

Supplementary Information

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1. Characterization of the ligand precursor HSiN (1)

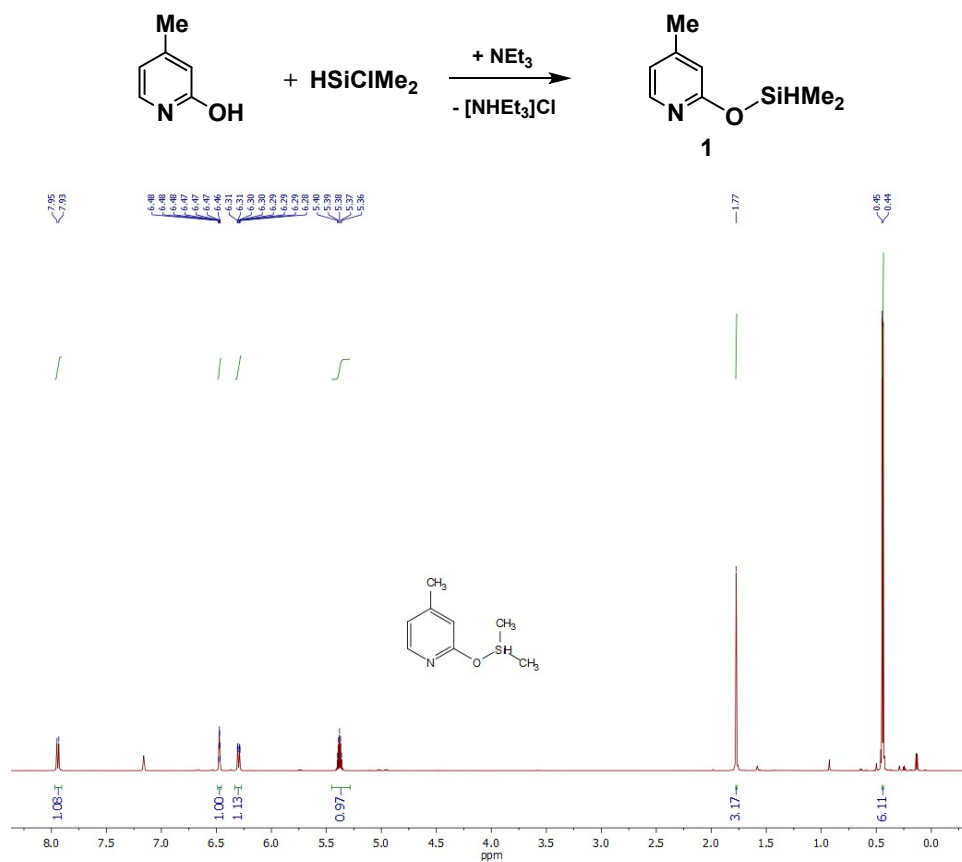


Figure S1. ^1H NMR spectrum of **1**

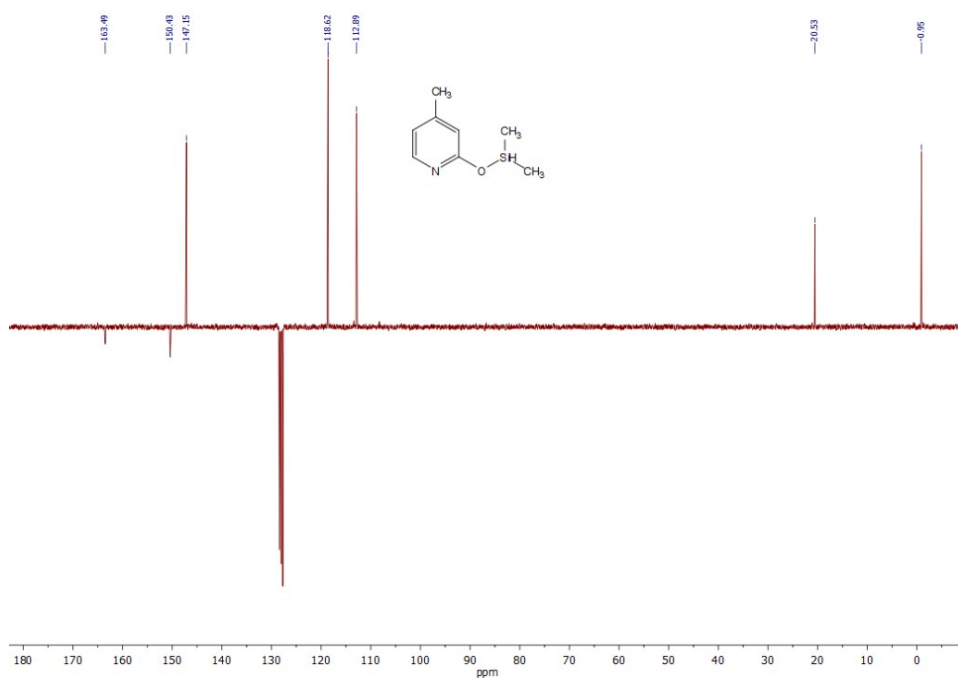


Figure S2. ^{13}C -APT NMR spectrum of **1**

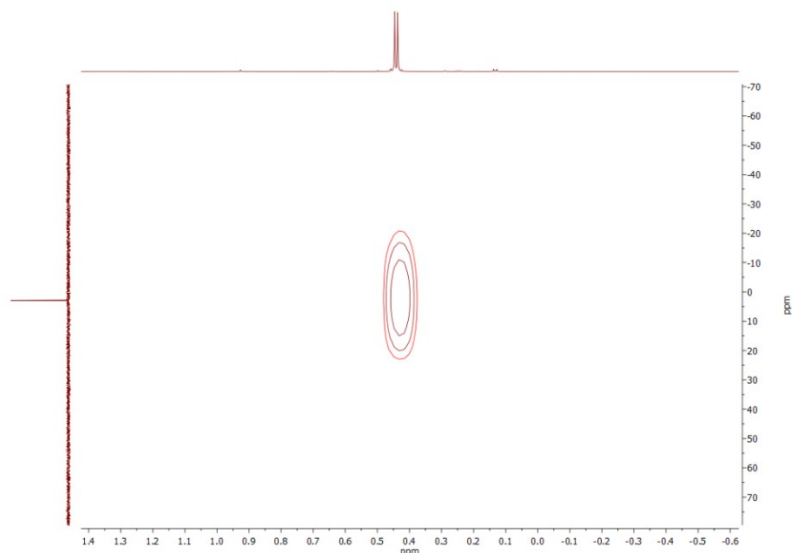


Figure S3. ^1H - ^{29}Si HMBC NMR spectrum of **1**

2. Characterization of complex $[\text{Ir}(\mu\text{-Cl})(\kappa^2\text{-NSi})_2]_2$ (**2**)

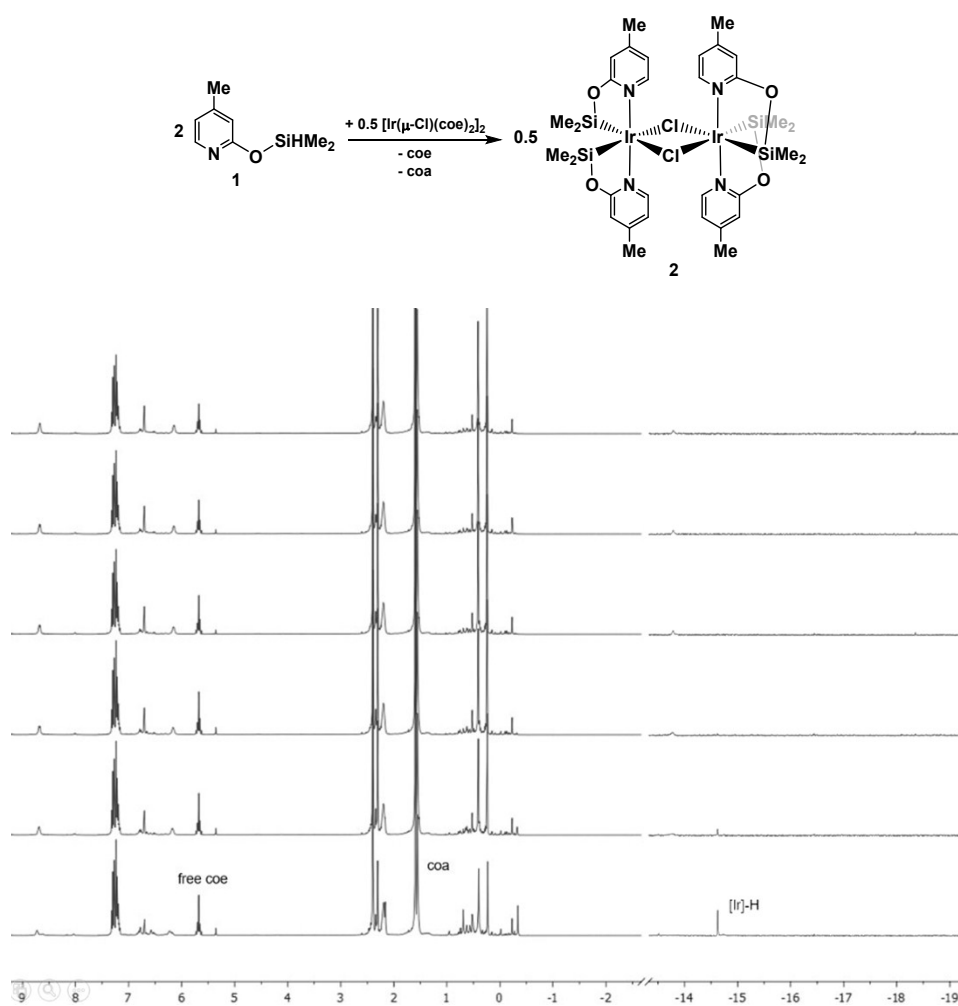


Figure S4. ^1H NMR spectra from the formation of **2**

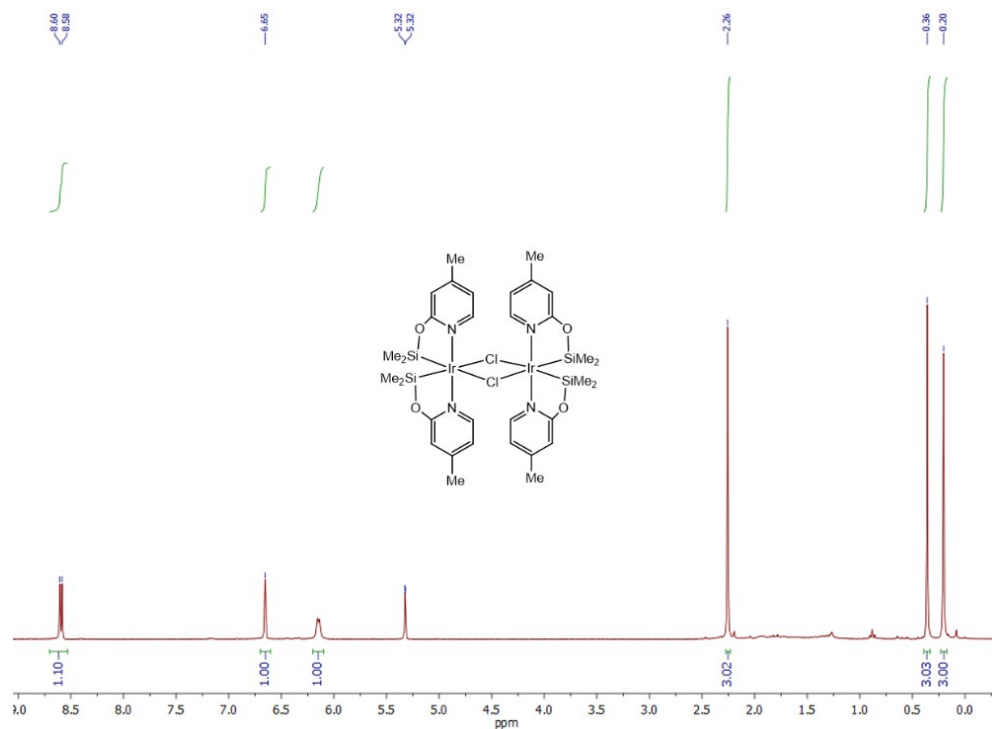


Figure S5. ^1H NMR spectrum of complex 2

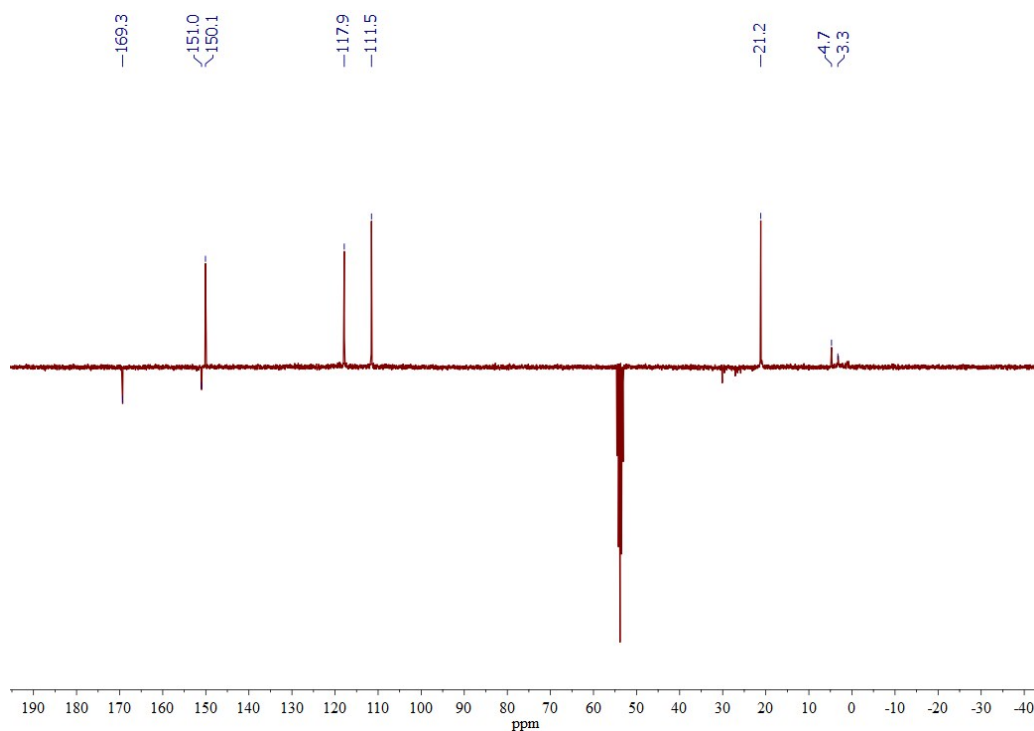


Figure S6. ^{13}C -APT NMR spectrum of complex 2

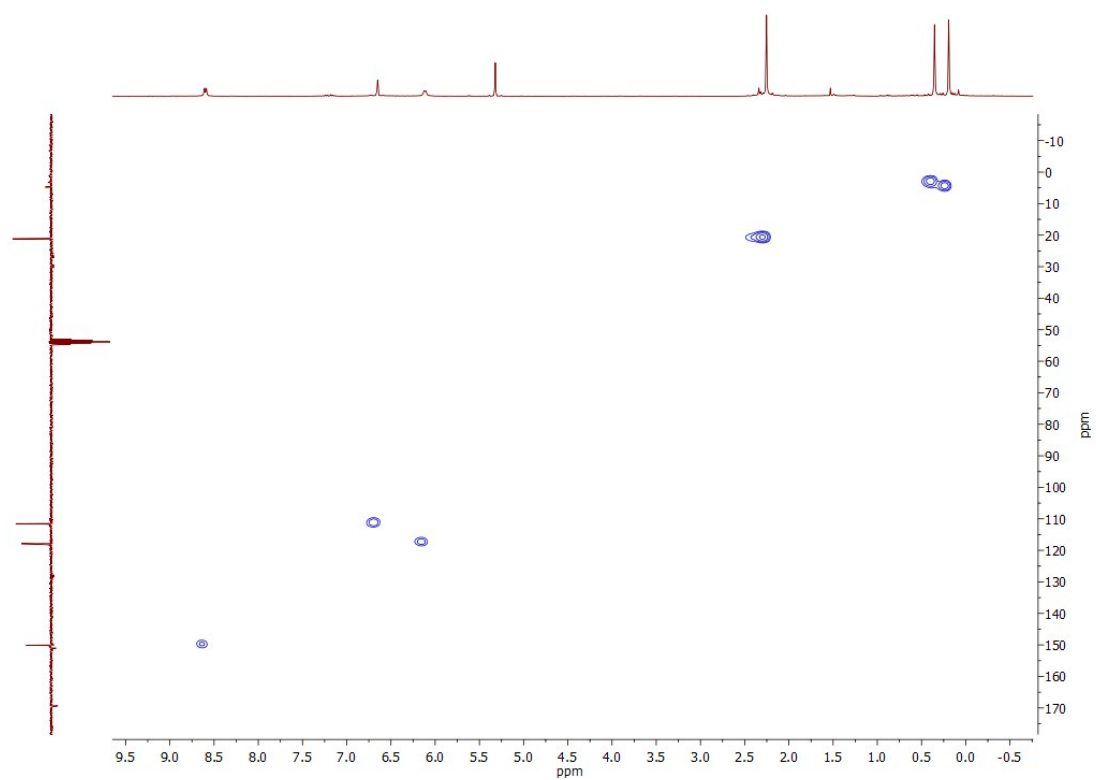


Figure S7. ^1H - ^{13}C HSQC NMR spectrum of complex **2**

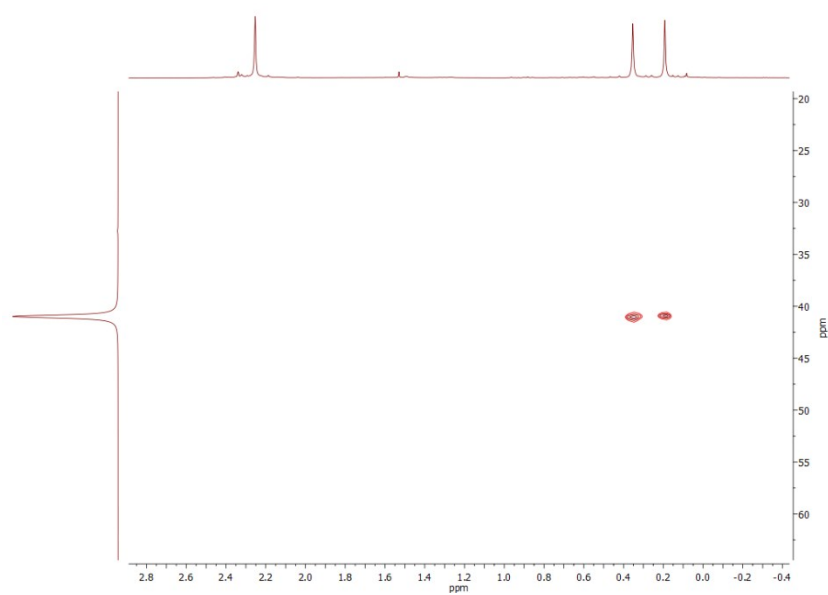


Figure S8. ^1H - ^{29}Si HMBC NMR spectrum of complex **2**

3. Characterization of complex $[\text{Ir}(\text{CF}_3\text{CO}_2)(\kappa^2\text{-NSi})_2]$ (**3**)

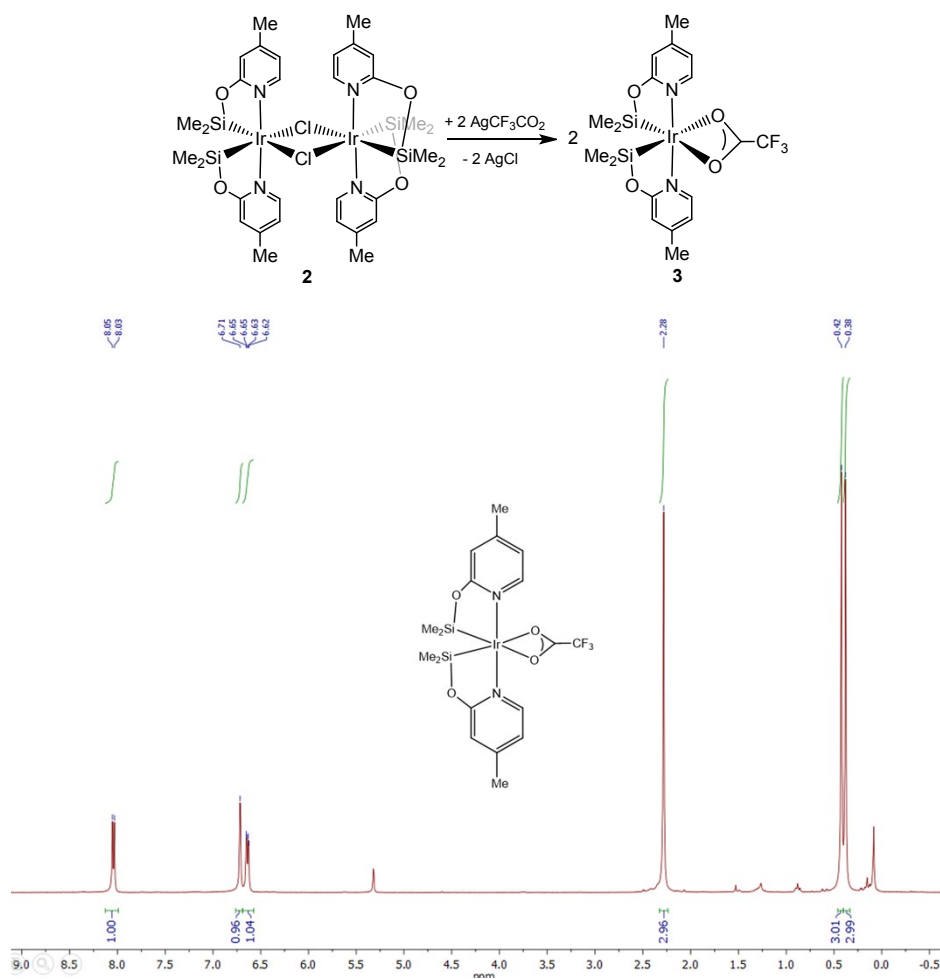


Figure S9. ^1H NMR spectrum of complex **3**

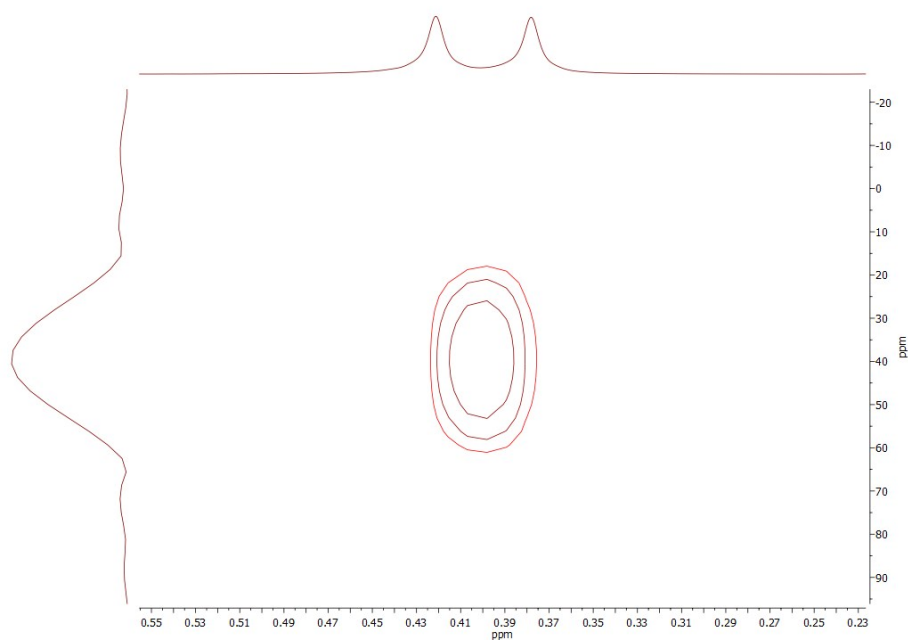


Figure S10. ^1H - ^{29}Si HMBC NMR spectrum of complex **3**

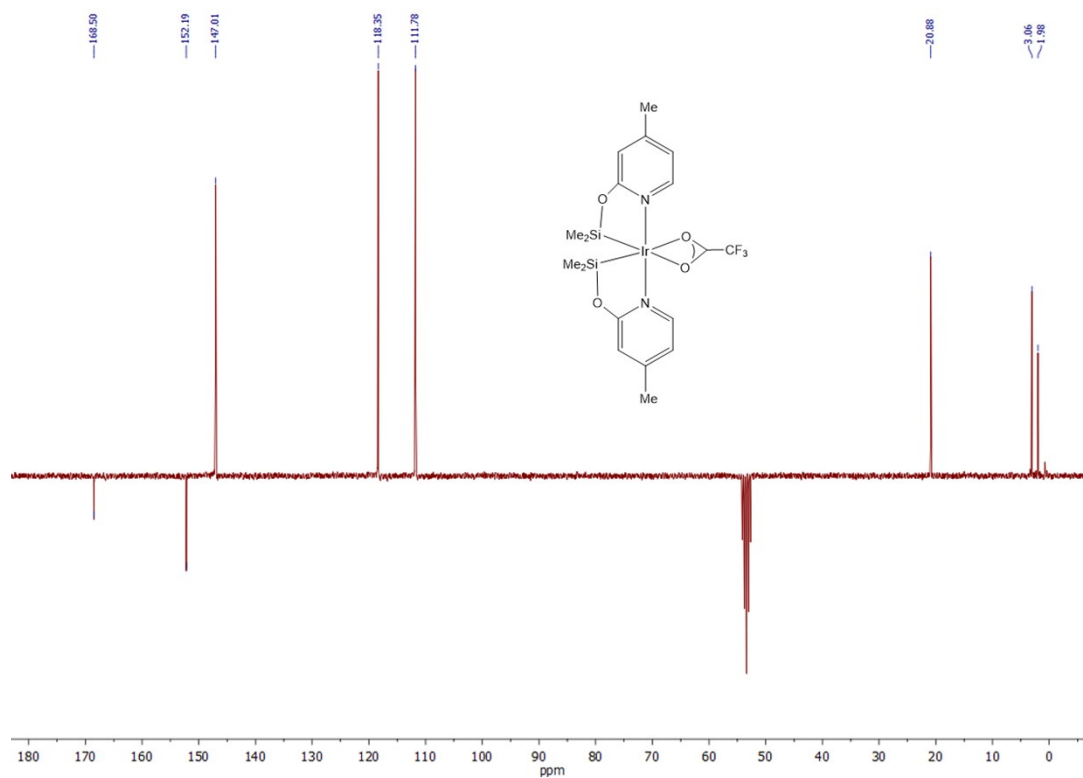


Figure S11. ¹³C-APT NMR spectrum of complex 3

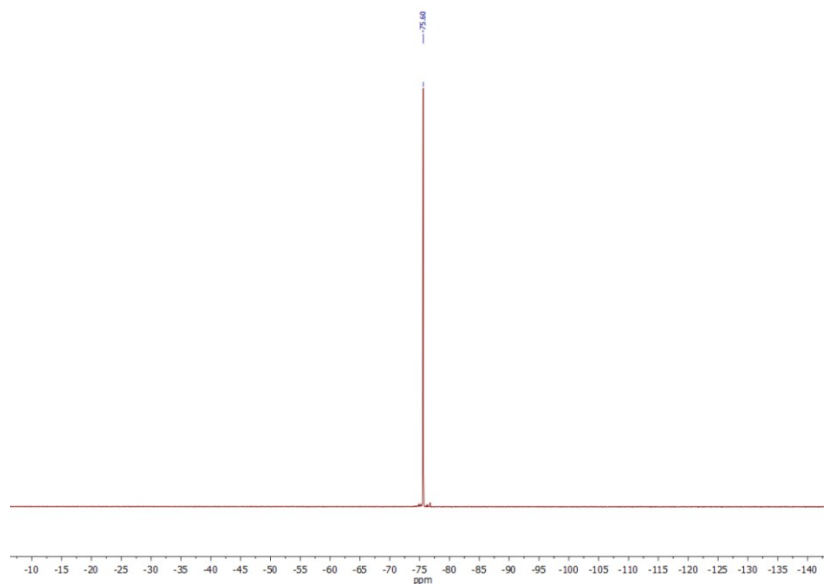
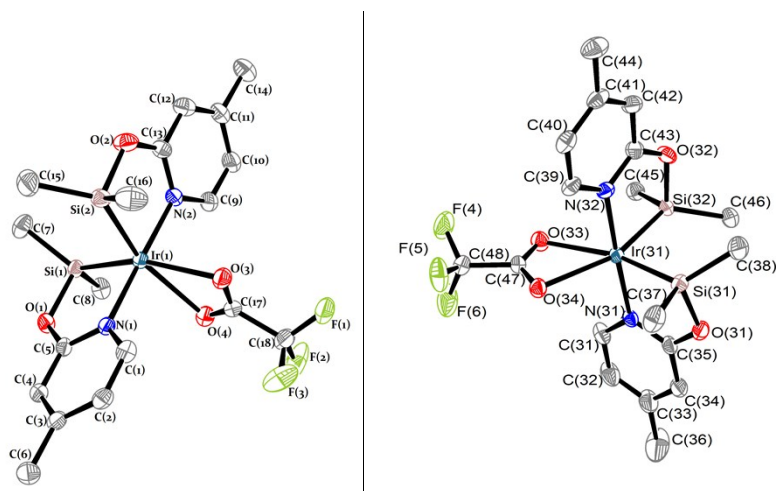


Figure S12. ¹⁹F NMR spectrum of complex 3

4. Selected X-ray details



Molecular scheme of both independent molecules of **3**

Selected bonds lengths (Å) and angles (°) for both independent molecules of complex **3**.

	Mole 1		Mole 2
Ir(1)-Si(1)	2.2645(10)	Ir(31)-Si(31)	2.2505(10)
Ir(1)-Si(2)	2.2505(11)	Ir(31)-Si(32)	2.2570(10)
