Supplementary Information

Reactivity of a stable N-heterocyclic silylene with a 1,1'-ferrocenediyl backbone towards carbonyl compounds, including carbon suboxide

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Table of Contents

I Experimental Section

A Compound Synthesis

General considerations

All reactions involving air-sensitive compounds were performed in an inert atmosphere (argon or dinitrogen) by using standard Schlenk techniques or a conventional glovebox. Starting materials were procured from standard commercial sources and used as received. N-heterocyclic silylene **1**,[S1] carbon suboxide[S2] and diphenylketene[S3] were synthesised by adapted versions of the published procedures. NMR spectra were recorded at ambient temperature with Varian NMRS-500 and MR-400 spectrometers operating at 500 and 400 MHz, respectively, for ^{1}H. Elemental analyses were carried out with a HEKAtech Euro EA-CHNS elemental analyser at the Institute of Chemistry, University of Kassel, Germany.

Synthesis of 2

Carbon suboxide was prepared from a thorough mixture of malonic acid (200 mg, 1.92 mmol), phosphorus pentoxide (2.00 g, 7.0 mmol P_4O_{10}) and calcined sand (4 g) and was condensed under static vacuum into a 100 mL flask fitted with a Young's tap containing a frozen solution of silylene **1** (50.0 mg, 89 μmol) in toluene (7 mL) immersed in liquid dinitrogen. The flask was sealed immediately after removing the cooling bath and allowed to warm to room temperature, which took ca. 30 min. After a further 15 min, the colour of the solution had changed from light yellow to orange brown. Volatile components were removed under vacuum. The solid residue was taken up in a minimal amount of benzene. Slow evaporation of part of the solvent afforded the product as yellow crystals. The mother liquor was decanted off and the crystals were dried under vacuum. Yield 12.0 mg (22 %).

$C_{73}H_{84}N_4Fe_2O_3Si_2$ (1233.34): calcd. C 71.09, H 6.86, N 4.54 %; found C 71.20, H 7.16, N 4.70 %.

^{1}H NMR (500 MHz, C_6D_6): δ = 7.05 – 7.00 (m, 8H, C_6H_3), 6.80 – 6.78 (m, 4H, C_6H_3), 4.64, 4.26 (2 s, br, 2 × 2H, C_5H_4), 4.22 (s, br, 4H, C_5H_4), 4.10, 4.07 (2 sept, 2 × 2H, $^{3}J_{HH}$ = 6.7 Hz, C*H*Me$_2$), 3.76, 3.72 (2 s, br, 2 × 2H, C_5H_4), 3.70 – 3.68 (m, 4H, C_5H_4), 3.64, 3.52 (2 sept, 2 × 2H, $^{3}J_{HH}$ = 6.7 Hz, C*H*Me$_2$), 1.70, 1.61, 1.46, 1.39, 1.06, 0.96, 0.49, 0.30 ppm (8 d, 8 × 6H, $^{3}J_{HH}$ = 6.7 Hz, CH*Me*$_2$). ^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ = 212.7, 187.4 (2 × CO), 174.3 (O=C*C*$_2$C=C=O), 148.9, 148.5, 147.0, 146.8 (4 × *C*CHMe$_2$), 142.2, 139.7 (2 × C_{ipso} Dipp), 125.7, 125.6, 125.4, 124.9 (4 × CH Dipp), 113.3 (O=C*C*$_2$C=C=O), 101.3, 100.9 (2 × C_{ipso} C_5H_4),

70.4, 70.2, 68.8, 68.7, 68.5, 67.9, 66.8, 64.8 (8 × CH C_5H_4), 33.0 (*C*=C=O), 28.7, 28.7, 28.7, 28.0 (4 × *C*HMe$_2$), 27.3, 27.0, 26.3, 26.0, 25.7, 25.6, 25.6, 25.2 ppm (8 × CH*Me*$_2$). ^{29}Si{^{1}H} NMR (99 MHz, C_6D_6): δ = –46.7, –59.7 ppm.

Synthesis of 3

The product was obtained quantitatively by storing crystalline **2** under aerobic conditions for several days. As described in the main text and in Section I B (vide infra), we observed a single-crystal-to-single-crystal transformation for this gas–solid chemical reaction. The solubility of **3** thus obtained was not sufficient for a meaningful NMR spectroscopic analysis. **3** can also be obtained from **2** by hydrolysis in benzene solution, albeit not in analytically pure form, when a substantial excess of water is avoided, as was revealed by experiments performed on an NMR tube scale. NMR spectroscopic analysis was cumbersome due to the poor solubility of **2**. In a typical experiment, **2** (3.0 mg, 2.4 μmol) was dissolved in C_6D_6 (0.7 mL) and moist THF-d_8 (0.1 mL, water content 0.1 μL, corresponding to 5.5 μmol of H_2O) was added. A ^{13}C{^{1}H} NMR spectrum was recorded after 3 h. Due to the very low concentration, data acquisition for the spectrum shown in Fig. S12 took 5 d, after which time the solution was still clear (no turbidity or signs of precipitate formation). A comparison with the ^{13}C{^{1}H} NMR spectrum of **2** (Fig. S10) reveals, apart from many similarities, pertinent differences, which are in accord with, but do not prove, the formation of **3**. In particular, substantial changes can be made out for characteristic signals due to the C_5O_2 unit. More specifically, the spectrum of **2** exhibits three low-field signals at δ = 212.7, 187.4 (2 × CO) and 174.3 ppm (O=C*C*$_2$C=C=O). After hydrolysis, the three signals at lowest field are located at δ = 181.0, 165.2 and 164.7 ppm. The only previously reported stable methyleneketene contains an N–C=C=C=O moiety (in contrast to the O–C=C=C=O moiety present in **3**), giving rise to ^{13}C NMR signals at δ = 173.1 (N–C), 76.4 and 160.6 ppm (C=O) in $CDCl_3$.[S4] This suggests that the signal at δ = 181.0 ppm and one of the two signals at $\delta \approx$ 165 ppm are due to the O–C and C=O unit, respectively, of **3**. The spectrum shows several signals of comparatively low intensity not attributable to **3**, most likely indicating decomposition of this product in solution over time. In a separate experiment performed with the same amounts of reactants and volumes of solvents, volatile components were removed under vacuum after 1 d. Crystallisation of the residue from benzene afforded crystals composed of a 2:3 mixture of **2** and **3** according to XRD.

$C_{73}H_{86}N_4Fe_2O_4Si_2$ (1251.35): calcd. C 70.07, H 6.93, N 4.48 %; found C 70.13, H 7.02, N 4.65 %.

Synthesis of 4

Silylene **1** (26.1 mg, 46 μmol) was added to a solution of diphenylketene (9.0 mg, 46 μmol) in C_6D_6 (0.8 mL) placed in an NMR tube. After 24 h yellow crystals had formed. The supernatant was decanted off and the product dried under vacuum. Yield 22.4 mg (64 %).

$C_{48}H_{52}N_2FeOSi$ (756.87): calcd. C 76.17, H 6.92, N 3.70 %; found C 75.66, H 6.84, N 3.62 %. ^{1}H NMR (500 MHz, C_6D_6): δ = 7.20 – 7.18 (m, 2H, Ph), 7.12 – 7.01 (m, 11H, Ph and C_6H_3), 6.95 – 6.92 (m, 1H, Ph), 6.88 – 6.85 (m, 2H, Ph), 4.65, 4.57 (2 s, br, 2 × 2H, C_5H_4), 4.03, 3.92 (2 sept, 2 × 2H, $^3J_{HH}$ = 6.8 Hz), 3.87 – 3.86 (m, 4H, C_5H_4), 1.45, 1.28, 1.25, 1.04 ppm (4 d, 4 × 6H, $^3J_{HH}$ = 6.8 Hz, CH*Me*$_2$). ^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ = 160.3 (CO), 148.8, 148.1 (2 × *C*CHMe$_2$), 140.4 (*C*Ph$_2$), 139.2 (C_{ipso} Dipp), 138.2 (C_{ipso} Ph), 130.1, 129.0, 128.6 (3 × CH Ph), 128.2 (CH Dipp), 127.9 (C_{ipso} Ph), 126.5, 126.3 (2 × CH Ph), 125.0, 124.7 (2 × CH Dipp), 124.4 (CH Ph), 98.9 (C_{ipso} C_5H_4), 69.2, 69.1, 68.6, 68.5 (4 × CH C_5H_4), 28.9, 28.7 (2 × *C*HMe$_2$), 26.0, 25.8, 25.2, 25.1 ppm (4 × CH*Me*$_2$). ^{29}Si{^{1}H} NMR (99 MHz, C_6D_6): δ = –64.8 ppm.

Synthesis of 5

An excess of acetone (1 drop) was added to a stirred solution of silylene **1** (25.0 mg, 44 μmol) in *n*-hexane (2 mL). The solvent was allowed to evaporate almost completely after 24 h, affording the product as yellow crystals. Yield 16.8 mg (61 %).

$C_{37}H_{48}N_2FeOSi$ (620.72): calcd. C 71.59, H 7.79, N 4.51 %; found C 71.33, H 7.74, N4.40 %. ^{1}H NMR (500 MHz, C_6D_6): δ = 7.15 – 7.11 (m, 4H, C_6H_3), 7.06 – 7.03 (m, 2H, C_6H_3), 5.47 (s, 1H, SiH), 4.62, 4.55 (2 s, br, 2 × 2H, C_5H_4), 4.19, 3.97 (2 sept, 2 × 2H, $^3J_{HH}$ = 6.8 Hz, C*H*Me$_2$), 3.92 (s, br, 4H, C_5H_4), 3.75, 3.12 (2 s, 2 × 1H, CH_2), 1.49 (d, 6H, $^3J_{HH}$ = 6.8 Hz, CH*Me*$_2$), 1.39 – 1.36 (2 d, 2 × 6H, $^3J_{HH}$ = 6.8 Hz, CH*Me*$_2$), 1.22 (d, 6H, $^3J_{HH}$ = 6.8 Hz, CH*Me*$_2$), 0.99 ppm (s, 3H, OC*Me*). ^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ = 154.4 (O*C*Me), 149.9, 148.8 (2 × *C*CHMe$_2$), 140.5 (C_{ipso} Dipp), 127.6, 124.8, 124.7 (3 × CH Dipp), 100.3 (C_{ipso} C_5H_4), 94.6 (CH_2), 70.9, 68.0, 67.6, 67.1 (4 × CH C_5H_4), 28.7, 28.6 (2 × *C*HMe$_2$), 26.2, 25.7, 25.2 (two closely spaced signals) (4 × CH*Me*$_2$), 21.5 ppm (OC*Me*). ^{29}Si NMR (99 MHz, C_6D_6): δ = –48.7 ppm (d, $^1J_{SiH}$ = 264.1 Hz).

