1.11089042396098	0.74913025468283	-1.17840473502840
O	1.09357956494182	0.10197551146734	1.26110348392070
N	-0.61722512093006	-1.55058097034415	0.01741384473848
C	-0.88090509936098	-2.66110445545480	0.02663725937606
C	-1.21434811359090	-4.06382576726293	0.03696644882885
C	-2.45670060241874	1.50170403413050	0.67499658280794
C	-2.58405239539399	1.16872268949130	-0.67441556072161
C	2.30474056442660	0.15778024839576	0.70582091933002
C	2.32093731930449	0.52564709638662	-0.64020450659871
C	-3.78006623343984	1.37544722997588	-1.33475557975639
C	-4.85867328343445	1.93259162634189	-0.63719732736004
C	-4.72582449514218	2.27052929053558	0.71022014585378
C	-3.51209397196120	2.05004631114159	1.37400766117723
C	3.50836259060954	0.62956633033255	-1.33455831399524
C	4.71064390877408	0.35827436333791	-0.66870827879173
C	4.69795544812010	-0.01515313815410	0.67579902263025
C	3.48537710814969	-0.11778184010599	1.36848302311080
H	-2.06789008787029	-4.22872961100463	0.69250576269963
H	-1.46966496442917	-4.38699646938139	-0.97078027477992
H	-0.36553065396166	-4.64110208572671	0.39921405999228

Ge(cat^{Br})$_2$(THF)$_2$

Ge	-0.20821754356115	0.50400013170913	-0.03909823892905
Br	-6.32654951633587	3.07579055332561	-1.10157452658003
Br	-3.38022060765570	1.46510622097027	3.51988648526183
Br	3.56040927611157	-0.06176027916304	2.98159570132042
Br	6.20587933368051	0.46576381023926	-2.05337936216315

Br	3.21008390717653	0.66667828540083	-3.49602440897135
Br	-3.76016887530704	2.06373238080083	-2.96967816612832
Br	-6.13361881135119	2.77448216166263	2.17743340326907
Br	6.38337359999966	0.09624882394158	1.21932978936767
O	-0.62844624968019	-1.47208941054212	-0.21792110875012
O	0.22123538046936	2.52456131838958	0.14451913483851
O	1.15360197530836	0.13814006547199	1.12828706583649
O	1.01696075787126	0.40995827898671	-1.39967833957440
O	-1.55965777410428	0.92471692385670	-1.20076982490318
O	-1.41657921264066	0.68038368565139	1.32904010478176
C	0.36558782586408	-2.52577625655380	-0.15532720559639
C	-0.37536356436694	-3.75943197492937	-0.63225417418941
C	-1.80270988942835	-3.49311160522438	-0.16738184627275
C	-1.96153195875193	-2.00632460513852	-0.41668658207444
C	0.19957547189099	3.46521270761220	-0.95776514814759
C	0.56968728441768	3.17225847178570	1.39353070148845
C	0.47611287328436	4.65205689212570	1.07665693536300
C	0.87302012055159	4.70126603540639	-0.39519930112122
C	3.55154780548433	0.12942873646192	1.12316125596425
C	4.72545401280217	0.20381845498227	0.36147029049522
C	4.65022193451793	0.35921400059441	-1.02154069852645
C	3.40123190085872	0.44004653921731	-1.65158319200973
C	-3.58092627137196	1.65345030878482	1.67204390300695
C	-4.72614761315153	2.20769132624551	1.08473394355847
C	-4.80760668052717	2.33560127642842	-0.30084435780083
C	-3.74342309101180	1.91082587433584	-1.10772551103602
C	2.24679129485881	0.35371876210996	-0.89663891283955
C	2.32304340262394	0.20016858218018	0.49507124334953
C	-2.62211937278828	1.35422063505355	-0.52334816949187
C	-2.54078522065213	1.22285904508352	0.87040939353145
H	0.04895866424303	-4.66993421156603	-0.21173544268130
H	-0.33140814307391	-3.84016597920158	-1.71974278901942
H	1.20656042061103	-2.25523605096369	-0.79125191194997

H	0.70654435589368	-2.61625856864669	0.87634365328329
H	-1.91253419843229	-3.72055144547042	0.89437045852163
H	-2.54575268829635	-4.07319170926812	-0.71262077189638
H	-2.64290777602519	-1.52251559546560	0.28070271190088
H	-2.27212200090914	-1.78492042079600	-1.43814099641984
H	1.58303823671750	2.87428152495171	1.66828326433465
H	-0.11923039205823	2.83534460541530	2.16561768042882
H	-0.83939431056705	3.65409493618585	-1.23383543517796
H	0.71580027018193	3.01989758231035	-1.80591381710803
H	0.53867900151768	5.60679856723104	-0.89956321746184
H	1.95711418502397	4.63636705699811	-0.50621515484659
H	1.12936068443174	5.24290219902775	1.71721179763689
H	-0.54461945054404	5.01396983079481	1.21413460032797

Ge(cat^Br)_2(THF)

Ge	-0.30103180689433	1.18517493425011	-0.11908771841232
Br	-6.71215348263690	-0.78247505799231	-0.21359523292970
Br	-3.99335127617363	4.07455112796078	1.06048198143827
Br	3.48563995310586	-0.67162455075268	2.15389184763836
Br	5.67604371689613	0.70330395279344	-2.93392760986214
Br	2.64789617184536	1.73299180800728	-3.85275825189138
Br	-3.75131320312395	-2.16618523317417	-0.84709959504277
Br	-6.83895521295373	2.36642266700790	0.74984891692825
Br	6.09934005131591	-0.51037242675029	0.10056349710551
O	0.81631377190752	2.93065548828730	0.48088329596904
O	0.97881301322277	0.31072742834442	0.76616516256786
O	0.64601053727272	1.27565432721842	-1.62515994384695
O	-1.52159117251401	-0.11435605339404	-0.38754146923792
O	-1.62070830513242	2.29424124036720	0.34762387804065
C	0.82710801058924	4.14969618813569	-0.29183732426645
C	1.10431105541744	3.19284358561992	1.87320761011405
C	1.16013456606573	4.70705885737465	1.98139079657873
C	1.58627611167624	5.12962240458189	0.57951725112206
C	3.32674014985639	-0.03484156687676	0.40777480118791