Ir(1)-O(3)	2.363(3)	Ir(31)-O(33)	2.414(3)
Ir(1)-O(4)	2.418(3)	Ir(31)-O(34)	2.407(2)
Ir(1)-N(1)	2.052(3)	Ir(31)-N(31)	2.053(3)
Ir(1)-N(2)	2.056(3)	Ir(31)-N(32)	2.049(3)
Si(1)-Ir(1)-Si(2)	95.84(4)	Si(31)-Ir(31)-Si(32)	92.14(4)
Si(1)-Ir(1)-O(3)	159.28(7)	Si(31)-Ir(31)-O(33)	164.82(7)
Si(1)-Ir(1)-O(4)	104.53(7)	Si(31)-Ir(31)-O(34)	110.28(7)
Si(1)-Ir(1)-N(1)	82.22(8)	Si(31)-Ir(31)-N(31)	81.17(9)
Si(1)-Ir(1)-N(2)	99.02(9)	Si(31)-Ir(31)-N(32)	95.26(8)
Si(2)-Ir(1)-O(3)	104.47(7)	Si(32)-Ir(31)-O(33)	103.00(7)
Si(2)-Ir(1)-O(4)	159.54(7)	Si(32)-Ir(31)-O(34)	157.11(7)
Si(2)-Ir(1)-N(1)	97.71(9)	Si(32)-Ir(31)-N(31)	98.05(9)
Si(2)-Ir(1)-N(2)	82.24(9)	Si(32)-Ir(31)-N(32)	82.05(9)
O(3)-Ir(1)-O(4)	55.39(9)	O(33)-Ir(31)-O(34)	54.76(9)
O(3)-Ir(1)-N(1)	90.92(10)	O(33)-Ir(31)-N(31)	95.36(11)
O(3)-Ir(1)-N(2)	87.90(11)	O(33)-Ir(31)-N(32)	88.09(10)
O(4)-Ir(1)-N(1)	87.06(10)	O(34)-Ir(31)-N(31)	90.17(10)
O(4)-Ir(1)-N(2)	92.56(11)	O(34)-Ir(31)-N(32)	91.05(11)
N(1)-Ir(1)-N(2)	178.76(12)	N(31)-Ir(31)-N(32)	176.43(11)

Ring puckering parameters (Å,°) for Ir-Si-O-C-N metallacycles of complexes **2** and **3**.

		q	φ	conformation
Complex 2	Ir(1)-Si(1)-O(1)-C(5)-N(1)	0.050(4)	154(5)	⁵ T ₁ / ⁵ E
	Ir(1)-Si(2)-O(2)-C(13)-N(2)	0.154(3)	-148(2)	² E
	Ir(2)-Si(3)-O(3)-C(21)-N(3)	0.175(3)	-157(3)	² T ₁
Complex 3	Ir(2)-Si(1)-O(4)-C(29)-N(4)	0.120(3)	-164(2)°	² T ₁
	Ir(1)-Si(1)-O(1)-C(5)-N(1)	0.0212(1)	12.51(13)	¹ T ₂
	Ir(1)-Si(2)-O(2)-C(13)-N(2)	0.0700(1)	-141.93(5)	² E
	Ir(31)-Si(31)-O(31)-C(35)-N(31)	0.202(1)	-146.08(1)	² E
Ir(31)-Si(32)-O(32)-C(43)-N(32)	0.133(1)	-162.01(1)	² T ₁	

5. 3-Catalyzed (5 mol %) hydrosilylation of CO₂ (4 bar) at RT

a) Using HSiMe₂Ph as reductant.

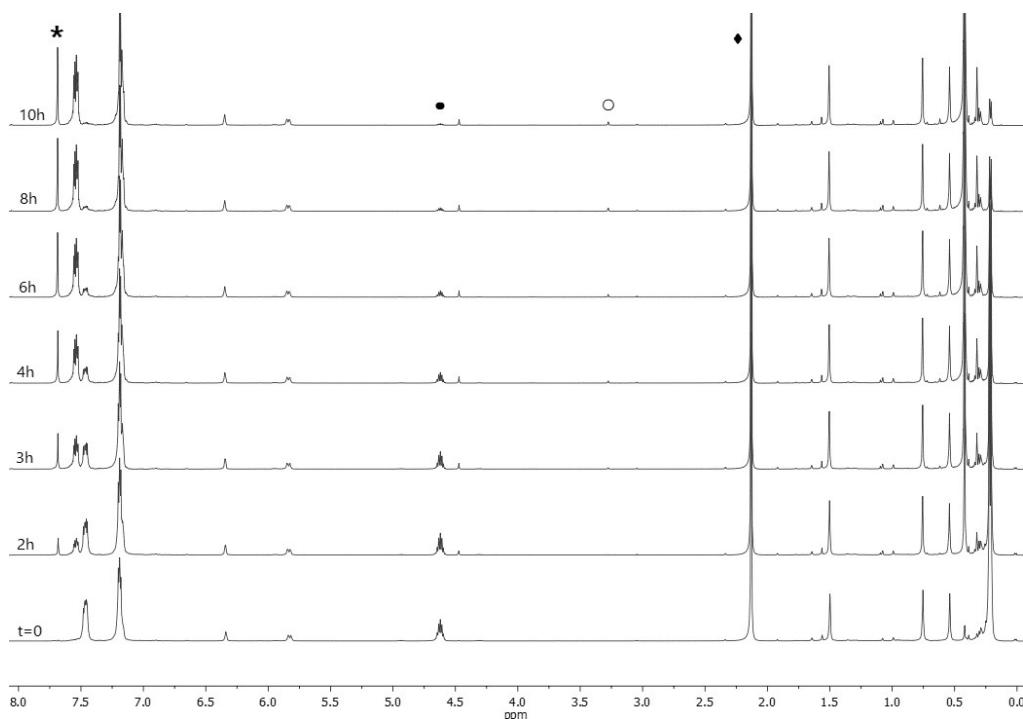


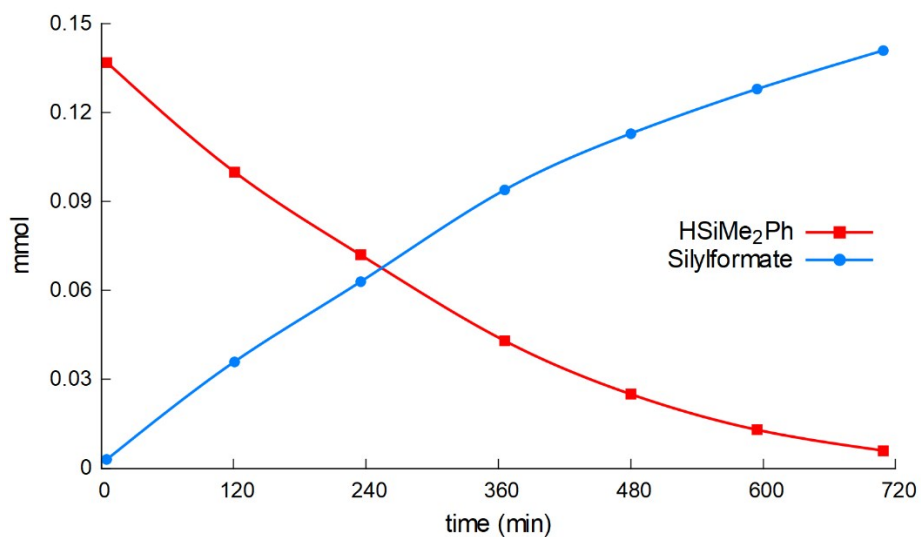
Figure S13. ¹H NMR spectra from the reaction of CO₂ with HSiMe₂Ph.

