Electronic Supplementary Information

Using soft X-ray absorption spectroscopy to evaluate the electronic structures of sp^2-hybridized carbons in organic solvents

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1. General Methods and Materials

Materials

Ph–Si(OCH_2CH_2O)$_2$[1] and Ph–Si(OMe)$_3$F[2] were prepared according to the previous literature procedures. Anhydrous THF was purchased from KANTO. Ethylene glycol (FUJIFILM Wako Pure Chemical Corporation) was degassed by three freeze-pump-thaw cycles. Other chemicals were obtained from commercial suppliers unless otherwise noted.

General Methods

All reactions with oxygen- or moisture-sensitive reagents were performed under a nitrogen atmosphere, nitrogen gas was dried by passage through P_2O_5. Elemental analyses were performed on a J-SCIENCE LAB MICRO CORDERJM10. ^{1}H, ^{13}C, ^{19}F, ^{31}P NMR spectra were recorded on JEOL JNM-ECZ400R/S1 spectrometer (396 MHz at ^{1}H, 100 MHz at ^{13}C, ^{19}F at 376 MHz ^{31}P at 160 MHz). Chemical shifts are reported in δ (ppm) referenced to an internal tetramethylsilane standard for ^{1}H NMR. Chemical shifts of ^{13}C NMR are given related to solvent peak as an internal standard ($CDCl_3$: δ 77.0 or DMSO-d_6: δ 39.5). Fluorine chemical shifts were referenced to the fluorine signals of CF_3CO_2H at −75.4 ppm ($CDCl_3$) and trifluoromethylbenzene (THF-d_8) at −63.5 ppm.[3] Chemical shifts of ^{31}P NMR were obtained related to PPh_3 (δ −4.20) in $CDCl_3$ as an external standard. ^{1}H, ^{13}C, ^{31}P, and ^{19}F NMR spectra were recorded in $CDCl_3$ or THF-d_8 at 25 °C. IR measurements were performed on JASCO FT/IR-460plus spectrometer in the ATR mode.

XAS experiments

Soft X-ray absorption spectroscopy (XAS) was measured at the soft X-ray beamline BL3U at the UVSOR-III Synchrotron.[4] The energy resolution of the incident soft X-rays were 0.14 eV at the C K-edge. The photon energies were precisely calibrated by measuring XAS of the polymer film before and after the sample measurements.[5] The detail of the transmission-type liquid cell for XAS of liquid samples was described previously.[6, 7] The liquid cell was in an ambient pressure of helium gas, where a liquid layer was sandwiched between two 100 nm-thick Si_3N_4 membranes. The thickness of the liquid layer was precisely controlled from 20 nm to 40 μm by adjusting the helium pressure around the liquid cell for appropriate absorbance of soft X-ray. XAS spectra were obtained using the Beer–Lambert law, $\ln(I_0/I)$, where I_0 and I were the transmission signals of the Si_3N_4 membranes and liquid samples confined by the Si_3N_4 membranes, respectively. The liquid samples were filled in the syringes under the argon-filled globe box and were introduced to the liquid cell with the typical flow rate of 200 ~ 500 μl/min using the syringe pump by preventing the air environment. The liquid cell was cleaned by flowing pure solvents before the sample measurements.

2. C K-edge XAS Spectra of Organic Solvents

Figure S1 shows C K-edge XAS spectra of organic solvents. Note that small spectral fluctuations around 286 eV come from the carbon contamination of the beamline. The XAS spectra were obtained by the Beer-Lambert law, $\ln(I_0/I)$, where the transmissions of Si_3N_4 membranes were measured as I_0 and those of liquid samples confined by the Si_3N_4 membranes were measured as I, respectively. Most of the carbon contamination peak was diminished in this procedure; however, small spectral fluctuations were sometimes observed because the I_0 and I intensities were not measured at the same time. The previous studies determined the energy thresholds (pre-edge features), where methanol is 287.6 eV,[8] ethanol is 286.5 eV,[9] and acetonitrile is 286.4 eV,[10] respectively. The energy threshold of hexane is 286.2 eV, that of tetrahydrofuran is 286.0 eV, that of ethylene glycol is 287.8 eV, that of dimethyl sulfoxide is 286.2 eV, that of acetic acid is 287.0 eV, that of *N,N*-dimethylformamide is 287.2 eV, and that of acetone is 286.2 eV, respectively.

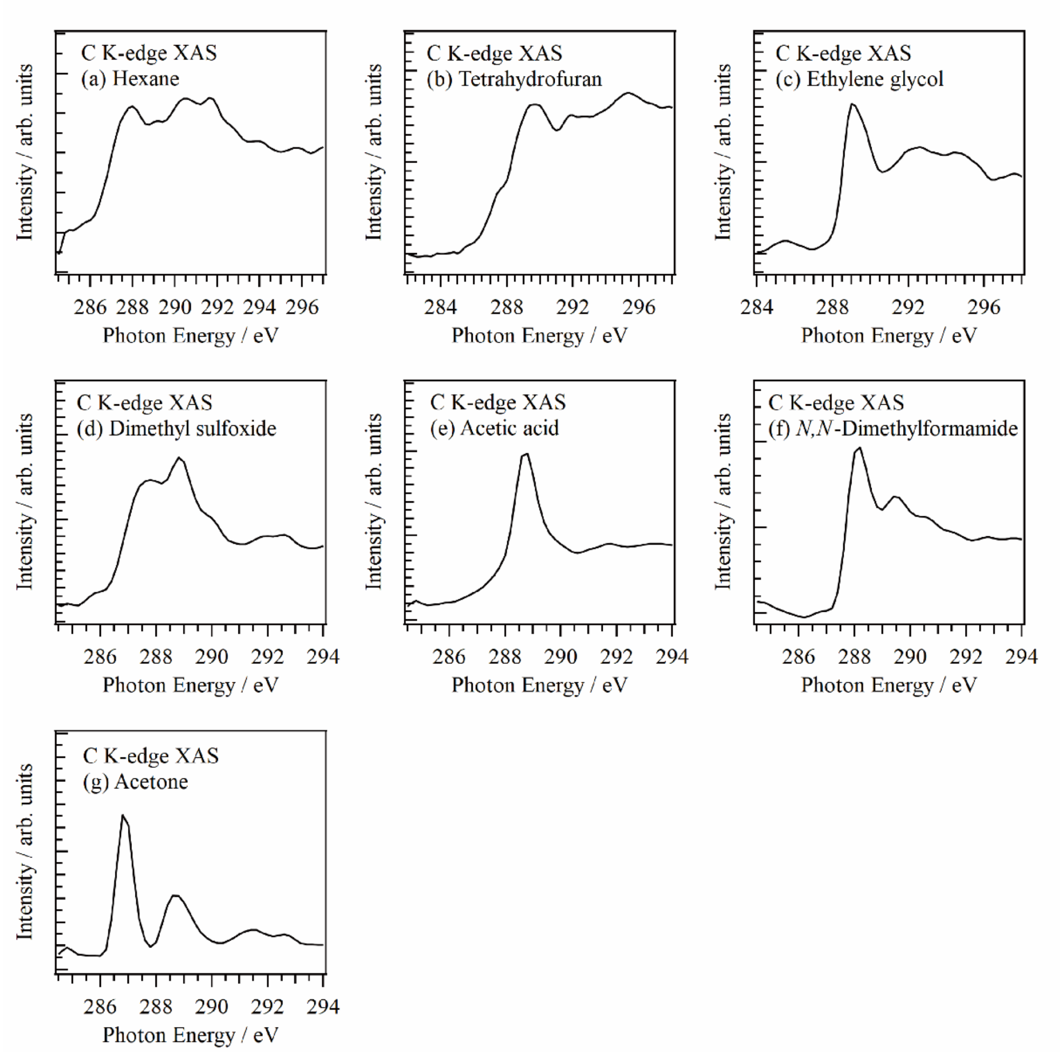


Figure S1. C K-edge XAS spectra of organic solvents. (a) hexane, (b) tetrahydrofuran, (c) ethylene glycol, (d) dimethyl sulfoxide, (e) acetic acid, (f) *N,N*-dimethylformamide, and (e) acetone.

3. C K-edge XAS Spectra of Organic Molecules Containing sp^2 Carbons

Figure S2 shows C K-edge XAS spectra of organic molecules containing sp^2 carbons in liquid phases. The previous studies determined that the energetic positions of the C=C π* peaks in benzene are 285.1 eV,[11] and those of ortho carbon and meta + para carbons of the pyridine are 285.5 eV and 285.0 eV, respectively.[12] The energetic positions of the C=C π* peaks in toluene are 285.2 eV, those in chlorobenzene is 285.2 eV, those in 1-hexene is 285.0 eV, those in 2,3-dimethyl-2-butene is 285.4 eV, and those in ethyl acrylate is 284.5 eV, respectively.

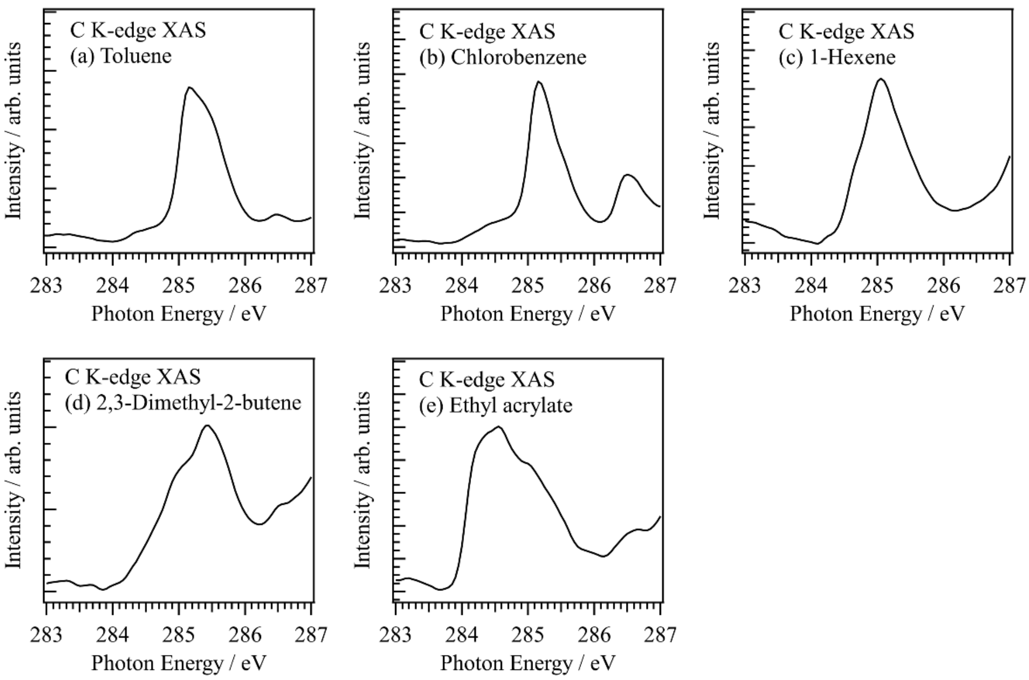


Figure S2. C K-edge XAS spectra of organic molecules containing sp^2 carbon in liquid phases. (a) Toluene, (b) chlorobenzene, (c) 1-hexene, (d) 2,3-dimethyl-2-butene, and (e) ethyl acrylate.

4. Preparations of Arylsilanes and Silicates

<u>100 mM Ph–Si(OMe)$_3$ in THF solution</u>

In a grove box, Ph–Si(OMe)$_3$ (1930 mg) (purchased from TCI) was dissolved in THF (98 mL).

<u>100 mM Ph–Si(OCH$_2$CH$_2$O)$_2$ in ethylene glycol solution</u>

In a grove box, Ph–Si(OCH$_2$CH$_2$O)$_2$ (1063 mg), prepared according to a published procedure[1], was dissolved in degassed ethylene glycol (39 mL).

<u>100 mM Ph–Si(OMe)$_3$F in THF solution</u>

Ph–Si(OMe)$_3$F was prepared according to the literature.[2] In a glove box, Ph–Si(OMe)$_3$ (1968 mg) and THF (90 mL) was added to a TBAF solution in THF (1 M, 10 mL, 1 equiv). The resulting mixture was stirred at room temperature for 30 minutes to afford the Ph–Si(OMe)$_3$F solution.

