Supporting Information

Rhodium(I)-Catalyzed Silylation of Aryl Iodides with Di(2-furyl)methylsilane

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General Considerations.

All experiments were carried out under a nitrogen atmosphere using oven-dried (120 °C) glassware. NMR spectra were recorded on a JEOL JNM-ECA600 (^{1}H, 600 MHz; ^{13}C, 150 MHz), a JEOL JNM-A500 spectrometer (^{1}H, 500 MHz; ^{13}C, 125 MHz) or a JEOL ECX-400 spectrometer (^{1}H, 400 MHz; ^{13}C, 100 MHz). Chemical shifts of ^{1}H NMR and ^{13}C NMR signals reported δ ppm referenced to the solvent or an internal $SiMe_4$. Mass spectra were obtained at an ionization potential of 70 eV with a JEOL JMS-T100GCV spectrometer. GLC analyses were carried out with a Shimadzu GC-14B equipped with a glass column (OV-17 on Chromosorb W, 2 m). GLC yields were determined using suitable hydrocarbons as internal standards.

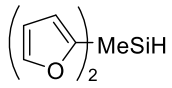
Materials.

N-Methylpyrrolidone (NMP) was distilled from CaH_2 prior to use. Other solvents were also distilled from suitable drying agent. $Rh(acac)(CO)_2$ (Aldrich), aryl halides **2**, and triethylamine (TCI) were purchased from commercial sources, and used without purification.

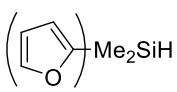
Synthesis of Di(2-furyl)methylsilane (1).

To a solution of furan (0.90 mL, 12 mmol) in ether (10 mL) was added dropwise a solution of *n*-butyllithium (1.6 M in hexanes, 6.5 mL, 10 mmol). The reaction mixture was refluxed for 2 h and then was transferred via cannula to a solution of dichloromethylsilane (0.52 mL, 5.0 mmol) in ether (10 mL) at -78 °C. After being stirred for 2 h at -78 °C, the solution was allowed to warm to rt overnight. The mixture was then filtered through a short silica pad with ether as eluent and concentrated in vacuo. The residue was purified by column chromatography (silica gel, eluent: hexane) to provide the title compound as a colorless liquid: (0.63 g, 70%).

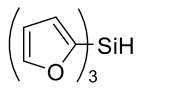
Tri(2-furyl)silane (81%, from trichlorosilane) and (2-furyl)dimethylsilane (57%, from chlorodimethylsilane) were prepared by the same procedures.



Di(2-furyl)methylsilane (1). ^{1}H NMR ($CDCl_3$): δ = 0.61 (s, 3H), 4.92 (m, 1H), 6.43 (dd, *J* = 1.4, 3.1 Hz, 2H), 6.81 (d, *J* = 3.1 Hz, 2H), 7.71 (d, *J* = 1.4 Hz, 2H). ^{13}C NMR ($CDCl_3$): δ = -6.38, 109.76, 122.79, 147.81, 153.35. HRMS (EI): *m*/*z* [M^+–H]: calcd for $C_9H_9O_2Si$: 177.0372; found 177.0354.



(2-Furyl)dimethylsilane. ^{1}H NMR ($CDCl_3$): δ = 0.35 (s, 6H), 4.43 (m, 1H), 6.40 (dd, *J* = 1.4, 3.1 Hz, 1H), 6.70 (d, *J* = 3.1 Hz, 1H), 7.67 (d, *J* = 1.8 Hz, 1H). ^{13}C NMR ($CDCl_3$): δ = -4.59, 109.51, 120.83, 147.03, 157.06. HRMS (EI): *m*/*z* [M+]: calcd for $C_6H_{10}OSi$: 126.0501; found 126.0508.

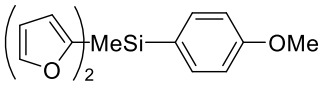


Tri(2-furyl)silane. ^{1}H NMR ($CDCl_3$): δ = 5.46 (s, 1H), 6.47 (dd, *J* = 1.4, 3.1 Hz, 3H), 6.95 (d, *J* = 3.0 Hz, 3H), 7.76 (d, *J* = 1.8 Hz, 3H). ^{13}C NMR ($CDCl_3$):

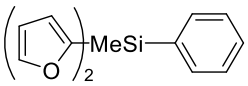
δ = 109.99, 124.75, 148.54, 150.06. HRMS (EI): *m*/*z* [M^+]: calcd for $C_{12}H_{10}O_3Si$: 230.0399; found 230.0399.

General Procedure for Catalytic Silylation.