Synthesis of 6

Benzophenone (3.2 mg, 18 μmol) was added to a stirred solution of silylene **1** (10.0 mg, 18 μmol) in toluene (3 mL). After 30 min the solvent was removed under vacuum, leaving a waxy

solid. Yield 13.2 mg (100 %). Unfortunately, attempts to obtain crystalline material were unsuccessful.

$C_{47}H_{52}N_2FeOSi$ (744.86): calcd. C 75.79, H 7.04, N 3.76 %; found C 75.93, H 7.28, N 3.77 %. ^{1}H NMR (500 MHz, C_6D_6): δ = 7.56 – 7.54 (m, 2H, Ph) 7.18 – 6.98 (m, 9H, Ph and C_6H_3), 6.45 – 6.42, 5.75 – 5.71, 5.58 – 5.53, 5.45 – 5.41 (4 m, 4 × 1H, SiCH-C*H*=C*H*-C*H*=C*H*), 4.97 – 4.96, 4.91 – 4.90, 4.60 – 4.59, 4.58 – 4.56 (4 m, 4 × 1H, C_5H_4), 4.30, 4.16, 4.15, 4.05 (4 sept, 4 × 1H, $^3J_{HH}$ = 6.7 Hz, C*H*Me$_2$), 4.01 – 3.98, 3.96 – 3.94 (2 m, 2 × 1H, C_5H_4), 3.94 – 3.93 (m, 2H, C_5H_4), 3.22 (s, br, 1H, SiCH), 1.49, 1.40, 1.35, 1.31, 1.21, 1.20, 1.19, 1.17 ppm (8 d, 8 × 3H, $^3J_{HH}$ = 6.7 Hz, CH*Me*$_2$). ^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ = 150.0, 149.4 (2 × *C*CHMe$_2$), 149.2 (CO), 148.0, 147.7 (2 × *C*CHMe$_2$), 142.2, 141.8 (2 × C_{ipso} Dipp), 134.9 (C_{ipso} Ph), 128.6, 128.0, 127.5 (3 × CH Ph), 128.2, 125.8, 125.0, 124.9, 124.4 (5 × CH Dipp), 124.0, 123.9, 123.7, 122.7 (SiCH-*C*H=*C*H-*C*H=*C*H), 114.9 (*C*CPh), 101.2, 99.8 (2 × C_{ipso} C_5H_4), 70.6, 68.9, 68.8, 68.4 (two closely spaced signals), 68.2, 67.9, 67.7 (8 × CH C_5H_4), 28.6, 28.5, 28.2 (two closely spaced signals) (4 × *C*HMe$_2$), 27.4, 27.3 (2 × CH*Me*$_2$), 26.9 (SiCH), 26.5, 25.9, 25.7 (two closely spaced signals) 25.6, 24.5 ppm (6 × CH*Me*$_2$). ^{29}Si{^{1}H} NMR (99 MHz, C_6D_6): δ = –19.9 ppm.

Synthesis of 7

Fluorenone (6.4 mg, 36 μmol) was added to a solution of silylene **1** (20.0 mg, 36 μmol) in C_6D_6 (0.8 mL). A rapid reaction was indicated by an almost immediate colour change from yellow to dark orange. After 10 min the product crystallised as fine needles, which were isolated by decanting the mother liquor off after centrifugation, washed with *n*-hexane (4 × 0.2 mL) and dried under vacuum. Yield 19.8 mg (75 %).

$C_{47}H_{50}N_2FeOSi$ (742.85): calcd. C 75.99, H 6.78, N 3.77 %; found C 76.10, H 6.99, N 3.41 %. ^{1}H NMR (500 MHz, C_6D_6): δ = 7.37 – 7.36 (m, 2H, C_6H_3), 7.20 – 7.14 (m, integral could not be determined due to overlap with solvent signal, required: 4H, C_6H_4), 6.96 – 6.92, 6.86 – 6.84 (2 m, 2 × 2H, C_6H_4), 6.61 – 6.57, 6.24 – 6.22 (2 m, 2 × 2H, C_6H_3), 4.60, 4.21 (2 s, br, 2 × 2H, C_5H_4), 4.09 (sept, 2H, $^3J_{HH}$ = 6.7 Hz, C*H*Me$_2$), 3.86 (s, br, 2H, C_5H_4), 3.79 – 3.74 (m, 4H, C_5H_4 and C*H*Me$_2$), 1.66, 1.19, 1.12, 0.77 ppm (4 d, 4 × 6H, $^3J_{HH}$ = 6.7 Hz, CH*Me*$_2$). ^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ = 147.9 (C_{ipso} Dipp), 147.3, 146.5 (2 × *C*CHMe$_2$), 143.0, 139.4 (2 × C_{quart} C_6H_4), 126.3, 125.9, 125.5 (3 × CH C_6H_4), 125.2 (CH Dipp), 124.0 (CH C_6H_4), 119.4 (CH Dipp), 103.0 (C_{ipso} C_5H_4), 68.9 (two closely spaced signals), 67.9, 67.3 (4 × CH C_5H_4), 29.5

(*C*HMe$_2$), 27.0, 26.1, 24.8, 22.8 ppm (4 × CH*Me*$_2$); C_{spiro} signal not detected. ^{29}Si{^{1}H} NMR (99 MHz, C_6D_6): δ = –62.1 ppm.

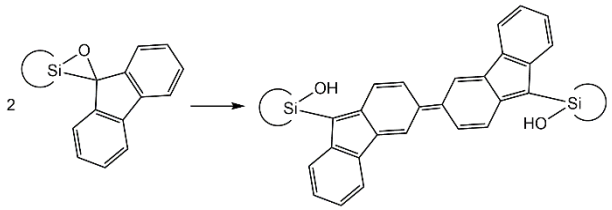
Synthesis of 8

Benzil (7.5 mg, 36 µmol) was added to a solution of silylene **1** (20.0 mg, 36 µmol) in C_6D_6 (0.8 mL). ^{1}H NMR spectroscopic monitoring revealed completion of the reaction after 5 min. The solvent was allowed to evaporate almost completely, leaving the product as a yellow crystalline solid. Yield 19.3 mg (69 %).

$C_{48}H_{52}N_2FeO_2Si$ (772.87): calcd. C 74.59, H 6.78, N 3.62 %; found C 74.27, H 6.76, N 3.58 %.

^{1}H NMR (500 MHz, C_6D_6): δ = 7.16 – 7.14 (m, integral could not be determined due to overlap with solvent signal, required: 4H, Ph), 7.08 – 7.03 (m, 6H, C_6H_3), 6.94 – 6.91 (m, 4H, Ph), 6.88 – 6.84 (m, 2H, Ph), 4.66 (s, br, 4H, C_5H_4), 4.19 (sept, 4H, $^3J_{HH}$ = 6.8 Hz, C*H*Me$_2$), 3.92 (s, br, 4H, C_5H_4), 1.38, 1.31 ppm (2 d, 2 × 12H, $^3J_{HH}$ = 6.8 Hz, CH*Me*$_2$). ^{13}C{^{1}H} NMR (101 MHz, C_6D_6): δ = 149.0 (*C*CHMe$_2$), 139.8 (C_{ipso} Dipp), 138.4 (C_{ipso} Ph), 133.3 (CO), 128.6, 128.5 (2 × CH Ph), 127.7 (CH Dipp), 127.6 (CH Ph), 124.7 (CH Dipp), 99.8 (C_{ipso} C_5H_4), 69.1, 68.3 (2 × CH C_5H_4), 28.6 (*C*HMe$_2$), 26.4, 25.6 ppm (2 × CH*Me*$_2$). ^{29}Si{^{1}H} NMR (99 MHz, C_6D_6): δ = –46.9 ppm.

Synthesis of 9 by dimerisation of 7



Scheme S1 Dimerisation of **7** to afford **9**.

A solution of **7** (19.8 mg, 27 µmol) in C_6D_6 (0.8 mL) was monitored daily by ^{1}H NMR spectroscopy, which revealed completion of the dimerization after 6 d. The solvent was allowed to evaporate to a residual volume of ca. 0.1 mL, leaving the product as a dark blue crystalline solid. Yield 8.6 mg (43 %).

$C_{94}H_{100}N_4Fe_2O_2Si_2$ (1485.69): calcd. C 75.99, H 6.78, N 3.77 %; found C 76.21, H 6.93, N 3.35 %.

^{1}H NMR (500 MHz, C_6D_6): δ = 7.29 – 7.25 (m, 4H, CH aryl), 7.11 – 7.07 (m, 6H, CH aryl), 7.04 – 7.00 (m, 4H, CH aryl), 6.98 – 6.95 (m, 2H, CH aryl), 6.76 – 6.69 (m, 4H, CH aryl), 5.65,

5.63, 5.47 (3 s, 3 × 2H, olefinic CH), 4.52, 4.43, 3.89, 3.85 (4 s, 4 × 4H, C_5H_4), 4.14, 3.99 (2 sept, 2 × 4H, $^3J_{HH}$ = 6.8 Hz, C*H*Me$_2$), 2.41 (s, 2 H, OH), 1.35, 1.20, 1.16, 1.11 ppm (4 d, 4 × 12H, $^3J_{HH}$ = 6.8 Hz, CH*Me*$_2$). $^{13}C\{^1H\}$ NMR (101 MHz, C_6D_6): δ = 149.3, 149.0 (2 × *C*CHMe$_2$), 144.5, 142.8, 139.9 (3 × C_{quart} aryl), 127.2, 125.9, 125.7, 125.4, 119.3 (5 × CH aryl), 101.4 (C_{ipso} C_5H_4), 76.8, 70.4, 67.9, 67.8, 66.4 (4 × CH C_5H_4), 28.5, 28.3 (2 × *C*HMe$_2$), 26.2, 25.6, 25.2, 25.0 ppm (4 × CH*Me*$_2$). $^{29}Si\{^1H\}$ NMR (99 MHz, C_6D_6): δ = –65.6 ppm.

B X-Ray Crystallography

For each data collection a single crystal was mounted on a micro-mount by using commercial perfluoropolyether oil (Alfa Aesar Fomblin YR-1800) and transferred in the cold gas stream. All geometric and intensity data were taken from this sample at 100(2) K. Data collection for **7**·C_6H_6 was carried out on a Stoe IPDS2 diffractometer equipped with a 2-circle goniometer and an imaging plate detector. All other diffraction experiments were performed with a Stoe StadiVari diffractometer equipped with a 4-circle goniometer and a DECTRIS Pilatus 200K detector. CuK_α radiation (λ = 1.54186 Å) was used for **9**·2 C_6H_6, **2**·1.5 C_6H_6 and **3**·1.5 C_6H_6. MoK_α radiation (λ = 0.71073 Å) was used in all other cases.