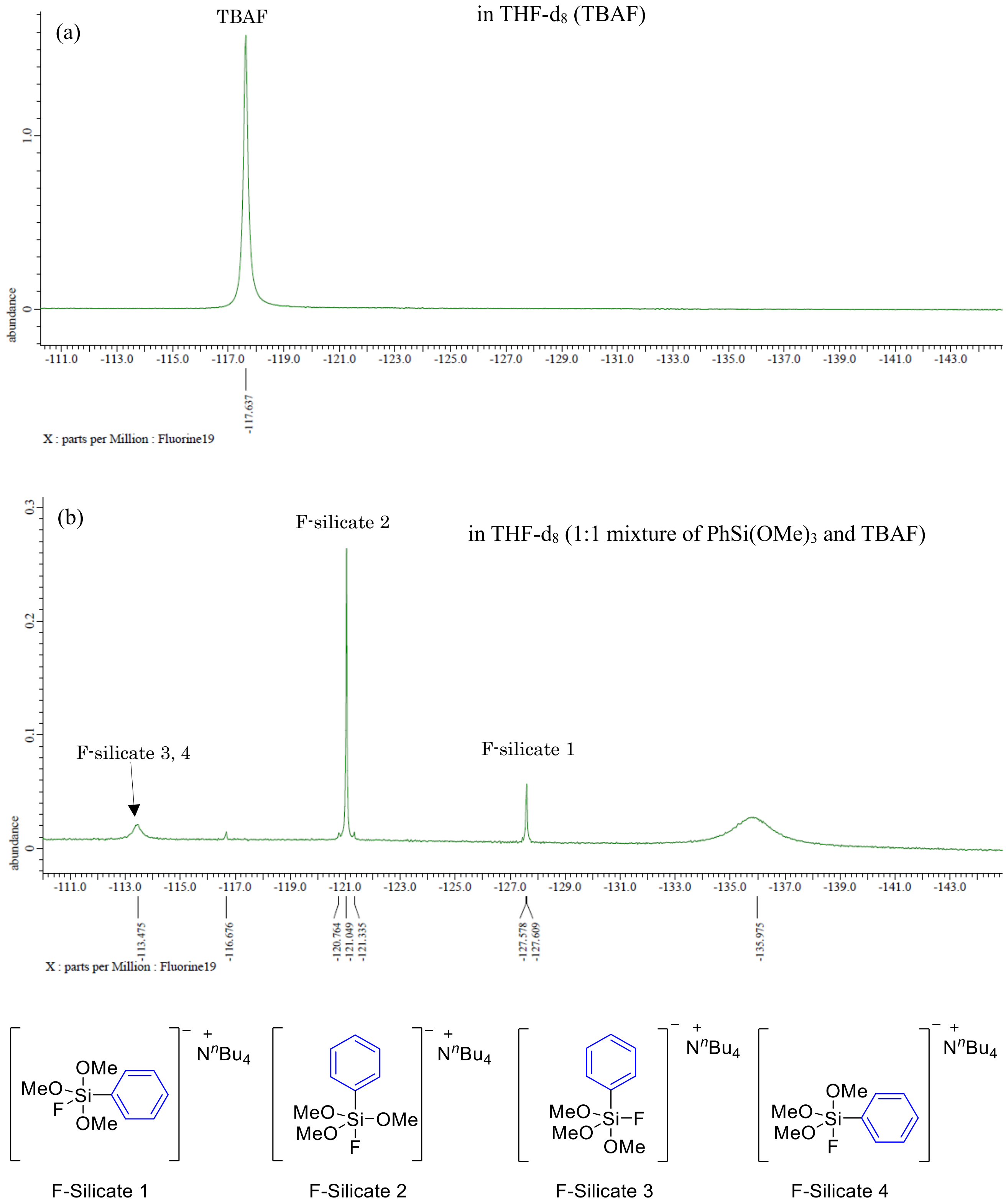
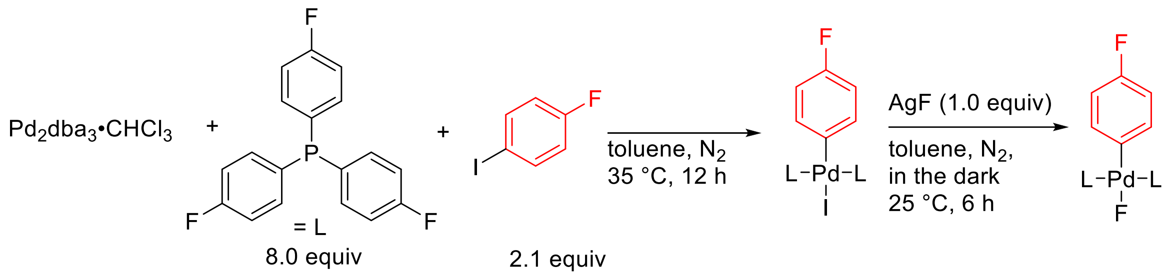


Figure S3. [19]F NMR spectra in THF-d_8 of (a) TBAF and (b) Ph-Si(OMe)$_3$F.

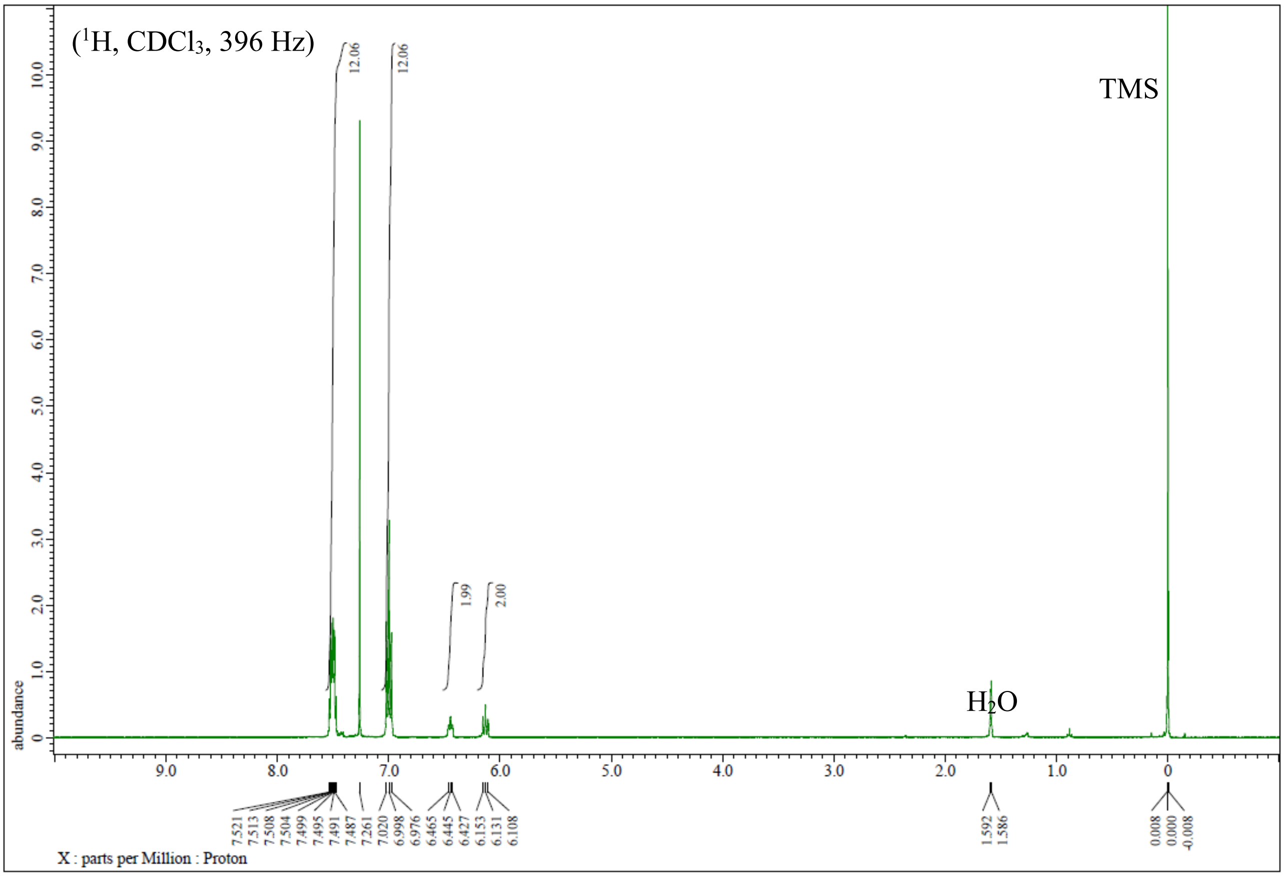
5. Stoichiometric Reactions

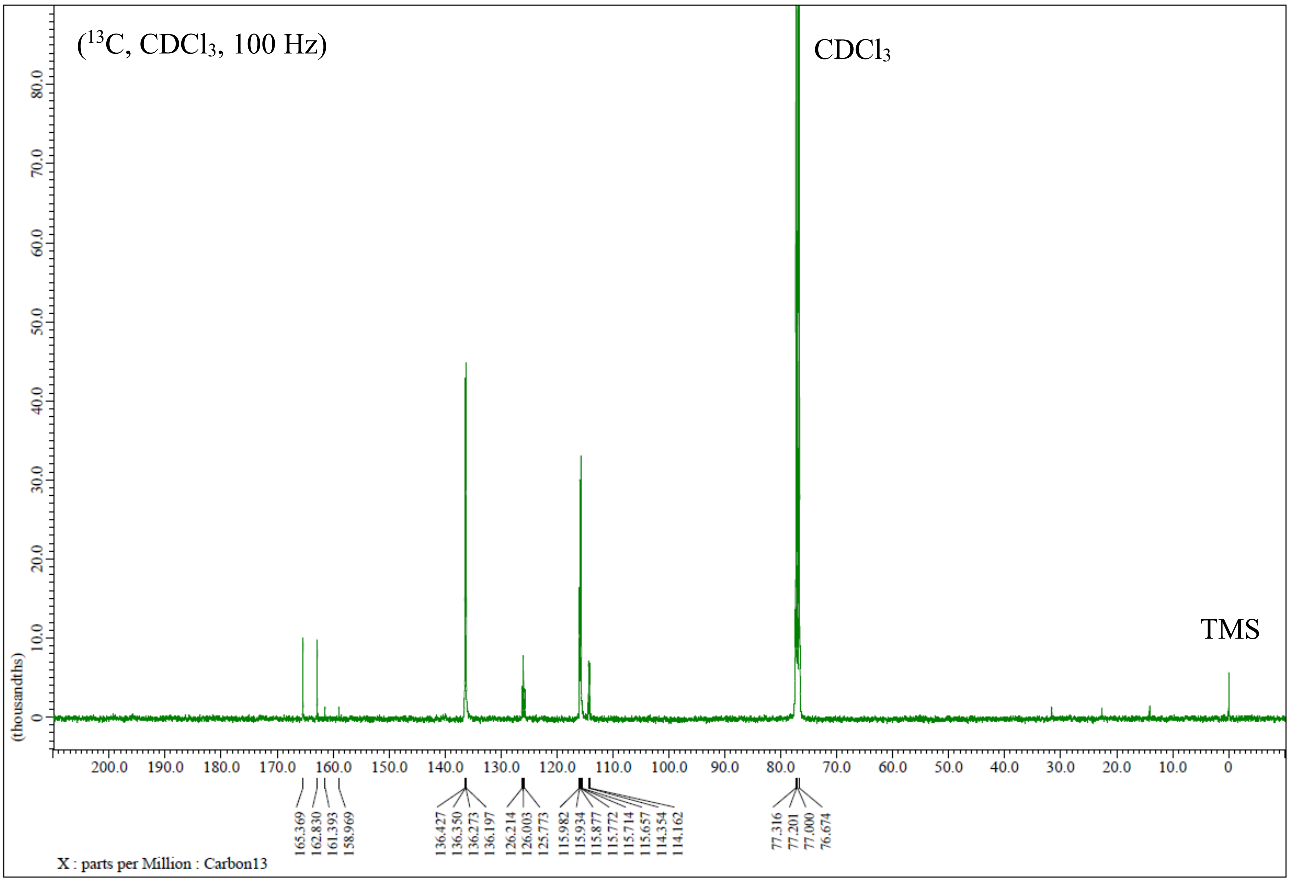
5-1. Synthesis of Palladium Complex [Bu_4N][*p*-F-C_6H_4-PdF(PPh_3)] 1