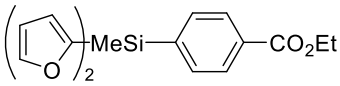
In a glove box, $Rh(acac)(CO)_2$ (1.9 mg, 7.5 μmol) was placed in a screw-capped 5-mL vial with a stir bar. NMP (1 mL), Et_3N (0.10 mL, 0.75 mmol), aryl iodide **2** (0.250 mmol), and **1** (66.8 mg, 0.375 mmol) were added to the vial. The vial was sealed with a cap and removed from the glove box. The reaction mixture was then stirred at 80 °C for 2 h. After the reaction, the mixture was diluted with toluene, washed three times with water to remove NMP, and dried over Na_2SO_4. The solvent was removed under reduced pressure, and the residue was purified by flash column chromatography to give the desired product **3**.



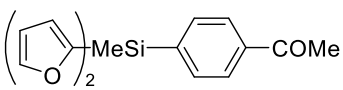
(4-Methoxyphenyl)di(2-furyl)(methyl)silane (3a). ^{1}H NMR ($CDCl_3$): δ = 0.78 (s, 3H), 3.81 (s, 3H), 6.42 (dd, *J* = 1.8, 3.0 Hz, 2H), 6.76 (d, *J* = 3.0 Hz, 2H), 6.93 (d, *J* = 8.5 Hz, 2H), 7.54 (d, *J* = 8.5 Hz, 2H), 7.72 (d, *J* = 1.8 Hz, 2H). ^{13}C NMR ($CDCl_3$): δ = -4.24, 55.05, 109.61, 113.79, 122.79, 124.52, 136.24, 147.72, 155.38, 161.14. HRMS (EI): *m*/*z* [M^+]: calcd for $C_{16}H_{16}O_3Si$: 284.0868; found 284.0840.



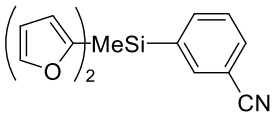
(Phenyl)di(2-furyl)(methyl)silane (3b). ^{1}H NMR ($CDCl_3$): δ = 0.81 (s, 3H), 6.43 (dd, *J* = 2.6, 1.7 Hz, 2H), 6.77 (d, *J* = 2.6 Hz, 2H), 7.3-7.4 (m, 3H), 7.61 (d, *J* = 8.1 Hz, 2H), 7.73 (d, *J* = 1.7 Hz, 2H). ^{13}C NMR ($CDCl_3$): δ = -4.48, 109.63, 122.97, 127.96, 129.95, 133.84, 147.80, 154.95. HRMS (EI): *m*/*z* [M^+]: calcd for $C_{15}H_{14}O_2Si$: 253.0685; found 253.0679.



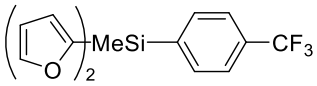
(4-Ethoxycarbonylphenyl)di(2-furyl)(methyl)silane (3c). ^{1}H NMR ($CDCl_3$): δ = 0.83 (s, 3H), 1.38 (t, *J* = 7.2 Hz, 3H), 4.38 (q, *J* = 7.2 Hz, 2H), 6.44 (dd, *J* = 3.3, 1.5 Hz, 2H), 6.79 (d, *J* = 3.3 Hz, 2H), 7.69 (d, *J* = 8.3 Hz, 2H), 7.74 (d, *J* = 1.5 Hz, 2H), 8.02 (d, *J* = 8.2 Hz, 2H). ^{13}C NMR ($CDCl_3$): δ = -4.63, 14.29, 61.00, 109.74, 123.30, 128.65, 131.67, 134.60, 139.90, 148.04, 154.14, 166.58. HRMS (EI): *m*/*z* [M+]: calcd for $C_{18}H_{18}O_4Si$: 326.0974; found 326.0983.



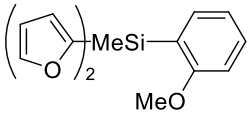
(4-Acetylphenyl)di(2-furyl)(methyl)silane (3d). ^{1}H NMR ($CDCl_3$): δ = 0.83 (s, 3H), 2.60 (s, 3H), 6.45 (dd, *J* = 2.0, 3.5 Hz, 2H), 6.80 (d, *J* = 3.5 Hz, 2H), 7.72 (d, *J* = 7.8 Hz, 2H), 7.74 (d, *J* = 2.0 Hz, 2H), 7.94 (d, *J* = 7.8 Hz, 2H). ^{13}C NMR ($CDCl_3$): δ = -4.66, 26.64, 109.75, 123.34, 127.37, 134.88, 137.97, 140.42, 148.06, 154.00, 198.26. HRMS (EI): *m*/*z* [M^+]: calcd for $C_{17}H_{16}O_3Si$: 296.0869; found 296.0861.