C	4.41336753501844	0.05538243418919	-0.46990640803148
C	4.23429092721557	0.56946260803078	-1.75445992205761
C	2.96737715366900	0.99625892221745	-2.16925226212493
C	-4.02020618063432	2.28802889869109	0.52056188423019
C	-5.20045007343293	1.54854782543609	0.38282095254898
C	-5.14404050908914	0.21423553705922	-0.02575482446283
C	-3.91238441039853	-0.39320125947184	-0.29989117183244
C	1.89627265499253	0.88267714247773	-1.30544923416353
C	2.07550127151686	0.36595233509566	-0.01704037766712
C	-2.75366235839187	0.34728863930726	-0.16118390527667
C	-2.81635426213045	1.67695750210704	0.24604577217572
H	2.05737316934965	2.71992804905501	2.11579657073018
H	0.32583645039621	2.75116989876010	2.49554690505669
H	-0.20128864787454	4.47494992419696	-0.46510907658329
H	1.30445722320795	3.94229101605016	-1.24864713793136
H	1.32844882020744	6.16208191432386	0.34803528080850
H	2.66332616152135	5.01380932704235	0.44575338946158
H	1.85221792665032	5.03191638756939	2.75690142405201
H	0.17500966016412	5.11172907625359	2.21964364206632

Ge(cat^{Br})$_2$

Ge	-0.30238604626443	0.71799447246471	0.08057810093298
O	-1.44870452184273	1.68695870533160	1.00033814420409
O	-1.55999528169687	-0.12962768775273	-0.81210091670894
O	0.937207151102335	1.55981816943465	-0.84238984764429
O	0.86209664165224	-0.24382497406978	0.98470280199913
C	-2.69670779037834	1.32867532899042	0.60233138891606
C	-2.75715711047678	0.34450004890551	-0.37945496272131
C	2.10206376048530	0.11383696920876	0.56165013060354
C	2.14287325407458	1.09101673581571	-0.42807318928899
C	-3.97001024960063	-0.10204321896469	-0.86339687002693
C	-5.14574932323201	0.45391475849052	-0.34726906270900
C	-5.08515290436210	1.44205916312101	0.63968388073773
C	-3.84827144826111	1.88510246463516	1.12104011673697

C	3.34599209089935	1.53679492333596	-0.93645104863835
C	4.53190228688151	0.98693147295547	-0.43736611397403
C	4.49100289588648	0.00560630459796	0.55739668074137
C	3.26383882770408	-0.43658608319892	1.06372761002676
Br	-3.67489779328968	3.19444922480998	2.43218416373435
Br	-6.79192961169024	-0.14047091457303	-0.99292862462284
Br	-6.64942140357433	2.18681111341051	1.33160971254998
Br	3.11655666358613	-1.73695780078699	2.38694919737619
Br	6.16508309553262	1.58021895803554	-1.11617114652446
Br	6.06894205447297	-0.73096737826468	1.22663382340852
Br	3.30722373224452	2.84628848324013	-2.25838882631018
Br	-3.95746896977395	-1.42096923917281	-2.17645514279835

ACN

N	-2.91598372023246	0.46160253874396	0.00000735435015
C	-2.97758951298266	1.60908832137919	-0.00000965345602
C	-3.05542132591543	3.05829118134895	-0.00000039175509
H	-2.19302285515126	3.48351611323346	-0.50992196067509
H	-3.95802837409244	3.38872256757766	-0.51057078460075
H	-3.07608782562574	3.43608027961679	1.02049669443680

THF

O	-6.22377652708292	3.50894113924272	-0.00327783072972
C	-4.97763524681156	4.15830562140470	-0.15504853063773
C	-5.20459308839107	5.61885795399477	0.21837295126915
C	-7.25814161826486	4.45869905996542	0.15698780959056
C	-6.65788557570859	5.81391597570245	-0.19993059443893
H	-4.63189662389681	4.07471653105655	-1.19327161820590
H	-4.23209646856422	3.67130503636690	0.47887729120479
H	-7.61594609923491	4.45623979454221	1.19447679165567
H	-8.10343007573637	4.18985849134202	-0.48181718765805
H	-4.51228849499671	6.29511453009128	-0.28280420217783
H	-5.09392460537543	5.76770298588703	1.29494386006117
H	-6.72422708791566	5.99871687166726	-1.27457880103682
H	-7.15094701602086	6.64139463733668	0.30991499640364

Styrene

C	-3.37168473241895	5.81893049726451	0.00000003203160
C	-4.52932917186881	5.16349755849830	-0.00000008058496
C	-4.73013335804996	3.71162934920579	-0.00000010803407
C	-3.67513842956313	2.79639448956100	-0.00000027376346
C	-3.91726495547273	1.43489060426253	-0.00000028338993
C	-5.22014950328438	0.95214894193476	-0.00000018195201
C	-6.27793423685541	1.84696477643273	-0.00000005971628
C	-6.03191630767565	3.21114164076429	0.00000001091718
H	-3.34807239837424	6.89919673711776	0.00000002975616
H	-2.41034731855681	5.32233579381406	0.00000012821773
H	-5.44337744572938	5.74931376997370	-0.00000016791037
H	-2.65142111506185	3.14773953993637	-0.00000039729432
H	-3.08472114937936	0.74353148742580	-0.00000041326973
H	-7.29734848805969	1.48412638796051	0.00000000520432
H	-5.40616961863859	-0.11364098367349	-0.00000021899467
H	-6.86538245171103	3.90368187122136	0.00000010288279

Ge(cat^{Br})$_2$(styrene)

Br	-2.53810425589012	4.72863320288723	1.40366887916337
Br	-7.39288346830008	2.10655516628280	-0.05857975621335
Br	1.97078547401434	-2.08163834439457	2.92462655746158
Br	4.83872517185579	-2.03402818375730	-2.00714153613318
Br	4.65140320146568	-2.94093454451454	1.15334524908673
Br	-5.60128095286593	-0.59431754117247	-0.81413527375939
Br	-5.84769463873860	4.79117602303127	1.05926199044700
Br	2.34796849750477	-0.27062514434524	-3.33199524050191
Ge	-0.97987212383111	0.38050748517933	0.05676465702255
O	-1.43975930168916	2.00762619585398	0.56762066378577
O	-2.64271606329175	-0.07405988090617	-0.30739038587341
O	0.19068845811671	0.24687765303825	-1.25121701124421
O	0.03021295234346	-0.48743178172174	1.20632982837188
C	-2.27406014872795	-2.93879564526469	2.11739780536654
C	-2.78436925669981	2.11686839498057	0.45341218856618