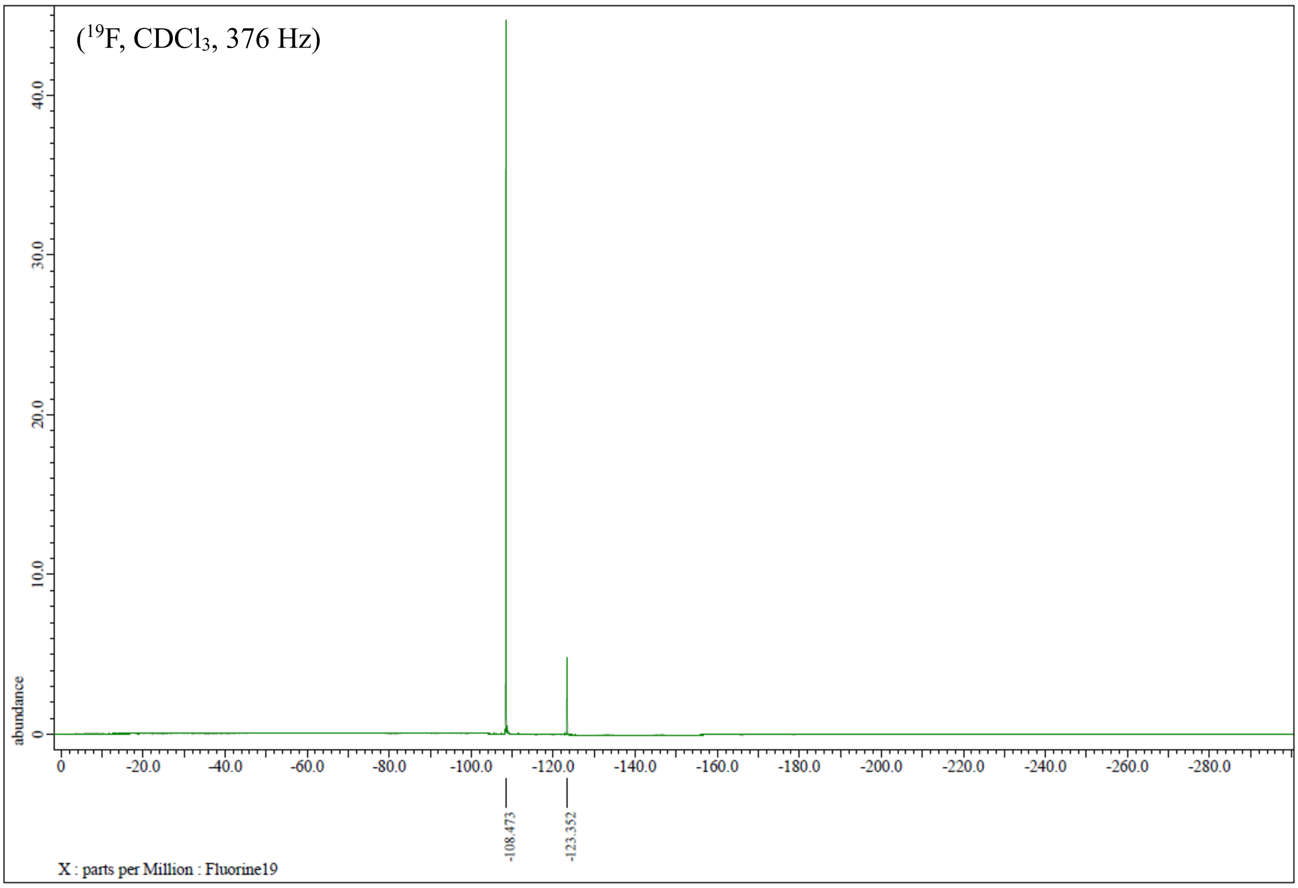


To a mixture of Pd_2dba_3•$CHCl_3$ (200 mg, 0.194 mmol) and tris(4-fluorophenyl)phosphine (492 mg, 1.55 mmol) in dry toluene (5.0 mL) was added 4-fluoroiodobenzene (46 µL, 0.4 mmol) under N_2. The mixture was stirred at 35 ºC for 12 h under N_2. After the mixture was cooled to 25 ºC, the resulting solution was concentrated under reduced pressure to give a crude product that was purified by recrystallization from hot hexane to give a white solid (297 mg). In a glove box, the white solid (200 mg) was dissolved in dry toluene (8.0 mL), and silver fluoride (79 mg, 0.62 mmol) was added to the solution. The mixture was stirred vigorously at 25 ºC in the dark. After 6 h, the resulting mixture was passed through a pad of Celite®. The resulting solution was concentrated under reduced pressure, and the obtained yellow solid was redissolved in minimum amount of $CHCl_3$ (ca. 0.5 mL). The solution was added dropwise into hexane (20 mL) to give a colorless solid which was subsequently filtered and washed with hexane (1 mL× 3) to furnish the titled product **1** (107 mg, 0.13 mmol) in 64% yield. [CAS: none] Colorless solid. Mp. 100-105 ºC (decomp.). ^{1}H NMR (396 MHz, $CDCl_3$) δ 7.54–7.47 (m, 12H), 7.00 (t, J = 8.8 Hz, 12H), 6.45 (t, J = 8.0 Hz, 2H), 6.13 (t, J = 8.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.10 (d, J = 253.9 Hz), 160.18 (d, J = 242.4 Hz), 136.31 (dd, J = 7.7, 7.7 Hz), 126.00 (dd, J = 23.0 Hz), 115.82 (ddd, J = 79.4, 5.7, 5.7 Hz), 114.26 (d, J = 19.2 Hz). Other two peaks overlapped.^{19}F NMR (372 MHz, $CDCl_3$) δ −108.47, −123.35. ^{31}P NMR (160 MHz, $CDCl_3$) δ 18.17. IR (ATR): 3073, 1588, 1493, 1394, 1228, 1160, 1096, 1012, 811, 725 cm^{-1}. Anal. Calcd for $C_{42}H_{28}F_8P_2Pd\cdot 1/2H_2O$: C, 58.52: H, 3.39. Found: C, 58.23: H, 3.39.

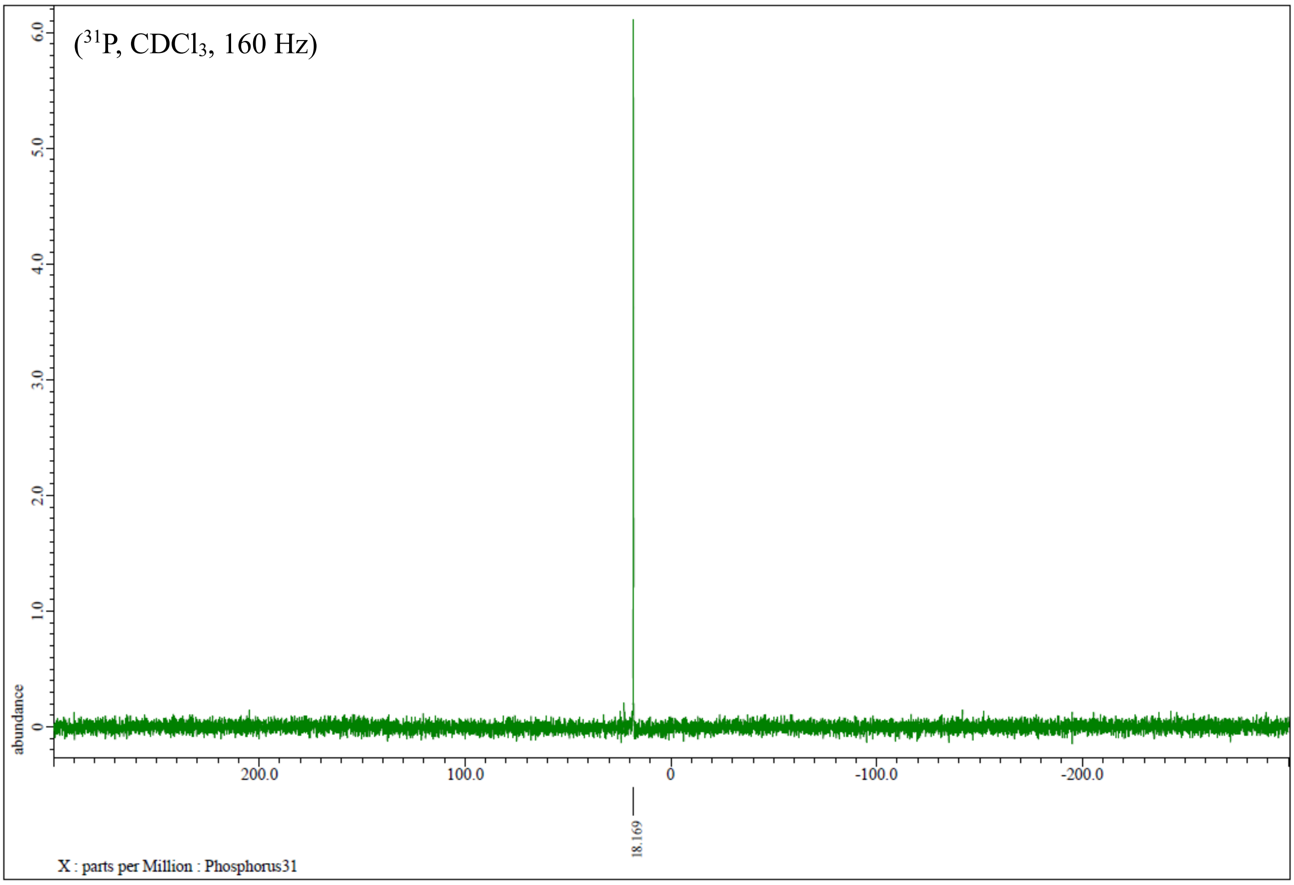
^{1}H, ^{13}C, ^{19}F, and ^{31}P NMR charts





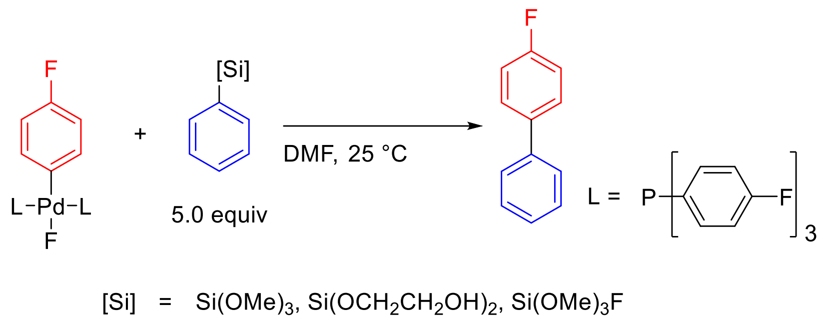


(19F, CDCl3, 376 Hz)
abundance
0
10.0
20.0
30.0
40.0
0
-20.0
-40.0
-60.0
-80.0
-100.0
-120.0
-140.0
-160.0
-180.0
-200.0
-220.0
-240.0
-260.0
-280.0
-108.473
-123.352
X : parts per Million : Fluorine19



(31P, CDCl3, 160 Hz)
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
200.0
100.0
0
-100.0
-200.0
18.169
X : parts per Million : Phosphorus31

5-2. Stoichiometric Reactions between $[Bu_4N][p\text{-}F\text{-}C_6H_4\text{-}PdF(PPh_3)]$ (1) and Silicon Reagents



Arylpalladium fluoride **1** (4.11 mg, 0.005 mmol) and 4-trifluoromethylbiphenyl (1.11 mg, 0.005 mmol) were charged into a J-Young tube and transferred into a glove box. A silicon reagent (Ph–Si(OMe)$_3$, Ph–Si(OCH$_2$CH$_2$O)$_2$, or Ph–SiF(OMe)$_3$, 0.025 mmol) and dry DMF (0.5 mL) were sequentially added into the J-Young tube. After shaken the reaction mixture vigorously, the reaction progress was measured by ^{19}F NMR at 25 ºC. NMR yields of 4-fluoromethylbiphenyl (δ = −116.17 ppm) were determined related to the integration of 4-trifluoromethylbiphenyl (δ = −61.40 ppm) as an internal standard.