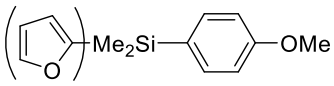
(3-Benzonitrile)di(2-furyl)(methyl)silane (3e). ^{1}H NMR ($CDCl_3$): δ = 0.82 (s, 3H), 6.46 (dd, *J* = 2.4, 3.5 Hz, 2H), 6.82 (d, *J* = 3.5 Hz, 2H), 7.48 (t, *J* = 7.8 Hz, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 2.4 Hz, 2H), 7.82 (d, *J* = 7.4 Hz, 1H), 7.86 (d, *J* = 2.0 Hz, 1H). ^{13}C NMR ($CDCl_3$): δ = -4.70, 109.85, 112.33, 118.95, 123.66, 128.51, 133.21, 136.48, 138.16, 138.63, 148.31, 153.30. HRMS (EI): *m*/*z* [M^+]: calcd for $C_{16}H_{13}NO_2Si$: 279.0716; found 279.0737.



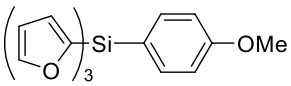
(4-Trifluoromethylphenyl)di(2-furyl)(methyl)silane (3f). ^{1}H NMR ($CDCl_3$): δ = 0.83 (s, 3H), 6.45 (dd, *J* = 3.3, 1.7 Hz, 2H), 6.81 (d, *J* = 3.3 Hz, 2H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.73 (d, *J* = 8.3 Hz, 2H), 7.75 (d, *J* = 1.7 Hz, 2H). ^{13}C NMR ($CDCl_3$): δ = -4.72, 109.81, 123.5, 124.19 (q, *J* = 225 Hz), 124.51 (q, *J* = 4 Hz), 131.85 (q, *J* = 26 Hz), 135.00, 139.12, 148.14, 153.94. HRMS (EI): *m*/*z* [M^+]: calcd for $C_{16}H_{13}F_3O_2Si$: 322.0637; found 322.0587.



(2-Methoxyphenyl)di(2-furyl)(methyl)silane (3g). ^{1}H NMR ($CDCl_3$): δ = 0.82 (s, 3H), 3.74 (s, 3H), 6.42 (dd, *J* = 3.3, 1.3 Hz, 2H), 6.77 (d, *J* = 3.3 Hz, 2H), 6.85 (d, *J* = 8.3 Hz, 1H), 6.92 (t, *J* = 7.0 Hz, 1H), 7.29 (d, *J* = 7.2 Hz, 1H), 7.38 (t, *J* = 7.7 Hz, 1H), 7.70 (d, *J* = 1.3 Hz, 2H). ^{13}C NMR ($CDCl_3$): δ = -4.07, 55.19, 109.56, 120.71, 122.33, 123.18, 129.47, 131.95, 136.61, 147.21, 155.67, 164.53. HRMS (EI): *m*/*z* [M^+]: calcd for $C_{16}H_{16}O_3Si$: 284.0868; found 284.0889.



(4-Methoxyphenyl)(2-furyl)dimethylsilane (4-OMe). ^{1}H NMR ($CDCl_3$): δ = 0.54 (s, 6H), 3.77 (s, 3H), 6.40 (dd, *J* = 3.5, 1.7 Hz, 1H), 6.68 (d, *J* = 9.2 Hz, 2H), 6.72 (d, *J* = 3.5 Hz, 1H), 7.55 (d, *J* = 9.0 Hz, 2H), 7.68 (d, *J* = 1.7 Hz, 1H). ^{13}C NMR ($CDCl_3$): δ = -3.36, 55.28, 109.52, 116.33, 121.25, 127.71, 138.17, 147.23, 156.67, 159.43. HRMS (EI): *m*/*z* [M^+]: calcd for $C_{13}H_{16}O_2Si$ 232.0920; found 232.0914.



(4-Methoxyphenyl)tri(2-furyl)silane (4-OMe). ^{1}H NMR ($CDCl_3$): δ = 3.82 (s, 3H), 6.46 (dd, *J* = 3.3, 1.7 Hz, 3H), 6.87 (d, *J* = 3.3 Hz, 3H), 6.95 (d, *J* = 8.8 Hz, 2H), 7.62 (d, *J* = 8.6 Hz, 2H), 7.77 (d, *J* = 1.7 Hz, 3H). ^{13}C NMR ($CDCl_3$): δ = 55.02, 109.79, 113.91, 124.64, 125.05, 137.03, 148.36, 152.54, 161.54. HRMS (EI): *m*/*z* [M^+]: calcd for $C_{19}H_{16}O_4Si$: 336.0818; found 336.0793.

Computational Details.