C -3.43912189989568   0.98369873521377   -0.01872856421578

C 1.15977817107030   -0.85614610098949   0.55316087192887

C 1.24489498929691   -0.46210534901311   -0.77865233428884

C -4.80960741212322   0.96657256725906   -0.17448023810977

C -5.53862021946431   2.11580800422425   0.14989385500268

C -4.88216684734324   3.25498052465184   0.62396839724299

C -3.49102685299981   3.25713675571184   0.77827443674912

C 2.33910528369897   -0.79935935485923   -1.54733141949237

C 3.37053660904131   -1.54113076344637   -0.96457280059645

C 3.28938286022415   -1.92845100336444   0.37498000308640

C 2.17377144440963   -1.58175479003116   1.14218914289386

C -2.38638931032434   -3.04022025908391   0.79555075247085

C -1.28252039875494   -3.27925216337215   -0.14232132078277

C -1.39567780230606   -2.84646147427530   -1.46591689538613

C -0.35753605621841   -3.03066064737799   -2.36760514311376

C 0.80515581249718   -3.67188706706876   -1.96830038359497

C 0.91960137817664   -4.13215050926106   -0.66304979123401

C -0.11120489572027   -3.93684491450275   0.24010836718740

H -3.14252039009756   -2.76348863995389   2.73658213581044

H -1.32255805077109   -3.01146743179701   2.62838108036780

H -3.36493158391677   -2.91006879313806   0.34542105931893

H 1.61541341149408   -3.81890715462679   -2.67045317011761

H -0.01483539492337   -4.31849431587159   1.24834430225333

H 1.81671933238030   -4.64958875772885   -0.34843961069592

H -2.31004179206679   -2.36546988838466   -1.79265147140762

H -0.45895181722966   -2.67438371469070   -3.38412118682281

cis-Ge(cat^Br)₂(styrene)(ACN)

Br 2.47617208421489   3.91357133068248   -2.15035179917271

Br -7.21792842465876   0.47530183723395   -1.79446927020756

Br -2.86967319225950   -1.79504474777100   -4.72149775784420

Br 6.04323437118862   -0.26126612782609   -0.59093447158561

Br 5.57823341266672   2.83915223313549   -1.60772000014008

Br 3.39728644626000   -2.23020522812550   -0.14916112448209

Br -6.14085822197850   -1.27100107909791   -4.37439740642761

Br -5.00045674836557   1.66456081192447   0.38807258551780

Ge -0.56352369409593   0.35873693232002   -1.02779090484336

O   0.84463513064283   -0.74693960387430   -0.85537588359462

O   0.47456797390431   1.69158966412599   -1.61093607197818

O -1.34893342201452   -0.43502528964570   -2.44472501237672

O -2.17651329774410   0.89051712153336   -0.46384044918282

N -0.10776143707422   0.92642994532741   1.00121794067016

C   0.44735109549289   1.63346919260445   3.42499485052682

C   0.13755624192271   1.21968782794246   2.07713811947067

C -1.08725954955569   -2.46737281542037   0.92172689702554

C -1.97554324428705   -2.64937453010291   -0.12677408600341

C -3.32449650648696   -2.35049120638697   0.03596909921241

C -3.77464571601940   -1.85900462080901   1.25056480391877

C -2.88430183676237   -1.67710509854130   2.29721824856234

C -1.53041473488944   -1.97737221053708   2.15335597191377

C -0.63033783420363   -1.79346374636139   3.29481024547986

C   3.22369718339341   -0.46637328691442   -0.73871085283242

C   4.32108677045090   0.38164526085414   -0.92630498409677

C   4.12341857274631   1.69425846419153   -1.35547248264505

C   2.82789947959750   2.16838801162699   -1.59644141764629

C -4.47780675414196   0.69913202534463   -1.12033186056470

C -5.39001241033529   0.17582669163062   -2.04383333737823

C -4.93301467391966   -0.56467137370459   -3.13580761518688

C -3.56189207249563   -0.78768010612019   -3.31379785252476

C   1.75144159757124   1.32059878009044   -1.42099518280311

C   1.95009912740224   0.00050422931901   -0.99842880462275

C -2.66983630837575   -0.25628950736917   -2.40291708763907

C -3.13074050924716   0.47774088953112   -1.31071578093320

C   0.70224683833631   -1.77956811268739   3.26894862756424

H   1.27202855223157   -1.67292358045535   4.18204957578496

H   1.27465121077562   -1.89708087457849   2.35712877408236

H -0.31430853353266   1.25843518797269   4.10457614679488

H	1.41314441145787	1.22945864182228	3.71999174088180
H	0.47753569797214	2.72066671953258	3.47457959453312
H	-4.82107918707052	-1.62034000590044	1.38457985749474
H	-3.24908842749754	-1.30131045543604	3.24610839618276
H	-1.61907727351525	-3.05204145237564	-1.06601991305149
H	-0.05013771211567	-2.74325485922507	0.78600978693730
H	-4.01994173036474	-2.51382527734324	-0.77722049749746
H	-1.12501382722027	-1.66349351783643	4.25368966800684

trans-Ge(cat^Br^)₂(styrene)(ACN)

Br	2.71251120391968	2.87123956146559	-2.88879258788378
Br	-6.41258153962015	-3.42383383960162	-1.07274178362516
Br	-4.37144063081370	1.79748680432881	-2.15210479219482
Br	6.33351100015721	-1.54285720729743	-2.99852373140326
Br	5.81858206948521	1.70792560405282	-3.18100592086626
Br	3.73237622555357	-3.56768661227873	-2.52695944713544
Br	-6.96168960271973	-0.21006586220686	-1.55958012569173
Br	-3.29772849571419	-4.57923859539112	-1.26693251762264
Ge	-0.31745721922767	-0.88051067556333	-2.27960890633979
O	1.15741249730564	-1.94193166569872	-2.36174895463483
O	0.76039107444011	0.56034100027051	-2.50236557060279
O	-1.78098180271965	0.19041131349533	-2.15004235195251
O	-1.36325631962315	-2.28767772705651	-1.81989501087055
N	-0.65411364898934	-1.13272187352036	-4.31362133893205
C	-1.12403725992794	-1.46758156610719	-6.83268016999421
C	-0.86211928727607	-1.28035213409230	-5.42596838789510
C	-1.78472604737787	-2.17573776163261	1.50098073222516
C	-2.98364339635570	-2.74230070758844	1.89086635693147
C	-4.14566954309522	-1.98086202408775	1.90651724724924
C	-4.09860700062362	-0.64337657307825	1.54543044410399
C	-2.89547851319915	-0.07418123275119	1.16265684834192
C	-1.72598037162959	-0.83339844613644	1.12146251120800
C	-0.49450663610616	-0.19929490176901	0.65489660395698
C	3.52858175915067	-1.71656200314587	-2.65269863471391