Table S1. Results for the Stoichiometric reaction of Arylpalladium fluoride **1** with Silicon Reagents

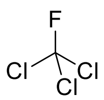
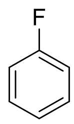
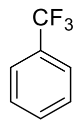
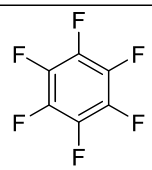
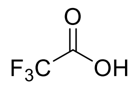
Time / min	NMR yield /%		
	Ph–Si(OMe)$_3$	Ph–Si(OCH$_2$CH$_2$O)$_2$	Ph–SiF(OMe)$_3$
0	0	0	0
5	6	74	0
9	9	85	2
12	12	85	4
16	15	85	4
19	16	85	5
24	18	85	5
27	19	85	5
30	21	85	5
40	32	85	6
50	38	85	9
60	43	85	11

6. DFT predicted ^{19}F NMR

All calculations were carried out with the Gaussian16 program.[13] Geometry optimizations and frequency calculations for all molecules were performed at the M062X/6-31+G(d)[14-17] and SMD implicit solvation (THF). The magnetic shielding tensors were calculated with the gauge including Atomic Orbital (GIAO)[18, 19] theory at the M062X/6-31+G(d) and SMD implicit solvation (THF). The computations were also performed using Research Center for Computational Science, Okazaki, Japan.

To determine the linear regression scaling factor, the magnetic shielding tensors of fluorinated compounds S1-S5 as training set molecules were calculated with GIAO theory at the M062X/6-31+G(d)[14-17] and SMD implicit solvation (THF). Geometries of these compounds were optimized at the same level of theory (Table S2). The linear fit for computed 13C isotropic shielding constants plotted against corresponding experimental chemical shifts[3] for S1-S5 was observed. The correlation coefficient, slope and intercept were found to be 0.9986, -1.0359 and 188.29 respectively (Figure S4).[20]

Table S2. Experimental ^{19}F chemical shifts and calculated shielding tensors of compounds S1-S5.

	Chemical Shift /ppm				
	 **S1**	 **S2**	 **S3**	 **S4**	 **S5**
Experimental chemical shifts[3]	−0.93	−114.31	−63.47	−164.51	−76.93
Calculated shielding tensors	186.83	308.64	256.51	356.14	268.54

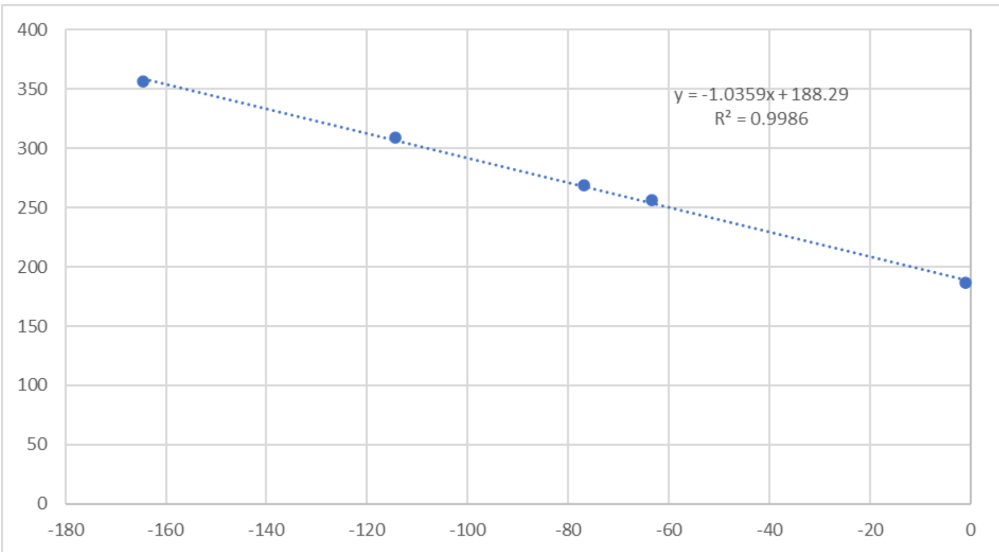


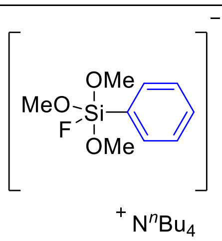
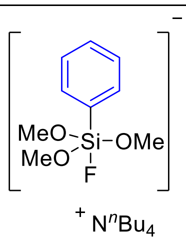
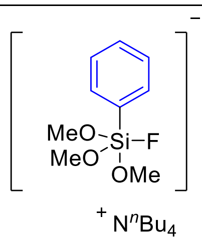
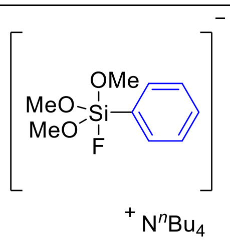
Figure S4. Linear regression between experimental chemical shifts and calculated shielding tensors of compounds S1-S5.

The geometries of F-silicate 1–4 were optimized at the M062X/6-31+G(d)[14-17] and SMD implicit solvation (THF) (Table S3). The magnetic shielding tensors σ were calculated with GIAO theory at the same level of theory. Using the linear regression data, scaled ^{19}F NMR chemical shifts δ were determined with eq. (1).

$$\delta = \frac{intercept - \sigma}{-slope} \tag{1}$$

(*slope*: -1.0359, *intercept*: 188.29)

Table S3. Calculated ^{19}F chemical shifts of F-Silicates 1-4.

	 F-Silicate 1	 F-Silicate 2	 F-Silicate 3	 F-Silicate 4
Calculated shielding tensors /ppm	318.1755	312.1286	299.5590	300.1847
Scaled NMR shifts /ppm	−125.38	−119.55	−107.41	−108.02
Experimental NMR shifts /ppm	−127.609	−121.049	−113.475	−113.475

7. Inner-shell Calculations

7-1. Methods for Molecular Dynamics Simulations

Molecular dynamics (MD) simulations were performed using the program package GROMACS 2022.4.[21] The potentials of molecules were described by the OPLS-AA force field, generating using the LigParGen server.[22-24] The cubic boxes of the MD simulations included one arylsilane molecule, 1000 solvent molecules of THF or EG, and several Na^+ ions for the charge neutralization. The temperature was controlled using the Nosé-Hoover thermostat method.[25, 26] The pressure was adjusted using the Parrinello-Rahman method.[27] The simulations were performed at a time step of 1 fs with periodic boundary conditions and the partial-mesh Ewald method.[28] The isothermal compressibility of THF and EG were taken from the previous study.[29] The equilibrium structures were obtained by the simulations, which run during 100 ps at −173.15 °C in the canonical ensemble, 100 ps at −73.15 °C and 1 atm and 2 ns at 25 °C and 1 atm in the isobaric-isothermal ensemble. The equilibrium structures were sampled at a time step of 1 ps at 25 °C and 1 atm for a simulation time of 10 ns.

7-2. Radial Distribution Functions

Figure S5(a) shows radial distribution function (RDF) of the Si atoms of various arylsilanes with the O atoms of solvent THF and the C atoms of solvent EG. The first coordination shells of solvent THF and EG molecules in the arylsilanes can be formed by selecting the solvent THF and EG molecules within 6.5 Å of the Si atoms. Figure S5(b) shows the RDF of the Si atoms of various arylsilanes with Na^+ ions. Because the Si – Na^+ distances are approximately 3.4 Å, the Na+ ions can be selected within 6.5 Å of the Si atoms.

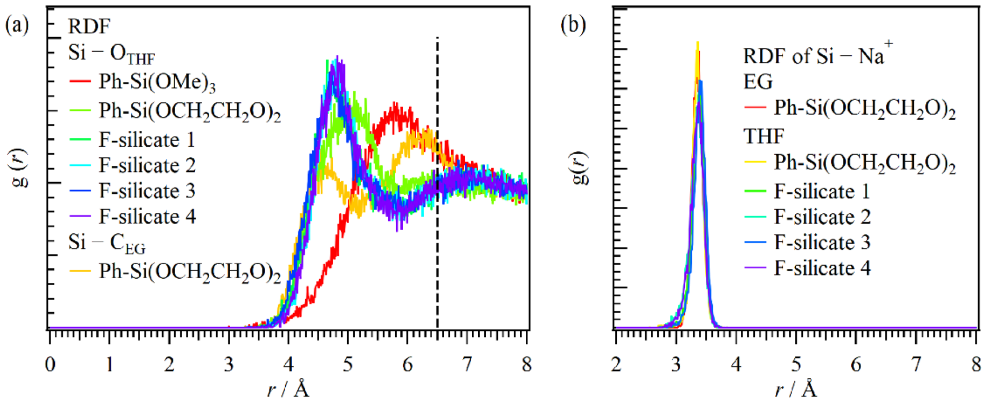


Figure S5. (a) RDF of the Si atoms of various arylsilanes with the O atoms of solvent THF and the C atoms of solvent EG. The dashed line shows the position at r = 6.5. (b) RDF of the Si atoms of various arylsilanes with Na^+ ions in EG and THF.

7-3. Methods for Inner-Shell Calculations

C K-edge inner-shell spectra of arylsilanes in solvent THF and EG were calculated using the GSCF3 code.[30, 31] The molecular structures of arylsilanes with solvent molecules and Na^+ ions were extracted from the snapshots obtained by the MD simulations, as described in Sec. 7-1. The solvent molecules and Na^+ ions were extracted within 6.5 Å of Si atoms, considering the RDF described in Sec. 7-2: The molecular distances of THF were determined from the O atoms of THF and Si atoms of arylsilanes, and those of EG were determined from the C atoms of EG with the Si atoms.

In the C K-edge inner-shell calculation, the ground and core excited states were obtained within the Hartree-Fock method, namely, ΔSCF (self-consistent field). The core hole was localized on specified C atoms. The zero point vibrational energy and electron correlation involving van der Waals interactions were ignored in the present calculations. Primitive basis functions were taken from the contracted Gaussian-type functions of Huzinaga et al., (73/7) for C, O, and F, (533/53) for Si, (6) for H, and (43/4) for Na^+.[32] The contraction schemes of excited C atoms were (3111121/3112/1*) with the polarization function ζ_d = 0.600. The other contraction schemes were (51121/52) for nonexcited C, O, and F, (5321/521/1*) with polarization function ζ_d = 0.262 for Si, and (42) for H atoms. Diffuse functions were not explicitly included because Rydberg states were not considered in the present calculations.

The molecular structures obtained from the snapshots of the MD simulations include the deviation of liquid structures.[33] The inner-shell spectra of arylsilanes including the deviation of solvent molecules are Na^+ ions were obtained by averaging 1100 inner-shell spectra of the extracted molecular structures during the 10 ns production run of the MD simulations. The calculated spectra were convoluted by Gaussian profiles with the width of 0.35 eV.

7-4. Inner-shell Calculation of Ph–Si(OCH_2CH_2O)$_2$ in Different Solvents

Figure S6 shows the calculated C K-edge inner-shell spectra of Ph–Si(OCH_2CH_2O)$_2$ in EG and THF obtained from the molecular structures by the MD simulations. Table S4 shows the energetic positions of *ipso*, *ortho*, *meta*, and *para* carbons. The energy shift of the *ipso* site in THF (−0.137 eV) is a little bit lower than that in EG (−0.112 eV). The energy shifts of the *meta* and *para* sites in THF are higher than those in EG and are close to F-silicate 2. The energetic positions of Ph–Si(OCH_2CH_2O)$_2$ are changed with different solvent molecules, but these energy differences are relatively smaller than those of F-silicate derivatives in THF.