All calculations were performed using Gaussian 03 and 09 program suite.[1] Geometries were fully optimized at the PBE0[2]/def2-SVP[3] level. Frequency calculations were performed at this level of theory to identify the optimized stationary points (minima or transition states) and to estimate thermodynamic corrections at 298 K and 1 atm. The electronic energies were then improved by the PBE0/def2-TZVPP[3] single-point calculations, which took the solvent effects of DMF into account by using the SMD solvation model[4]. Gibbs energies in solution can be obtained from adding the gas-phase Gibbs energy corrections of the solute (the PBE0/def2-SVP level) to the single-point energies (the PBE0/def2-TZVPP level).

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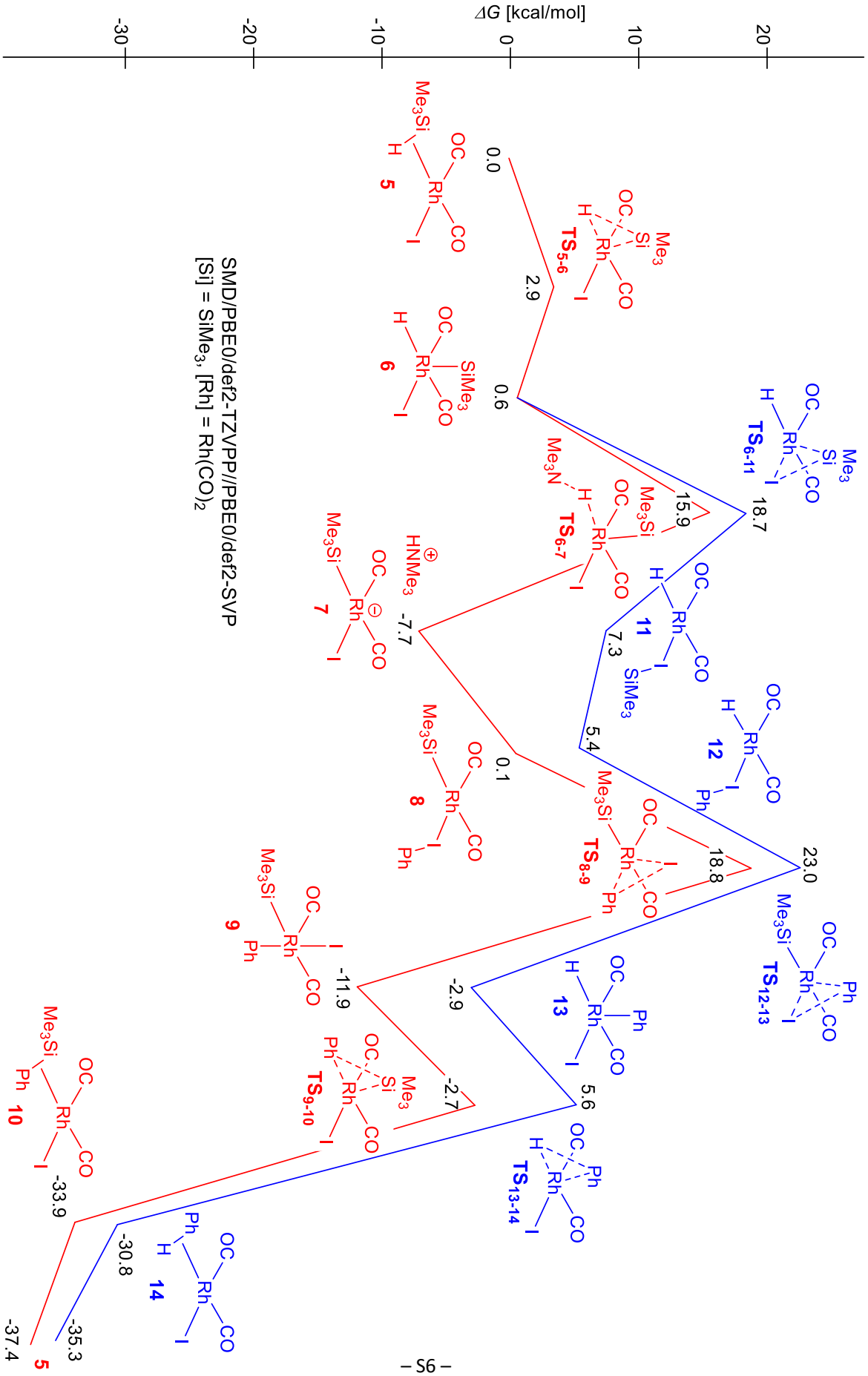
1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, Revision A.02; Gaussian, Inc.: Wallingford, CT, 2009.
2. (a) Perdew, J. P.; Burke, K.; Ernzerhof, M. *Phys. Rev. Lett.* **1996**, *77*, 3865; (b) Adamo, C.; Barone, V. *J. Chem. Phys.* **1999**, *110*, 6158.
3. Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.
4. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378.