C	4.60657569189813	-0.84386533146966	-2.84580876677535
C	4.38878293614940	0.53187898577508	-2.92281427662951
C	3.09098704452368	1.04553869222405	-2.80684498705875
C	-3.69385475689887	-2.77334429572962	-1.51804073055432
C	-4.99738303916811	-2.26498387832434	-1.45924751184960
C	-5.22892808305491	-0.90647954690654	-1.66294642658576
C	-4.15763177928943	-0.04337105070459	-1.92134764323838
C	2.03176727071962	0.17702810158545	-2.62556438119257
C	2.24992998540539	-1.20301685090391	-2.54820050666773
C	-2.87394804134159	-0.54839993243576	-1.95819105138417
C	-2.64245913510865	-1.91400748271724	-1.76335334769075
C	0.66922990789102	-0.80523671102585	0.37327575627002
H	-1.81780688096925	-2.29528678958571	-6.96827823326291
H	-1.56089403511072	-0.56146287797951	-7.24825214756966
H	-0.19404963844448	-1.69007881951093	-7.35257624645698
H	1.54739733116489	-0.22108934656496	0.13200297252300
H	0.81818100449867	-1.87118950282542	0.48754996452381
H	-5.00069374176917	-0.04617662571306	1.54771326044669
H	-2.86461808189508	0.96820463719011	0.86773657586128
H	-3.01758737019159	-3.78601964631692	2.17177915354047
H	-0.89142911978193	-2.78572131884067	1.48884690234725
H	-5.08585925993430	-2.43242910883729	2.19355771106936
H	-0.54413889038558	0.87847475760820	0.53162053587697

phenylacetylene

C	-6.98761875575464	5.23909764390422	0.00009591028875
C	-8.20527330819041	4.58064748424564	0.00007972524715
C	-8.24950429885359	3.19359491951808	-0.00002162971191
C	-7.06845840144096	2.46483455531116	-0.00010769170523
C	-5.84733699670827	3.11677445350757	-0.00009198849081
C	-5.79589311674879	4.51193428803079	0.00000936298918
C	-4.54019347560120	5.18645264328379	0.00002071498481
C	-3.48053030634859	5.75380589558236	-0.00001339142042
H	-2.54492557072925	6.25848546317177	-0.00003284738204

H	-6.94955567020334	6.31996623076856	0.00017449573996
H	-9.20254281469515	2.68155131794650	-0.00003398014926
H	-9.12349357408589	5.15272932944123	0.00014679310050
H	-7.09824746316154	1.38339303575007	-0.00018733821002
H	-4.92499823467836	2.55195979653824	-0.00015975828066

trans-Ge(cat^Br)₂(PhCCH)(ACN)

Br	-3.32803086993068	-4.55609567342666	-1.36968626624676
Br	-6.93488500020177	-0.13056880602669	-1.45815088478867
Br	3.75053815508885	-3.54339559806437	-2.33272900171223
Br	5.82621232338845	1.67182720921775	-3.38090097647279
Br	6.34570750580414	-1.55616349878540	-2.96552525226588
Br	-4.32654055929395	1.86082119587988	-2.02423352129218
Br	-6.42321190256815	-3.36622069324566	-1.08815943575530
Br	2.72050866244903	2.85143419199804	-3.15590724580951
Ge	-0.30060673589197	-0.85270143164874	-2.24074590916521
O	-1.36795369417507	-2.26908351698529	-1.83995924551138
O	-1.75861748981492	0.22305472725205	-2.10692239380532
O	0.77420642914525	0.57422685695964	-2.58769609865373
O	1.17526113203240	-1.91311712157083	-2.26750350307758
N	-0.63282083355924	-1.14440804928149	-4.28384778610479
C	0.59309542772432	-0.34615856415087	0.20974485177410
C	-2.64117284123121	-1.88329611643384	-1.77751203124775
C	-2.85748372305514	-0.50906411829431	-1.92937679019821
C	2.26398052098533	-1.18789065104908	-2.51432168710012
C	2.04318704169362	0.18341174307704	-2.69162367239505
C	-4.13425895018996	0.01103274748278	-1.85820623227184
C	-5.21341970808916	-0.84601944181427	-1.61165958466225
C	-4.99792061707270	-2.21376412942944	-1.45747923639400
C	-3.70245807213602	-2.73684963519678	-1.55173671368502
C	3.10192309996761	1.03725809593506	-2.94194406399665
C	4.39893707068835	0.51719266195287	-3.02857029061254
C	4.61874056299884	-0.84957122258558	-2.85252283675879
C	3.54366875007533	-1.70665270484960	-2.58858144030838

C	-0.47745167563025	-0.70076224021702	0.64716323258648
C	-1.74078051975266	-1.13623407279190	1.12947533225933
C	-2.80544829157201	-0.23613777562104	1.21579938679719
C	-4.04816709204889	-0.68183767773835	1.62668758938841
C	-4.23223326724673	-2.01675092819192	1.96223356003137
C	-3.17166770827714	-2.90942751815394	1.89264591833972
C	-1.92709173932689	-2.47630663042899	1.47268221764531
C	-0.82163042221622	-1.30267607544563	-5.39825725915234
C	-1.06051012391709	-1.50292970856116	-6.80763080171254
H	1.59110529675003	-0.00225352558490	0.05144891665746
H	-5.21014048740440	-2.36469699321465	2.26674547281912
H	-1.10189932333322	-3.16927192644747	1.38566718166177
H	-3.32120018915339	-3.95014095258773	2.14420262908989
H	-2.65542663793764	0.79880529997439	0.93827904009726
H	-4.87909247001849	0.00913342262264	1.66966528827544
H	-0.23798414797835	-2.06771499304303	-7.24246075361179
H	-1.13801216566534	-0.53915839519934	-7.30729263029833
H	-1.98796892700282	-2.05521376618594	-6.94714975495554

para-tolualdehyde

O	0.19777698124044	-0.87507039166112	0.00793253151958
C	-0.91258636467423	-1.33738708693362	-0.00009903728504
C	-3.29786908879386	1.56661297579643	0.00970799776627
C	-2.12047964710336	0.84807847075052	0.00979088703918
C	-2.15431121264994	-0.54618508848792	0.00003187079209
C	-3.38164615442405	-1.19572734877033	-0.00969966584254
C	-4.56155049177592	-0.46876702601926	-0.00972206455200
C	-4.53740120558812	0.92124678558086	-0.00003554309212
C	-5.80501745533497	1.72150387033159	0.00006530430556
H	-1.07438780092342	-2.43451887984404	-0.00843438117501
H	-1.16538800722199	1.35699223066845	0.01738818871690
H	-3.41665133365831	-2.27944964124301	-0.01731684956313
H	-5.51208687392602	-0.98753301686091	-0.01735460133669
H	-3.26306051722655	2.64959547359158	0.01732794653089