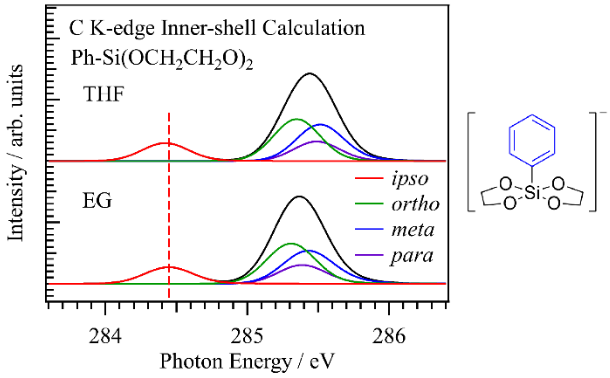


Figure S6. Calculated C K-edge inner-shell spectra of Ph–Si(OCH_2CH_2O)$_2$ in EG and THF, obtained by the snapshots from the MD simulations. The energies of the *ipso*, *ortho*, *meta*, and *para* carbons in the phenyl groups were obtained. The dashed line shows the energetic position of the ipso carbons of Ph–Si(OCH_2CH_2O)$_2$ in EG.

Table S4. The energetic positions of *ipso*, *ortho*, *meta*, and *para* carbons obtained from C K-edge inner-shell calculations of Ph–Si(OCH_2CH_2O)$_2$ in EG and THF. The energy shifts (ΔE) from Ph–Si(OMe)$_3$ are also shown.

eV	*Ipso*	ΔE	*Ortho*	ΔE	*Meta*	ΔE	*Para*	ΔE
Solvent EG	284.448	−0.112	285.310	−0.034	285.436	−0.013	285.389	0.021
Solvent THF	284.423	−0.137	285.349	0.005	285.517	0.068	285.490	0.122

7-5. Inner-shell Calculation of Different Forms of Ph–Si(OMe)$_3$F

Figure S7 shows the calculated C K-edge inner-shell spectra of F-silicate 1, F-silicate 2, F-silicate 3, and F-silicate 4 in THF. Table S5 shows the energetic positions of *ipso*, *ortho*, *meta*, and *para* carbons of these F-silicate derivatives.

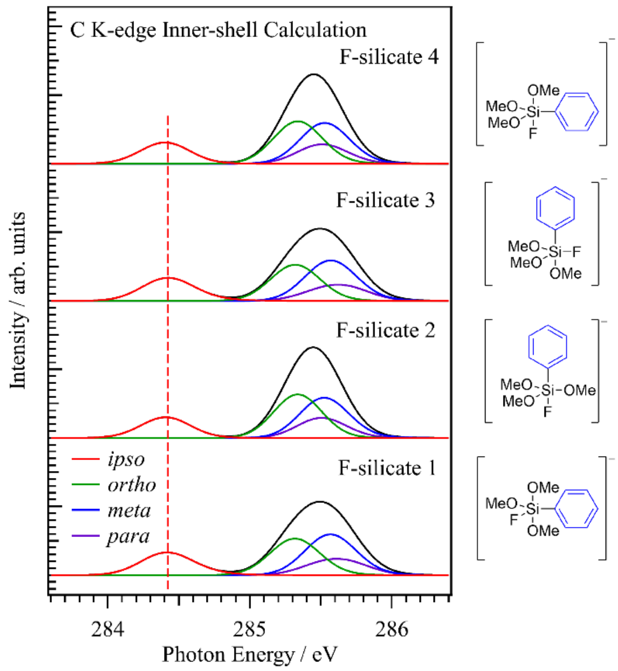


Figure S7. Calculated C K-edge inner-shell spectra of F-silicate 1, F-silicate 2, F-silicate 3, and F-silicate 4 in THF, obtained by the snapshots from the MD simulations. The energies of the *ipso*, *ortho*, *meta*, and *para* carbons in the phenyl groups were obtained. The dashed line shows the energetic position of the ipso carbons of F-silicate 1 in THF.

Table S5. The energetic positions of *ipso*, *ortho*, *meta*, and *para* carbons obtained from C K-edge inner-shell calculations of F-silicate 1, F-silicate 2, F-silicate 3, and F-silicate 4. The energy shifts (ΔE) from Ph–Si(OMe)$_3$ are also shown.

eV	*Ipso*	ΔE	*Ortho*	ΔE	*Meta*	ΔE	*Para*	ΔE
F-silicate 1	284.424	−0.136	285.318	−0.026	285.570	0.121	285.608	0.240
F-silicate 2	284.406	−0.154	285.338	−0.006	285.526	0.077	285.508	0.140
F-silicate 3	284.430	−0.130	285.320	−0.024	285.572	0.123	285.615	0.247
F-silicate 4	284.402	−0.158	285.339	−0.005	285.529	0.080	285.513	0.145

7-6. Evaluation of Solvent Effects in Inner-shell Calculation

Figure S8(a) shows the calculated C K-edge inner-shell spectrum of Ph–Si(OMe)$_3$ with no solvent THF molecules, together with that with THF molecules. The inner-shell spectrum of Ph–Si(OMe)$_3$ without solvent molecules was obtained by averaging 1100 inner-shell spectra of the extracted Ph–Si(OMe)$_3$ molecules removing solvent THF molecules from the snapshots of the MD simulations. Although the energetic position of the ipso carbons without THF molecules show a slightly higher energy shift than that with THF molecules, these energy shifts are sufficiently small relative to the energy shifts between different silicate molecules. It means that the energetic position of the ipso carbons in Ph–Si(OMe)$_3$ is not influenced with solvent THF molecules.

Figure S8(b) shows the calculated C K-edge inner-shell spectra of F-silicate 1 with no solvent THF molecules and with no Na^+ ions and THF molecules, together with that with Na^+ ions and THF molecules. These inner-shell spectra were also obtained by averaging 1100 inner-shell spectra of extracted molecular structures removing solvent molecules. The inner-shell spectrum of F-silicate 1 without solvent THF molecules is nearly the same spectral shape as that with solvent THF molecules, indicating the solvent molecules do not affect the inner-shell spectrum of F-silicate 1. By contrast, the inner-shell spectrum of F-silicate 1 without Na^+ ions shows different spectral shape relative to that with solvent molecules: The energetic position of the ipso carbons shows a lower energy shift and the spectral shape related to the ortho, meta, and para carbons is changed. It means that the charge neutralization of F-silicate 1 with Na^+ ions is important for calculating the inner-shell spectrum of F-silicate 1. The inner-shell spectrum of F-silicate 1 is not influenced by solvent THF molecule with neutral charges.

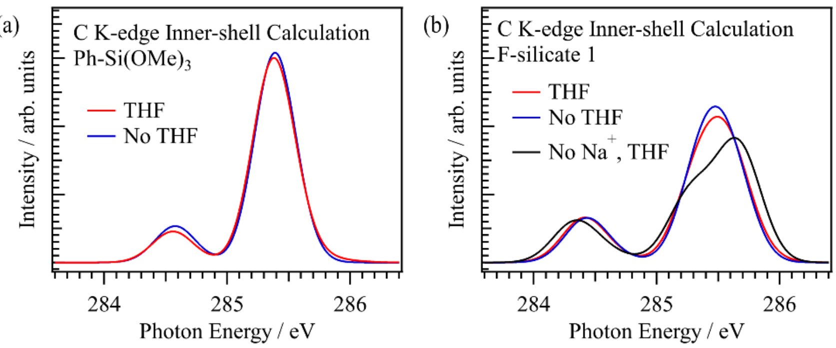
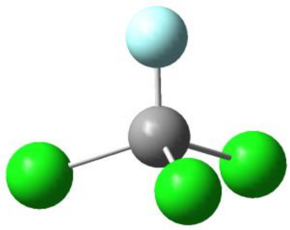


Figure S8. Calculated C K-edge inner-shell spectrum of Ph–Si(OMe)$_3$ with no solvent THF molecules, together with that with THF molecules. (b) Calculated C K-edge inner-shell spectra of F-silicate 1 with no solvent THF molecules and with no Na^+ ions and solvent THF molecules, together with that with Na^+ ions and THF molecules.

8. Cartesian Coordinates

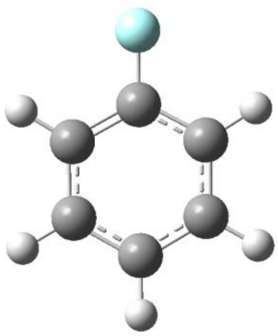
$CFCl_3$ S1



Zero-point correction=	0.011454 (Hartree/Particle)
Thermal correction to Energy=	0.016569
Thermal correction to Enthalpy=	0.017513
Thermal correction to Gibbs Free Energy=	-0.018557
Sum of electronic and zero-point Energies=	-1518.367397
Sum of electronic and thermal Energies=	-1518.362282
Sum of electronic and thermal Enthalpies=	-1518.361338
Sum of electronic and thermal Free Energies=	-1518.397408

C	0.00035200	-0.00004700	0.23687400
F	0.00104600	-0.00059100	1.57961000
Cl	-0.74123400	1.50926600	-0.30621500
Cl	-0.93743900	-1.39583300	-0.30657400
Cl	1.67799400	-0.11310400	-0.30707800

C_6H_5-F S2

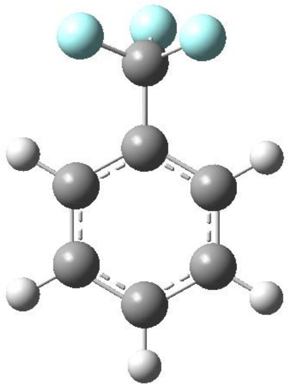


Zero-point correction=	0.093239 (Hartree/Particle)
Thermal correction to Energy=	0.098360
Thermal correction to Enthalpy=	0.099304
Thermal correction to Gibbs Free Energy=	0.064420
Sum of electronic and zero-point Energies=	-331.272684
Sum of electronic and thermal Energies=	-331.267563
Sum of electronic and thermal Enthalpies=	-331.266619
Sum of electronic and thermal Free Energies=	-331.301503

C	-1.13283300	1.20847800	-0.00000500

C	-1.83102100	0.00000100	0.00001000
C	-1.13285100	-1.20846300	-0.00002000
C	0.26224400	-1.21900500	0.00001200
C	0.92181000	-0.00001400	0.00003300
C	0.26224200	1.21899800	-0.00000200
H	-1.67255100	2.15095800	-0.00001000
H	-2.91679400	0.00001900	0.00000600
H	-1.67254700	-2.15095600	-0.00002600
H	0.83145600	-2.14324100	0.00000400
H	0.83150300	2.14320600	-0.00001500
F	2.27793100	0.00000400	-0.00001400

C_6H_5–CF_3 S3

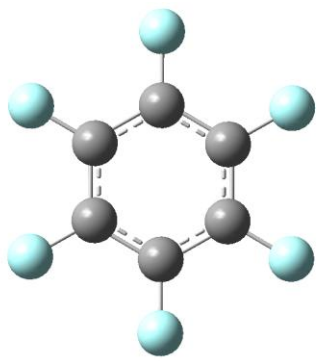


Zero-point correction= 0.106447 (Hartree/Particle)
Thermal correction to Energy= 0.114273
Thermal correction to Enthalpy= 0.115217
Thermal correction to Gibbs Free Energy= 0.072372
Sum of electronic and zero-point Energies= -569.003271
Sum of electronic and thermal Energies= -568.995445
Sum of electronic and thermal Enthalpies= -568.994500
Sum of electronic and thermal Free Energies= -569.037346

C	-2.13505100	1.20957900	0.00234600
C	-2.83019600	0.00000700	0.01171500
C	-2.13509700	-1.20956000	0.00195400
C	-0.74204900	-1.21426300	-0.01865500
C	-0.05586400	-0.00002300	-0.03171300
C	-0.74202800	1.21425400	-0.01826300
H	-2.67651100	2.15072200	0.00847500
H	-3.91641700	0.00003900	0.02514400
H	-2.67654900	-2.15071000	0.00777700

H	-0.19567600	-2.15275800	-0.02789900
H	-0.19560100	2.15272100	-0.02721000
C	1.44369800	-0.00000800	-0.00440300
F	1.97067400	-1.08155600	-0.60881200
F	1.92982200	0.00014900	1.25741000
F	1.97064600	1.08141500	-0.60906200