* Silylformate • Silane ○ Methoxysilane ♦ Hexamethylbenzene

time (min)	Integral (6H)	Silane (mmol)	Integral (6H)	Silylformate (mmol)
5	2.11	0.14	0.04	0.00
121	1.54	0.10	0.56	0.04
235	1.11	0.07	0.97	0.06
366	0.67	0.04	1.46	0.09
480	0.39	0.03	1.75	0.11
594	0.19	0.01	1.97	0.13
709	0.10	0.01	2.18	0.14

0.022 mmol of hexamethylbenzene added

Integrals are relative to that of the hexamethylbenzene signal, taken as one. Considering the number of protons responsible for each signal and the amount of mmol of C₆Me₆ added to the solution (which is about 0.018 mmol), the amount of mmol of the different molecules can be obtained.



b) Using HSiMePh₂ as reductant.

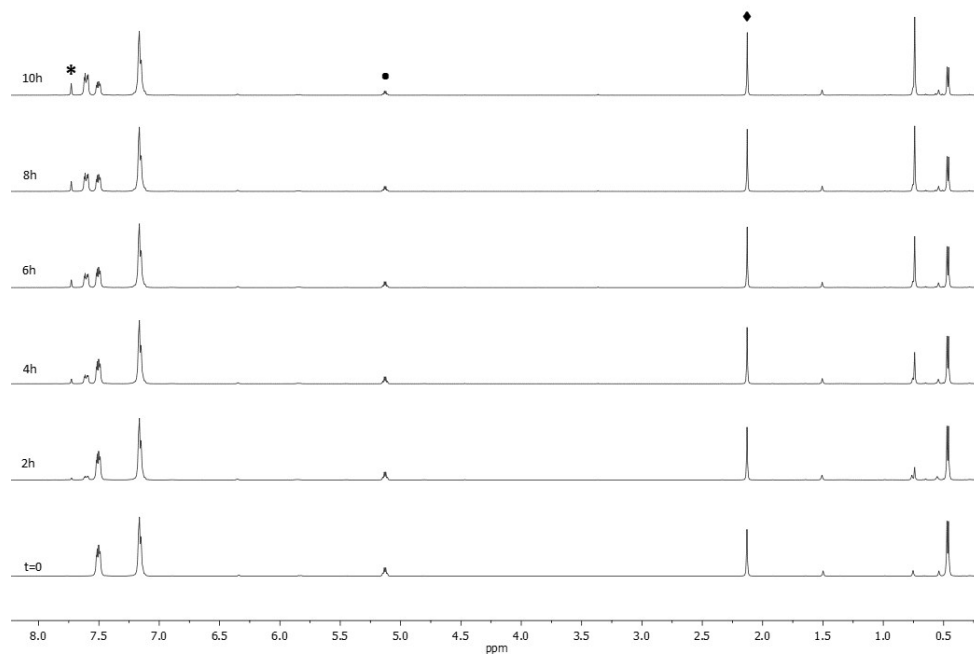
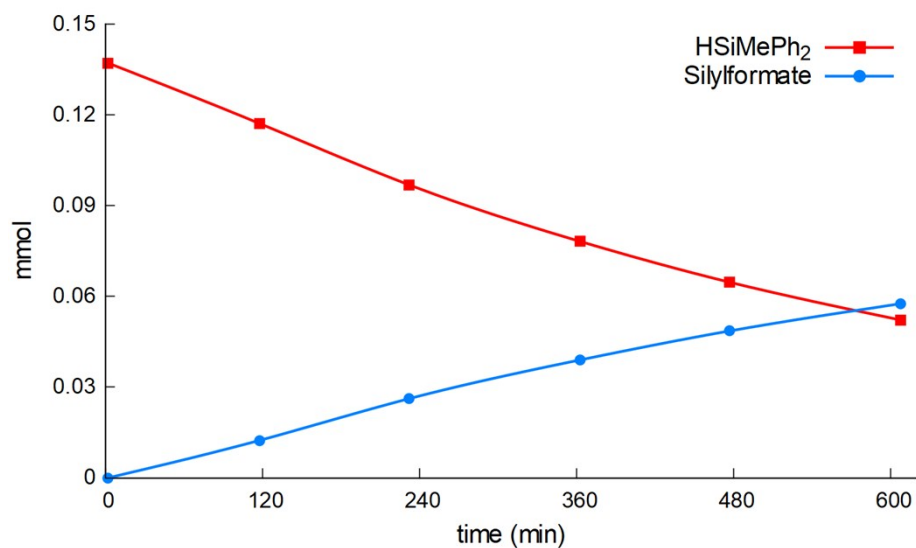


Figure S14. ¹H NMR spectra from the reaction of CO₂ with HSiMePh₂.
* Silylformate • Silane ♦ Hexamethylbenzene

time (min)	Integral (3H)	Silane (mmol)	Integral (3H)	Silylformate (mmol)
2	1.57	0.14	0.00	0.00
118	1.34	0.12	0.14	0.01
232	1.11	0.10	0.30	0.03
363	0.89	0.08	0.45	0.04
477	0.74	0.06	0.55	0.05
608	0.60	0.05	0.66	0.06

0.015 mmol of hexamethylbenzene added



c) Using HSiMe(OSiMe₃)₂ as reductant.

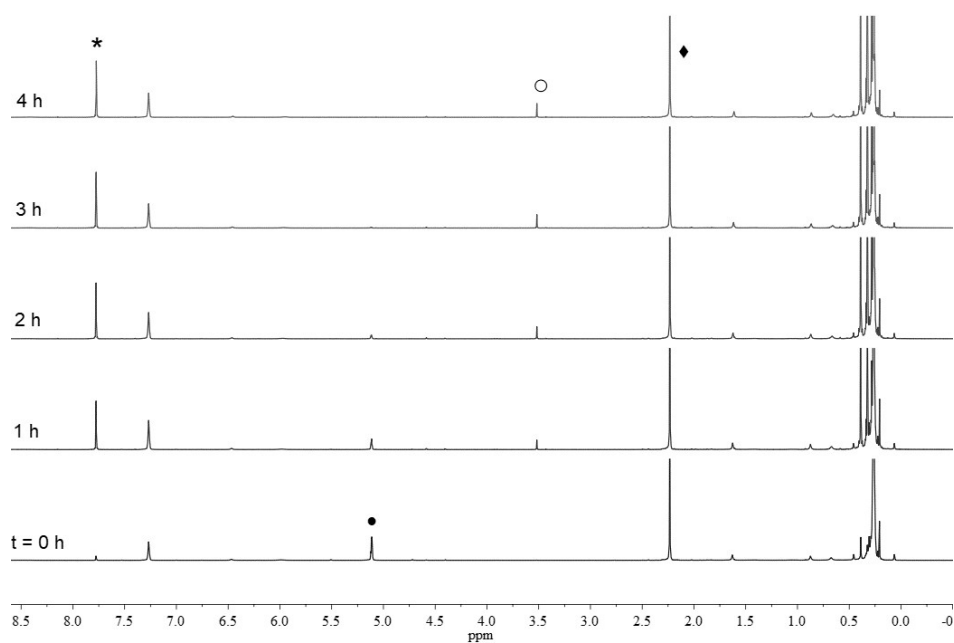
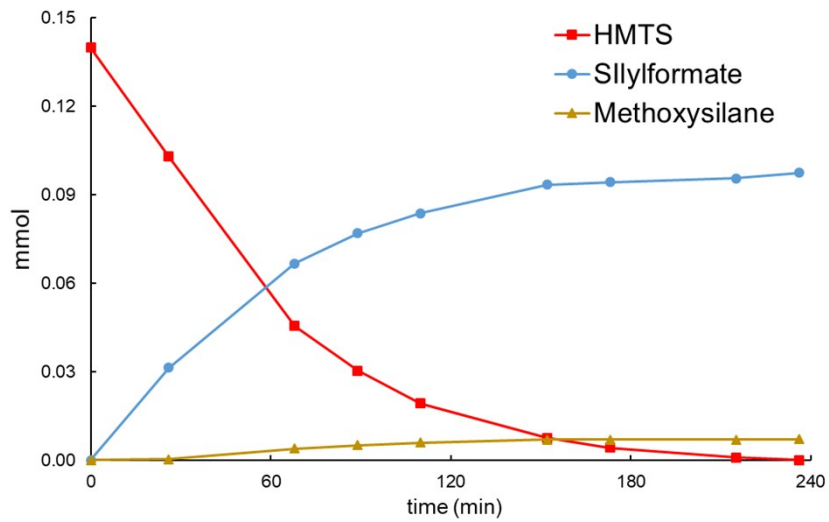


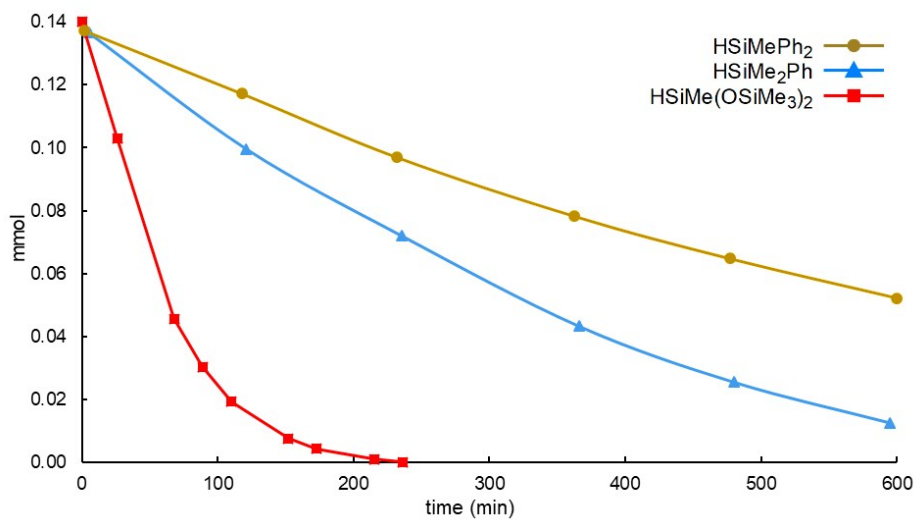
Figure S15. ¹H NMR spectra from the reaction of CO₂ with HSiMe(OSiMe₃)₂.
 * Silylformate • Silane ○ Methoxysilane ◆ Hexamethylbenzene

time (min)	Integral(1H)	Silane (mmol)	Integral(1H)	Silylformate (mmol)	Integral(3H)	Methoxysilane (mmol)
0	0.40	0.14	0.00	0.00	0.00	0.00
26	0.27	0.10	0.08	0.03	0.00	0.00
68	0.12	0.05	0.18	0.07	0.03	0.00
89	0.08	0.03	0.20	0.08	0.04	0.01
110	0.05	0.02	0.22	0.08	0.05	0.01
152	0.02	0.01	0.25	0.09	0.06	0.01
173	0.01	0.00	0.25	0.09	0.06	0.01
215	0.00	0.00	0.25	0.10	0.06	0.01
236	0.00	0.00	0.26	0.10	0.06	0.01

0.021 mmol of hexamethylbenzene added



d) 3-Catalyzed (5 mol %) hydrosilylation of CO₂ (4 bar) at RT



Variation of the concentration of the different silanes over time. HMTS = HSiMe(OSiMe₃)₂.

6. 3-Catalyzed (1 mol %) hydrosilylation of CO₂ (3 bar) at RT

a) Using HSiMe₂Ph as reductant.

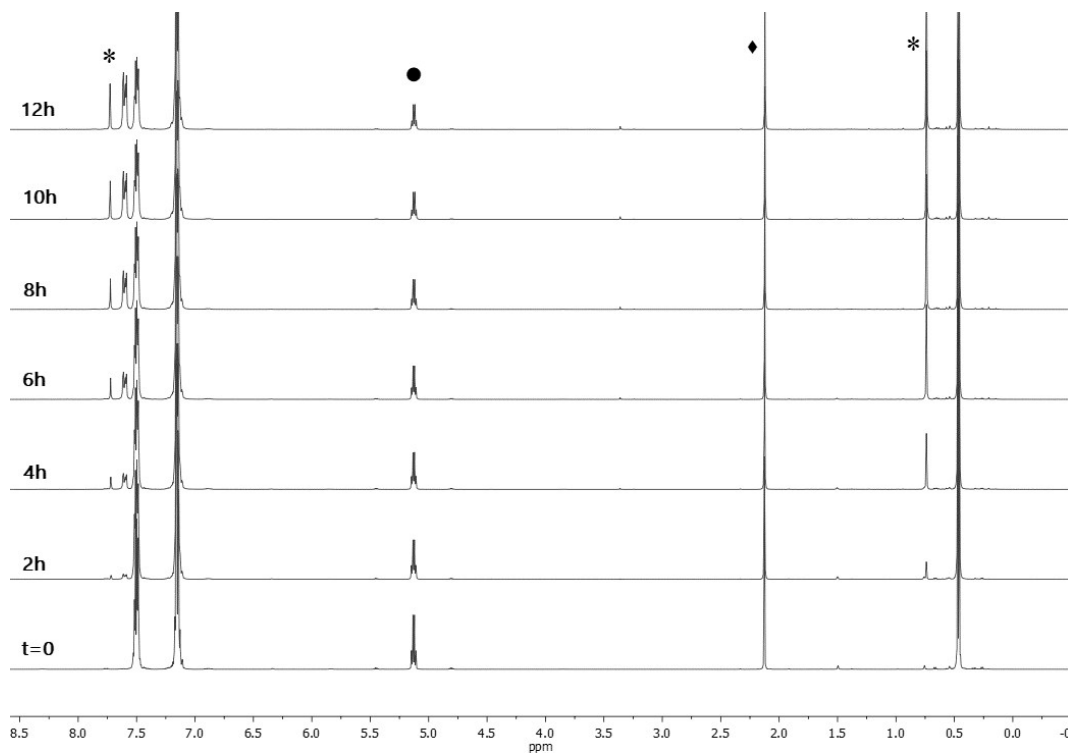
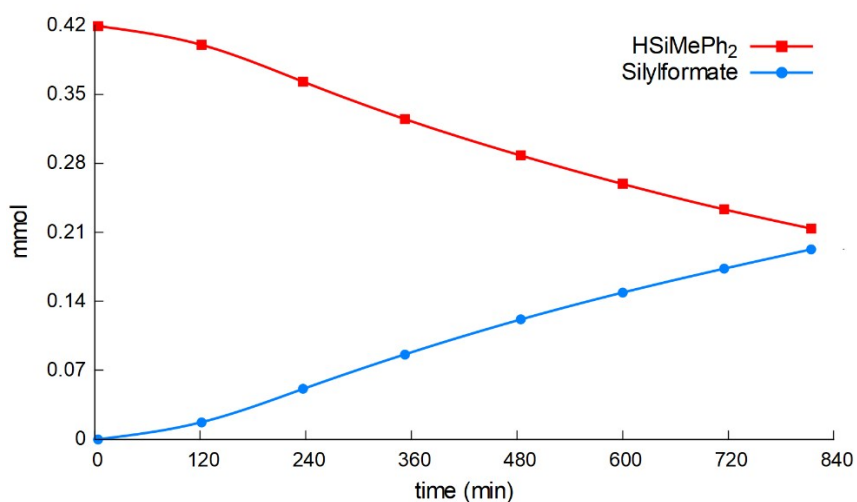


Figure S16. ¹H NMR spectra from the reaction of CO₂ with HSiMePh₂.
* Silylformate ● Silane ◆ Hexamethylbenzene

time (min)	Integral (3H)	Silane (mmol)	Integral (3H)	Silylformate (mmol)
4	3.96	0.42	0.00	0.00
122	3.78	0.40	0.16	0.02
237	3.43	0.36	0.48	0.05
353	3.07	0.32	0.81	0.09
485	2.72	0.29	1.15	0.12
600	2.45	0.26	1.40	0.15
716	2.20	0.23	1.63	0.17
749	2.14	0.23	1.70	0.18
782	2.08	0.22	1.76	0.19
815	2.02	0.21	1.82	0.19

0.018 mmol of hexamethylbenzene added



b) Using HSiMePh₂ as reductant.