H	-5.86699337929768	2.36103054897259	0.88175322526951
H	-5.85967727020142	2.37284520488013	-0.87342110322125
H	-6.68662283134058	1.08266759744803	-0.00791821667219

trans-Ge(cat^{Br})₂(_para_-tolualdehyde)(ACN)

trans-Ge(cat^{Br})$_2$(*para*-tolualdehyde)(ACN)

Br	2.47781483479685	0.08493108987730	-3.50982911769560
Br	-6.78451705956199	1.97997278201583	2.58616173448771
Br	-4.55358618888868	1.31466464121762	-2.62897758274143
Br	5.97846091374538	-0.27242374021823	0.98823507610262
Br	5.55003691416553	-0.29731119738135	-2.28158965082896
Br	3.32842040357312	0.12939768709185	2.96252621662559
Br	-7.18636596733833	1.93991767472368	-0.68692324291165
Br	-3.76297387528248	1.38501280991241	3.85081264310024
Ge	-0.64469353331114	0.61212661940738	0.19678157559859
O	-0.99406589792847	-1.38041258614654	0.24051332968046
O	0.80383414501850	0.42395260105626	1.28510361581388
O	0.47446225513644	0.42100802963282	-1.24257239552732
O	-2.07203157119451	0.87153258831756	-0.92314678003530
O	-1.76620249267811	0.87989263266327	1.60735922316596
N	-0.27585358446157	2.72831470748780	0.14774659228784
C	0.19074066217453	5.27194470192072	0.14425888993357
C	-0.07010810329811	3.85119016410038	0.14535244395729
C	-2.25827674796767	-7.68553392936763	-0.61919094909404
C	-1.46218079884575	-4.16899380262003	0.51498304557523
C	-1.70850375887163	-5.52220422605268	0.52442427335330
C	-1.99468247437872	-6.21309405764952	-0.65915950968459
C	-2.02714860458028	-5.50788545008028	-1.85950518962953
C	-1.78089916246852	-4.14854674982184	-1.88190623355135
C	-1.49714638978053	-3.46835163309088	-0.69734404605534
C	-1.24879775492450	-2.05406519711145	-0.76177274202480
C	3.17154111020735	0.10447260627644	1.10189670850486
C	4.27237065578989	-0.06293688311999	0.25072784038934
C	4.09238327414097	-0.07237208753117	-1.13066312530481
C	2.80924229632671	0.08850532957263	-1.67003923377848

C	-4.07384444608727	1.38515232844672	2.00932631900155
C	-5.33668610312627	1.63178437767025	1.45387442706419
C	-5.50722088101104	1.61685115375001	0.07132814721651
C	-4.41339578252003	1.35864639406256	-0.76547059028108
C	1.72818174461655	0.25596049797882	-0.82681153891797
C	1.90807569632132	0.26078001418657	0.56414975996415
C	-3.17009387161513	1.12070971269374	-0.21321879575634
C	-2.99920794493049	1.12895397688306	1.17894892328986
H	-1.29358891054722	-1.57997988801609	-1.74880444302196
H	-0.17678128908596	5.71399886310862	-0.77969354825623
H	-0.31237963830718	5.73838074356022	0.98906135114569
H	1.26162201945826	5.44876967437188	0.22417365782485
H	-1.39423972271202	-8.22452470528297	-0.22796809837370
H	-3.10091967624329	-7.91246669405432	0.03545018374992
H	-2.48338065378105	-8.08624911728669	-1.60553599632667
H	-2.24731372684176	-6.02939088433506	-2.78177529409465
H	-1.80886163913794	-3.60944272462058	-2.82131514844627
H	-1.68139276136338	-6.06332956405773	1.46197503283817
H	-1.24268530900030	-3.64499493744124	1.43564857226672

HSiEt₃

Si	-3.29638235618199	0.96236643459578	0.09354523098166
C	-1.41358955497644	1.08979808405629	0.20981041370591
C	-3.99263084423205	2.34857751070453	-0.98735775330339
C	-3.80908978944146	-0.72866476099756	-0.57910619501682
C	-0.92347689235911	2.42333668418980	0.77310475287066
C	-5.51581280760574	2.32292533107657	-1.11000697522672
C	-3.30358289224391	-1.90080968413376	0.26136077373888
H	-3.86231885402641	1.11102334513536	1.46969567155474
H	-0.98477035594455	0.92386681561198	-0.78381302808632
H	-1.04115597550099	0.26908842855399	0.83005386715430
H	-1.22355328176165	3.26287405827479	0.14446995848382
H	0.16429678064213	2.45387016738499	0.85089454373246
H	-1.32449808422295	2.60840058767293	1.77083117877598

H	-3.67239263038736	3.31130758641764	-0.57798982062486
H	-3.53680439042660	2.28665629067577	-1.98088464057170
H	-5.99771701943864	2.39808134737092	-0.13396513844050
H	-5.86873789488550	1.40056250956573	-1.57338731317296
H	-5.88631745859113	3.14942286929833	-1.71816712925434
H	-3.44938667391284	-0.82490568432553	-1.60869861565478
H	-4.90046326811193	-0.76709353526229	-0.64558665560612
H	-2.21375208498081	-1.93181785590375	0.29828417965436
H	-3.63813622598242	-2.85900052736451	-0.13886464858146
H	-3.65925973012762	-1.83833062299800	1.29098227718720

SiEt₃⁺

Si	-3.06735107899382	0.95263275386031	-0.18400718007993
C	-3.06279628288363	-1.89687674538827	0.16091423225622
C	-5.41438114951241	2.27615687781812	-1.17389845395916
C	-0.72807327661783	2.48159062670305	0.47082832356241
C	-3.89452595906549	-0.69107156197578	-0.28129702950013
C	-3.97633333999027	2.47351823311108	-0.68986473713247
C	-1.33087592177950	1.07609207284691	0.42011018309215
H	-2.76158743441635	-1.82679634700400	1.20492410920730
H	-3.64629141681731	-2.80911764073701	0.05549082571401
H	-2.16393919384304	-2.01912575382551	-0.44138585029840
H	-4.82556233732054	-0.61589336201440	0.29723559766385
H	-4.25020339083506	-0.80984370575657	-1.31405870977302
H	-5.84806980425180	3.23500629535410	-1.45009425732399
H	-5.46795510866648	1.63454236852177	-2.05203236829858
H	-6.05125346655352	1.84539043501844	-0.40291027180497
H	-3.36430010856691	2.97308951997095	-1.45347836707369
H	-3.93393902103984	3.16916156987783	0.15951740172050
H	-1.27698523644080	3.13937819042748	1.14286953874236
H	0.29627262737406	2.43334243099213	0.83436190892138
H	-0.69867666471124	2.95181455622563	-0.51085368532584
H	-1.29958252473645	0.59365536387318	1.40670603486458
H	-0.72577064753172	0.40579568540055	-0.20582320717458