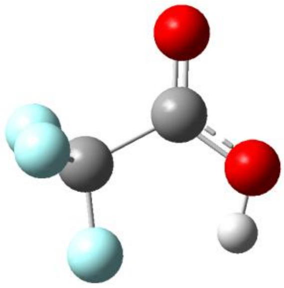
C_6F_6 S4



Zero-point correction= 0.052688 (Hartree/Particle)
Thermal correction to Energy= 0.062265
Thermal correction to Enthalpy= 0.063210
Thermal correction to Gibbs Free Energy= 0.017673
Sum of electronic and zero-point Energies= -827.317029
Sum of electronic and thermal Energies= -827.307452
Sum of electronic and thermal Enthalpies= -827.306508
Sum of electronic and thermal Free Energies= -827.352045

C	1.31147800	0.45387700	0.00009500
C	1.04856200	-0.90880700	0.00004600
C	-0.26292200	-1.36321100	-0.00007600
C	-1.31148900	-0.45384200	0.00005100
C	-1.04858600	0.90877800	0.00018800
C	0.26295900	1.36320300	0.00000000
F	-2.05518600	1.77964200	-0.00006600
F	-2.56973700	-0.88808400	0.00002900
F	-0.51494900	-2.67029500	-0.00008000
F	2.05524800	-1.77957300	0.00000600
F	2.56976700	0.88799700	-0.00000900
F	0.51485500	2.67031300	-0.00008300

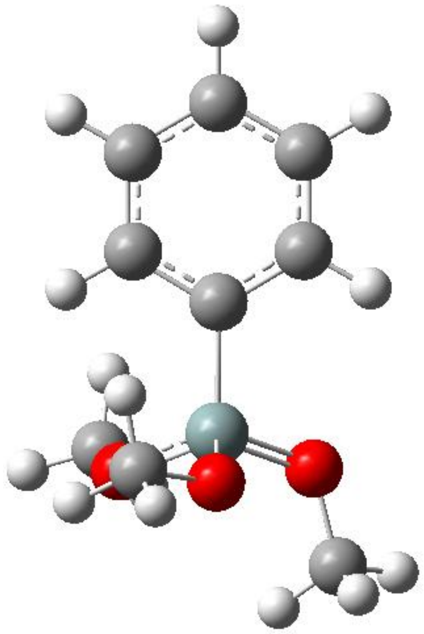
CF_3COOH S5



Zero-point correction= 0.039419 (Hartree/Particle)
Thermal correction to Energy= 0.045626
Thermal correction to Enthalpy= 0.046570
Thermal correction to Gibbs Free Energy= 0.008034
Sum of electronic and zero-point Energies= -526.594434
Sum of electronic and thermal Energies= -526.588227
Sum of electronic and thermal Enthalpies= -526.587282
Sum of electronic and thermal Free Energies= -526.625819

C	0.96146300	0.15026300	-0.00685200
O	1.44728400	1.24345200	-0.00393700
C	-0.58041800	-0.00358800	-0.00213100
O	1.66560100	-0.97193300	0.00170600
F	-1.11786300	0.71330400	-0.98464900
F	-1.07738500	0.42933400	1.15697500
F	-0.94842100	-1.28499600	-0.16242100
H	1.10366900	-1.77098400	-0.01739100

Ph–Si(OMe)$_3$

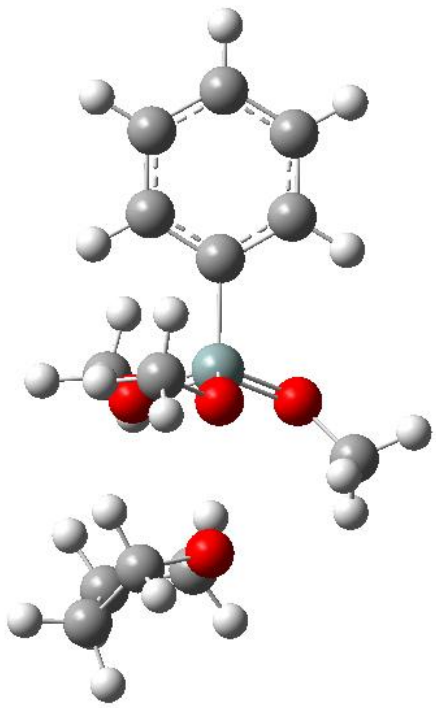


Zero-point correction=	0.222375 (Hartree/Particle)
Thermal correction to Energy=	0.238045
Thermal correction to Enthalpy=	0.238989
Thermal correction to Gibbs Free Energy=	0.177164
Sum of electronic and zero-point Energies=	-866.187938
Sum of electronic and thermal Energies=	-866.172268
Sum of electronic and thermal Enthalpies=	-866.171324
Sum of electronic and thermal Free Energies=	-866.233149

C	0.92501500	0.14142400	-0.03797900
C	1.68418900	-0.96354600	0.38007100
C	3.07808300	-0.91155400	0.40158300
C	3.73539700	0.25429400	0.00751000
C	2.99772000	1.36413000	-0.40696400
C	1.60446400	1.30553100	-0.42986500
H	1.18175000	-1.87593000	0.69842000
H	1.03947200	2.17774800	-0.75104200
H	3.50807800	2.27425700	-0.71042900
H	4.82107800	0.29896400	0.02590400
H	3.64961800	-1.77625000	0.72778800
Si	-0.92804600	0.02513000	-0.10133200
O	-1.52368000	1.54484600	0.08173300
O	-1.50204700	-0.56923400	-1.52587600
O	-1.46999900	-1.01515000	1.06218100
C	-2.91817000	1.81308600	-0.02808600

H	-3.50503000	1.14188800	0.61044300
H	-3.08689200	2.84297500	0.29506000
H	-3.25258400	1.70389900	-1.06493100
C	-1.23292200	-1.90404600	-1.93537400
H	-1.66946600	-2.04569500	-2.92691100
H	-0.15292700	-2.08835500	-1.99899900
H	-1.68100300	-2.62442100	-1.24213200
C	-1.25434700	-0.75893500	2.44425300
H	-1.52297700	-1.66045200	3.00022200
H	-0.20430600	-0.51705700	2.65165500
H	-1.88292200	0.07062100	2.78841400

Ph–Si(OMe)$_3$-THF

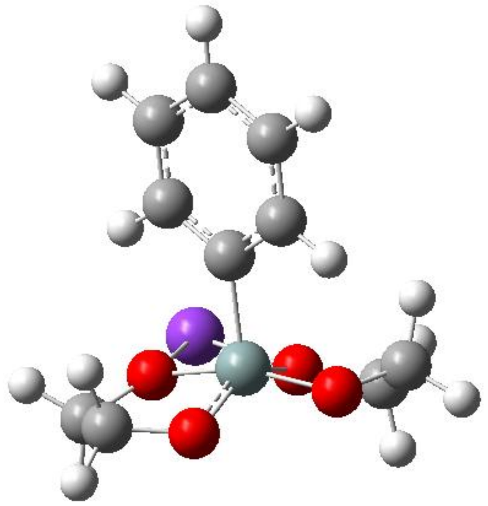


Zero-point correction= 0.342472 (Hartree/Particle)
Thermal correction to Energy= 0.364054
Thermal correction to Enthalpy= 0.364998
Thermal correction to Gibbs Free Energy= 0.290276
Sum of electronic and zero-point Energies= -1098.424178
Sum of electronic and thermal Energies= -1098.402597
Sum of electronic and thermal Enthalpies= -1098.401653
Sum of electronic and thermal Free Energies= -1098.476374

Si	-0.28826800	0.30391500	0.10573400
C	-2.12534000	0.00960500	-0.07764100
C	-3.01358900	1.06938400	-0.31486400

C	-4.39016700	0.85365700	-0.39481600
C	-4.90308500	-0.43417500	-0.23776500
C	-4.03720100	-1.50374200	-0.00357900
C	-2.66261200	-1.27969600	0.07307700
H	-1.99724800	-2.12475400	0.24772300
H	-2.62280900	2.07661800	-0.44428700
H	-5.06137800	1.68775200	-0.58187000
H	-4.43268100	-2.50899300	0.11555400
H	-5.97450200	-0.60531600	-0.30065300
O	0.03842700	1.71713000	-0.65119400
O	0.13873600	0.41938900	1.69063100
O	0.48329900	-1.01573200	-0.52167200
O	2.76234000	0.71669300	0.28750000
C	3.17438900	-0.38734400	1.09284700
H	2.32145500	-1.05953500	1.25119900
H	3.50604000	0.00259700	2.06032400
C	3.15852700	0.50324200	-1.06993500
H	3.90552800	1.26300800	-1.33885900
H	2.28240300	0.63188800	-1.71579400
C	3.75513400	-0.90339700	-1.13282500
H	2.97199700	-1.64012300	-1.34131400
H	4.53368500	-0.99170100	-1.89553900
C	4.27301300	-1.08475600	0.29740700
H	5.22940800	-0.56474500	0.42769700
H	4.40141200	-2.13200900	0.58473100
C	0.78647400	2.81969600	-0.16085500
H	1.71270000	2.91882700	-0.73454900
H	1.03992900	2.69604100	0.89479900
H	0.18412500	3.72467400	-0.29190300
C	0.25029600	-1.49818300	-1.83479000
H	-0.80397200	-1.40626700	-2.12538800
H	0.52734900	-2.55578200	-1.86511400
H	0.86075600	-0.95010100	-2.56266100
C	-0.14659200	-0.62151300	2.61214600
H	0.42033300	-0.42709900	3.52663800
H	0.14883700	-1.60201000	2.21829200
H	-1.21550100	-0.64428600	2.85814600

Ph–Si(OCH_2CH_2O)$_2$

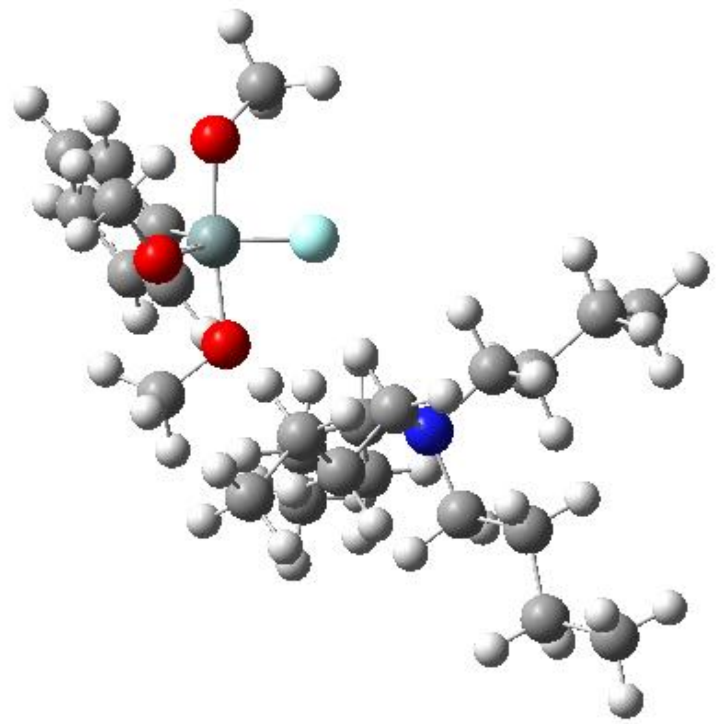


Zero-point correction= 0.226236 (Hartree/Particle)
Thermal correction to Energy= 0.241708
Thermal correction to Enthalpy= 0.242652
Thermal correction to Gibbs Free Energy= 0.181299
Sum of electronic and zero-point Energies= -1578.853676
Sum of electronic and thermal Energies= -1578.838205
Sum of electronic and thermal Enthalpies= -1578.837261
Sum of electronic and thermal Free Energies= -1578.898613

C	1.27648500	-0.03386400	-0.02871400
C	1.57937100	-1.30666200	0.48466200
C	2.87103400	-1.65299700	0.89007700
C	3.90721700	-0.72550100	0.78210900
C	3.63952600	0.54254700	0.26375100
C	2.34323400	0.87628500	-0.13255000
O	-0.62010900	0.27794000	-2.28809500
O	-0.25545400	2.16877200	-0.82896400
C	-1.44345100	-1.83073300	-1.64527800
C	-0.37336000	2.89296400	0.36323700
H	-1.42706700	2.39820500	2.21987300
H	-2.48622700	2.62896900	0.80339800
O	-1.44065500	0.85760500	0.84006400
Si	-0.48078000	0.45775900	-0.58529900
C	-0.62108600	-1.06970900	-2.68846800
H	-1.12954400	-2.88089700	-1.57373300
H	-2.51245900	-1.80736500	-1.90830800
H	-0.57677900	3.94911600	0.14982100