The diffraction experiments of **2**·1.5 C_6H_6 and **3**·1.5 C_6H_6 may be regarded as reflecting the starting and end point, respectively, of a hydrolysis reaction of one and the same individual single crystal. A single crystal of **2**·1.5 C_6H_6 was prepared and subjected to a diffraction experiment as described above. Subsequently, the crystal was allowed to warm to room temperature and stored in the air for 2 d. The crystal remained intact with no obvious changes in colour and shape. The whole dataset was recorded again. The lattice parameters were almost unchanged. The results of the structure refinement revealed a second set of atomic positions in the sterically shielded space between the two [Fe(η^5-C_5H_4–NDipp)$_2$] moieties (ca. 50% occupation of the two Si2 positions). This procedure was repeated several times, showing a continuous increase of the occupancies of the second set of atomic positions, accompanied by a decrease of the occupancies of the atomic positions of the starting material. After 7 days no further changes were detected, as was confirmed by a final diffraction experiment after an additional 9 days.

All data sets were corrected for absorption, Lorentz and polarization effects. The structures were solved by direct methods (SHELXT 2014/7) and refined using alternating cycles of least-squares refinements against F^2 (SHELXL 2017/1).[S5] C-bonded H atoms were included to the models in calculated positions, heteroatom-bonded H atoms have been found in the difference Fourier lists. All H atoms were treated with the 1.2 fold or 1.5 fold isotropic displacement parameter of their bonding partner. Experimental details for the diffraction experiments are given in Table S1. CCDC 2073362 – 2073368 contain the supplementary crystallographic data for this paper. These data are provided free of charge by The Cambridge Crystallographic Data Centre.

Table S1 X-ray crystallographic details

	7·C_6H_6	**4**	**5**	**8**	**9**·2 C_6H_6	**2**·1.5 C_6H_6	**3**·1.5 C_6H_6
Chemical formula	$C_{53}H_{56}FeN_2OSi$	$C_{48}H_{52}FeN_2OSi$	$C_{37}H_{48}FeN_2OSi$	$C_{48}H_{52}FeN_2O_2Si$	$C_{106}H_{112}Fe_2N_4O_2Si_2$	$C_{82}H_{93}Fe_2N_4O_3Si_2$	$C_{82}H_{95}Fe_2N_4O_4Si_2$
Formula mass	820.93	756.85	620.71	772.85	1641.87	1350.48	1368.49
Crystal system	monoclinic	monoclinic	monoclinic	triclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/m$	$C2/c$	P-1	$P2_1/c$	$P2_1/c$	$P2_1/c$
a/Å	17.6006(11)	9.9638(5)	35.2084(15)	11.3202(7)	22.7412(9)	15.180(3)	15.3738(6)
b/Å	9.5335(4)	17.1476(5)	11.2249(4)	11.3024(6)	10.0006(3)	22.128(2)	22.1555(6)
c/Å	25.8773(17)	12.4864(6)	17.4082(7)	16.7461(9)	23.1761(10)	20.694(4)	20.5912(8)
α/°	90	90	90	84.184(4)	90	90	90
β/°	105.878(5)	110.840(4)	107.998(3)	70.145(5)	114.070(3)	96.132(14)	95.588(3)
γ/°	90	90	90	88.898(5)	90	90	90
U/Å^3	4176.4(4)	1993.80(16)	6543.3(5)	2004.6(2)	4812.5(3)	6911.5(19)	6980.3(4)
Z	4	2	8	2	2	4	4
μ/mm^{-1}	0.433	0.447	0.529	0.448	3.027	4.108	4.085
F(000)	1744	804	2656	820	1744	2868	2908
Crystal size/mm^3	0.29 × 0.02 × 0.01	0.24 × 0.14 × 0.06	0.22 × 0.2 × 0.03	0.23 × 0.2 × 0.19	0.09 × 0.05 × 0.02	0.33 × 0.19 × 0.06	0.33 × 0.19 × 0.06
Absorption correction	multi-scan	integration	multi-scan	multi-scan	multi-scan	multi-scan	multi-scan
T_{min}/T_{max}	0.7087/0.9955	0.9357/0.9767	0.6090/0.9468	0.5092/0.9218	0.2962/0.8974	0.1813/0.6211	0.2195/0.6709
θ range/°	2.512 – 51.992	4.222 – 55.0	3.826 – 51.998	3.622 – 53.0	4.256 – 141.952	5.866 – 141.804	5.776 – 141.716
Reflections measured	18192	14675	13729	15109	18069	24200	25742
Independent reflections	8185	4729	6338	8203	8840	12476	12639
[R_{int}]	[0.0931]	[0.0326]	[0.0231]	[0.0413]	[0.0403]	[0.0316]	[0.0355]
Parameters	531	275	397	495	532	854	863
Final R_1 (wR_2) [$I > 2\sigma(I)$]	0.0851 (0.1469)	0.0450 (0.1113)	0.0469 (0.1081)	0.0494 (0.1285)	0.0549 (0.1255)	0.0641 (0.1554)	0.0727 (0.1694)
Final R_1 (wR_2) [all data]	0.1741 (0.1943)	0.0552 (0.1203)	0.0665 (0.1188)	0.0603 (0.1362)	0.0835 (0.1391)	0.0854 (0.1725)	0.1016 (0.1914)
Goodness of fit	1.085	1.092	1.019	1.026	1.032	1.042	1.031
Residual electron density/eÅ^{-3}	0.45/–0.45	1.17/–0.59	1.85/–1.07	0.67/–0.53	0.49/–0.33	2.00/–0.68	2.73/–1.32
CCDC No.	2073362	2073363	2073364	2073365	2073366	2073367	2073368

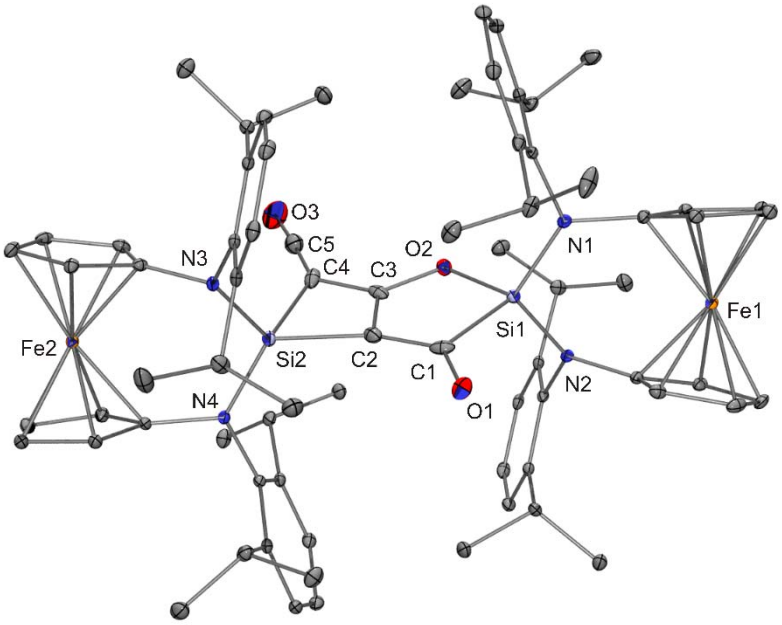


Fig. S1 Molecular structure of **2**·1.5 C_6H_6 in the crystal (ORTEP with 30 % probability ellipsoids; H atoms and solvent molecules omitted for clarity). Selected interatomic distances [Å] and angles [°]: Si1–O1 1.725(3), Si1–N1 1.709(3), Si1–N2 1.717(3), Si1–C1 1.961(5), Si2–N3 1.720(3), Si2–N4 1.715(3), Si2–C2 1.894(5), Si2–C4 2.017(5), O1–C3 1.378(5), O2–C1 1.246(6), O3–C5 1.152(7), C1–C2 1.398(7), C2–C3 1.379(6), C3–C4 1.396(7), C4–C5 1.286(7); O1–Si1–C1 91.2(2), N1–Si1–N2 110.15(16), N4–Si2–N3 110.91(15), C2–Si2–C4 72.7(2), Si–O1–C3 108.8(3), Si1–C1–C2 105.8(3), C1–C2–C3 112.3(4), O1–C3–C2 121.8(4), Si2–C2–C3 89.6(3), C2–C3–C4 113.4(4), Si2–C4–C3 84.3(3), O3–C4–C5 176.7(6).

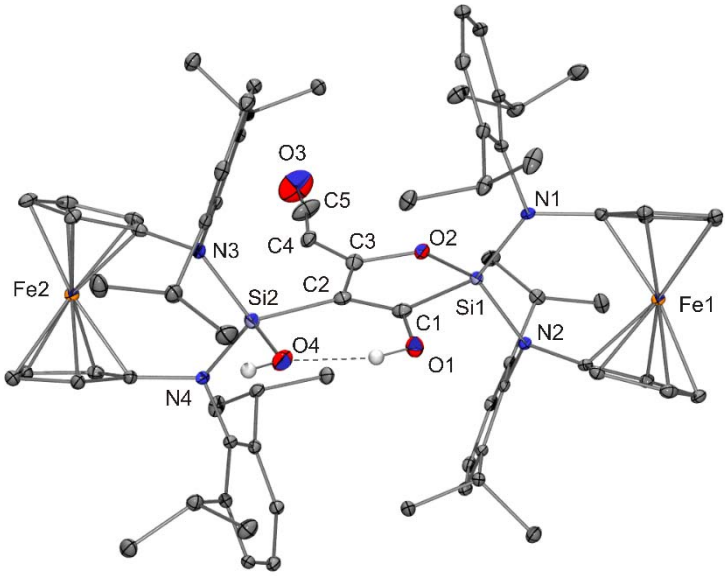


Fig. S2 Molecular structure of **3**·1.5 C_6H_6 in the crystal (ORTEP with 30 % probability ellipsoids; H atoms and solvent molecules omitted for clarity). Selected interatomic distances [Å] and angles [°]: Si1–O2 1.665(4), Si1–N1 1.711(4), Si1–N2 1.714(4), Si1–C1 1.909(6), Si2–O4 1.686(4), Si2–N3 1.747(4), Si2–N4 1.737(4), Si2–C2 1.900(6), O1–C1 1.363(6), O2–C3 1.412(6), O3–C5 1.180(8), C1–C2 1.364(8), C2–C3 1.419(8), C3–C4 1.306(7), C4–C5 1.350(9); O2–Si1–C1 89.6(2), N1–Si1–N2 109.8(2), N4–Si2–N3 107.4(2), O4–Si2–C2 90.3(2), Si1–O2–C3 113.8(3), Si1–C1–C2 109.8(4), C1–C2–C3 111.7(5), O2–C3–C2 115.0(4), C3–C4–C5 137.7(6), O3–C5–C4 171.7(9).