ACN--SiEt₃⁺

Si	-3.28218583404361	0.97080465001983	0.10786982414197
N	-4.04339826615922	1.15880667389944	1.82083540915366
C	-5.08275460069755	1.40920161707696	4.17236724806286
C	-4.50539039561173	1.26863344423170	2.86108648374357
C	-1.45990477480805	1.11274153045367	0.47856909447686
C	-4.03932944806311	2.40643192399121	-0.81068944829673
C	-3.88038900526479	-0.72256980347590	-0.39524267724645
C	-1.01274348496691	2.48000173755388	0.99966901917045
C	-5.55430352170477	2.31952142612705	-1.00589483758898
C	-3.33181588215164	-1.87635335079883	0.44658201256617
H	-5.89201385320369	0.69008349510220	4.29646293582547
H	-4.32073274924274	1.22709696295184	4.92974058539497
H	-5.47650019921522	2.41801116069791	4.29367802567728
H	-0.93225439961010	0.87982015076265	-0.45306910579621
H	-1.16731723839934	0.32058024080211	1.17353832318926
H	-1.22853645479160	3.27842760888507	0.29040223260427
H	0.06146364241938	2.49123556096720	1.17676740739813
H	-1.49271848199643	2.73911984696310	1.94427379629625
H	-3.76749516075092	3.34116472762112	-0.31222027678072
H	-3.54141124847017	2.45107086552916	-1.78571778988510
H	-6.09295812644949	2.30253754496396	-0.05753340170893
H	-5.84402273922695	1.43063830831518	-1.56540221214320
H	-5.92003740787259	3.18095778292393	-1.56230275333752
H	-3.59109314067848	-0.85750866457502	-1.44344247534123
H	-4.97397924271305	-0.73503221313799	-0.40095807642491
H	-2.24431172993530	-1.93002442658707	0.40743260680069
H	-3.71228135053209	-2.83036537923451	0.08530595111835
H	-3.62051184425972	-1.79643824702987	1.49544365772975

Ge(cat^Br)₂H⁻

Ge	-0.37586420780018	-0.58290571765468	0.62429698438466
O	-1.38857865038741	0.68255202346988	1.47761370457119
O	-1.81990793515461	-0.68539358330436	-0.60481938335951

O	0.72962943101808	-0.17400648645706	-0.77783749077918
O	1.08991778262550	-0.08294399960002	1.72339464722519
C	-2.55107129884454	0.90487765259887	0.88045468806733
C	-2.78057967953978	0.14169394882204	-0.28253341943489
C	2.11860848900292	0.28958396887159	1.00657313634003
C	1.92853722850870	0.23732011127750	-0.38941945522507
C	-3.96764936616331	0.30239911431128	-0.97821748551272
C	-4.93135260804059	1.21510377956107	-0.52537237841140
C	-4.69952914242266	1.96396733057979	0.62174953598831
C	-3.49623815266877	1.80394772385592	1.32780252427079
C	2.94491884459710	0.59528480882188	-1.25000216237412
C	4.18209977554910	1.01585585109430	-0.73569646381120
C	4.37568569234622	1.06915111396787	0.63911703334904
C	3.33972471476152	0.70525905307657	1.51159019290869
Br	-3.10577558866343	2.77137998795284	2.88167590029941
Br	-6.53302336543097	1.41073575315864	-1.48249641633361
Br	3.52663999320520	0.74687162104069	3.37357890062527
Br	5.55662434246056	1.49708799753710	-1.91763377530771
Br	6.02142089582042	1.62477575553405	1.34800960367955
Br	-4.20969629523003	-0.74342710846162	-2.51167000012095
H	-0.45580151814280	-2.02968922244749	1.09835368596704
Br	-5.97764634927596	3.18789440133666	1.24325525530728
Br	2.60233696786972	0.49197412105670	-3.08710736231346

Ge(cat^{Br})_2(ACN)H^-

Br	-6.12605974196628	0.01420330935886	-1.42869275135228
Br	-3.21420365283119	1.02322807362404	3.38606103710525
Br	3.60037909358634	0.39908596785962	3.28020181198510
Br	6.03154228393083	-1.28282362296895	-1.61209642219624
Br	3.40732552856073	-0.02387802325955	-3.23526529472223
Br	-3.35422833768660	0.72249815609613	-3.13727672700239
Br	-6.05729844993113	0.17238306725462	1.86948456228156
Br	6.12922511633425	-1.06801199729575	1.68118755284061
Ge	0.26031689249041	1.89613785624596	0.00507625489675

H	0.39244226318023	3.41527537772325	-0.07653868324895
O	1.51421805191379	1.36244894296239	1.27084523834077
O	1.44106165224113	1.20054525541329	-1.24902552006354
O	-1.11400321392460	1.49512626657157	-1.21452159815638
O	-1.05357109079693	1.59108499690861	1.30655155282808
N	-0.01418518592317	-1.18279332100160	0.13590030707814
C	3.62010956359592	0.24063114611691	1.41441634458641
C	4.67303503287501	-0.37584267624261	0.72044483366246
C	4.63227874982173	-0.46608201700812	-0.66457668212895
C	3.53798385310719	0.06013840614384	-1.36894015668150
C	-3.34266543328693	0.94486886268845	1.52046113078143
C	-4.52881629682565	0.58068790054312	0.86000044261676
C	-4.56021553488674	0.52133924442873	-0.52719657911668
C	-3.40680940740423	0.82830158837788	-1.26771183745865
C	2.50464812421128	0.67061210272958	-0.68596352120694
C	2.54478969337630	0.76098048702000	0.72078883849910
C	-2.24249820761570	1.20310407258525	-0.62161372216176
C	-2.20945771467340	1.25735087538460	0.79166709874506
C	-2.33823728600440	-2.28039204929142	-0.25193811023447
C	-1.04144063282688	-1.66962017058071	-0.03269373888500
H	-2.28312940147117	-3.35476432745467	-0.08497416968686
H	-2.66869151976047	-2.09556048779492	-1.27248308463449
H	-3.07338154060960	-1.85425022013841	0.42904826068985

Ge(cat^Br)$_2$(H)(SiEt$_3$)

Br	-3.92417877197886	2.49947363055950	1.79261614774001
Br	-5.63114518457656	1.41958343141748	-3.54444375742721
Br	2.95813901684658	-2.23359894887443	1.46646684118906
Br	6.60690399125771	2.13341509990388	1.03349770713525
Br	6.02101570070226	-0.99657684440227	1.87190700337635
Br	-2.46887029831480	0.73273343649861	-4.32054134507678
Br	-6.36565164585468	2.30651304609503	-0.45939103519663
Br	4.11857212370767	3.97358602601415	-0.19053498415510
Ge	0.17503971033249	1.23337238672471	-0.35007756709640