H	0.55839700	2.83594600	0.95286400
O	-1.23930300	-1.16353500	-0.42348500
H	0.78711500	-2.04977100	0.55431100
K	-2.20846200	-1.31950700	1.91794700
H	2.14945600	1.86665800	-0.53916100
H	-1.04781000	-1.15992300	-3.69375800
H	0.41011200	-1.45718400	-2.71600300
C	-1.51503200	2.23751000	1.13869500
H	3.07019900	-2.64739700	1.28312500
H	4.44197100	1.27010800	0.16646600
H	4.91488000	-0.98974400	1.09301100

F-silicate 1



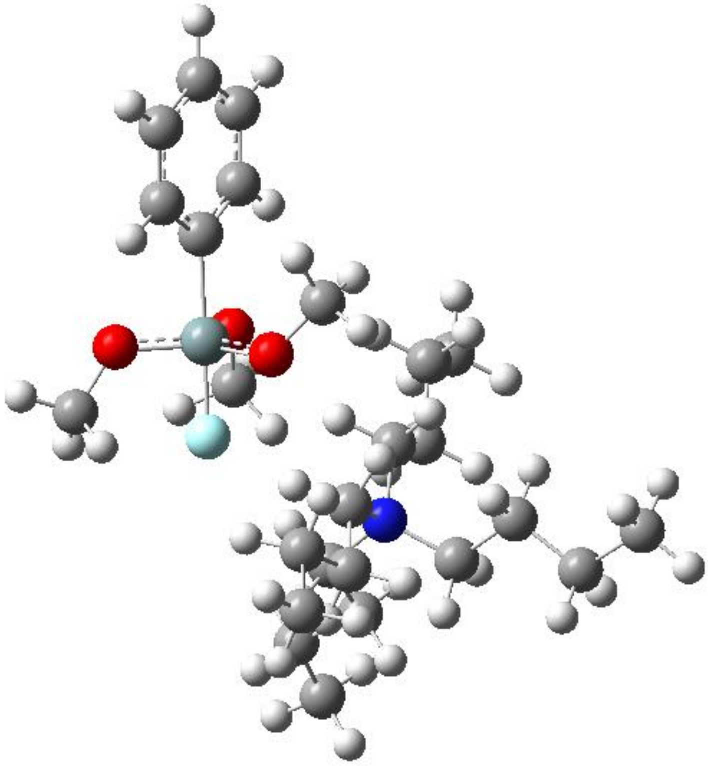
Zero-point correction= 0.736693 (Hartree/Particle)
Thermal correction to Energy= 0.776651
Thermal correction to Enthalpy= 0.777595
Thermal correction to Gibbs Free Energy= 0.660804
Sum of electronic and zero-point Energies= -1651.316135
Sum of electronic and thermal Energies= -1651.276177
Sum of electronic and thermal Enthalpies= -1651.275232
Sum of electronic and thermal Free Energies= -1651.392024

F	1.25596600	0.42382600	1.64938400
N	-2.22864900	-0.01543000	0.10853500

C	-2.44375100	-0.66969400	1.45681500
H	-3.13408300	-0.02396500	2.00500600
H	-1.47207700	-0.62112100	1.95722200
C	-2.95585500	-2.10066200	1.44118500
H	-3.87410700	-2.18469600	0.84634300
H	-2.20844100	-2.76866800	0.99813500
C	-3.24380200	-2.55727600	2.87393100
H	-4.00559000	-1.90283300	3.31692900
H	-2.33625700	-2.44128900	3.48004800
C	-3.71580600	-4.00740100	2.92606800
H	-4.63466100	-4.14253000	2.34368500
H	-3.92148800	-4.31983200	3.95487700
H	-2.95572100	-4.68199100	2.51585900
C	-1.22135500	-0.82022200	-0.71148200
H	-0.63417900	-0.09479000	-1.27615100
H	-0.53874800	-1.25973000	0.02244700
C	-1.77870300	-1.88061900	-1.65456500
H	-2.33436500	-1.40686300	-2.47222800
H	-2.46776500	-2.56389100	-1.14740400
C	-0.62045700	-2.68726400	-2.24773000
H	0.07694200	-2.00515500	-2.75214300
H	-0.05826600	-3.16660300	-1.43547100
C	-1.10715000	-3.74516300	-3.23411600
H	-1.64559100	-3.28447100	-4.07037000
H	-1.78657500	-4.45395400	-2.74668100
H	-0.26876900	-4.31475300	-3.64815300
C	-1.59232500	1.33662800	0.41124300
H	-0.57383000	1.10493700	0.73186000
H	-2.14783700	1.75968300	1.25204700
C	-1.55487100	2.32243000	-0.74478800
H	-2.56572200	2.65586500	-1.01460300
H	-1.11010700	1.86271200	-1.63609700
C	-0.71161600	3.53652000	-0.34625100
H	0.30529900	3.19369900	-0.11984000
H	-1.11933100	3.97736200	0.57380200
C	-0.68189600	4.59233200	-1.44809900
H	-0.04290500	5.43706100	-1.17027000
H	-1.68645200	4.98299400	-1.65100600
H	-0.29196700	4.17197200	-2.38281700
H	-3.89945000	-0.84956600	-0.86527100
C	-3.52432800	0.14990300	-0.64302000
H	-3.26426800	0.62535900	-1.59265200
C	-4.59695500	0.94736000	0.08636700

H	-4.19551400	1.88763200	0.48228900
H	-4.98316600	0.37319000	0.93739400
C	-5.75047600	1.25844000	-0.87018500
H	-5.37352300	1.86559000	-1.70344900
H	-6.12488600	0.32285300	-1.30606300
C	-6.89047800	1.99324100	-0.17121400
H	-7.70454300	2.21610000	-0.86833000
H	-6.54261200	2.94182900	0.25368700
H	-7.30326100	1.39088700	0.64607000
Si	2.55262400	0.88563500	0.66390200
C	3.46156300	-0.60184300	-0.13905700
C	4.80056700	-2.79834800	-1.33998600
C	4.81227600	-0.87899700	0.13232600
C	2.80770500	-1.46702100	-1.03206100
C	3.45478600	-2.55614100	-1.61921800
C	5.48063200	-1.95108200	-0.46381900
H	5.34694200	-0.24274100	0.83505700
H	1.76489600	-1.27097300	-1.27290700
H	2.91336500	-3.21154200	-2.29882800
H	6.52971600	-2.13060100	-0.23989800
H	5.31435300	-3.63880700	-1.80011100
O	1.33017300	0.98601900	-0.60473900
O	3.57425800	0.92745200	2.08637800
O	3.04997600	2.45559100	0.24998100
C	4.14894600	3.15099200	0.78542300
H	4.00323600	3.39613500	1.84327400
H	4.26069700	4.08397500	0.21845600
H	5.08168800	2.57897500	0.69841200
C	3.53693100	-0.09987800	3.03192200
H	2.74950400	0.06529800	3.78274900
H	4.50083600	-0.14366600	3.55905000
H	3.36118300	-1.09181900	2.58345500
C	1.66440900	1.45366900	-1.87587700
H	1.61859400	2.55178400	-1.93463300
H	0.95864200	1.03997000	-2.61601300
H	2.67707200	1.15375300	-2.19142800

F-silicate 2



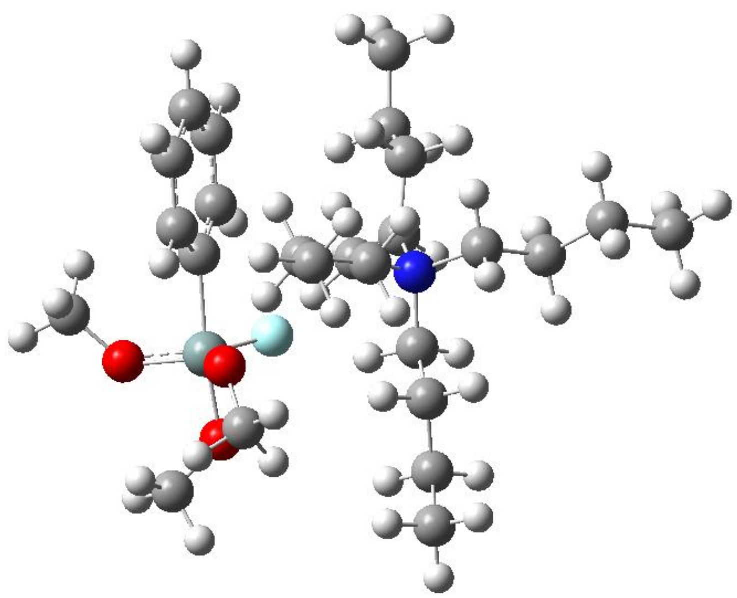
Zero-point correction= 0.736950 (Hartree/Particle)
Thermal correction to Energy= 0.777137
Thermal correction to Enthalpy= 0.778081
Thermal correction to Gibbs Free Energy= 0.660610
Sum of electronic and zero-point Energies= -1651.315644
Sum of electronic and thermal Energies= -1651.275458
Sum of electronic and thermal Enthalpies= -1651.274513
Sum of electronic and thermal Free Energies= -1651.391984

Si	-2.35543100	0.00746300	0.82100500
F	-0.88391000	-0.09919600	1.77554000
N	2.18097300	0.09046100	-0.05045900
C	1.14612600	-0.62464000	-0.89799000
H	1.05262600	-0.04201200	-1.81852000
H	0.20811800	-0.51424200	-0.34642700
C	1.41002100	-2.08384800	-1.22648000
H	2.36227100	-2.21266100	-1.75716100
H	1.45508300	-2.68604400	-0.31212400
C	0.26278400	-2.60451900	-2.09803900
H	0.23955500	-2.04239700	-3.04107800
H	-0.69065800	-2.40648300	-1.58949500
C	0.39582400	-4.09675400	-2.38627800

H	1.33577800	-4.31656000	-2.90622900
H	-0.42693200	-4.45375400	-3.01402900
H	0.38361400	-4.67660700	-1.45589200
C	2.30206800	-0.58953100	1.30816600
H	2.52833800	0.19953000	2.02773600
H	1.29575100	-0.95445500	1.53296800
C	3.34816800	-1.68975400	1.45426100
H	4.35559400	-1.25707400	1.43865100
H	3.29791700	-2.41966300	0.64036700
C	3.13129900	-2.41194300	2.78653300
H	3.12694500	-1.67892500	3.60383900
H	2.13927700	-2.88222100	2.78284600
C	4.20301300	-3.46681500	3.04557400
H	5.19978000	-3.01269600	3.08666200
H	4.21045200	-4.22157300	2.25068800
H	4.02959900	-3.98210900	3.99572700
C	1.60166100	1.47820200	0.19115500
H	0.73452500	1.31233700	0.83672600
H	1.21764500	1.82473400	-0.77092800
C	2.55992200	2.50948300	0.76767200
H	3.33241900	2.77466600	0.03472000
H	3.07674200	2.13041500	1.65796900
C	1.77638200	3.77000700	1.14540100
H	1.02642800	3.51354600	1.90401800
H	1.22299200	4.12986300	0.26800500
C	2.68822400	4.87565500	1.66883200
H	2.11349500	5.76692400	1.94047000
H	3.42537400	5.16905100	0.91237000
H	3.23472100	4.54467100	2.55959800
H	3.88698800	-0.85738300	-0.83657700
C	3.51933100	0.16481800	-0.73688400
H	4.18741100	0.68927800	-0.04762100
C	3.50685600	0.83905500	-2.10215100
H	2.99381100	1.80718900	-2.06408200
H	2.97117400	0.21511400	-2.82803800
C	4.94233000	1.05242600	-2.58805900
H	5.46962500	1.70340400	-1.87855100
H	5.47370300	0.09168300	-2.58937400
C	4.98758400	1.66768700	-3.98362100
H	6.01932200	1.82467000	-4.31408100
H	4.47758700	2.63773900	-4.00080700
H	4.49540300	1.01705800	-4.71543100
C	-4.00425300	0.12867300	-0.23204100