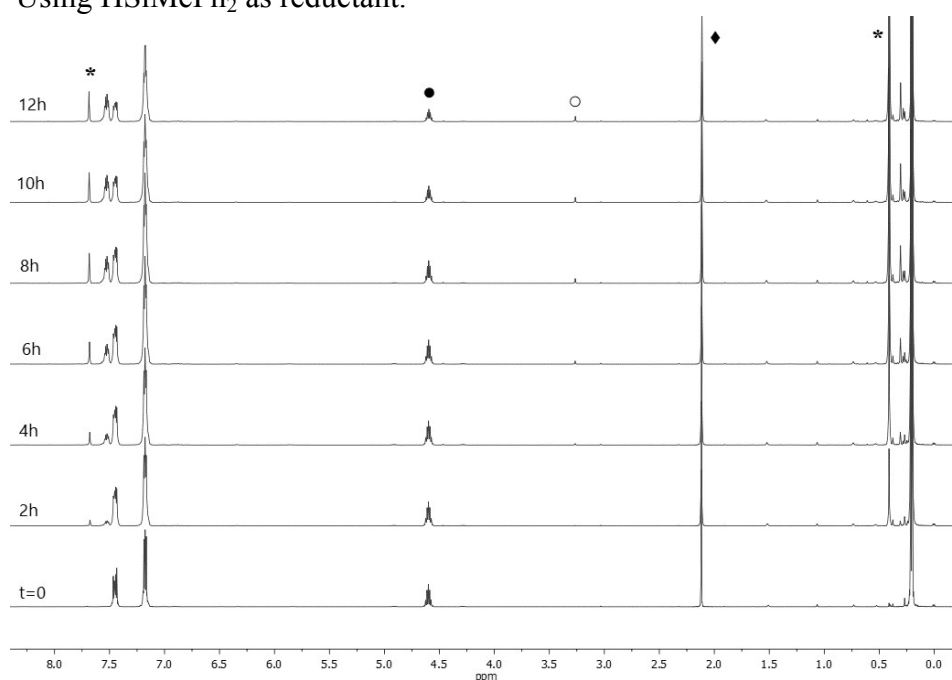
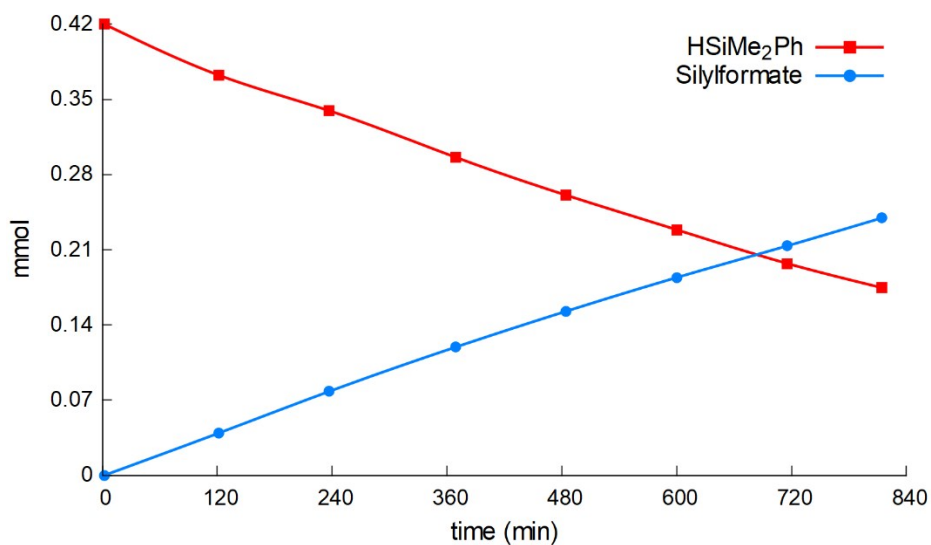


Figure S17. ¹H NMR spectra from the reaction of CO₂ with HSiMe₂Ph.
 * Silylformate • Silane ◯ Methoxysilane ♦ Hexamethylbenzene

time (min)	Integral (6H)	Silane (mmol)	Integral (6H)	Silylformate (mmol)
2	6.89	0.42	0.00	0.00
122	6.11	0.37	0.64	0.04
237	5.56	0.34	1.28	0.08
369	4.86	0.30	1.96	0.12
485	4.28	0.26	2.50	0.15
600	3.75	0.23	3.02	0.18
716	3.23	0.20	3.50	0.21
782	2.99	0.18	3.73	0.23
815	2.86	0.17	3.93	0.24

0.020 mmol of hexamethylbenzene added



c) Using HSiMe(OSiMe₃)₂ as reductant.

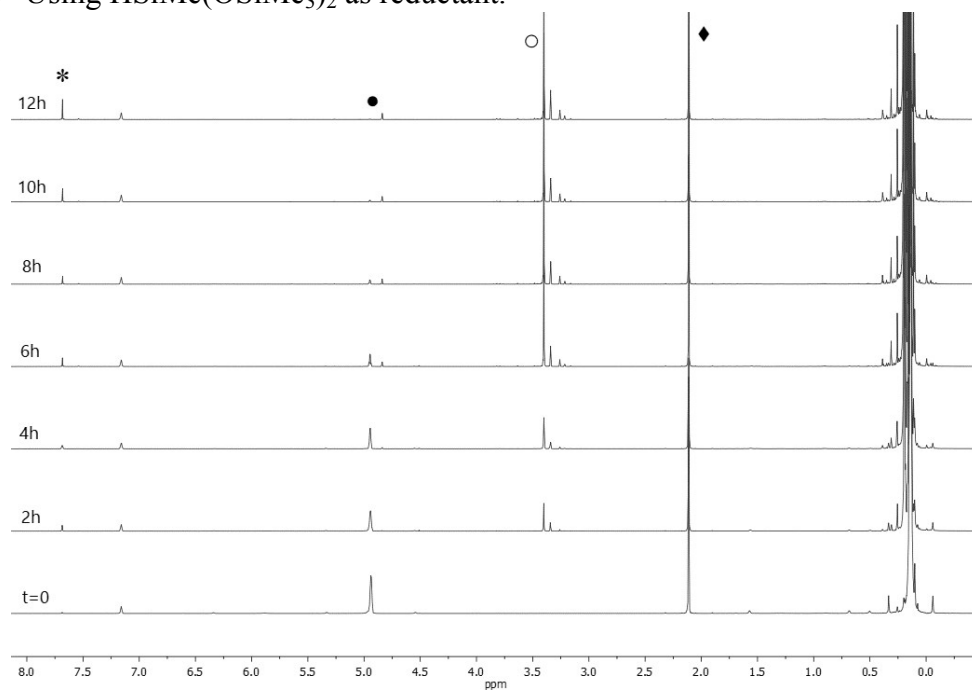
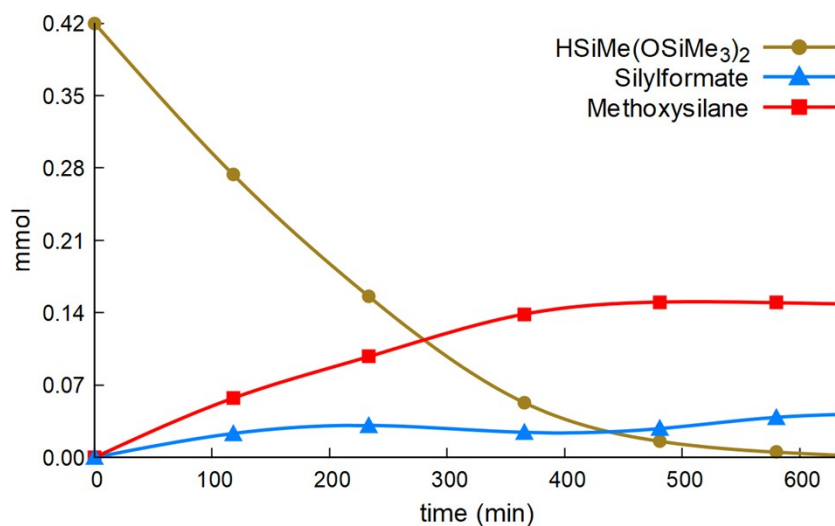


Figure S18. ¹H NMR spectra from the reaction of CO₂ with HSiMe(OSiMe₃)₂.
 * Silylformate • Silane ○ Methoxysilane ◆ Hexamethylbenzene

time (min)	Integral (1H)	Silane (mmol)	Integral (1H)	Silylformate (mmol)	Integral (1H)	Methoxysilane (mmol)
0	1.22	0.42	0.01	0.00	0.00	0.00
118	0.80	0.27	0.07	0.02	0.50	0.06
234	0.45	0.16	0.09	0.03	0.85	0.10
366	0.15	0.05	0.07	0.02	1.21	0.14
481	0.05	0.02	0.08	0.03	1.31	0.15
580	0.01	0.01	0.11	0.04	1.31	0.15
646	0.00	0.00	0.12	0.04	1.30	0.15

0.019 mmol of hexamethylbenzene added



7. 3-Catalyzed (1 mol %) hydrosilylation of ¹³CO₂ (2.6 bar) with HSiMe(OSiMe₃)₂ at 298K

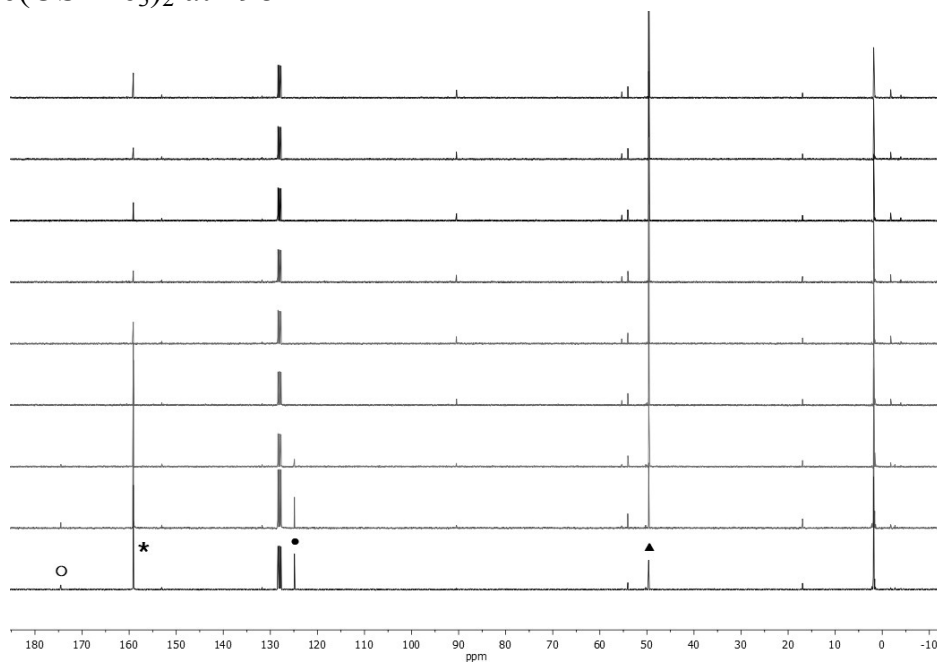


Figure S19. ¹³C NMR spectra from the reaction of ¹³CO₂ with HSiMe(OSiMe₃)₂.
 ○ Iridium-Formate * Silylformate • Free ¹³CO₂ ▲ Methoxysilane



Figure S20. ^1H - ^{13}C HSQC NMR spectrum from the reaction of $^{13}\text{CO}_2$ with $\text{HSiMe}(\text{OSiMe}_3)_2$

8. Selected NMR spectra of the reaction products of the **3**-catalyzed hydrosilylation of CO_2 (1 bar) with $\text{HSiMe}(\text{OSiMe}_3)_2$ in C_6D_6

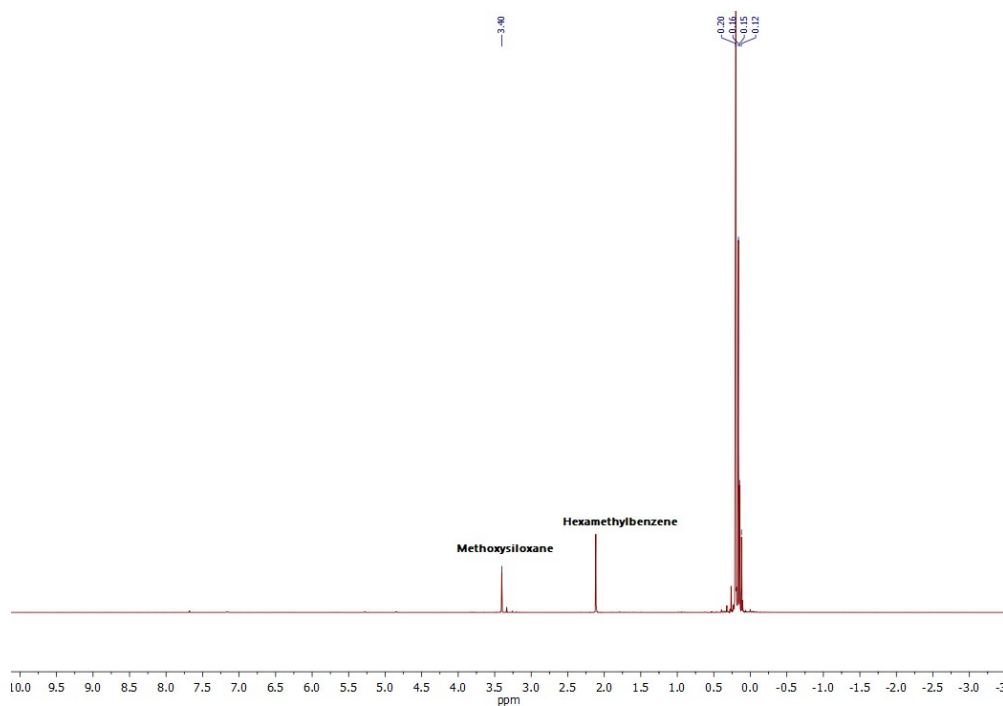


Figure S21. ^1H NMR spectra from the reaction of CO_2 with $\text{HSiMe}(\text{OSiMe}_3)_2$

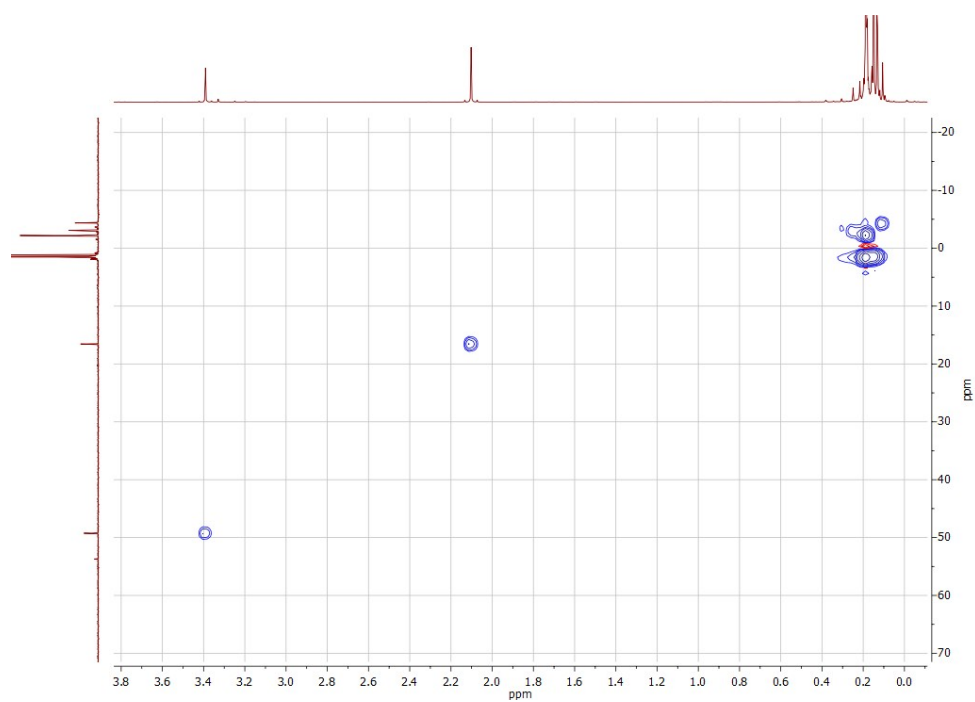


Figure S22. ^1H - ^{13}C HSQC NMR spectrum from the reaction of CO_2 with $\text{HSiMe}(\text{OSiMe}_3)_2$

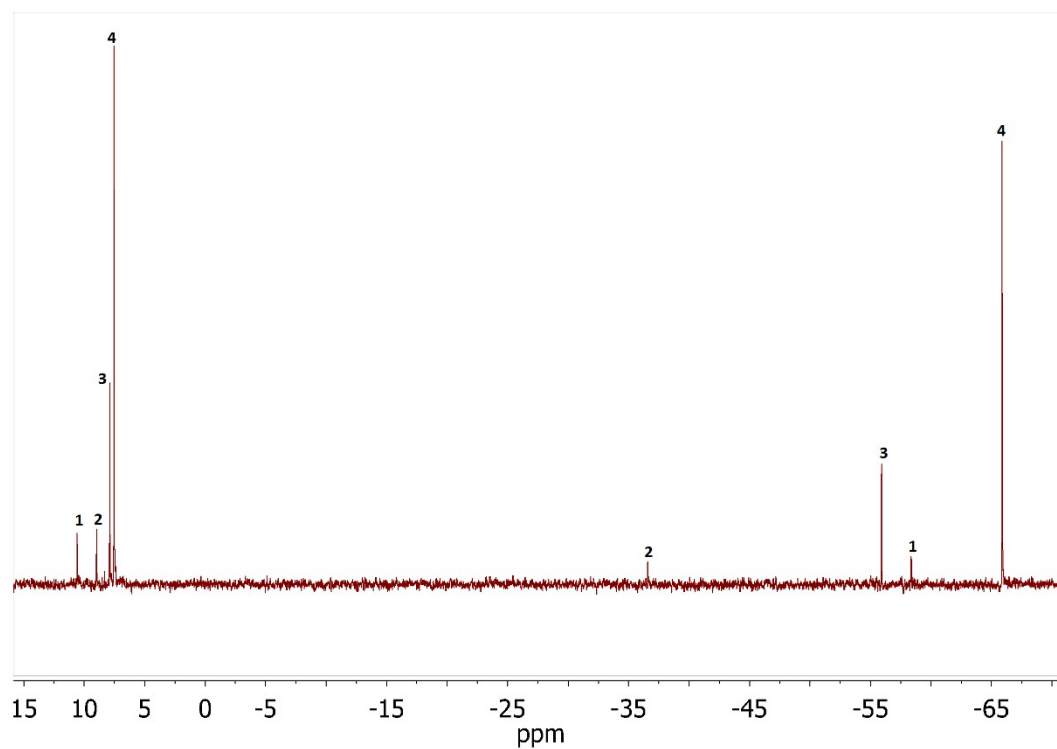


Figure S23. ^{29}Si DEPT 45 NMR spectrum from the reaction of CO_2 with $\text{HSiMe}(\text{OSiMe}_3)_2$: silylformate, **1**; starting $\text{HSiMe}(\text{OSiMe}_3)_2$, **2**; Methoxysilane **3**; $\text{O}\{\text{SiMe}(\text{OSiMe}_3)_2\}_2$, **4**.