Reaction Pathway with Calculated Relative Free Energies.



Cartesian Coordinates

5

Rh	-0.19358	0.84969	-0.15934
C	1.18315	2.00348	0.36502
C	-1.44737	2.21093	-0.28625
O	-2.21408	3.05453	-0.37607
O	2.01753	2.71230	0.67388
I	1.63245	-1.06942	-0.08098
Si	-2.21760	-1.08413	0.14421
C	-3.91229	-0.37188	-0.22907
C	-1.99547	-2.78560	-0.59721
C	-1.84471	-1.04694	1.97787
H	-1.29199	-0.26840	-0.87772
H	-0.84485	-1.44988	2.19292
H	-1.91515	-0.03523	2.40261
H	-2.59601	-1.68219	2.47974
H	-4.02550	0.65063	0.16151
H	-4.11138	-0.35184	-1.31151
H	-4.68611	-0.99887	0.24346
H	-2.27615	-2.79709	-1.66118
H	-0.94782	-3.11030	-0.50929
H	-2.63266	-3.51003	-0.06441

TS_{5-6}

Rh	-0.48975	-0.64077	-0.35194
C	-0.00836	-1.85642	1.14370
C	-2.15395	-1.35976	-0.75486
O	-3.15592	-1.81954	-1.04982
O	0.25185	-2.47964	2.05411
I	1.94746	0.35444	-0.18261
Si	-1.50497	1.41964	0.37926
C	-3.36537	1.37859	0.08080
C	-1.16600	1.40752	2.23199
C	-0.83194	2.99529	-0.38932
H	-0.79036	0.47897	-1.43886
H	-3.61097	1.33017	-0.99104
H	-3.86370	0.54047	0.59038
H	-3.79398	2.31410	0.47920
H	0.26033	3.06242	-0.28933
H	-1.08520	3.06251	-1.45831
H	-1.28798	3.85805	0.12563
H	-1.57205	0.51051	2.72332
H	-0.08679	1.46295	2.43591
H	-1.65269	2.29096	2.68164

6

Rh	-0.48365	-0.65710	-0.34614
C	-0.22787	-1.56784	1.41667
C	-2.14451	-1.32423	-0.83890
O	-3.14062	-1.74950	-1.19790
O	-0.08469	-2.02493	2.44393
I	1.97893	0.26637	-0.18759
Si	-1.47562	1.41876	0.33022
C	-3.35519	1.30970	0.23851
C	-0.96988	1.67212	2.12521
C	-0.90652	2.85659	-0.73270
H	-0.58275	0.18231	-1.67675
H	-3.71766	1.16825	-0.79082
H	-3.76393	0.50371	0.86660
H	-3.76791	2.26403	0.60901
H	0.18900	2.94553	-0.73351
H	-1.24491	2.74260	-1.77349
H	-1.33897	3.78895	-0.33056
H	-1.32727	0.86237	2.77940
H	0.12258	1.74781	2.22402
H	-1.42091	2.61445	2.48263

TS_{6-7}

Rh	-0.43042	0.27686	-0.66710
C	-1.95109	-0.74400	-1.47203
C	-0.58317	2.03194	-1.15721
O	-0.69099	3.11955	-1.52433
O	-2.84003	-1.18931	-2.02704

I	0.84987	-1.90454	0.26123
Si	-1.70412	0.84675	1.23972
C	-3.04053	2.12367	0.85253
C	-2.55711	-0.71591	1.85639
C	-0.60695	1.52258	2.61569
H	1.09999	1.06181	-0.08807
N	2.46291	1.54122	0.10878
C	2.96043	1.09092	1.40279
C	3.21000	0.95665	-0.99707
C	2.39955	2.99174	0.02117
H	-2.62323	3.10557	0.58344
H	-3.69131	1.79297	0.02820
H	-3.67371	2.25805	1.74631
H	-3.24587	-1.13635	1.10817
H	-1.82594	-1.49213	2.12339
H	-3.14862	-0.45837	2.75252
H	-0.11338	2.46243	2.32583
H	-1.22893	1.72838	3.50397
H	0.15982	0.78551	2.89577
H	1.98131	3.29092	-0.94931
H	1.74669	3.38339	0.81415
H	3.40087	3.44680	0.13037
H	3.17314	-0.13852	-0.91768
H	2.74535	1.25056	-1.94981
H	4.26225	1.29482	-0.99416
H	2.34228	1.51814	2.20332
H	2.88987	-0.00365	1.45497
H	4.00947	1.40633	1.55586