C	-6.34232000	0.46327500	-1.83306100
C	-4.87060400	1.22641100	-0.07134000
C	-4.36694100	-0.79765400	-1.22486100
C	-5.51024400	-0.64121100	-2.01585100
C	-6.01679100	1.40031800	-0.85023400
H	-4.64087500	1.96684300	0.69300500
H	-3.73620300	-1.67051800	-1.37987100
H	-5.75368900	-1.38463500	-2.77249400
H	-6.65892200	2.26409100	-0.68951100
H	-7.23390800	0.58975000	-2.44266500
O	-2.23343900	-1.65152500	0.46528500
O	-3.18390000	0.59176100	2.17952700
O	-1.47072000	1.11104100	-0.14391500
C	-1.39136000	-2.58718900	1.08733600
H	-0.32763700	-2.35526700	0.94990400
H	-1.59013400	-3.57180700	0.64520200
H	-1.58067100	-2.65392900	2.16723700
C	-2.61938000	0.94845600	3.41742500
H	-2.19611700	0.08326300	3.94281300
H	-3.41679300	1.37247700	4.03985700
H	-1.82893900	1.70251200	3.31034100
C	-1.72507300	1.42187000	-1.48842500
H	-1.78424800	0.52274300	-2.12009600
H	-0.89696400	2.04201800	-1.85758700
H	-2.65624500	1.98740900	-1.62319700

F-silicate 3



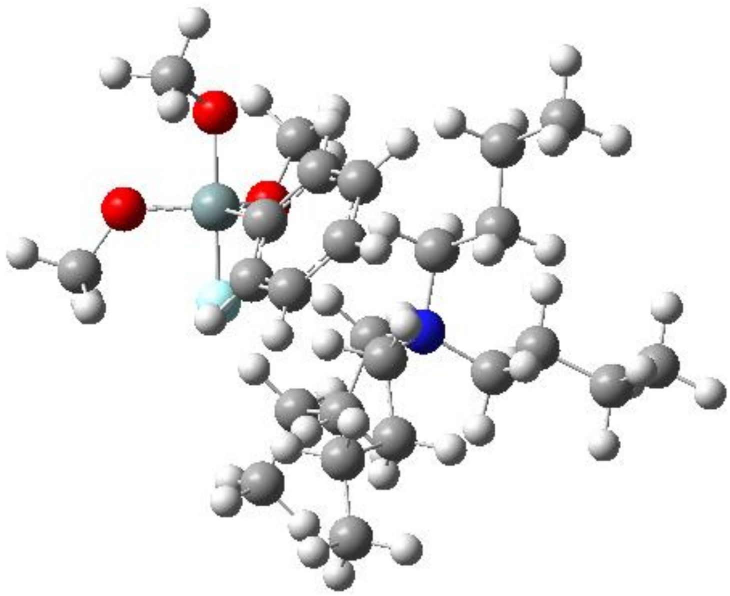
Zero-point correction= 0.736594 (Hartree/Particle)
Thermal correction to Energy= 0.776791
Thermal correction to Enthalpy= 0.777735
Thermal correction to Gibbs Free Energy= 0.661075
Sum of electronic and zero-point Energies= -1651.311699
Sum of electronic and thermal Energies= -1651.271502
Sum of electronic and thermal Enthalpies= -1651.270558
Sum of electronic and thermal Free Energies= -1651.387218

F	-1.38976500	0.00543400	-1.94003100
N	1.79150700	-0.13741900	-0.05816800
C	1.42383700	-1.38033500	-0.84760200
H	2.10298600	-1.41035200	-1.70321400
H	0.41543100	-1.18898700	-1.22772600
C	1.45689600	-2.70099200	-0.09843500
H	2.43690300	-2.88007500	0.36185800
H	0.70768700	-2.70195100	0.69971900
C	1.13881800	-3.84349400	-1.06721500
H	1.92540900	-3.90566400	-1.83026500
H	0.20356900	-3.61949600	-1.59655300
C	1.00994300	-5.17952800	-0.34160700
H	1.93512200	-5.43034100	0.19060100
H	0.79410300	-5.99250700	-1.04222100
H	0.19781500	-5.14618600	0.39454600
C	0.83275800	0.04026300	1.11536000
H	0.71778900	1.11705100	1.25955600
H	-0.13246100	-0.34952200	0.77661600
C	1.22694900	-0.58917900	2.44739400
H	2.10777900	-0.09009200	2.86818400
H	1.47552600	-1.65038500	2.34285700
C	0.05679600	-0.44477800	3.42505300
H	-0.17339200	0.62031300	3.55873100
H	-0.83933700	-0.90096900	2.98420100
C	0.36279100	-1.08308200	4.77691300
H	1.24577700	-0.62531600	5.23834100
H	0.55971300	-2.15616400	4.66833200
H	-0.47647600	-0.96526800	5.47001600
C	1.56256000	1.01922800	-1.02052600
H	0.48091100	1.04420200	-1.18077800
H	2.03423200	0.73251000	-1.96380600
C	2.06993000	2.38243200	-0.57710300
H	3.14965000	2.36432700	-0.38553200
H	1.57618900	2.70751800	0.34670100

C	1.78223900	3.40816100	-1.67778200
H	0.71680000	3.37211800	-1.93732200
H	2.33698900	3.13256200	-2.58411300
C	2.16051600	4.82215900	-1.24751700
H	1.94987600	5.54777200	-2.03981500
H	3.22803300	4.88803500	-1.00629500
H	1.59716000	5.12278200	-0.35617400
H	3.30287100	-1.02530100	1.10176400
C	3.21897700	-0.17535500	0.42281600
H	3.36338700	0.73295100	1.01465000
C	4.27442900	-0.28243700	-0.66928900
H	4.14603900	0.50190500	-1.42494000
H	4.19762300	-1.24816000	-1.18317700
C	5.67005400	-0.15571500	-0.05307800
H	5.75851400	0.81954900	0.44314500
H	5.79493400	-0.91868700	0.72632300
C	6.77105900	-0.30293100	-1.09927500
H	7.76302000	-0.20291400	-0.64722600
H	6.67734100	0.46353000	-1.87721800
H	6.72068000	-1.28322600	-1.58674400
Si	-2.62514300	-0.38550300	-0.85305300
C	-2.21910800	1.31014600	0.08344400
C	-1.63056300	3.77363300	1.40606000
C	-2.38487600	1.47353800	1.47096500
C	-1.75714700	2.44272500	-0.61150500
C	-1.46329600	3.65292900	0.02617100
C	-2.09904200	2.67327400	2.12769300
H	-1.61160600	2.38085200	-1.68929200
H	-1.10410600	4.50098500	-0.55471400
H	-2.23662400	2.74981000	3.20479700
H	-1.40244800	4.70946600	1.91082500
H	-2.72912500	0.62557100	2.06003400
O	-2.81329100	-1.83072000	-1.81461400
O	-4.25286200	0.01126600	-1.15594500
O	-2.18008100	-1.22066100	0.57200300
C	-2.08029900	-2.60864100	0.77396800
H	-3.04340100	-3.03705200	1.08377300
H	-1.36371300	-2.78963900	1.58745300
H	-1.74142300	-3.13621100	-0.12557500
C	-5.02156400	1.02968000	-0.56664000
H	-5.07498300	0.93078600	0.52593700
H	-6.04021400	0.95239200	-0.96524500
H	-4.63773700	2.03174000	-0.79725800

C	-3.94825400	-2.63724300	-1.70773800
H	-3.67221600	-3.68283800	-1.91315800
H	-4.72089100	-2.34142100	-2.43301200
H	-4.41691500	-2.60575500	-0.71208400

F-silicate 4



Zero-point correction= 0.736131 (Hartree/Particle)
Thermal correction to Energy= 0.776607
Thermal correction to Enthalpy= 0.777551
Thermal correction to Gibbs Free Energy= 0.659401
Sum of electronic and zero-point Energies= -1651.325231
Sum of electronic and thermal Energies= -1651.284755
Sum of electronic and thermal Enthalpies= -1651.283811
Sum of electronic and thermal Free Energies= -1651.401961

Si	-2.63187000	-0.50677600	-0.93723100
F	-1.67571300	-1.72111200	-0.10508200
N	1.76367700	-0.02207300	-0.01194000
C	1.55270900	-1.19904700	-0.94937200
H	2.15597300	-0.98857400	-1.83640600
H	0.49658100	-1.15008000	-1.23623400
C	1.88230900	-2.57658400	-0.39908900
H	2.90706200	-2.62411900	-0.00833800
H	1.19798600	-2.83286900	0.41790600
C	1.72123100	-3.61327100	-1.51461600
H	2.40761200	-3.37300100	-2.33724400
H	0.70362400	-3.54727000	-1.92034200

C	1.98674700	-5.03162000	-1.01836600
H	3.00501500	-5.12629900	-0.62299200
H	1.87077400	-5.76217000	-1.82552400
H	1.28857300	-5.30205800	-0.21807900
C	0.93440900	-0.21920600	1.25509600
H	0.61925000	0.77576600	1.58116400
H	0.03927300	-0.75850700	0.92911900
C	1.62003700	-0.92392200	2.42243200
H	2.39732900	-0.28077800	2.85192800
H	2.10600200	-1.85321500	2.10987100
C	0.58756000	-1.24465900	3.50504500
H	0.09525000	-0.31746600	3.82363000
H	-0.19638100	-1.88460500	3.07887800
C	1.22331900	-1.93284700	4.70987500
H	1.99168500	-1.29737800	5.16554600
H	1.69831900	-2.87658300	4.41760100
H	0.47583400	-2.15763000	5.47759600
C	1.19677000	1.17950200	-0.75258000
H	0.11647200	1.00720000	-0.78522400
H	1.57149700	1.11560800	-1.77796400
C	1.51427100	2.54669400	-0.16546600
H	2.59569400	2.72958600	-0.15323800
H	1.15604400	2.62850600	0.86822800
C	0.84512900	3.63268100	-1.01265700
H	-0.23714300	3.45655400	-1.04112100
H	1.20399900	3.55716600	-2.04770600
C	1.12540800	5.03060400	-0.46896800
H	0.63888300	5.79794900	-1.07959300
H	2.20130000	5.24070000	-0.45903600
H	0.75455300	5.13260000	0.55755800
H	3.55164900	-0.71792700	0.84683100
C	3.21926000	0.17887100	0.32316700
H	3.25868300	1.00832700	1.03508400
C	4.13604400	0.44034200	-0.86484900
H	3.75212900	1.24750800	-1.49991200
H	4.21323900	-0.45733300	-1.48985900
C	5.53184400	0.82186100	-0.36570000
H	5.46272800	1.73896300	0.23365100
H	5.90765700	0.03603900	0.30253800
C	6.51190000	1.03121500	-1.51643100
H	7.50320900	1.31176800	-1.14637300
H	6.16568500	1.82671600	-2.18629500
H	6.62098000	0.11643300	-2.11007100

C	-2.46965800	0.62187400	0.60478900
C	-2.10139700	2.33278500	2.84027700
C	-2.50016700	0.13057200	1.92000500
C	-2.26685600	2.00361600	0.45135700
C	-2.05968600	2.84950500	1.54390800
C	-2.33996200	0.96958600	3.02527000
H	-2.64365700	-0.93546600	2.08644600
H	-2.27891400	2.42362500	-0.55307500
H	-1.88402300	3.91183800	1.38570200
H	-2.38797600	0.55891900	4.03149800
H	-1.95930600	2.98653000	3.69736000
O	-3.50849900	0.68637900	-1.86332700
O	-3.94051000	-1.57741700	-1.03214900
O	-1.35082100	-0.47711300	-2.05724300
C	-1.23264600	0.37464300	-3.16873900
H	-2.04172400	0.22390600	-3.89159900
H	-0.27682900	0.14983900	-3.66153300
H	-1.23636100	1.43526700	-2.88158800
C	-4.02417700	-2.85078000	-0.44293200
H	-3.27865900	-3.54455000	-0.85062400
H	-5.02188600	-3.25364500	-0.65580400
H	-3.89598700	-2.81471100	0.64675800
C	-4.80757300	1.05204600	-1.50593900
H	-4.94231200	1.13800900	-0.41418500
H	-5.54837200	0.32604200	-1.87089900
H	-5.04147000	2.03270400	-1.94483400

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