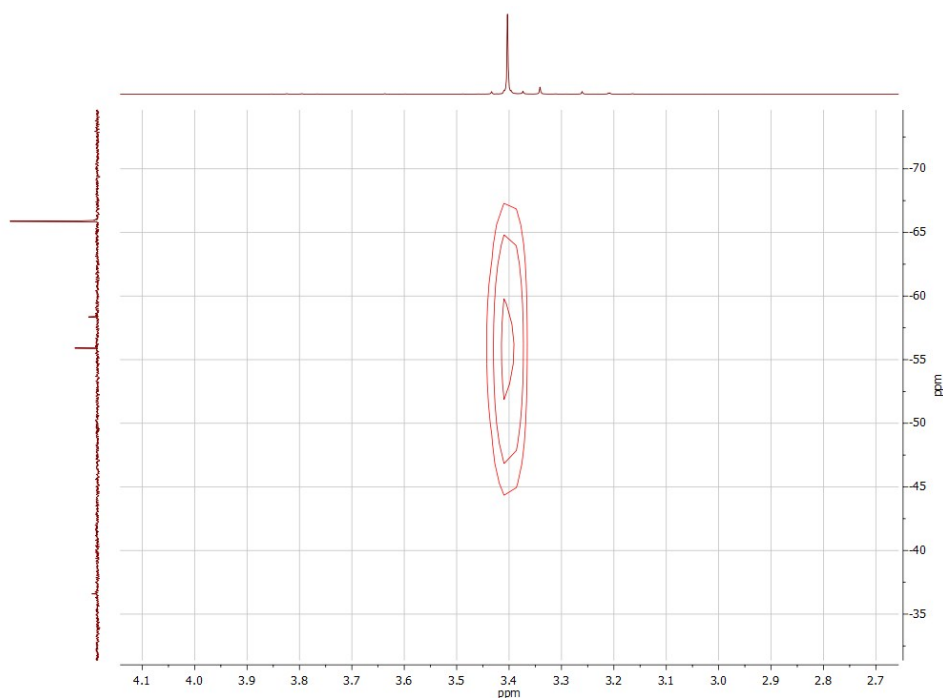


Figure S24. ^1H - ^{29}Si HMBC NMR spectrum from the reaction of CO_2 with $\text{HSiMe}(\text{OSiMe}_3)_2$. Correlation between the methoxy group and the silicon $\text{CH}_3\text{OSiMe}(\text{OSiMe}_3)_2$.

9. Comparison of the catalytic activity of complex **3 (1 mol %) with 1 vs 3 bar of CO_2 at RT in C_6D_6**

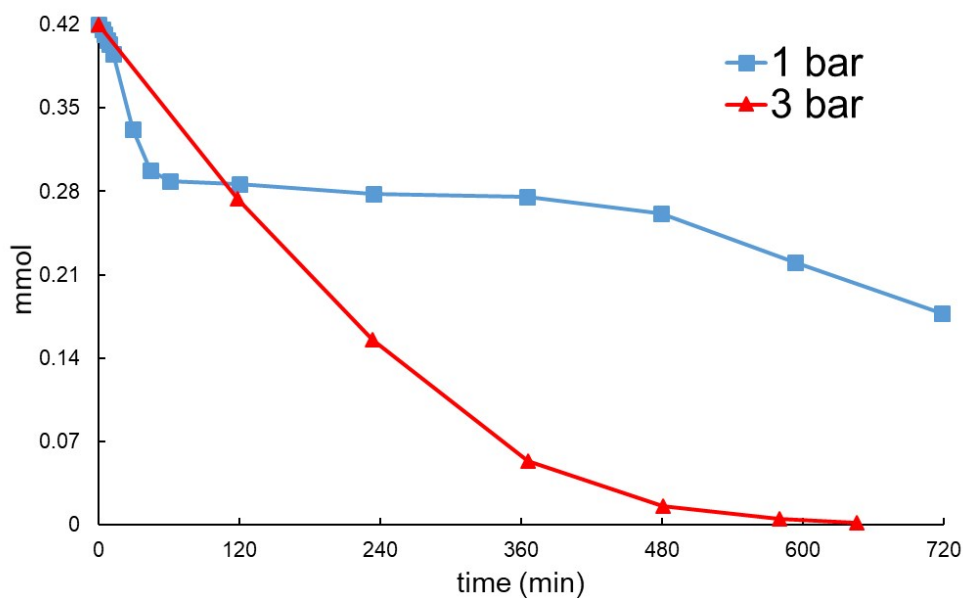


Figure S25. Representation of the consumption of the starting siloxane from the **3**-catalyzed (1 mol%) reaction of $\text{HSiMe}(\text{OSiMe}_3)_2$ with CO_2 (1 versus 3 bar) in C_6D_6 at 298K

10. Comparison of the catalytic activity of complex **3** and NSiN complex

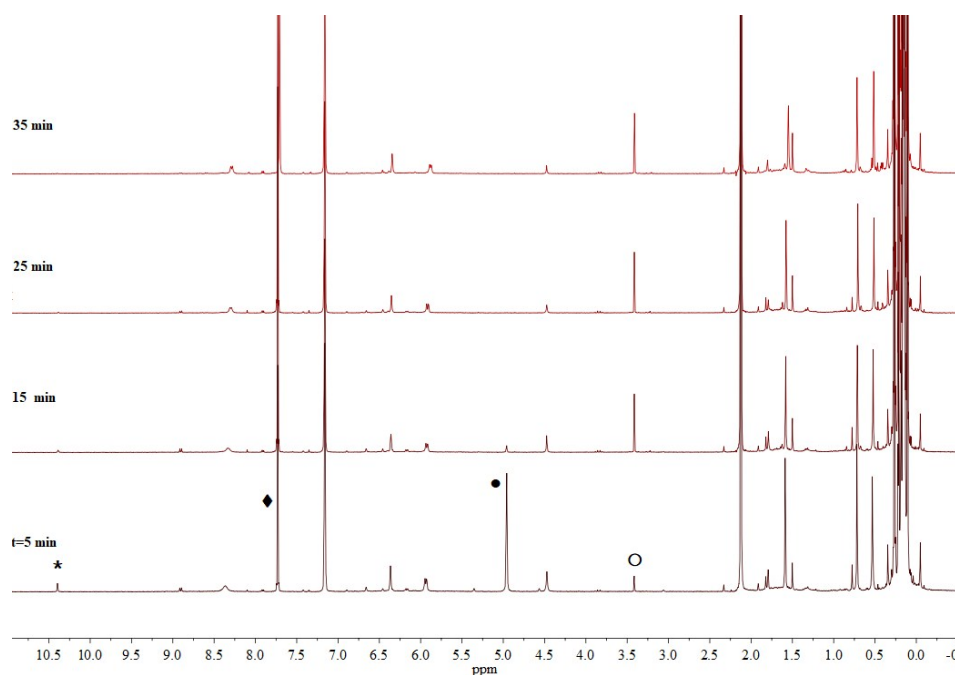


Figure S26. ¹H NMR spectra from the **3**-catalyzed (10 mol%) reaction of CO₂ (3 bar) with HSiMe(OSiMe₃)₂ at 328K in C₆D₆. * Iridium-formate ♦ Silylformate • Silane ○ Methoxysilane

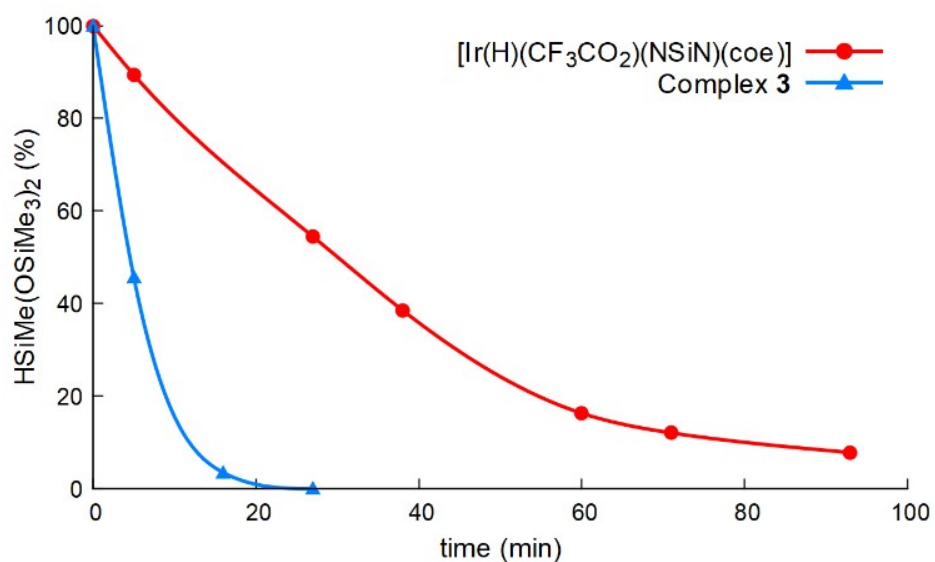


Figure S27. Representation of the consumption of the starting siloxane from the reaction of CO₂ (3 bar) with HSiMe(OSiMe₃)₂ in C₆D₆ at 328K in presence of catalytic amounts of complexes **3** or [Ir(H)(CF₃CO₂)(NSiN)(coe)] (10 mol% relative to Si-H)

11. Selected ^{19}F NMR spectra from different reactions conditions after the catalytic process

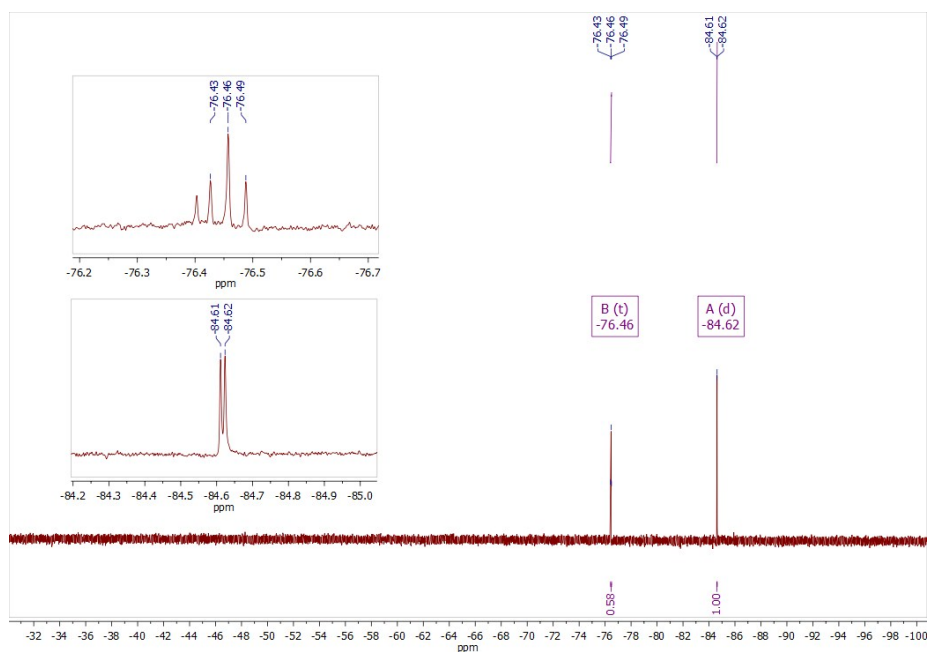


Figure S28. ^{19}F NMR spectrum after the reaction of CO_2 with $\text{HSiMe}(\text{OSiMe}_3)_2$.

12. High-Resolution Mass-Spectrum of the complexes **2** and **3**

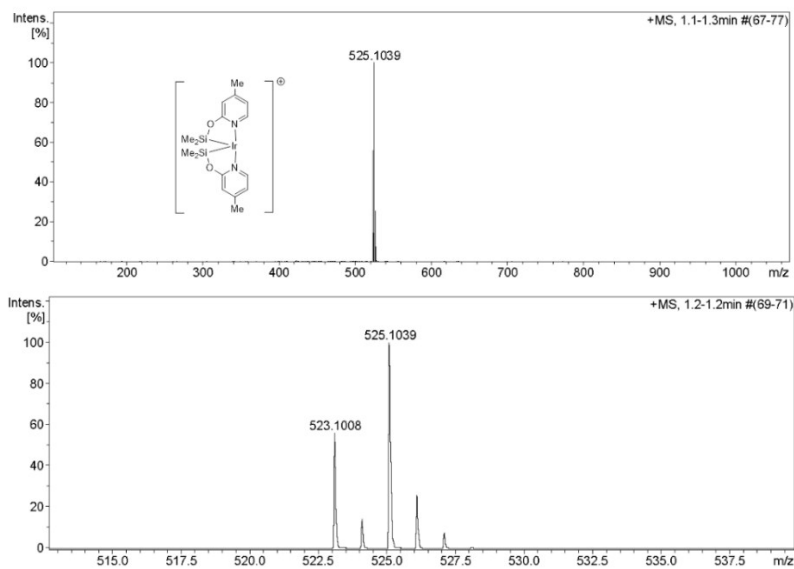


Figure S29. HR-MS of complex **2**

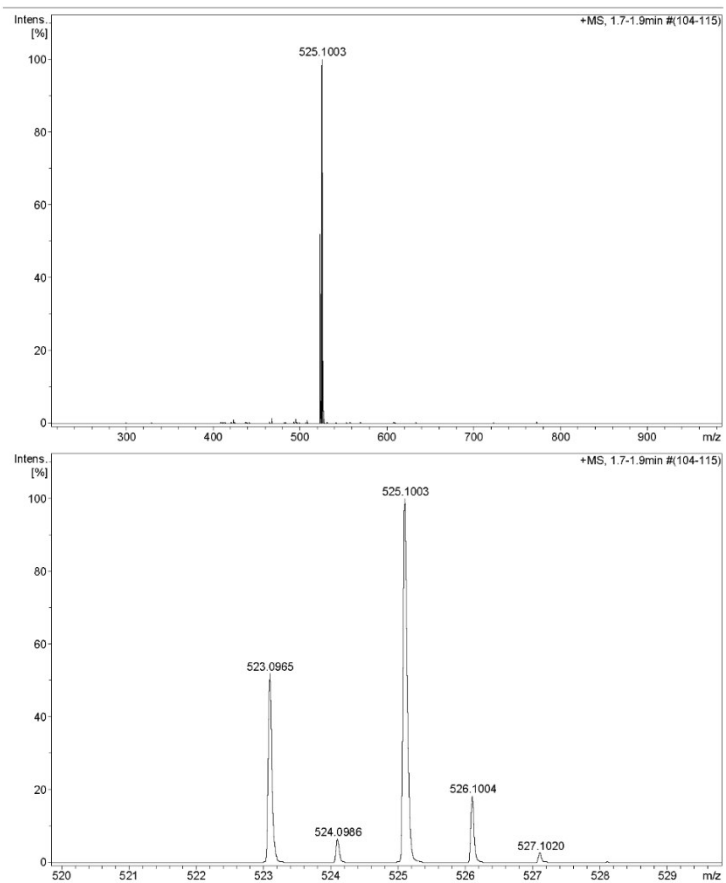


Figure S30. HR-MS of complex 3

13. DFT Calculations

Energetic values for all DFT calculated structures. Geometrical optimizations and thermochemistry corrections calculated using the def2-SVP, E(DZ), basis set. Single point energies using the def2-TZVP basis set, E(TZ). G and Gtrans are Gibbs free energy corrections calculated with and without translational contribution to the energy, correspondingly. All absolute energies in a.u. while relative energies relative to **A** and isolated molecules in kcal mol⁻¹.

	E(DZ)	G	Gtrans	E(TZ)	DG(TZ)trans
A	-2092.9430	0.3317	0.3532	-2094.7761	0
B	-2502.6855	0.4420	0.4637	-2504.7555	-6.6
TSBC	-2502.6581	0.4455	0.4672	-2504.7288	12.3
C	-2502.6626	0.4437	0.4653	-2504.7329	8.5
D	-1756.1059	0.3251	0.3465	-1757.5366	5.4
TSDE	-1756.1009	0.3267	0.3480	-1757.5313	9.7
E	-1756.1504	0.3343	0.3557	-1757.5772	-14.3
F	-2165.8879	0.4438	0.4653	-2167.5532	-19.4
TSFG	-2165.8617	0.4480	0.4695	-2167.5277	-0.7
G	-2165.8742	0.4429	0.4644	-2167.5429	-13.5
D'	-1756.1059	0.3251	0.3465	-1757.2115	-16.8
TSDE'	-1756.1009	0.3267	0.3480	-1757.2046	-12.5
E'	-1756.1504	0.3343	0.3557	-1757.2429	-36.5
TSGH	-2165.8654	0.4424	0.4639	-2167.5364	-9.7
H	-2165.8932	0.4485	0.4700	-2167.5623	-22.1
I	-2575.6287	0.5571	0.5787	-2577.5374	-27.2
TSIJ	-2575.6244	0.5609	0.5826	-2577.5341	-22.7
J	-2575.6389	0.5590	0.5806	-2577.5511	-34.5
TSJK	-2985.3210	0.6699	0.6917	-2987.4803	-9.3
K	-2461.1900	0.5296	0.5512	-2462.9687	-65.9
TSKD	-2461.1761	0.5321	0.5537	-2462.9544	-55.3
D''+ O(SiMe3)2	-2280.3202	0.4421	0.4823	-2282.1338	-75.9
TSJM	-2575.6008	0.5615	0.5832	-2577.5086	-6.3
TSIM	-2575.5902	0.5595	0.5811	-2577.5037	-4.5
M	-1682.0978	0.3483	0.3696	-1683.4407	-38.7
J_{OMe}	-2876.4169	0.5813	0.6031	-2878.7050	-44.9
TSJK_{OMe}	-3436.4859	0.6942	0.7162	-3439.2080	-27.6
CO2	-188.4447	-0.0089	0.0088	-188.6715	
SiHMe3	-409.7222	0.0879	0.1064	-409.9647	
SiHMe(OMe)2	-560.0962	0.0933	0.1123	-560.5299	
CF3CO2SiMe3	-934.9880	0.0977	0.1175	-935.8627	
CF3CO2SiMe(OMe)2	-1085.3676	0.1049	0.1249	-1086.4332	
O(SiMe3)2	-893.5273	0.1843	0.2038	-894.1098	
CH2(OSiMe3)2	-1007.9632	0.2125	0.2323	-1008.6764	
HCO2SiMe3	-598.2068	0.1066	0.1166	-598.6730	
CH3OSiMe3	-524.2143	0.1170	0.1359	-524.5972	

14. Other mechanistic alternatives for conversion of **I** and **J**

Path a) **TSJK**, S_N2 nucleophilic attack of hydride to the carbon atom of bis(silyl)acetal.

Path b) **TSIM**, concerted silyl transfer from silane to the oxygen lone pair while the C-O bond is broken forming formaldehyde and bis(silyl)ether intermediate (**M**).