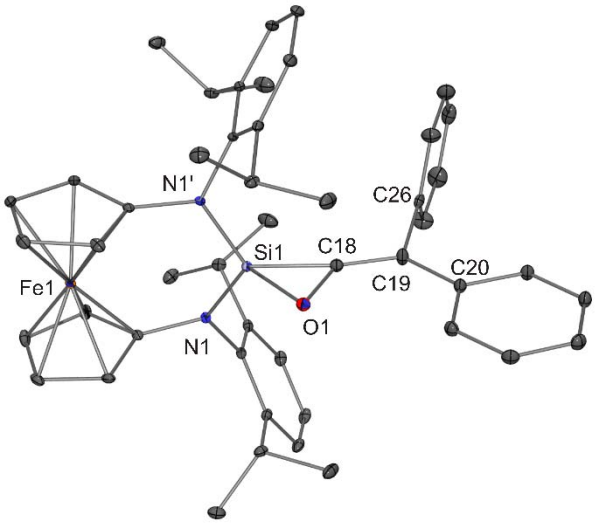


Fig. S3 Molecular structure of **4** in the crystal (ORTEP with 30 % probability ellipsoids; H atoms omitted for clarity). Selected interatomic distances [Å] and angles [°]: Si1–O1 1.712(2), Si1–N1 1.6984(15), Si1–C18 1.781(3), O1–C18 1.453(4), C18–C19 1.342(4); N1–Si1–N1 115.14(11), O1–Si1–C18 49.13(12), Si1–O1–C18 67.90(15), Si1–C18–O1 62.97(14), C18–C19–C20 125.8(3), C18–C19–C26 115.7(3), C20–C19–C26 116.8(2).

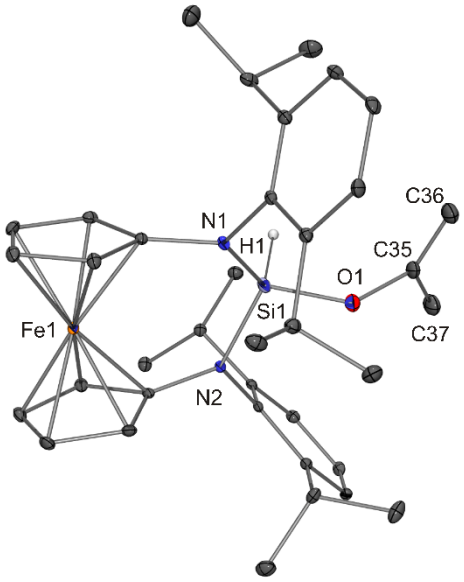


Fig. S4 Molecular structure of **5** in the crystal (ORTEP with 30 % probability ellipsoids; H atoms omitted for clarity). Si1–O1 1.625(2), Si1–N1 1.717(2), Si1–N2 1.720(2), O1–C35 1.397(4), C35–C36 1.328(5), C35–C37 1.468(5); N1–Si1–N2 111.77(10), Si1–O1–C35 126.7(2), O1–C35–C36 118.5(3), C36–C35–C37 126.4(3).

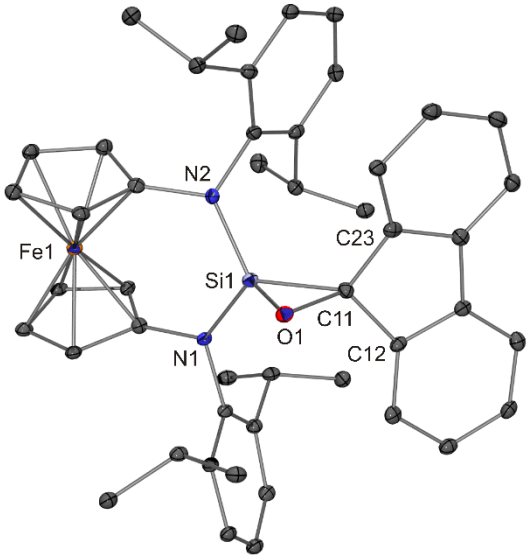


Fig. S5 Molecular structure of **7**·C_6H_6 in the crystal (ORTEP with 30 % probability ellipsoids; H atoms and solvent molecule omitted for clarity). Selected interatomic distances [Å] and angles [°]: Si1–O1 1.655(4), Si1–N1 1.707(5), Si1–N2 1.727(5), Si1–C11 1.852(6), O1–C11 1.525(7), C11–C12 1.511(8), C11–C23 1.469(8); N1–Si1–N2 112.7(2), O1–Si1–C11 51.2(2), Si1–O1–C11 71.1(3), Si1–C11–O1 57.7(3), C12–C11–C23 103.6(5).

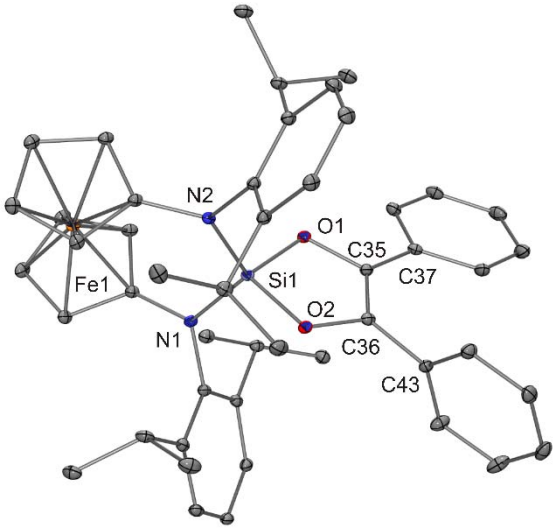


Fig. S6 Molecular structure of **8** in the crystal (ORTEP with 30 % probability ellipsoids; H atoms omitted for clarity). Selected interatomic distances [Å] and angles [°]: Si1–O1 1.6667(17), Si1–O2 1.6608(16), Si1–N1 1.7020(19), Si1–N2 1.699(2), O1–C35 1.398(3), O2–C36 1.401(3), C35–C36 1.350(3), C35–C37 1.466(3), C36–C43 1.481(3); N1–Si1–N2 112.98(10), O1–Si1–O2 95.33(8), Si1–O1–C35 108.96(13), Si1–O2–C36 108.22(13), O1–C35–C36 112.6(2), O2–C36–C35 114.1(2), C36–C35–C37 132.0(2), C35–C36–C43 129.6(2).

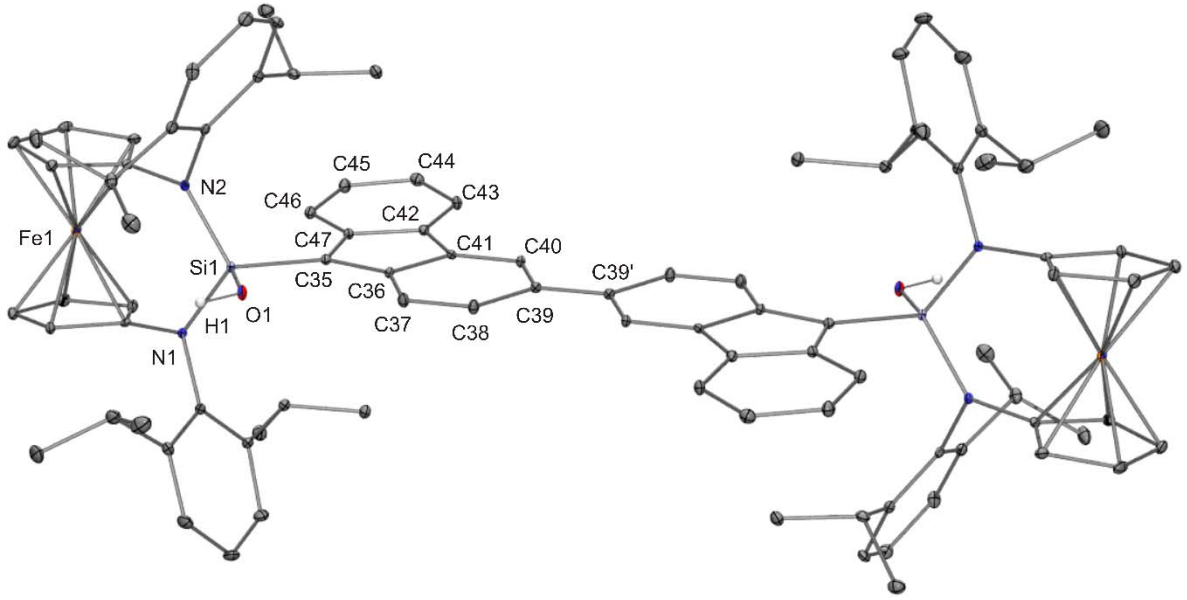


Fig. S7 Molecular structure of, **9**·2 C_6H_6 (i. e. the benzene solvate of the dimer of **7**) in the crystal (ORTEP with 30 % probability ellipsoids; H atoms and solvent molecule omitted for clarity). Selected interatomic distances [Å] and angles [°]: Si1–O1 1.635(2), Si1–N1 1.729(3), Si1–N2 1.730(2), Si1–C35 1.873(3), C35–C36 1.394(4), C35–C47 1.472(4), C36–C37 1.434(4), C36–C41 1.451(4), C37–C38 1.352(4), C38–C39 1.431(4), C39–C39' 1.421(6), C39–C40 1.439(4), C40–C41 1.368(4), C41–C42 1.456(4), C42–C43 1.377(4), C42–C47 1.425(4), C43–C44 1.393(5), C44–C45 1.399(5), C45–C46 1.385(5), C46–C47 1.394(4); N1–Si1–N2 111.69(12), O1–Si1–C35 102.34(13), C36–C35–C47 106.4(3).

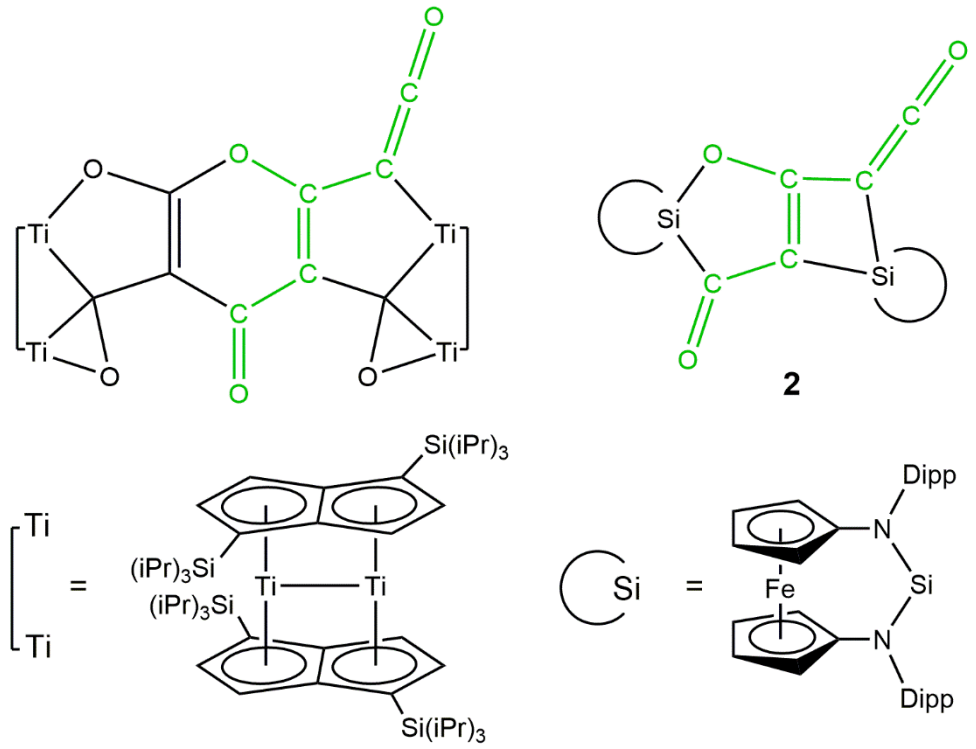


Fig. S8 [[Ti_2{μ:η^5,η^5-C_8H_4-1,4-(Si*i*Pr$_3$)$_3$}$_2$]$_2$(μ-C_9O_6)] (left), obtained from the reaction of C_3O_2 with [Ti_2{μ:η^5,η^5-C_8H_4-1,4-(Si*i*Pr$_3$)$_3$}$_2$];[S2] similar to **2** (right), this complex also contains a C_5O_3 subunit (green).