7

Rh	0.33668	0.83343	0.00000
C	-0.87714	2.31189	-0.00025
C	1.89871	1.74322	-0.00018
O	2.87004	2.37508	-0.00031
O	-1.55574	3.23857	-0.00054
I	-1.77009	-0.90006	0.00013
Si	1.85126	-1.10187	0.00003
C	3.74272	-0.78636	-0.00015
C	1.58192	-2.19974	1.53544
C	1.58171	-2.19995	-1.53519
H	0.53129	-2.52333	-1.59380
H	1.81590	-1.64406	-2.45782
H	2.23153	-3.09264	-1.49708
H	1.81624	-1.64375	2.45797
H	0.53151	-2.52313	1.59424
H	2.23172	-3.09245	1.49733
H	4.06096	-0.21444	-0.88718
H	4.06112	-0.21440	0.88679
H	4.29025	-1.74575	-0.00018

8

Rh	-0.97155	0.83734	-0.06141
C	0.32878	2.24101	-0.24373
C	-2.44850	1.90553	-0.08271
O	-3.34529	2.62469	-0.09291
O	1.01192	3.14522	-0.39001
I	0.71327	-1.21610	0.07595
Si	-2.87692	-0.77580	0.03652
C	-3.94423	-0.51642	1.58145
C	-3.98477	-0.62052	-1.49372
C	-2.35556	-2.60988	0.09000
C	2.68422	-0.43200	0.06415
C	3.05506	0.51694	1.01382
C	3.58551	-0.90434	-0.88740
C	4.88861	-0.40564	-0.88571
C	4.36079	1.00708	0.99963
C	5.27635	0.54805	0.05369
H	3.28118	-1.64655	-1.62827
H	5.60161	-0.76612	-1.63111
H	2.33837	0.87584	1.75551
H	4.66014	1.75450	1.73820
H	6.29710	0.93692	0.04813
H	-3.34585	-0.61886	2.50062
H	-4.40777	0.48194	1.59435
H	-4.75175	-1.26712	1.61661
H	-1.78694	-2.92199	-0.80110

H	-1.77216	-2.86807	0.98887
H	-3.27368	-3.22191	0.11678
H	-4.45406	0.37310	-1.55858
H	-3.40833	-0.77860	-2.41901
H	-4.78878	-1.37514	-1.46119

TS_{8-9}

Rh	-0.41245	0.38637	0.74437
C	0.40512	0.19729	2.52977
C	-0.95844	2.13973	0.85949
O	-1.17629	3.26264	0.94379
O	0.64012	0.12319	3.64338
I	0.57849	-1.86504	-0.29718
Si	-2.34190	0.33574	-0.77699
C	-3.45001	1.87142	-0.87100
C	-2.04641	-0.15700	-2.58435
C	-3.37503	-1.02812	0.04546
C	1.44375	0.28887	-0.54997
C	2.60488	0.54309	0.19569
C	1.24743	0.90068	-1.79424
C	2.15939	1.86307	-2.22619
C	3.50408	1.50584	-0.25641
C	3.28143	2.17604	-1.45992
H	0.38812	0.64080	-2.41037
H	1.98682	2.36508	-3.18151
H	2.79814	0.00088	1.12256
H	4.39443	1.72203	0.33935
H	3.99525	2.92434	-1.81122
H	-2.87431	-2.00642	-0.01032
H	-3.57061	-0.80770	1.10641
H	-4.34917	-1.10671	-0.46841
H	-1.65791	0.68571	-3.17799
H	-1.36619	-1.01403	-2.69905
H	-3.01861	-0.43910	-3.02360
H	-3.80465	2.19151	0.12083
H	-2.93739	2.72800	-1.33595
H	-4.33572	1.63706	-1.48539

9

Rh	0.15233	-0.29411	0.22528
C	0.13268	-2.28959	0.38476
C	0.29039	0.62196	1.76275
O	0.36307	1.07785	2.81451
O	0.11396	-3.39547	0.62730
I	-2.48362	-0.45866	-0.32814
Si	0.15062	2.14887	-0.31444
C	1.76204	3.00343	0.14403
C	0.04099	1.96279	-2.18531
C	-1.28925	3.12896	0.37780
C	2.17575	-0.39593	0.01168
C	2.54112	-0.73964	-1.29566
C	3.18042	-0.16515	0.95533
C	4.52529	-0.24627	0.58528
C	3.88572	-0.80982	-1.66633
C	4.88281	-0.56085	-0.72429
H	2.93262	0.08742	1.98903
H	5.29990	-0.05880	1.33376
H	1.77545	-0.96439	-2.04958
H	4.15027	-1.07196	-2.69412
H	5.93583	-0.62186	-1.00887
H	0.87704	1.37830	-2.59633
H	-0.90998	1.50638	-2.49323
H	0.10199	2.97992	-2.61235
H	-2.24929	2.63886	0.16204
H	-1.20067	3.26301	1.46663
H	-1.29172	4.12968	-0.08607
H	1.88179	3.10753	1.23322
H	2.63829	2.46896	-0.25059
H	1.75142	4.01830	-0.28853