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Si  -2.36142941251731   -1.91672358095858    0.62563514764569
O   -1.25641494492913    1.76824750593130    0.52669874779243
O   -0.67858709438826    1.08462946284637   -1.88238697758252
O    1.55880887231683    2.32588515360393   -0.34015792177407
O    1.10717529907648   -0.11558136895352    0.29739139966014
C   -2.29758443380812    1.73456275454101   -0.34110706259210
C   -1.98582185831622    1.35783930854559   -1.64484094498519
C    2.37715343803582    0.31849132177573    0.49813757466344
C    2.62243626500997    1.64306449165222    0.14968745840936
C   -2.96954919244516    1.26080744593035   -2.60720663153352
C   -4.29132029125524    1.55397414609716   -2.25250742424934
C   -4.60295771687269    1.93525878950269   -0.94516448228101
C   -3.59606689297201    2.02588956735825    0.02145551586912
C    3.87791341974597    2.19533825370726    0.30336140184599
C    4.90503823181879    1.39866589221556    0.82161367989937
C    4.65688735800099    0.06980471716356    1.17654548301170
C    3.37929313672097   -0.47719322396546    1.01454294771718
C   -1.81138277497058   -1.39672925912248    2.35594868009406
C   -1.96442323900643   -3.73659094695871    0.31778193742813
C   -4.19104821564447   -1.55023437430824    0.30487548904906
C   -2.46580831632681   -2.19542724824539    3.48330612151009
C   -5.15248026913928   -2.64665430054265    0.76691379337725
C   -0.49046678263288   -4.07550511153665    0.53672504113509
H   -1.55360276713775   -1.12730740013470   -0.35969346367277
H   -4.45315629076171   -0.60584937015384    0.79031649124110
H   -0.72266244859213   -1.49347323263712    2.41352111896429
H   -2.01931937823076   -0.33073680306929    2.48774197576412
H   -4.32700954187298   -1.37493334805549   -0.76661899652138
H   -2.26062044971619   -3.99207599034728   -0.70404765148782
H   -2.58975285427832   -4.35723511353204    0.96707051148771
H   -5.07146219846819   -2.83920873287393    1.83749391433529
H   -4.96370240687378   -3.59084672356251    0.25508987828540
H   -6.18928552037931   -2.37298762093304    0.56760795968168
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H	-2.27067236669632	-3.26518109036858	3.39003578545513
H	-3.54849537739269	-2.06344119261254	3.49635365037197
H	-2.09463432986278	-1.88593361954317	4.46122713002108
H	0.16091235820704	-3.47175638086296	-0.09659063415761
H	-0.28077137783067	-5.12308061904126	0.31616609033374
H	-0.18831033633622	-3.89636954048810	1.56987594049908

4-methylacetophenone

O	0.14675710448012	-0.60474296252898	0.00907948786621
C	-0.85437367447670	-2.73511945452452	-0.00939801771966
C	-5.85470515020612	1.79079055402102	0.00027057796633
C	-4.58888760876554	0.98806488246794	0.00019357963177
C	-4.61077511370544	-0.40035272203160	-0.00951931742956
C	-3.43426984882288	-1.13486884558350	-0.00950225897292
C	-2.19641828485384	-0.49994604764161	0.00026358103268
C	-2.17399557126443	0.89761125104748	0.01001555321046
C	-3.34647119420338	1.62381345514003	0.00997623325519
C	-0.89233486069951	-1.22230502563230	0.00090871124031
H	-0.29673396921467	-3.06717262501743	-0.88525415402456
H	-0.30344334089276	-3.07924212965096	0.86604074821703
H	-1.82128558034647	-3.22831611997645	-0.01648885822009
H	-6.73758071253787	1.15350900934029	-0.00784404831303
H	-5.90824131826957	2.44239486701549	-0.87314329192909
H	-5.91571905367503	2.43042716651608	0.88199955580921
H	-3.30147267293149	2.70653828619944	0.01767934817171
H	-5.56074273243573	-0.92050468595440	-0.01724752224956
H	-3.50584135201994	-2.21346109661410	-0.01728863280479
H	-1.22113543595872	1.40906837990809	0.01767772836236

trans-Ge(cat^{Br})$_2$(*para*-methylacetophenone)(ACN)

Br	-4.00916053019929	0.96373639158143	3.66610252416828
Br	-7.14066127781577	2.72096436899840	-0.77539250824444
Br	2.99573715587340	-0.63304393505974	2.81950515962830
Br	5.44010289723632	-0.33827834524508	-2.33441926005052
Br	5.70737119259611	-0.89440434925876	0.90594018221958

Br	-4.48622788257005	2.21397798513682	-2.72349756037746
Br	-6.89690269591302	2.09191315773254	2.45292655662455
Br	2.46501927359075	0.48100697487774	-3.59087461894297
Ge	-0.79554204422775	0.60970348655223	0.02689005308476
O	-1.96101789566068	0.70127367495202	1.42662907373068
O	-2.14269741695920	1.20792910669646	-1.06160793297766
O	0.39140622776238	0.62238302594698	-1.36915716698076
O	0.58721337322673	0.14866676734657	1.12593615576270
O	-1.22959558493980	-1.31726048474731	-0.25227961982385
N	-0.29297670605759	2.68377108869607	0.39868580733952
C	-1.44884162370037	-1.56099033750043	-2.62090184337244
C	-3.14299006155429	1.14959102910322	1.01980091251719
C	-3.24628483918343	1.42572414144915	-0.35130679463651
C	1.71284571419390	0.03130637469703	0.43229380144678
C	1.60515476793731	0.28486536700148	-0.94341841943194
C	-4.43342618646489	1.88850991417945	-0.88350528974753
C	-5.53792804402145	2.09080003240169	-0.04542156217525
C	-5.43445820074443	1.82332516873045	1.31783822171620
C	-4.22852197056832	1.34885685863989	1.85171084295611
C	2.70954363501311	0.16508886070998	-1.76378725756277
C	3.94898143083787	-0.18915536793545	-1.21471595278591
C	4.05991198986414	-0.42685084367132	0.15331827232499
C	2.93284891682331	-0.31868388789246	0.97974139526408
C	-1.39439300198108	-2.07437675337684	-1.22233897318072
C	-1.50595852628739	-3.50215871757464	-0.92925985764526
C	-1.55873190139691	-4.46389296544417	-1.93966686233900
C	-1.63135771131791	-5.80828010180384	-1.62685414641147
C	-1.66493071378191	-6.23429059122218	-0.30270292532273
C	-1.61395363654003	-5.26986879345011	0.70619008884629
C	-1.53007673270833	-3.92881902629727	0.40573648222217
C	-1.75411503465092	-7.68703709325168	0.04555571658592
C	-0.04324399880751	3.77234394609923	0.63574276422686
C	0.27374864558740	5.14915505520202	0.93757646118823