Path c) **TSJM** 1,2-elimination of bis(silyl)ether through transition state

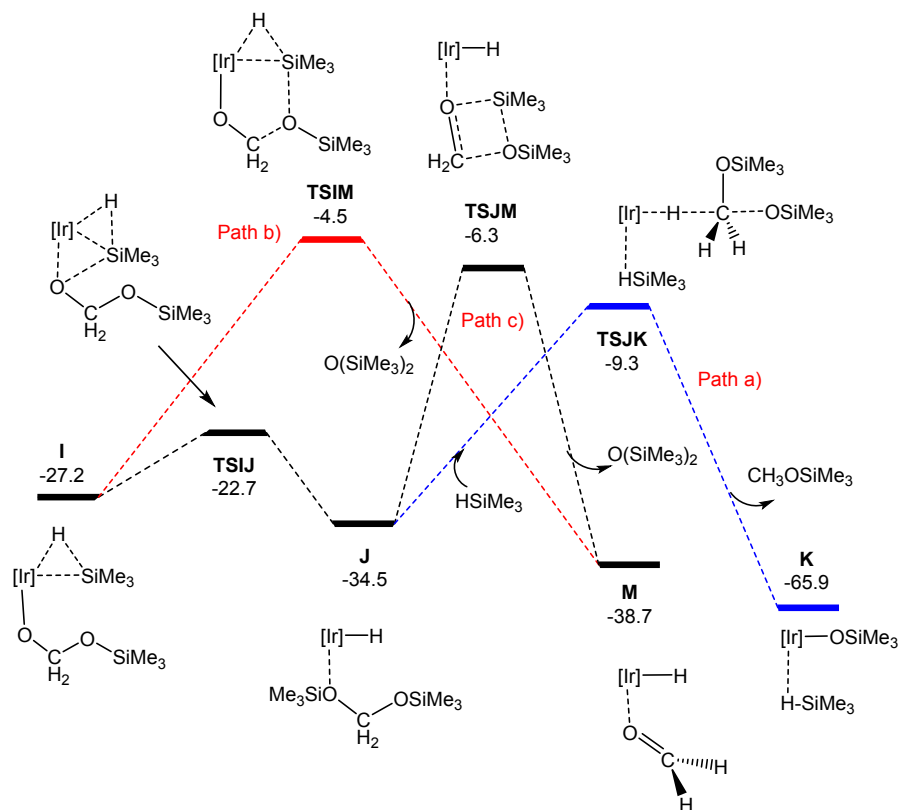


Figure S31. Other mechanistic alternatives for the conversion of **I** and **J**.

15. Comparison between Gibbs free energy profiles to the methoxysilane product step using HSiMe₃ and HSiMe(OMe)₂ silanes

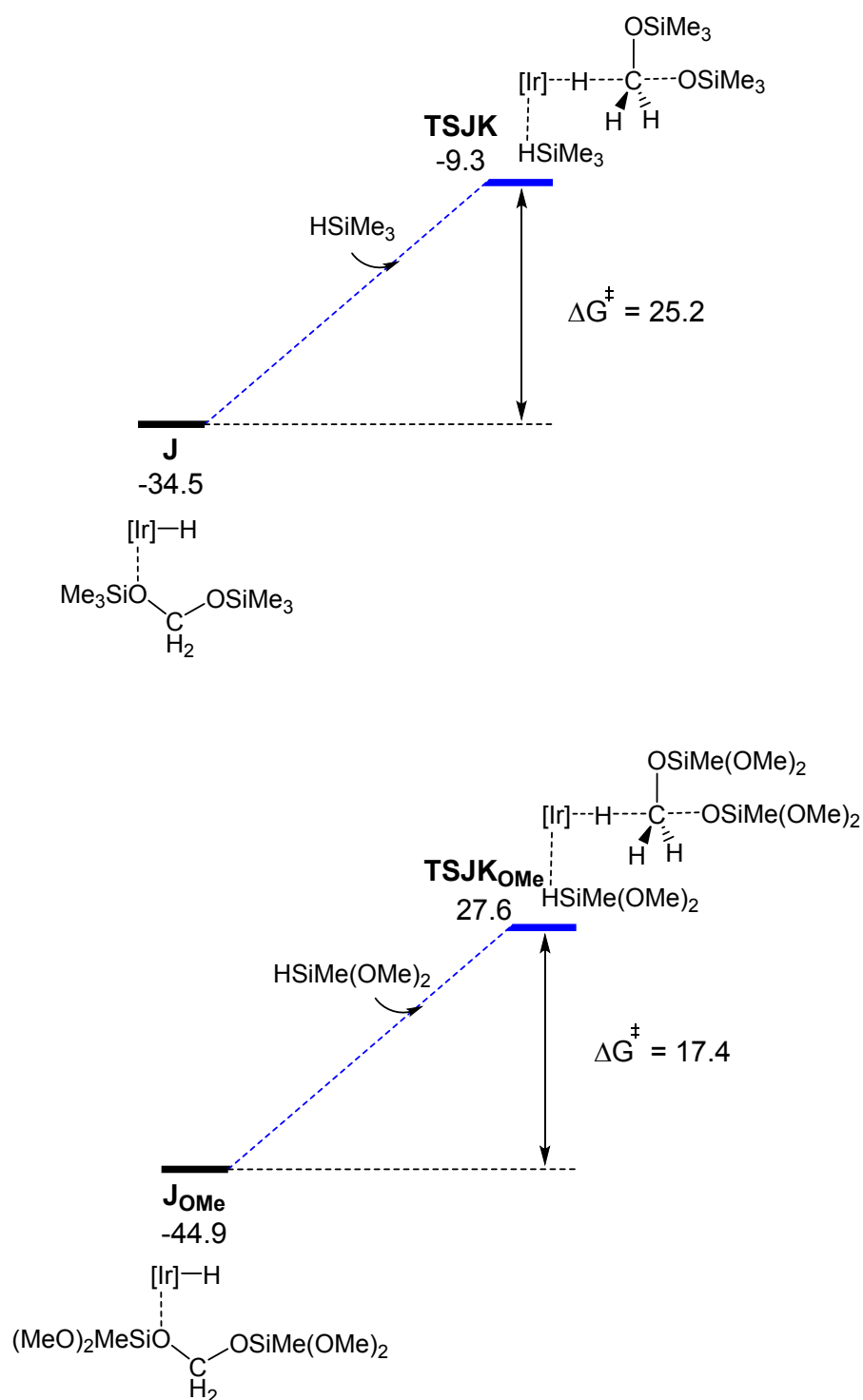
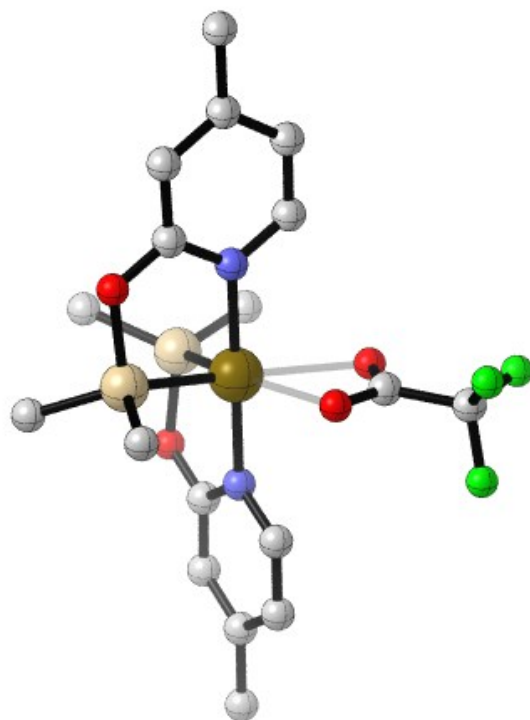


Figure S32. Comparison between Gibbs free energy profiles (in kcal mol⁻¹, relative to **A** and isolated molecules) for the key step leading to the methoxysilane, calculated using HSiMe₃ and HSiMe(OMe)₂ silanes.

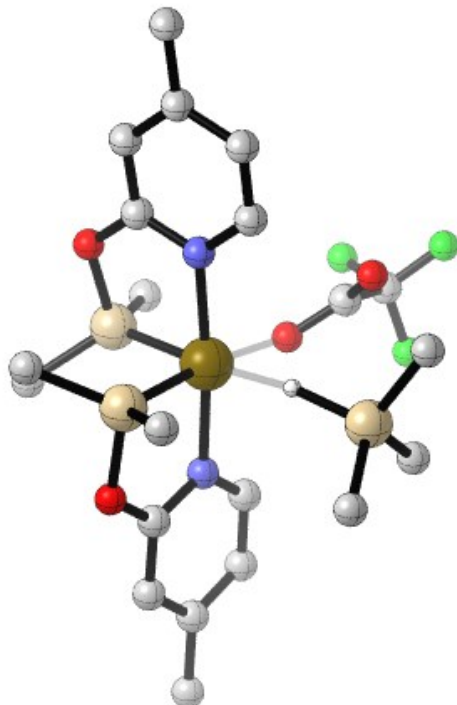
16. Full citation for the G09 program

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016

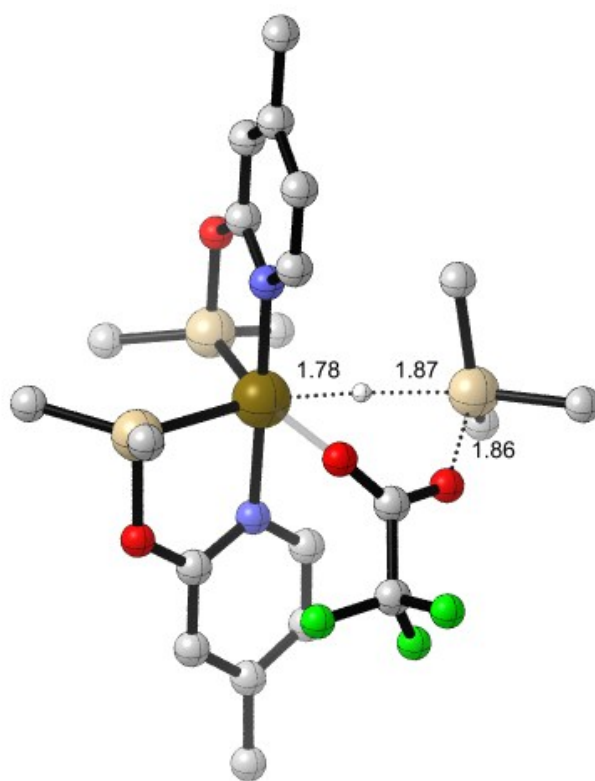
17. Geometrical Representation of all DFT optimized structures



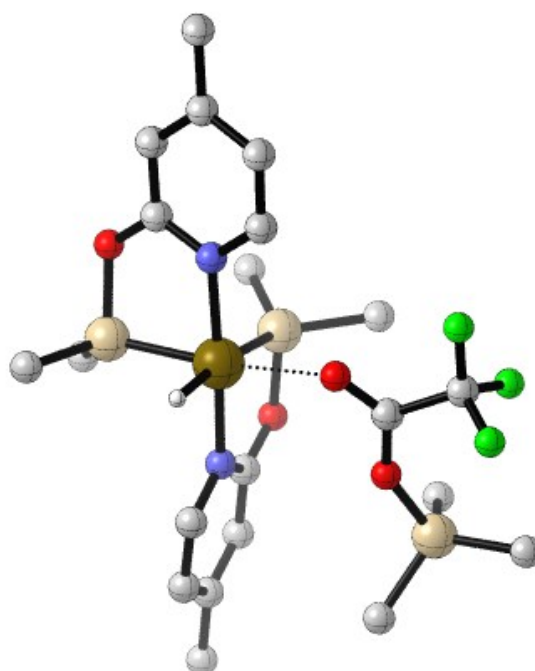
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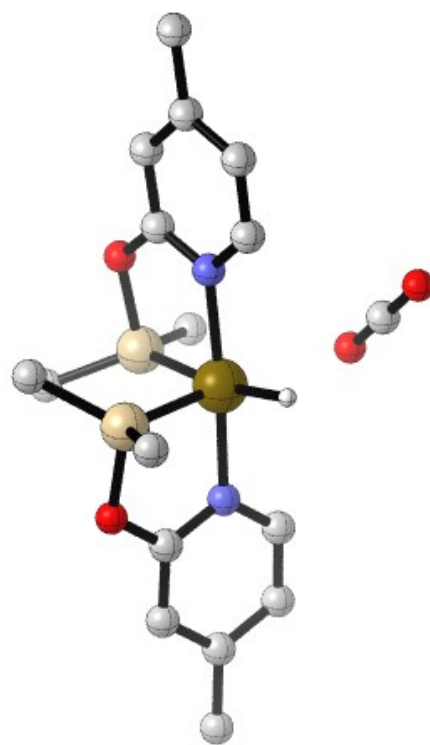
B