TS_{9-10}

Rh	-0.04003	0.35652	0.75487
C	-1.15687	-0.40149	2.31649
C	1.01460	1.43888	1.80411
O	1.58624	2.17269	2.46885
O	-1.71422	-0.92461	3.15021
I	-2.06113	-0.65434	-0.71372

Si	0.75466	1.56595	-1.22237
C	2.39327	2.48170	-1.00634
C	0.82953	0.65687	-2.86349
C	-0.60595	2.88529	-1.26112
C	1.62357	-0.65348	0.10162
C	1.39890	-1.81763	-0.65269
C	2.92673	-0.40131	0.55593
C	3.96465	-1.29719	0.29373
C	2.44226	-2.70893	-0.90705
C	3.72915	-2.45779	-0.43745
H	3.16394	0.49821	1.12539
H	4.96622	-1.07512	0.67144
H	0.40740	-2.03975	-1.04436
H	2.23380	-3.61096	-1.48852
H	4.54195	-3.15811	-0.64329
H	2.46041	3.05187	-0.06726
H	3.26064	1.80970	-1.07190
H	2.47038	3.20749	-1.83399
H	1.71229	0.00386	-2.91923
H	-0.07014	0.05197	-3.04351
H	0.90610	1.41030	-3.66581
H	-1.58339	2.45057	-1.51418
H	-0.70363	3.42629	-0.30699
H	-0.33515	3.62471	-2.03554

10

Rh	0.57324	0.76210	0.24285
C	1.81121	1.09397	1.56314
C	-0.51329	2.14970	0.83005
O	-1.14851	3.00813	1.23681
O	2.56317	1.32052	2.39005
I	2.26225	-1.20086	-0.40913
Si	-3.25662	-1.22352	0.54617
C	-2.73570	-0.78725	2.30118
C	-5.12316	-1.06423	0.36484
C	-2.69743	-2.96552	0.11420
C	-2.41207	0.00560	-0.63932
C	-1.11942	-0.26796	-1.16277
C	-3.01811	1.20417	-1.02157
C	-2.37351	2.12285	-1.86473
C	-0.45973	0.65455	-1.99694
C	-1.09650	1.86451	-2.33859
H	-4.02197	1.44556	-0.66016
H	-2.88108	3.04992	-2.14266
H	-0.67035	-1.25463	-1.01881
H	0.48804	0.37981	-2.46767
H	-0.59240	2.57516	-2.99731
H	-5.48307	-0.06745	0.66503
H	-5.44872	-1.24856	-0.67090
H	-5.62675	-1.80055	1.01158
H	-2.94474	-3.22390	-0.92737
H	-1.61154	-3.09171	0.25002
H	-3.19682	-3.69674	0.76987
H	-1.64135	-0.85643	2.40807
H	-3.03619	0.24044	2.55969
H	-3.19601	-1.47059	3.03275

$TS_{6\text{-}11}$

Rh	-1.10104	-0.25476	-0.30775
C	-1.48836	-0.96462	1.47587
C	-2.68896	0.60294	-0.66390
O	-3.64829	1.17395	-0.91538
O	-1.76843	-1.39796	2.49084
I	1.46568	-0.91941	-0.28844
Si	0.79606	1.66886	0.36325
C	-0.14082	2.01079	1.95976
C	2.60484	2.03747	0.76462
C	0.34633	2.76569	-1.09188
H	-0.84893	0.24602	-1.80105
H	-1.22834	2.06334	1.81979
H	0.08178	1.24924	2.72251
H	0.21768	2.98141	2.34611
H	0.78558	2.37185	-2.02039
H	-0.73770	2.85838	-1.23603
H	0.77630	3.76531	-0.90604
H	2.97971	1.41990	1.59444

H	3.25785	1.88063	-0.10675
H	2.67942	3.09771	1.06476

11

Rh	1.60569	-0.01491	-0.00013
C	1.20361	1.85604	-0.00004
C	3.42783	0.10845	-0.00037
O	4.57217	0.15372	-0.00051
O	1.03106	2.98841	-0.00010
I	-0.84899	-1.12233	0.00009
H	2.06775	-1.56729	-0.00029
Si	-2.56089	0.74382	0.00020
C	-2.29198	1.73860	1.55867
C	-2.29222	1.73856	-1.55834
C	-4.20498	-0.15056	0.00035
H	-1.30483	2.22280	-1.56690
H	-2.38026	1.10827	-2.45564
H	-3.05863	2.52993	-1.61631
H	-4.31924	-0.78380	-0.89232
H	-4.31911	-0.78373	0.89309
H	-5.02313	0.58910	0.00039
H	-2.37979	1.10833	2.45600
H	-1.30462	2.22293	1.56703
H	-3.05844	2.52992	1.61678