H	-1.91490956264842	-0.57966489010516	-2.66003715920278
H	-0.42942523385806	-1.44483494952906	-2.99815206060607
H	-1.98437716370769	-2.23056489871386	-3.28628742093904
H	-1.48516869033487	-3.20246391462414	1.20529612212561
H	-1.63676440689759	-5.58056357973326	1.74329839371169
H	-1.52752491211809	-4.17811825024521	-2.98153114876906
H	-1.66302273435238	-6.53842143886067	-2.42520992837831
H	-1.74892720920743	-8.31899100956132	-0.84050533225417
H	-2.66894814891665	-7.89834002127903	0.60107345862489
H	-0.91822718564080	-7.98919824963239	0.67775255793063
H	1.35145879597150	5.29526177461609	0.89949311820974
H	-0.08531127019220	5.39835621708349	1.93415902760388
H	-0.20208065198745	5.80529673878512	0.21112596349910

HBpin

O	-3.80939113745227	-3.99857346285660	0.57646955109246
O	-1.79394675575067	-2.95800502588033	0.73038776612347
C	-2.81494800829394	-5.70867251825211	1.91052393797869
C	-3.23073898076148	-6.07261380046281	-0.51278674823981
C	-1.25495731178235	-4.11673609930333	-1.28468164487951
C	-0.26870176379482	-4.82129589277709	0.88528269448606
C	-2.82988675665893	-5.04851779869759	0.53454020020301
C	-1.51245837225230	-4.26780034166774	0.21217998920290
B	-3.14604054950661	-2.83406850163743	0.80591598634214
H	-3.69572443394290	-1.80529500928407	1.04989428353418
H	-2.46175135274705	-6.83985070158492	-0.61494745871863
H	-4.15431290863305	-6.57087698779420	-0.21721666973875
H	-3.39537151548669	-5.62485152596453	-1.49101495400694
H	-3.81461492278628	-6.07075272692848	2.15135924162508
H	-2.13705294269268	-6.56200211912635	1.93813104796469
H	-2.51668497595430	-5.01616935381549	2.69884138825263
H	-0.07850885136816	-5.84538856889231	0.56048070294512
H	0.60230944906996	-4.22406228262147	0.61464787375158
H	-0.34707046002450	-4.81839235866285	1.97085564206757

H	-0.43705760788016	-3.41382529009952	-1.44408163314574
H	-0.97096957520099	-5.06569532456467	-1.74006046417603
H	-2.12616243189982	-3.73466670792605	-1.81849430066416

trans-Ge(cat^Br)_2(HBpin)(ACN)

Br	-5.04065208855046	0.46204537039224	2.77041621533099
Br	-7.05018199196681	0.39691746262264	-2.57563567912485
Br	1.84630942830673	-1.30077050946129	4.11343241751776
Br	5.39579683809438	-2.59159540598614	-0.17033077842048
Br	4.85075299390384	-2.28549200360123	3.06720983332065
Br	-3.99139644096648	-0.42284384873464	-3.61130101865269
Br	-7.57827177745232	0.84506697569938	0.64897039302982
Br	2.92952013151631	-1.90285934868201	-2.29689267112781
Ge	-1.04116455230169	-0.69011096569826	0.24553352654762
O	-1.58551509891060	-4.60418864230064	1.77859984119259
O	-1.45246219104359	-2.73286739425079	0.50749574547947
O	-2.50124674117352	-0.25687735023486	1.24960994273628
O	-2.09068018346344	-0.58738152747064	-1.24096024630638
O	0.43552345103285	-1.04071794826015	-0.76571615223424
O	0.01983540687950	-0.79395977666738	1.72868801275750
N	-0.61256504658288	1.38861544086955	0.08203427859836
C	0.29560278356239	-5.25904420080023	0.45639569248753
C	-1.92747950636353	-6.34798181978904	0.15356095096917
C	-3.15100818487679	-3.87950950180659	-0.76860629488465
C	-0.85350065081971	-3.70422282197887	-1.70655802594654
C	-1.21452914104595	-5.04434319885647	0.45910316468578
C	-1.66535207222872	-3.85748674049228	-0.43994050688979
C	-3.56306043793679	-0.08477726010910	0.46796994100226
C	-3.33817702088963	-0.26469294612445	-0.90324911846246
C	1.24411411747247	-1.19042616868397	1.39149322257654
C	1.47387303678844	-1.32434764729572	0.01539193213390
C	-4.37440207930303	-0.12874244190333	-1.80600683407591
C	-5.65462352183905	0.20648974321101	-1.34581234260962
C	-5.87730341573241	0.39376245564106	0.01705025572202

C	-4.82367165005188	0.24376940195742	0.92894326396323
C	2.70595886345954	-1.74459185038512	-0.44811060209306
C	3.72888992215193	-2.03159233179582	0.46582871948046
C	3.49859122665639	-1.90188926559433	1.83415134479153
C	2.24459260973931	-1.48221660623344	2.29860841462034
C	-0.40080284448814	2.50908165208119	0.03158244366044
C	-0.13327690426202	3.92687458407701	-0.03388719304379
B	-1.61401376659071	-3.26439314425461	1.80179513555838
H	-1.77782156272510	-2.61037041442939	2.77317462482940
H	-1.74192125005240	-6.65462309261962	-0.87644497746819
H	-1.55213191035933	-7.13801172265053	0.80350204137201
H	-3.00330432657925	-6.27811999739663	0.30198365519362
H	0.56233718855920	-5.95487089703548	1.25151064141719
H	0.63381377336754	-5.68782584306288	-0.48625068395026
H	0.85464546211136	-4.33673264464314	0.62352068862327
H	-0.98008209223036	-4.61311945590488	-2.29800152064814
H	-1.20882523205669	-2.87178749854594	-2.31004822983516
H	0.20940969383623	-3.57053722062948	-1.52975376388644
H	-3.44338530632217	-2.95782038369161	-1.26767613683872
H	-3.37226684182177	-4.69599967857553	-1.45500308359749
H	-3.78164682225131	-4.00339335748682	0.11254773703845
H	-0.17775716422103	4.26251269461946	-1.06815019526123
H	0.85729629246739	4.13307412892395	0.36699263455156
H	-0.87512596484621	4.46788787622846	0.55041204636981

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