C Plots of NMR Spectra

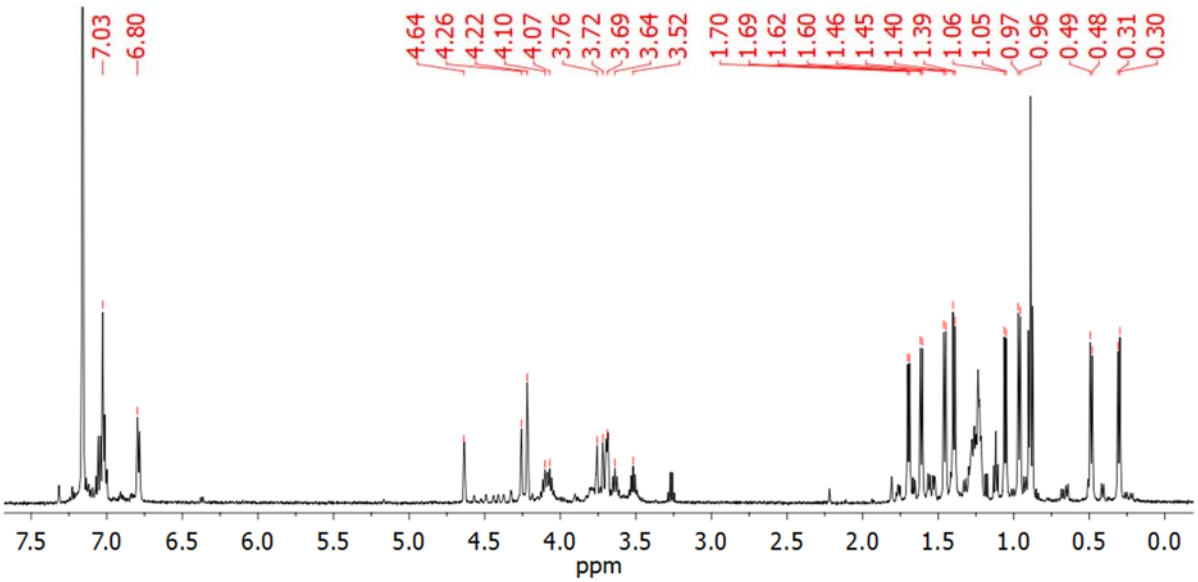


Fig. S9 ^{1}H NMR spectrum of crude **2** (C_6D_6, 499.7 MHz).

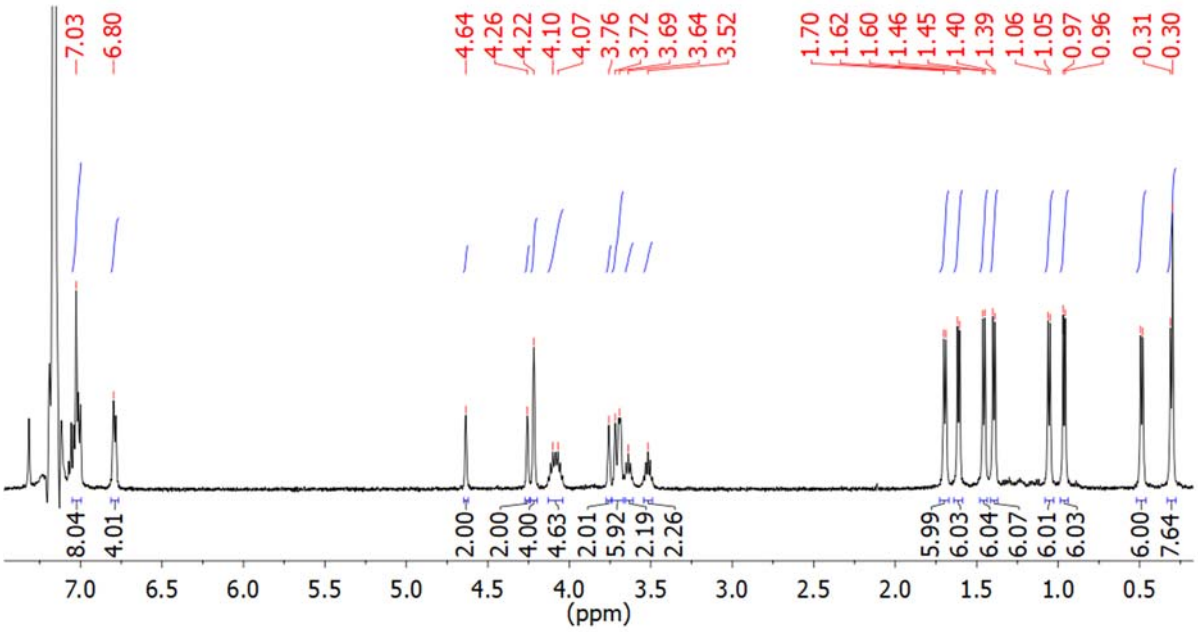


Fig. S10 ^{1}H NMR spectrum of **2** (C_6D_6, 499.7 MHz) after recrystallization.

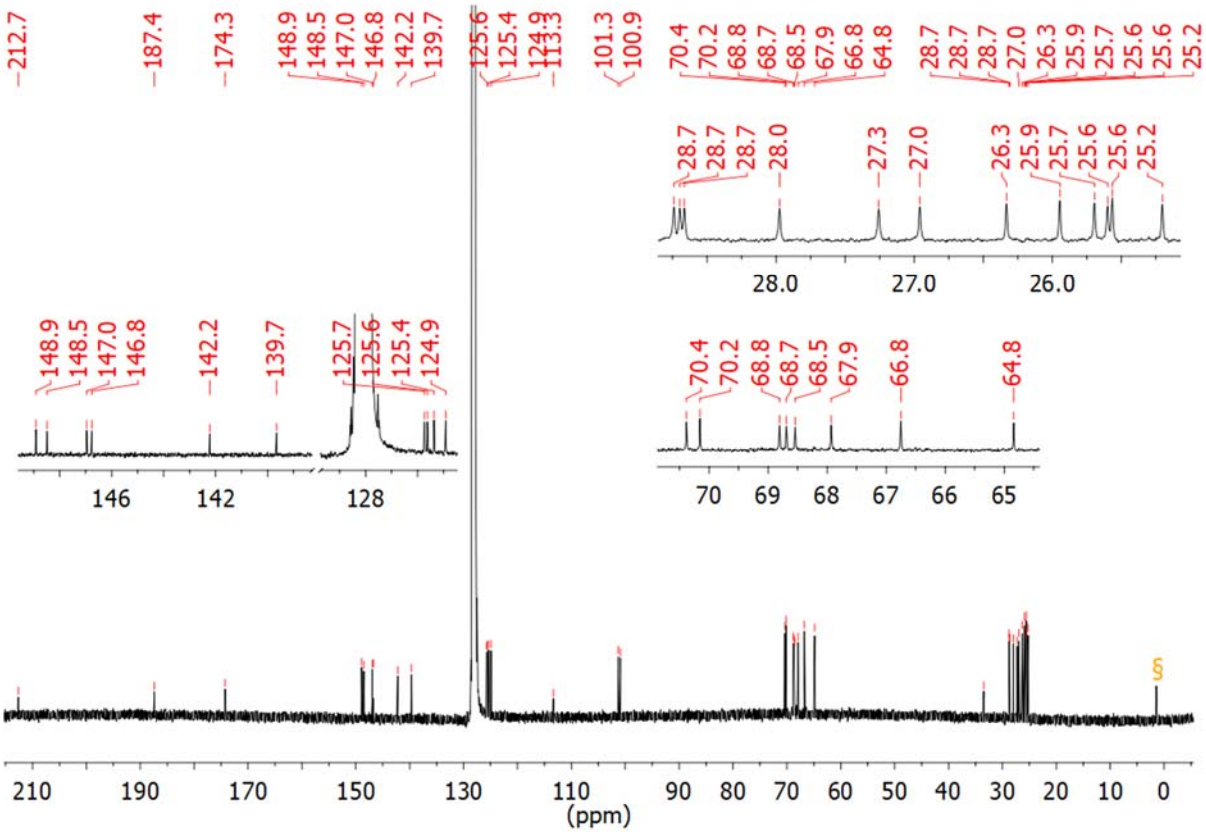


Fig. S11 $^{13}C\{^{1}H\}$ NMR spectrum of **2** (C_6D_6, 100.5 MHz). The signal marked belongs to silicon grease (§).

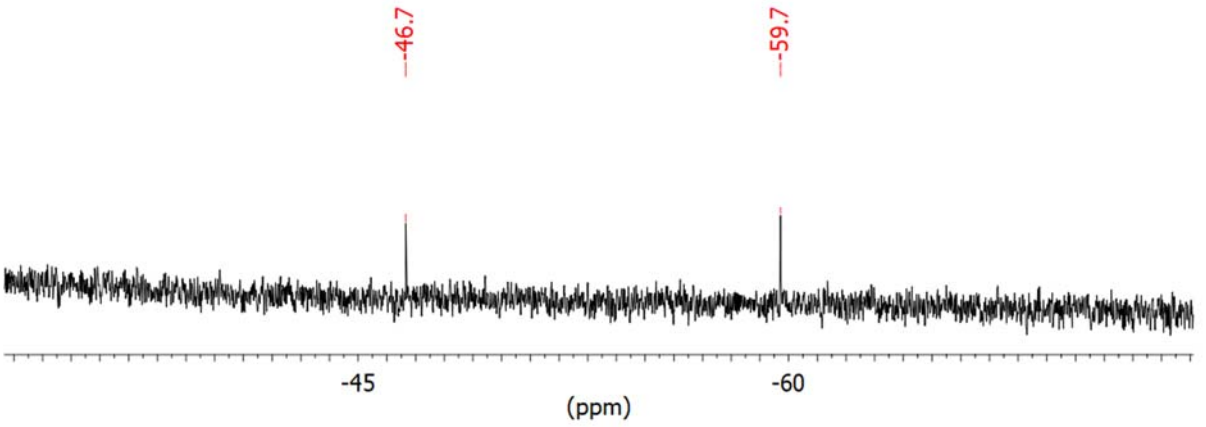


Fig. S12 $^{29}Si\{^{1}H\}$ NMR spectrum of **2** (C_6D_6, 99.3 MHz).