12

Rh	-1.71483	0.16825	-0.03942
C	-1.04335	1.95565	-0.24476
C	-3.50315	0.56740	-0.08151
O	-4.62704	0.78161	-0.10322
O	-0.69705	3.03488	-0.38538
I	0.47376	-1.29897	0.11960
H	-2.37356	-1.30876	0.09302
C	2.19562	-0.06162	0.04946
C	2.25593	1.08033	0.84397
C	3.24974	-0.42932	-0.78374
C	4.38989	0.37426	-0.81966
C	3.40134	1.87459	0.79261
C	4.46654	1.52392	-0.03564
H	3.18823	-1.32534	-1.40488
H	5.22069	0.09632	-1.47269
H	1.42379	1.35378	1.49603
H	3.45666	2.77462	1.40959
H	5.36041	2.15075	-0.07105

$TS_{12\text{-}13}$

Rh	-0.92594	0.65937	-0.26692
C	-1.52303	0.78627	1.59936
C	-1.21369	2.40902	-0.81497
O	-1.33198	3.48240	-1.18787
O	-1.96524	0.88923	2.64388
I	-0.07633	-1.84287	-0.18335
H	-0.67904	0.57734	-1.83834
C	1.24601	0.06439	0.05316
C	1.68258	0.33152	1.35823
C	2.04397	0.39774	-1.05067
C	3.22857	1.09899	-0.84001
C	2.87059	1.03587	1.54539
C	3.64192	1.42771	0.45184
H	1.72983	0.12959	-2.05970
H	3.83568	1.38593	-1.70228
H	1.10085	-0.00256	2.21896
H	3.19731	1.26698	2.56235
H	4.57639	1.97153	0.60666

13

Rh	-0.00217	0.84495	-0.32913
C	-0.18266	1.29669	1.65755
C	1.15099	2.15420	-0.98725
O	1.84486	2.93190	-1.44443
O	-0.31732	1.50130	2.76158
I	-1.96678	-0.87481	-0.02803
H	-0.01417	0.37206	-1.81661
C	1.64810	-0.29620	-0.08307
C	1.77317	-1.47634	-0.81912
C	2.62646	0.05857	0.84664

C	3.71963	-0.78544	1.06098
C	2.86873	-2.31192	-0.59169
C	3.84298	-1.97266	0.34508
H	2.55847	0.98934	1.41510
H	4.47781	-0.50078	1.79511
H	1.01865	-1.76170	-1.55232
H	2.95242	-3.24152	-1.16070
H	4.69813	-2.63110	0.51374

$TS_{13\text{-}14}$

Rh	0.01936	0.82052	-0.17523
C	-0.94175	1.54634	1.46868
C	1.08002	2.31940	-0.46921
O	1.68671	3.25703	-0.69802
O	-1.46233	1.85523	2.42389
I	-1.84569	-1.04846	-0.30607
H	0.60194	0.03642	-1.39748
C	1.75258	-0.28025	-0.06346
C	1.69254	-1.34786	0.84111
C	2.96612	0.02577	-0.68971
C	4.11845	-0.69554	-0.37375
C	2.85417	-2.05786	1.14955
C	4.06974	-1.73615	0.54946
H	3.03127	0.82335	-1.43182
H	5.05955	-0.43682	-0.86569
H	0.75143	-1.62883	1.31297
H	2.79473	-2.87912	1.86842
H	4.97225	-2.30106	0.79346

14

Rh	0.25321	0.57421	-0.00003
C	-0.86212	2.03723	0.00089
C	1.76642	1.65330	-0.00045
O	2.66458	2.35955	-0.00117
O	-1.53038	2.96099	0.00153
I	-2.04361	-0.78180	-0.00007
H	0.56367	-1.82136	-1.24686
C	1.43977	-1.45839	-0.70341
C	2.62055	-1.13022	-1.40147
C	1.44034	-1.45814	0.70450
C	2.62170	-1.12985	1.40149
C	3.78074	-0.83213	-0.70228
C	3.78132	-0.83199	0.70125
H	0.56463	-1.82078	1.24880
H	2.62181	-1.13949	2.49372
H	2.61975	-1.14017	-2.49370
H	4.69844	-0.59280	-1.24470
H	4.69947	-0.59257	1.24285