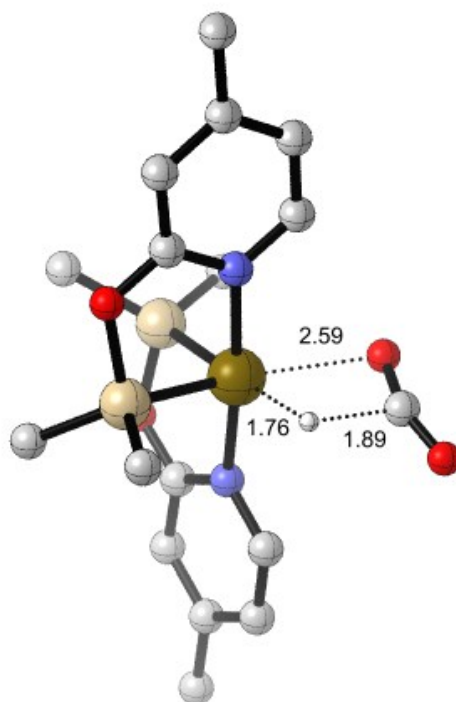
TSBC



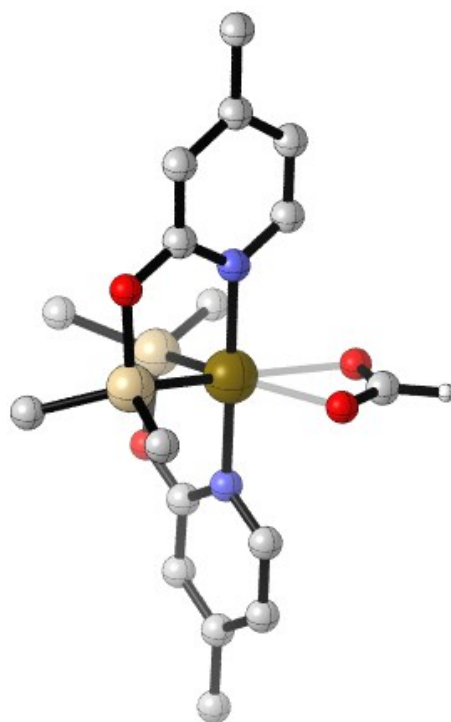
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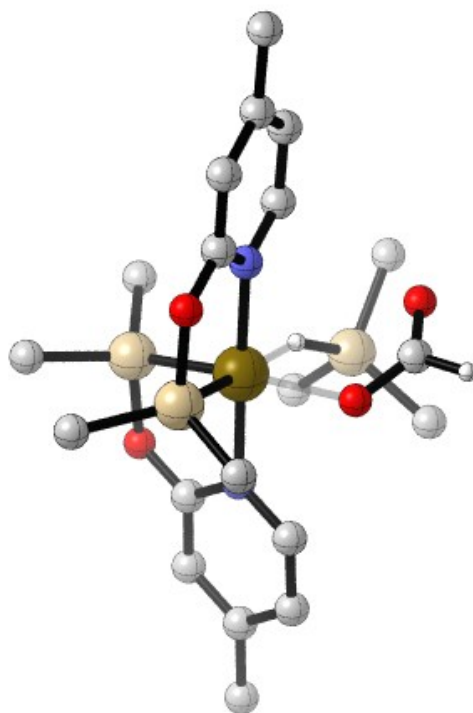
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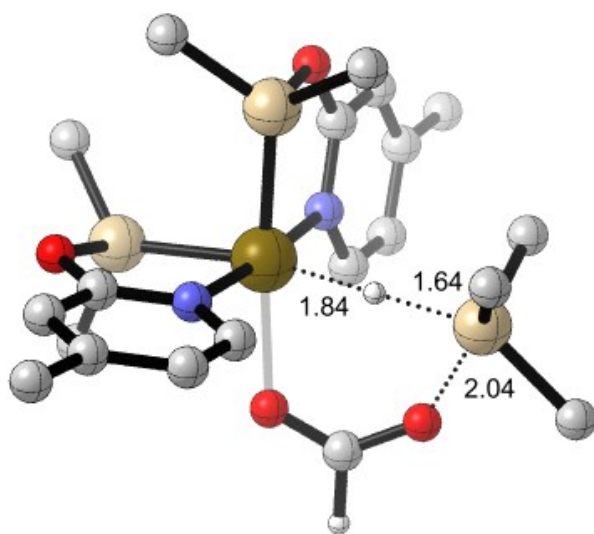
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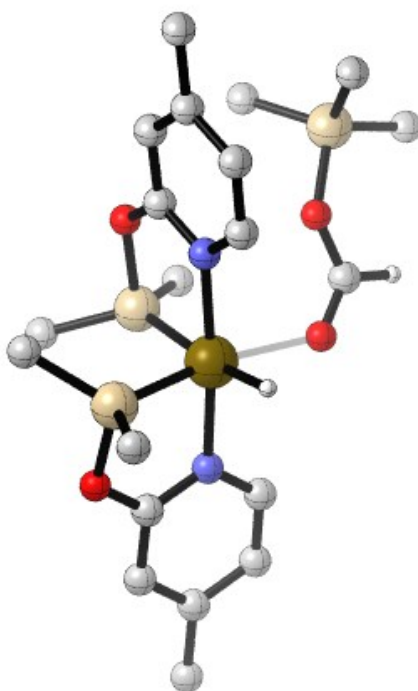
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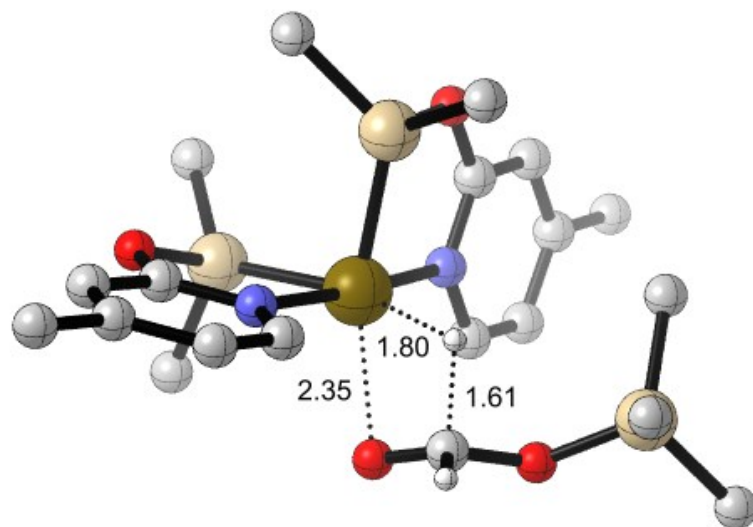
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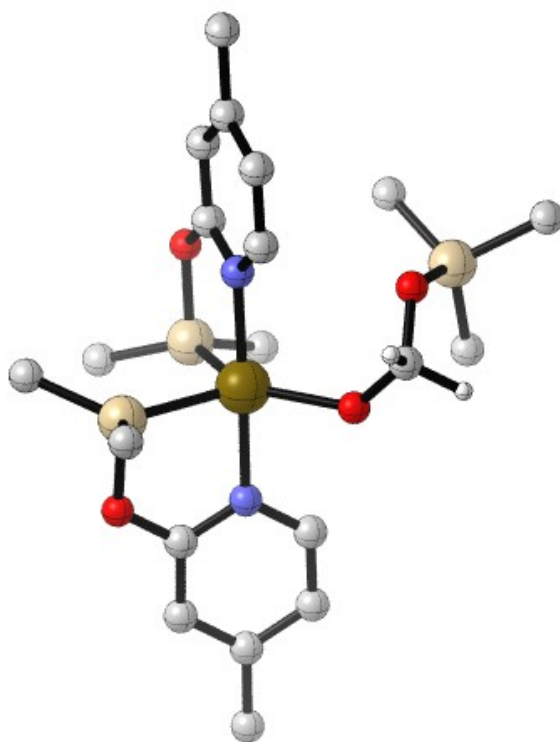
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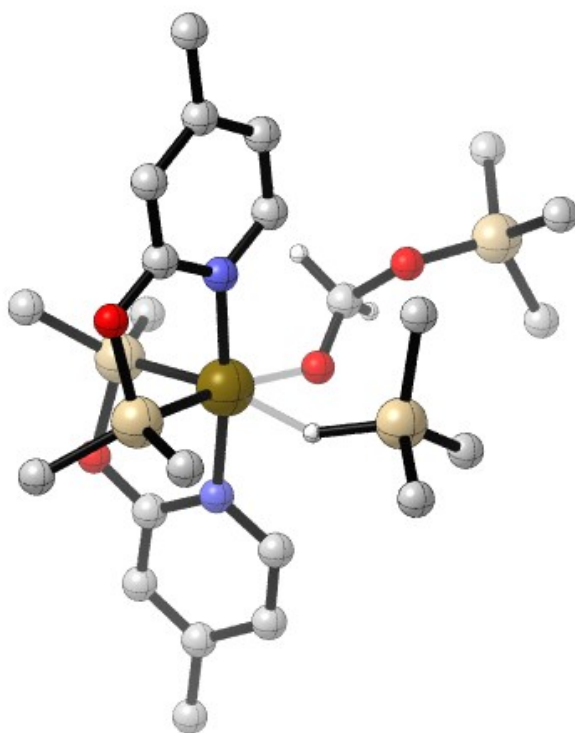
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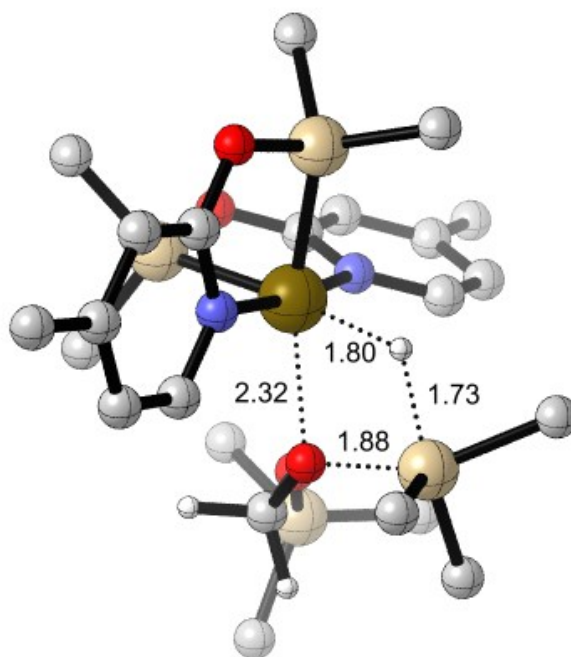
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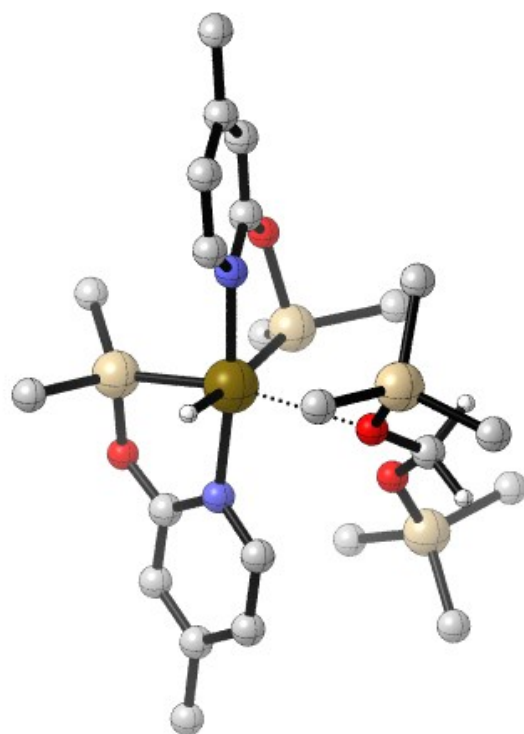
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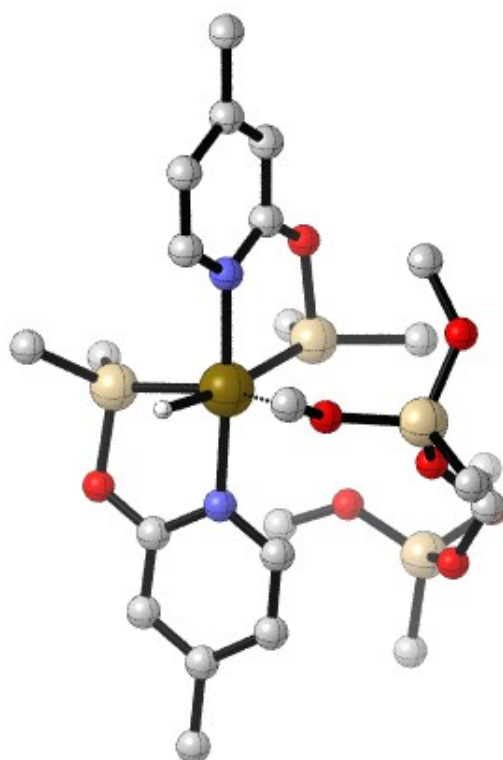
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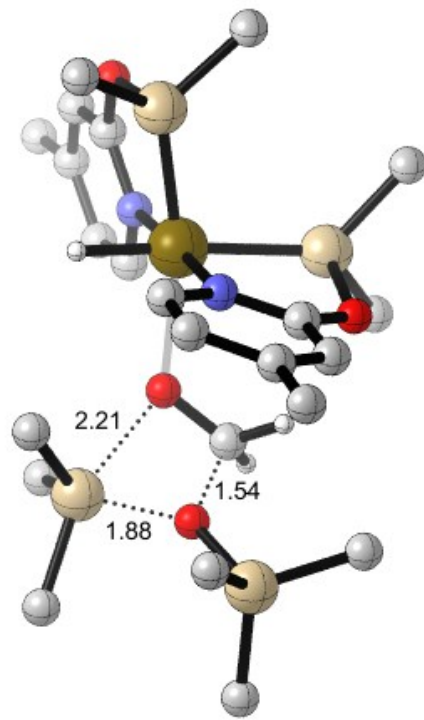
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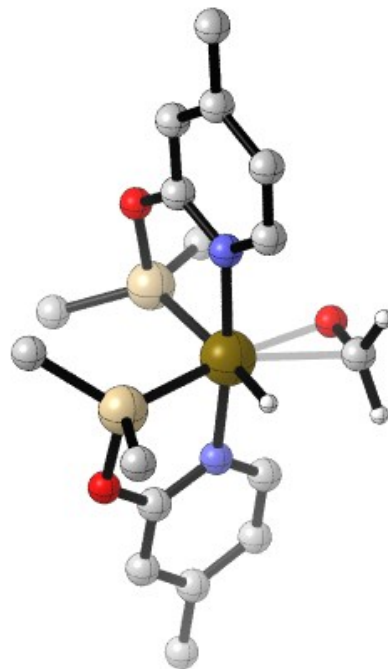
J



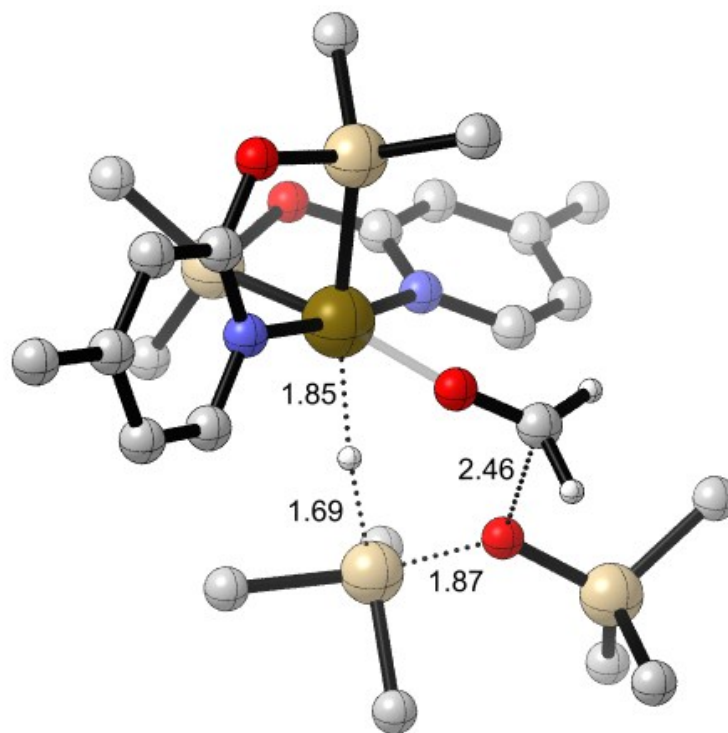
J_{OMe}



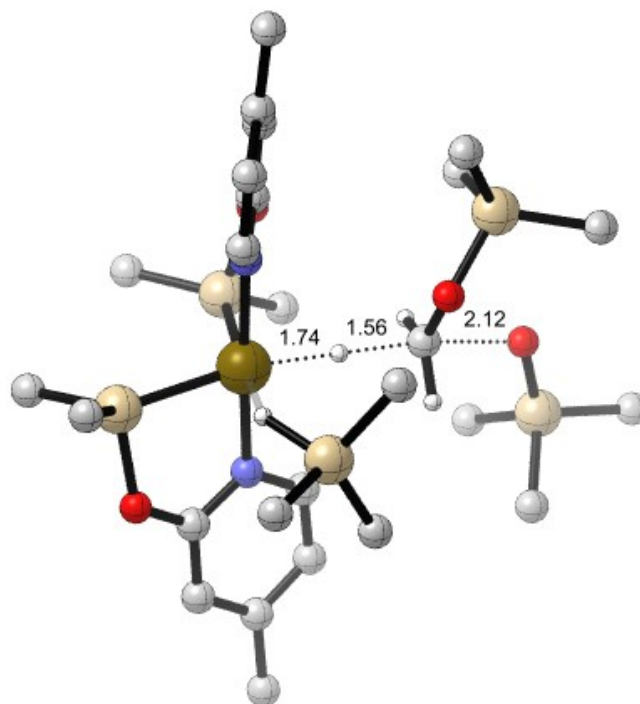
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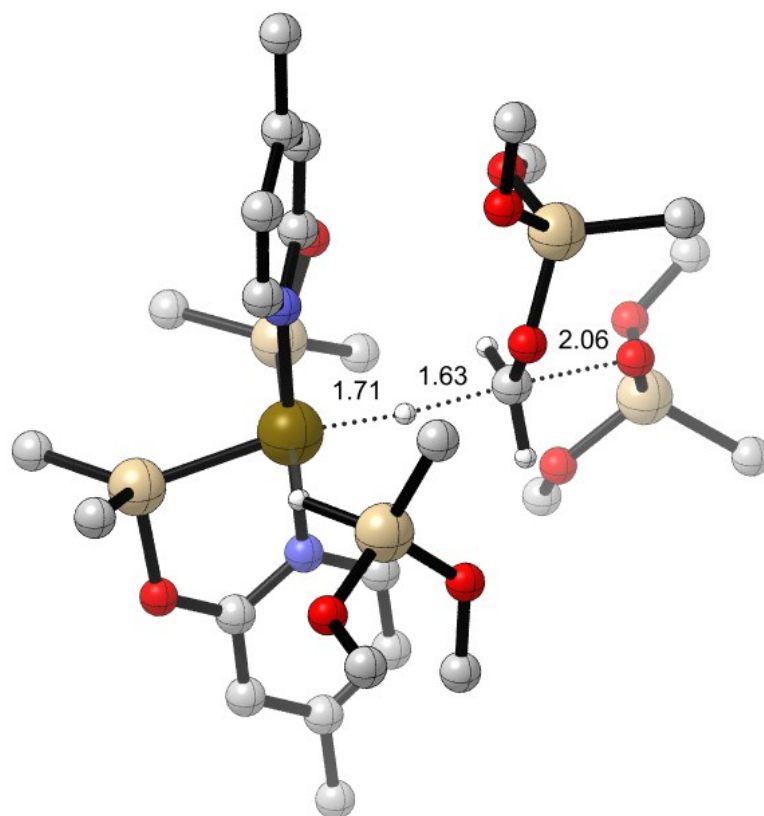
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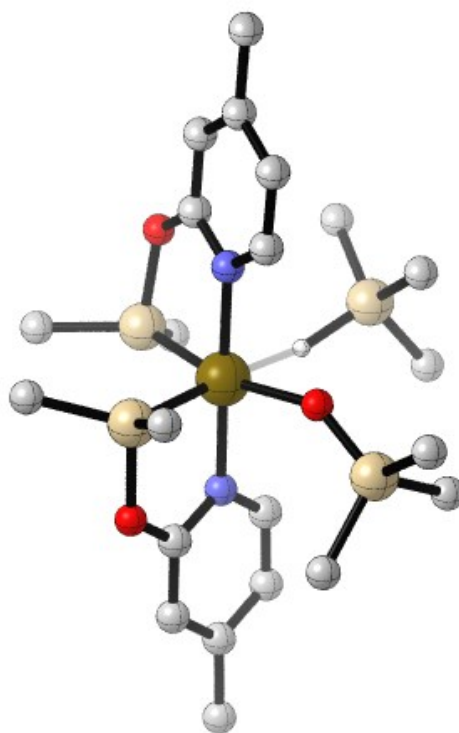
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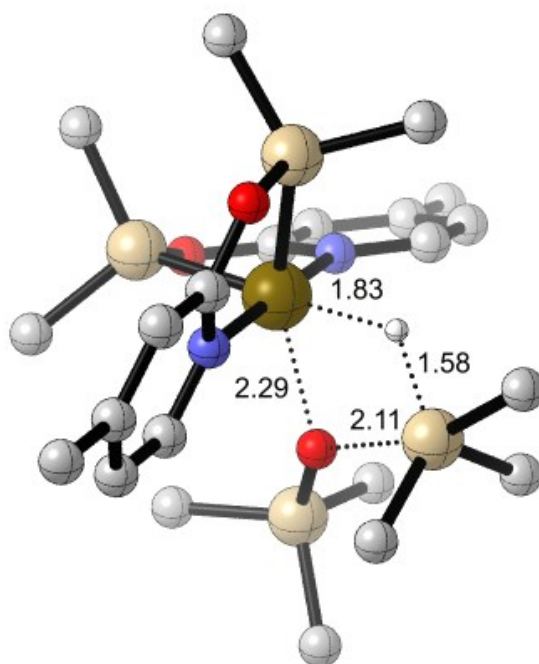
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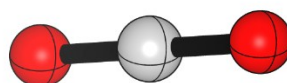
TSJK_{OMe}



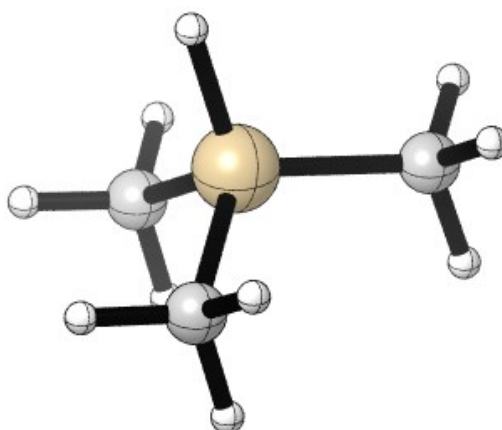
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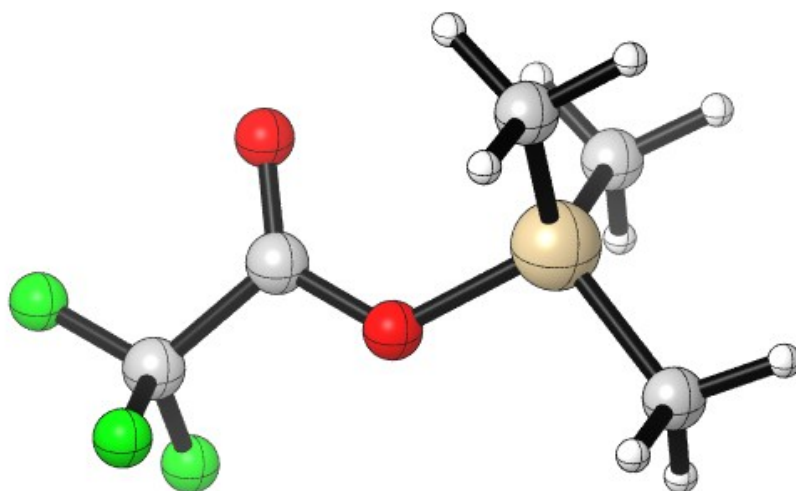
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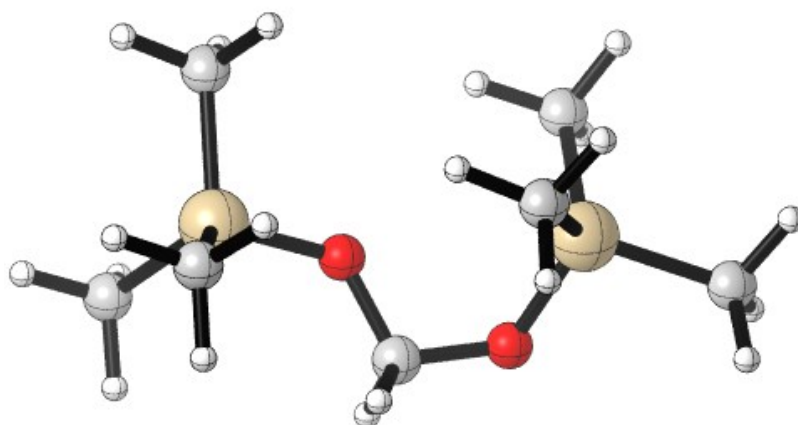
CO2