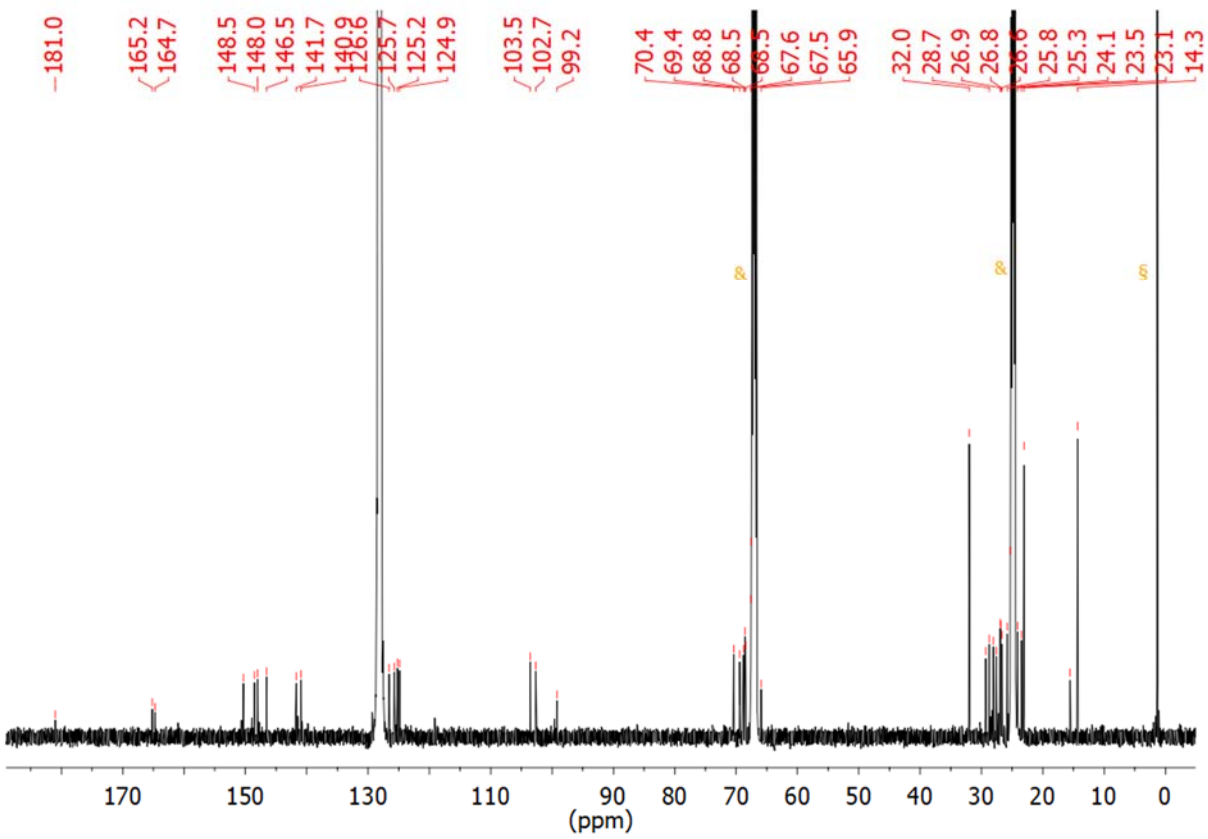


Fig. S13 $^{13}C\{^{1}H\}$ NMR spectrum of **3** (C_6D_6, 100.5 MHz). The signals marked belong to silicon grease (§) and THF (&).

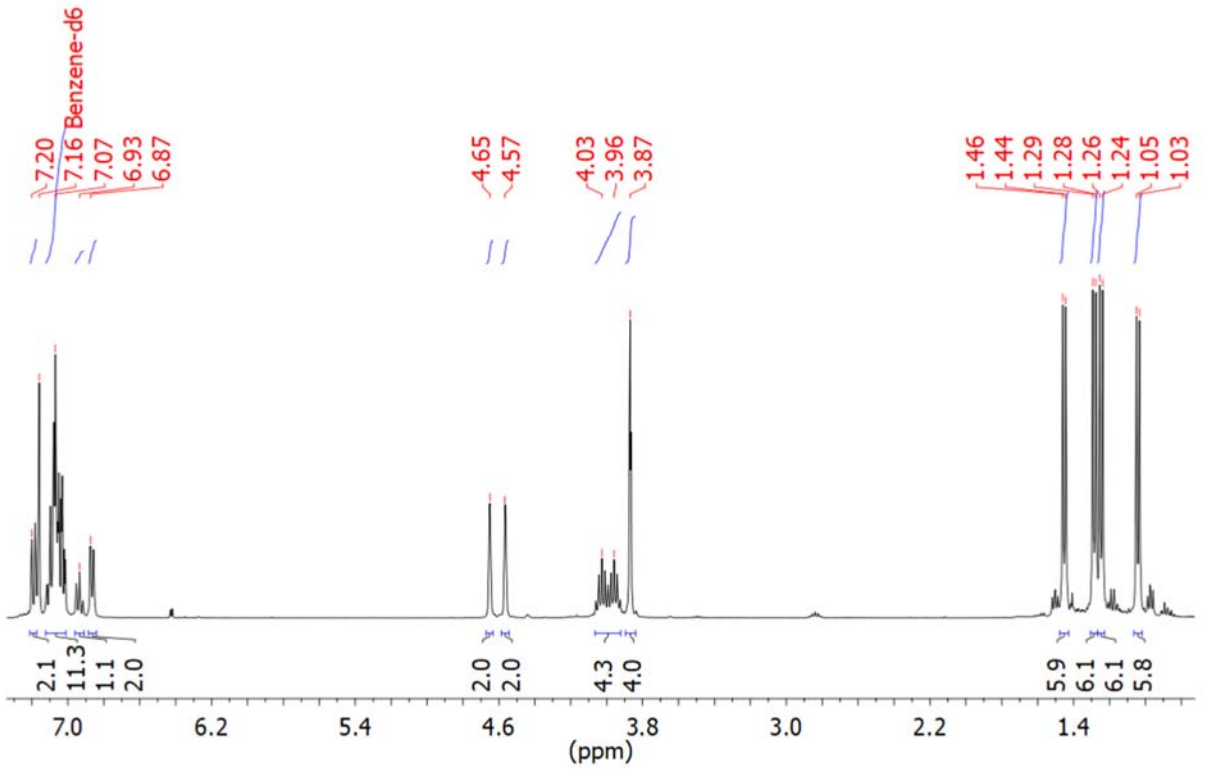


Fig. S14 ^{1}H NMR spectrum of **4** (C_6D_6, 499.7 MHz).

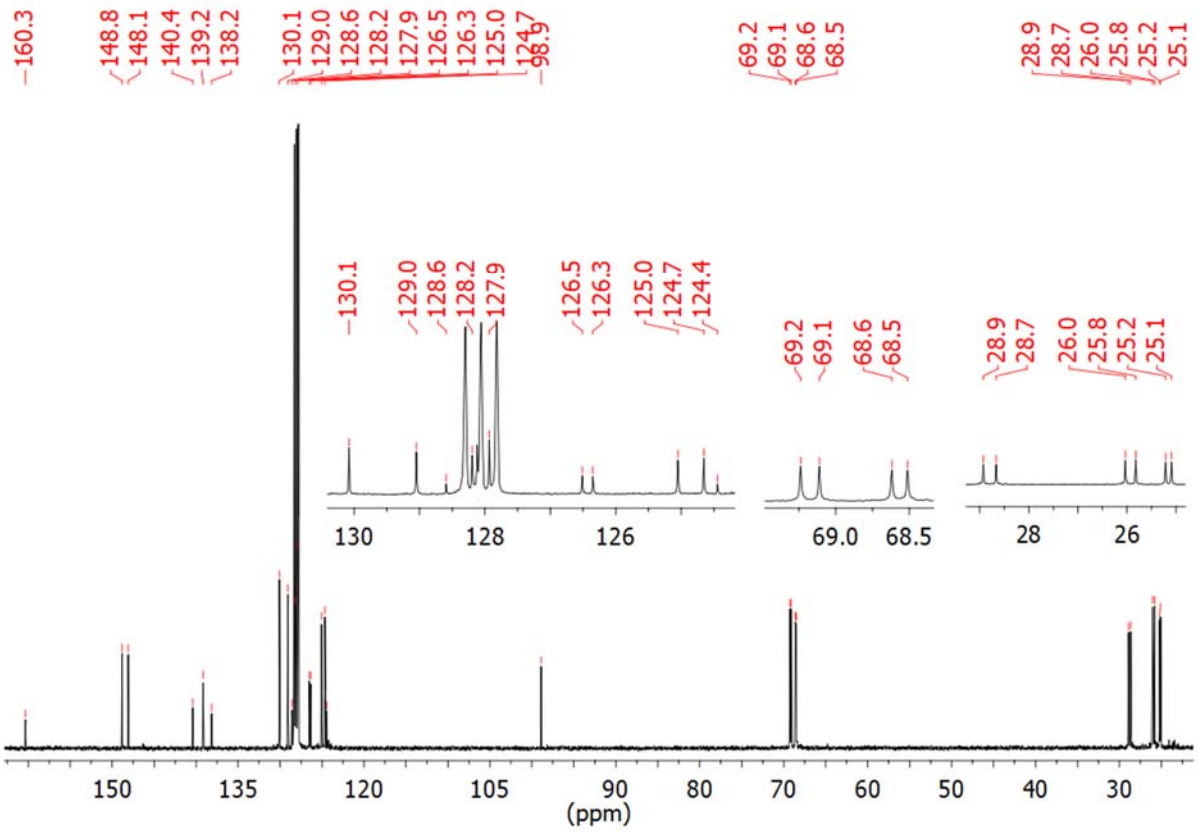


Fig. S15 $^{13}C\{^{1}H\}$ NMR spectrum of **4** (C_6D_6, 100.5 MHz).

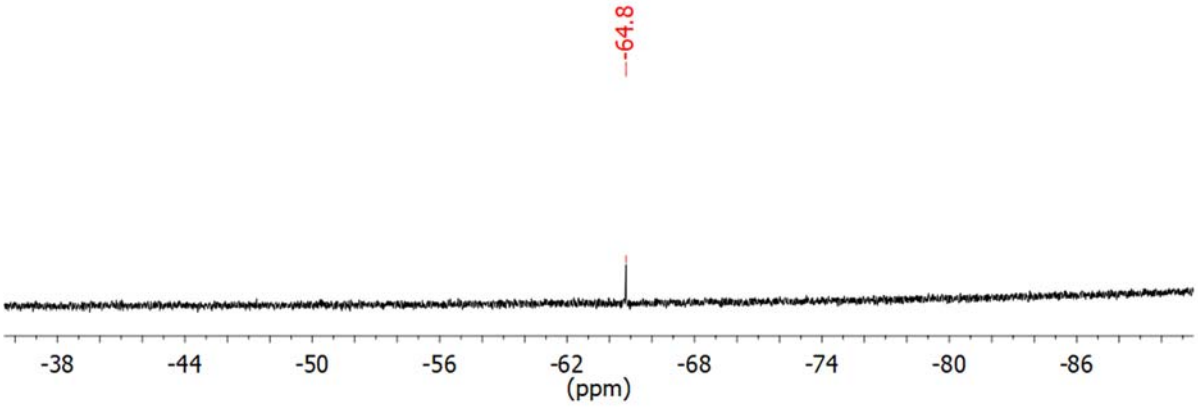


Fig. S16 $^{29}Si\{^{1}H\}$ NMR spectrum of **4** (C_6D_6, 99.3 MHz).

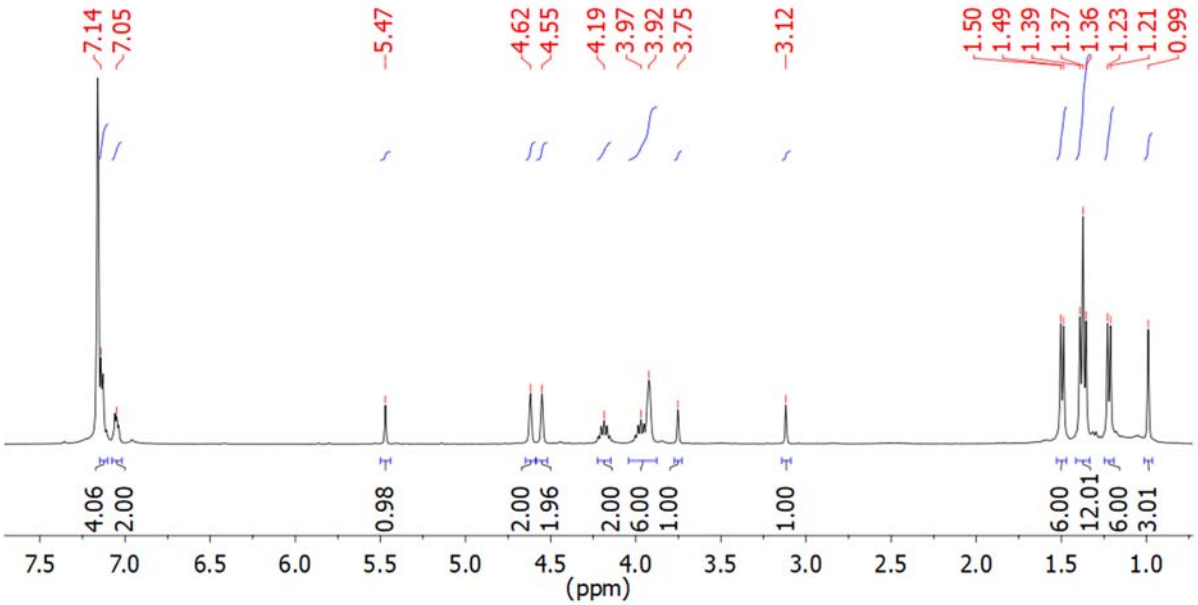


Fig. S17 ^{1}H NMR spectrum of **5** (C_6D_6, 499.7 MHz).

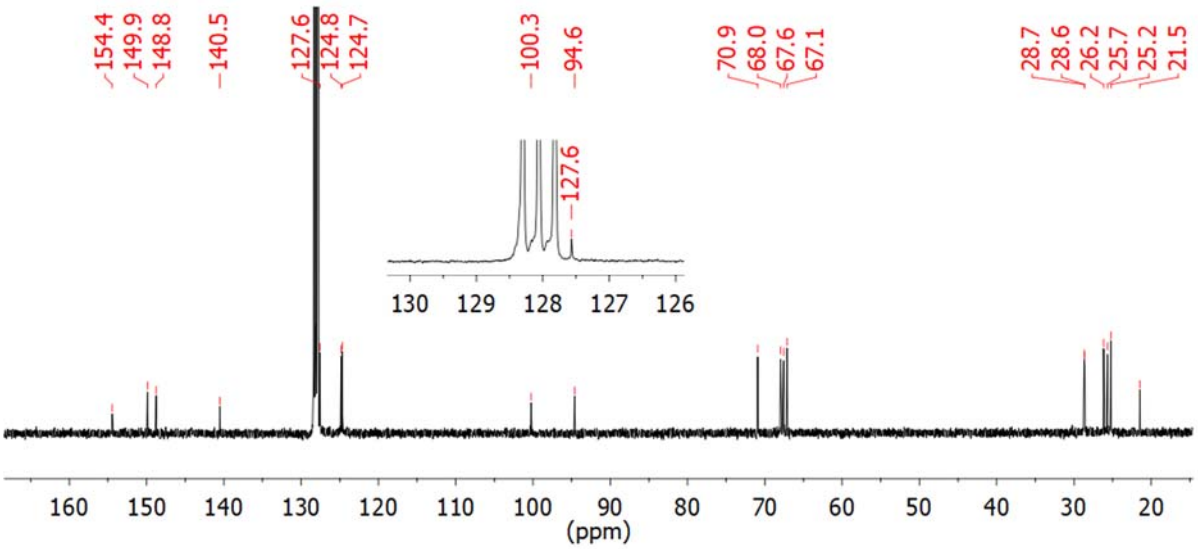


Fig. S18. ^{13}C{^{1}H} NMR spectrum of **5** (C_6D_6, 100.5 MHz).

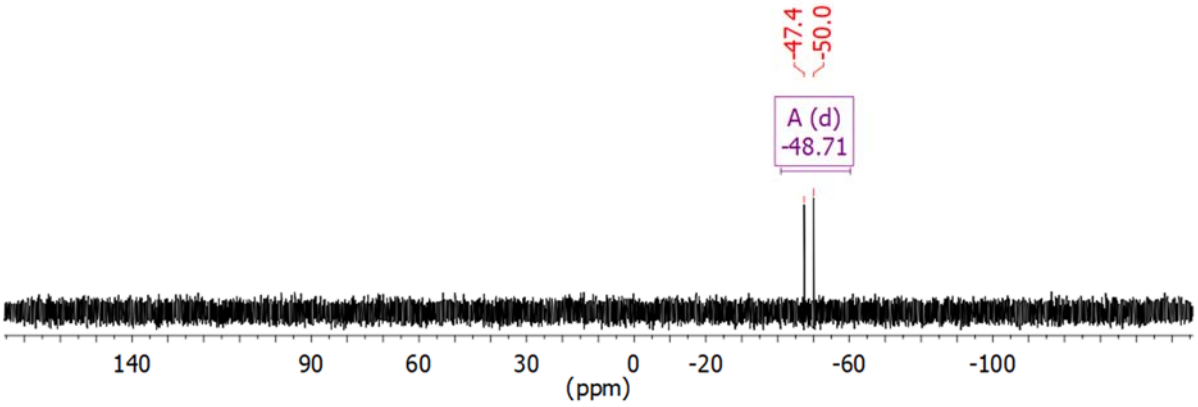


Fig. S19 ^{29}Si NMR spectrum of **5** (C_6D_6, 99.3 MHz).

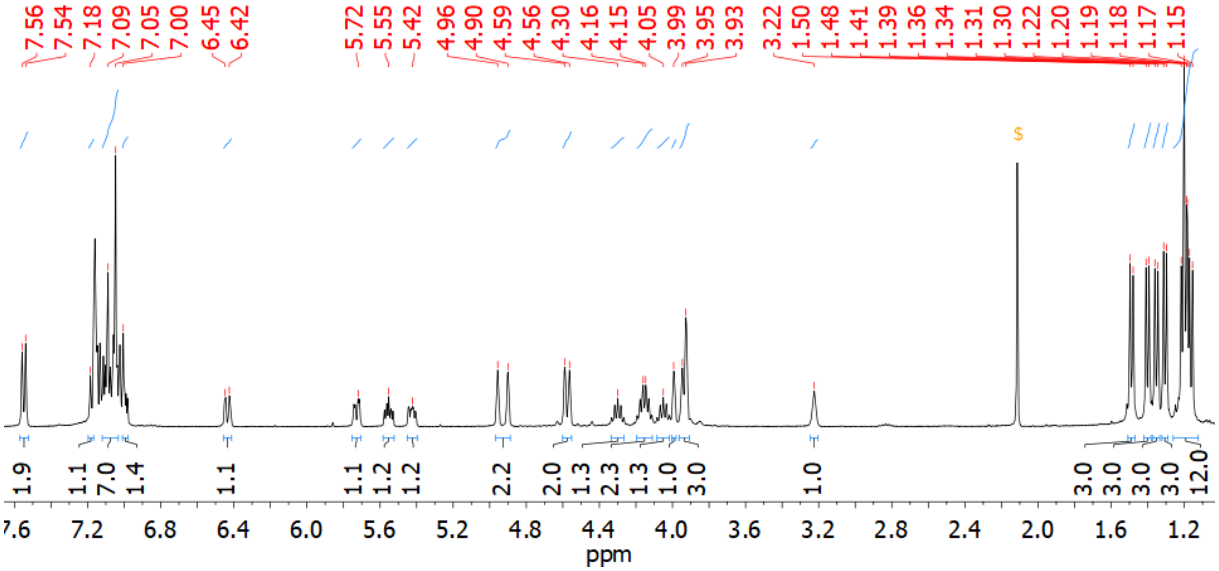


Fig. S20 ^{1}H NMR spectrum of **6** (C_6D_6, 499.7 MHz). The signal marked belongs to toluene ($).