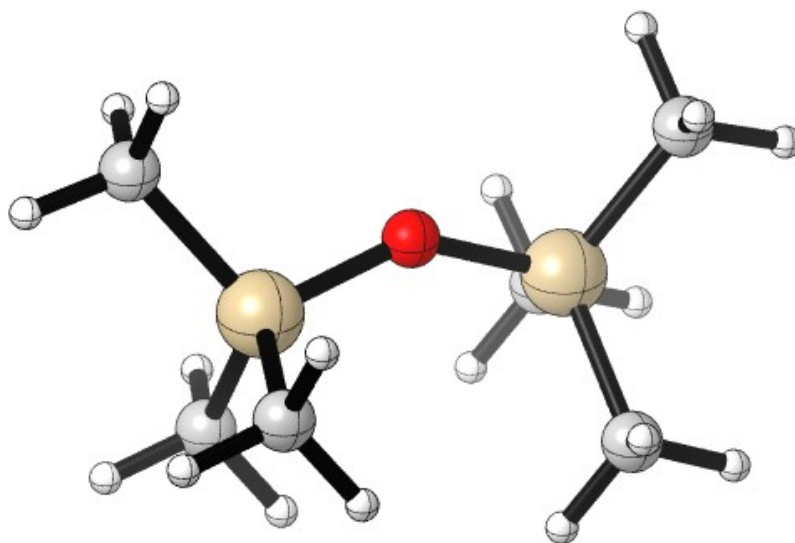
SiHMe3



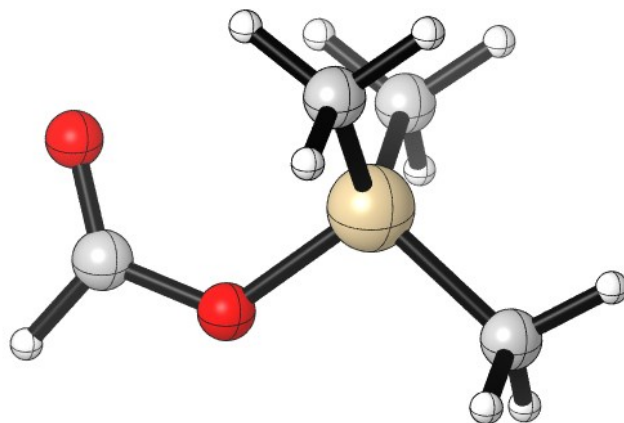
CF₃CO₂SiMe₃



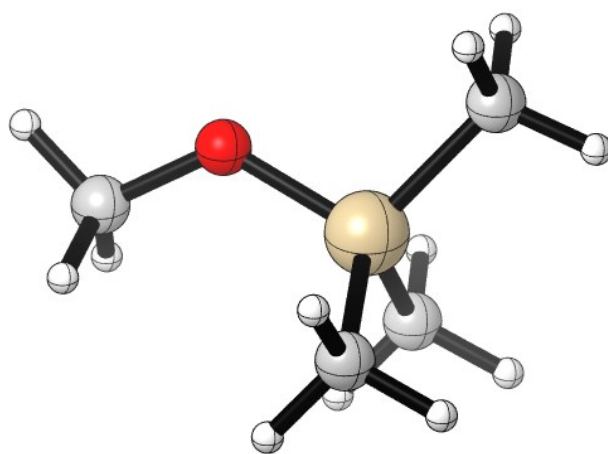
O(SiMe₃)₂



CH₂(OSiMe₃)₂



HCO₂SiMe₃



CH₃OSiMe₃

18. Cartesian coordinates (xyz, in Å) for all DFT optimized structures.

A	6 -0.839445	2.601303	-0.453521
77 -0.041908	-0.181191	-0.007979	6 -0.803843
14 0.210264	-1.783073	-1.608265	9 0.457974
14 -0.454817	-1.670765	1.663142	9 -1.588715
9 -0.418673	4.661253	0.852493	9 -1.184889
9 1.665656	4.280476	0.380106	7 2.075512
9 0.229788	4.613315	-1.211512	6 2.706990
8 1.955762	-2.065520	-1.433666	6 2.797606
8 -2.224183	-1.750887	1.520212	6 4.068934
8 0.021552	1.957600	1.068017	1 2.051946
8 0.144827	1.943509	-1.150643	6 4.191207
7 2.035107	-0.297372	0.046513	6 4.847164
7 -2.115339	-0.079807	-0.065188	1 4.525820
6 2.773239	0.547002	0.807748	1 4.723972
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6 4.149891	0.473878	0.877011	6 -2.789042
1 4.692633	1.180829	1.506445	6 -2.705052
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6 4.072053	-1.367828	-0.654195	1 -2.237299
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1 -2.104622	1.428400	-1.480339	1 1.470392
6 -4.133521	0.859727	-0.958432	6 -0.317469
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B			1 2.558074
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TSBC

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9 -3.777558 1.801658 -0.800071
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C

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 1 6.658152 0.270978 -1.196602
 6 -6.253326 0.372238 1.323341
 1 -6.470810 0.149184 2.380724
 1 -6.551189 1.419175 1.149306
 1 -6.884115 -0.274484 0.697744
 1 -0.432363 0.719879 -1.633989
 14 -1.211509 1.846319 -2.291250
 8 0.279958 1.536776 1.028056
 14 1.476210 2.606472 1.337185
 6 0.867764 3.811231 2.665493
 1 -0.059193 4.311433 2.338439
 1 0.642382 3.274141 3.602276
 1 1.612913 4.591895 2.894035
 6 1.942419 3.620177 -0.200306
 1 2.724186 4.363856 0.030117
 1 2.333351 2.962761 -0.994190
 1 1.071167 4.161451 -0.603279
 6 3.087535 1.816180 1.956842
 1 3.661190 1.374544 1.127481
 1 3.731170 2.574046 2.434928
 1 2.899087 1.019601 2.693511
 6 0.031185 2.676693 -3.439212
 1 -0.450531 3.486894 -4.011554
 1 0.863384 3.115012 -2.867969
 1 0.445318 1.955771 -4.162952
 6 -1.867615 3.011328 -0.978515
 1 -1.973869 4.034093 -1.374086
 1 -2.849589 2.676999 -0.611346
 1 -1.170106 3.010609 -0.127520
 6 -2.606987 1.049521 -3.273670
 1 -3.269613 1.830824 -3.682255
 1 -2.227328 0.450230 -4.115059
 1 -3.212049 0.386246 -2.637585
TSKD
 77 -0.135224 -0.440799 -0.111193
 7 -2.143749 -0.045284 0.251116

6	-2.512560	0.939584	1.100791	1	0.317335	2.111686	3.376226
6	-3.100051	-0.791410	-0.361887	6	1.289311	2.931997	-2.274668
6	-3.834156	1.225797	1.375982	1	1.197177	3.341255	-3.292669
1	-1.685552	1.508579	1.523315	1	1.543886	3.754729	-1.593618
6	-4.464551	-0.525984	-0.135621	1	2.135986	2.229087	-2.268019
6	-4.850975	0.483844	0.738135	6	-1.721952	3.135732	-1.109271
1	-4.076082	2.034519	2.067135	1	-1.862784	3.973665	-1.813251
1	-5.192948	-1.145657	-0.659329	1	-2.665653	2.568682	-1.101604
7	1.917058	-0.756556	-0.320324	1	-1.543975	3.537063	-0.105460
6	2.579346	-0.527261	-1.477470	6	-1.081495	1.720350	-3.546849
6	2.632147	-1.088396	0.789918	1	-1.332232	2.658994	-4.073205
6	3.953663	-0.599912	-1.583728	1	-0.380018	1.158821	-4.189400
1	1.952255	-0.274363	-2.331543	1	-2.007469	1.122933	-3.473582
6	4.037292	-1.174130	0.739311	CO2			
6	4.720028	-0.924792	-0.444416	6	0.000000	0.000000	0.000000
1	4.429567	-0.396460	-2.544083	8	0.000000	0.000000	1.163049
1	4.557214	-1.436437	1.660984	8	0.000000	0.000000	-1.163049
14	0.228870	-1.605158	1.866037	SiHMe3			
14	-1.008896	-2.225781	-1.277056	14	-0.000010	-0.000013	-0.384092
8	-2.730771	-1.768754	-1.154770	1	-0.000016	-0.000030	-1.882114
8	1.998430	-1.327359	1.914577	6	1.233663	-1.292683	0.225338
6	-0.498084	-0.900911	3.457229	1	0.964692	-2.300768	-0.130038
1	0.137722	-1.150770	4.322499	1	2.253247	-1.070906	-0.129817
1	-0.640642	0.185297	3.431362	1	1.258789	-1.319226	1.327630
1	-1.483168	-1.371731	3.616120	6	-1.736349	-0.422011	0.225341
6	0.202494	-3.474006	2.135341	1	-1.771838	-0.430680	1.327635
1	0.724505	-4.020127	1.337306	1	-2.474813	0.315122	-0.129875
1	0.711498	-3.689688	3.089992	1	-2.054219	-1.415787	-0.129962
1	-0.824613	-3.864023	2.205751	6	0.502695	1.714715	0.225327
6	-1.083035	-4.062027	-0.860978	1	1.510335	1.985652	-0.129816
1	-1.692478	-4.568715	-1.627646	1	-0.198959	2.486906	-0.130024
1	-0.079497	-4.516212	-0.872296	1	0.512861	1.749774	1.327623
1	-1.536083	-4.254485	0.120305	CF3CO2SiMe3			
6	-0.625170	-2.138545	-3.123663	6	0.777825	-0.479543	0.000080
1	0.426616	-2.425192	-3.295728	8	0.623768	-1.672725	0.000124
1	-1.261622	-2.832812	-3.696699	8	-0.164431	0.442094	-0.000025
1	-0.768953	-1.122129	-3.515954	14	-1.878619	0.084115	-0.000094
6	6.220393	-0.974586	-0.515560	6	-2.252260	-0.875001	1.559971
1	6.658448	-1.381901	0.406141	1	-3.332911	-1.079363	1.637922
1	6.556157	-1.590004	-1.365110	1	-1.716204	-1.835915	1.558494
1	6.628631	0.038469	-0.668766	1	-1.949413	-0.307456	2.454429
6	-6.300255	0.788071	0.998960	6	-2.252095	-0.875175	-1.560092
1	-6.526079	0.723533	2.075712	1	-3.332756	-1.079423	-1.638207
1	-6.543886	1.815107	0.680679	1	-1.949026	-0.307782	-2.454571
1	-6.964872	0.096057	0.463481	1	-1.716145	-1.836148	-1.558397
1	-0.185944	0.488290	-1.686695	6	-2.640515	1.788685	-0.000229
14	-0.320190	2.059900	-1.787834	1	-3.740803	1.720819	-0.000262
8	0.367978	1.775382	0.182849	1	-2.334224	2.358252	0.891420
14	1.383616	2.651382	1.162548	1	-2.334164	2.358142	-0.891929
6	0.846364	4.465700	1.184977	6	2.178903	0.175077	0.000095
1	0.817735	4.909230	0.177768	9	3.133845	-0.749241	0.000184
1	-0.161543	4.568202	1.620180	9	2.330921	0.945228	-1.085598
1	1.538210	5.066605	1.798740	9	2.330840	0.945352	1.085712
6	3.198643	2.562294	0.635140	O(SiMe3)2			
1	3.822549	3.106246	1.364641	8	0.000008	-0.000127	0.616297
1	3.553474	1.521462	0.608478	14	1.579604	-0.001448	0.073094
1	3.375448	3.004045	-0.355548	14	-1.579594	0.001482	0.073090
6	1.328331	2.038153	2.945384	6	2.665895	-0.517426	1.512700
1	1.667192	0.995163	3.030500	1	3.730654	-0.527939	1.226745
1	1.996475	2.661035	3.563934	1	2.547125	0.177719	2.359541

1	2.396858	-1.526476	1.864739	1	1.373939	1.785282	1.625925
6	1.740619	-1.221386	-1.352952	1	-0.409195	1.666973	1.562291
1	1.439826	-2.234455	-1.039807	1	0.540389	0.445754	2.455740
1	1.100797	-0.926466	-2.201178	6	0.524420	1.085519	-1.558454
1	2.778874	-1.274489	-1.720353	1	1.373810	1.785320	-1.626099
6	2.026036	1.731030	-0.508222	1	0.539664	0.446003	-2.455654
1	1.891683	2.462332	0.305458	1	-0.409348	1.667321	-1.561793
1	3.075490	1.784266	-0.842561	6	2.148055	-1.051565	-0.000139
1	1.386535	2.042075	-1.350170	1	3.071519	-0.449362	-0.000125
6	-1.739431	1.217303	-1.356606	1	2.163915	-1.698639	0.891293
1	-1.437677	2.231055	-1.046632	1	2.163879	-1.698526	-0.891657
1	-1.100039	0.919179	-2.204034	CH3OSiMe3 (dimer structure)			
1	-2.777701	1.270224	-1.724009	6	-0.950445	2.715293	0.000000
6	-2.027741	-1.732283	-0.503012	1	-0.839643	3.822507	0.000000
1	-1.387916	-2.046761	-1.343446	8	-0.008317	1.960253	0.000000
1	-1.894761	-2.461074	0.313145	8	-2.225458	2.365864	0.000000
1	-3.076996	-1.785472	-0.837961	14	-2.809264	0.716488	0.000000
6	-2.665395	0.522845	1.511132	6	-2.225458	-0.125723	1.562028
1	-3.730138	0.533539	1.225118	1	-2.752079	-1.086319	1.685968
1	-2.547328	-0.169898	2.360037	1	-1.151135	-0.345373	1.499309
1	-2.395394	1.532676	1.860181	1	-2.427459	0.494799	2.449663
CH2(OSiMe3)2				6	-2.225458	-0.125723	-1.562028
6	0.029909	-1.488708	-0.362796	1	-2.752079	-1.086319	-1.685968
1	-0.182724	-1.915051	0.641973	1	-2.427459	0.494799	-2.449663
1	-0.295103	-2.222266	-1.125889	1	-1.151135	-0.345373	-1.499309
8	1.389074	-1.283821	-0.518304	6	-4.663611	0.979925	0.000000
8	-0.668436	-0.281960	-0.525193	1	-5.191002	0.011735	0.000000
14	2.224990	0.093573	0.004290	1	-4.984871	1.541783	0.891752
14	-2.219281	0.103611	0.012200	1	-4.984871	1.541783	-0.891752
6	1.968625	1.524543	-1.183538	6	0.950445	-2.715293	0.000000
1	0.913329	1.834654	-1.189901	1	0.839643	-3.822507	0.000000
1	2.592263	2.390267	-0.904025	8	0.008317	-1.960253	0.000000
1	2.240578	1.226479	-2.209169	8	2.225458	-2.365864	0.000000
6	4.022144	-0.443303	-0.004041	14	2.809264	-0.716488	0.000000
1	4.684394	0.389057	0.286145	6	2.225458	0.125723	1.562028
1	4.192167	-1.276722	0.696275	1	2.752079	1.086319	1.685968
1	4.321984	-0.780580	-1.009356	1	1.151135	0.345373	1.499309
6	1.677162	0.559026	1.745245	1	2.427459	-0.494799	2.449663
1	1.728202	-0.308965	2.422975	6	2.225458	0.125723	-1.562028
1	2.326136	1.347829	2.160505	1	2.752079	1.086319	-1.685968
1	0.643055	0.935547	1.747286	1	2.427459	-0.494799	-2.449663
6	-2.378016	-0.289470	1.846130	1	1.151135	0.345373	-1.499309
1	-3.365576	0.026098	2.221862	6	4.663611	-0.979925	0.000000
1	-2.279489	-1.368962	2.045143	1	5.191002	-0.011735	0.000000
1	-1.609109	0.234867	2.435725	1	4.984871	-1.541783	0.891752
6	-2.379473	1.940888	-0.310135	1	4.984871	-1.541783	-0.891752
1	-2.227442	2.161384	-1.378805	HSiMe(OMe)2			
1	-3.376920	2.311671	-0.022859	14	0.011229	0.585193	-0.591438
1	-1.626856	2.506112	0.262563	1	0.020576	1.268969	-1.901020
6	-3.484955	-0.880139	-0.969576	6	-0.122886	1.771398	0.855787
1	-4.513341	-0.610382	-0.676910	1	-0.080307	1.251786	1.826947
1	-3.377582	-0.688677	-2.049526	1	0.703931	2.499371	0.831462
1	-3.365371	-1.963714	-0.804628	1	-1.072079	2.330229	0.816566
HCO2SiMe3				8	-1.303386	-0.436989	-0.615739
6	-1.950516	-0.727310	-0.000004	8	1.452781	-0.245629	-0.523856
1	-2.616276	-1.618511	0.000157	6	-1.910248	-1.090727	0.469623
8	-2.357738	0.407061	0.000066	1	-2.092790	-0.411457	1.323908
8	-0.671852	-1.090308	-0.000039	1	-2.883846	-1.492990	0.146542
14	0.640338	0.055903	-0.000015	1	-1.300553	-1.938249	0.835015
6	0.524656	1.085310	1.558585	6	1.903626	-1.068683	0.521962

1 1.367952 -2.036039 0.540932
1 2.975126 -1.280052 0.376245
1 1.786665 -0.595249 1.516068

CF₃CO₂SiMe(OMe)₂

6 1.104862 0.484940 0.090439
8 0.960419 1.679675 0.114666
8 0.160039 -0.426717 0.194898
14 -1.531851 -0.058808 0.356890
6 -1.824891 0.769890 1.980682
1 -2.893405 1.000417 2.113273
1 -1.507092 0.116889 2.807772
1 -1.252322 1.708300 2.034456
6 2.492555 -0.179442 -0.061096
9 3.440763 0.737430 -0.221323
9 2.776574 -0.902584 1.029969
9 2.503171 -0.996062 -1.121999
8 -1.978681 0.795768 -0.971643
8 -2.229582 -1.537800 0.314418
6 -2.012718 2.195512 -1.179971
1 -2.371029 2.382778 -2.203228
1 -2.706900 2.688937 -0.476713
1 -1.013784 2.642854 -1.059593
6 -2.134441 -2.467272 -0.749903
1 -2.554932 -2.051963 -1.681584
1 -1.085153 -2.755454 -0.934516
1 -2.703808 -3.367677 -0.475771