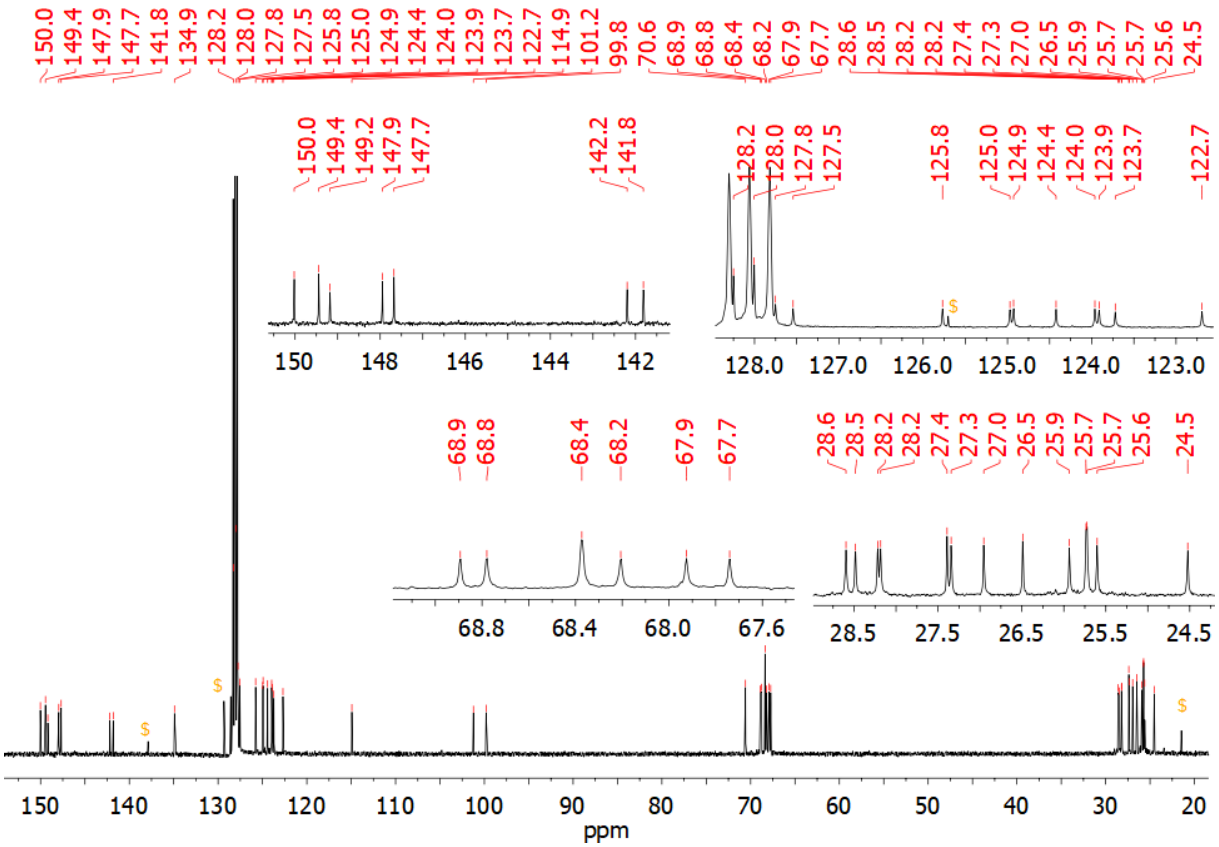


Fig. S21 ^{13}C{^{1}H} NMR spectrum of **6** (C_6D_6, 100.5 MHz). Signals marked belong to toluene ($).

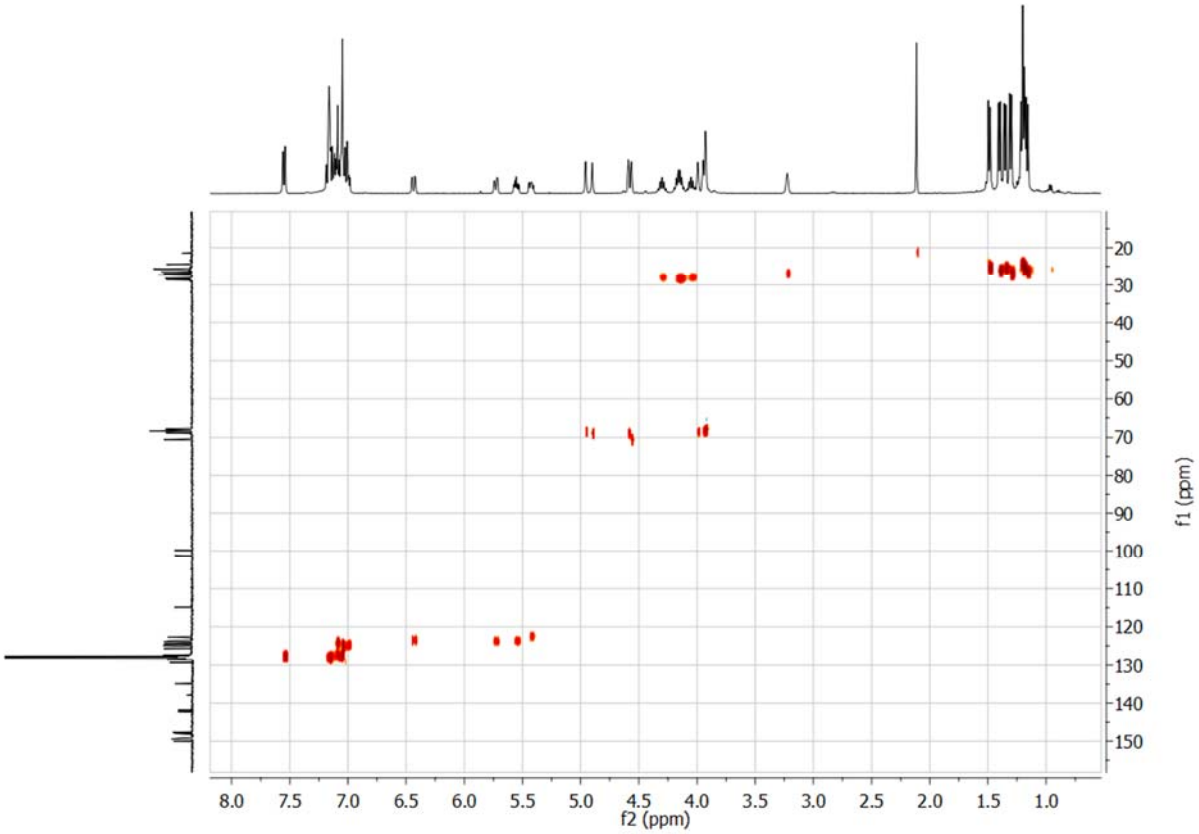


Fig. S22 ^{1}H-^{13}C HSQC NMR spectrum of **6** (C_6D_6).

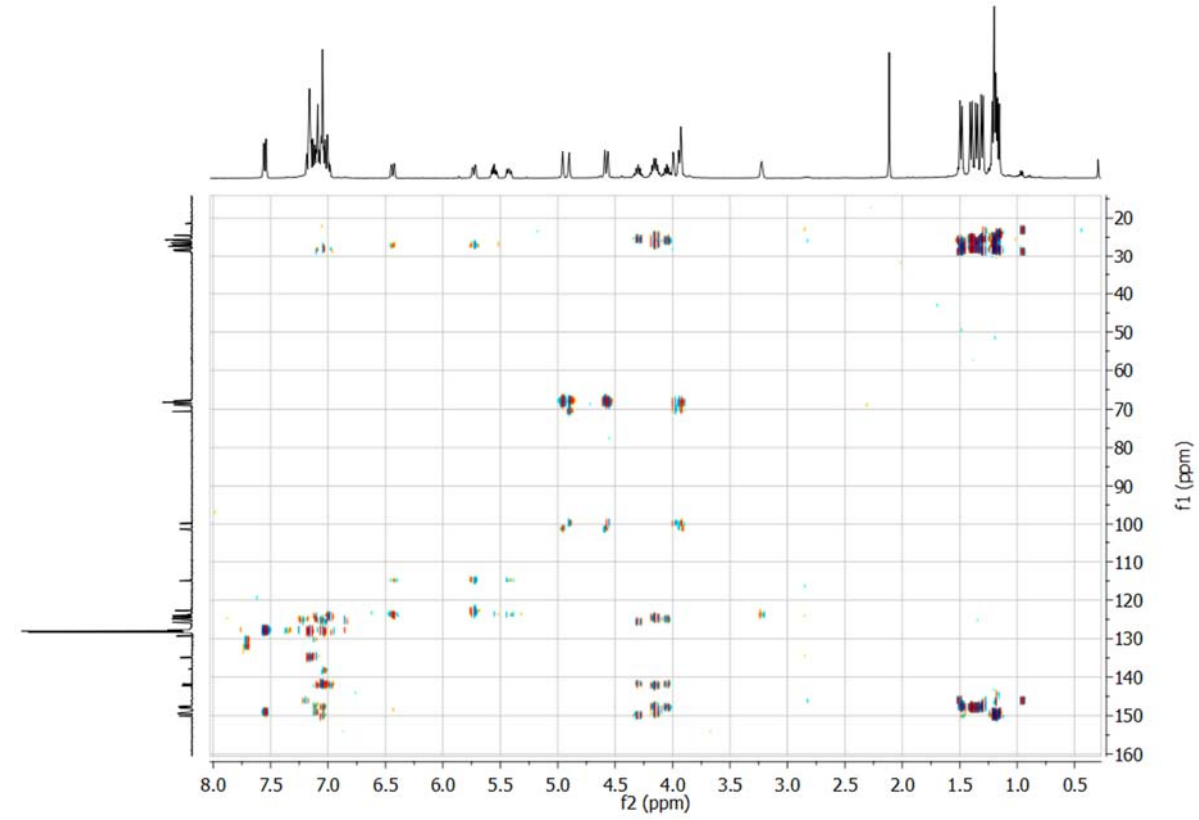


Fig. S23 ^{1}H-^{13}C HMBC NMR spectrum of **6** (C_6D_6).

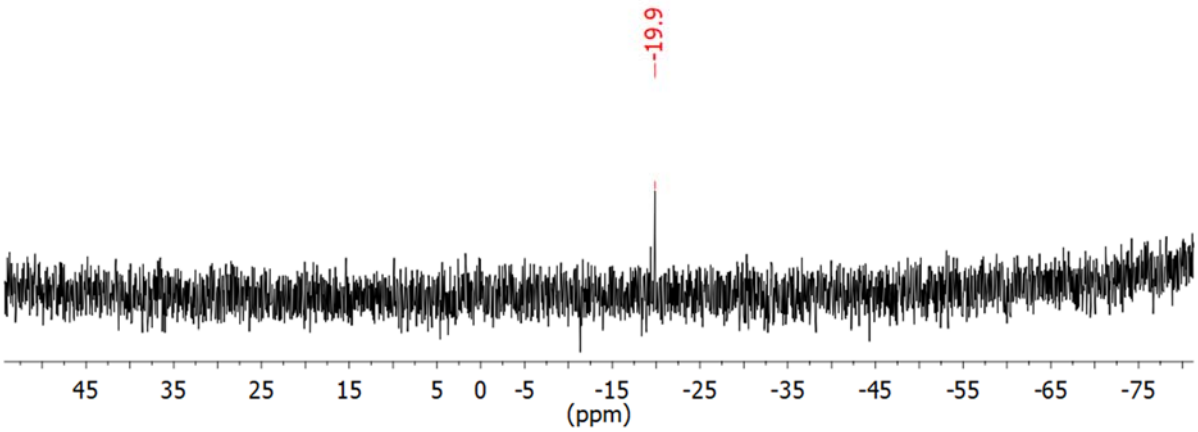


Fig. S24 $^{29}Si\{^{1}H\}$ NMR spectrum of **6** (C_6D_6, 99.3 MHz).

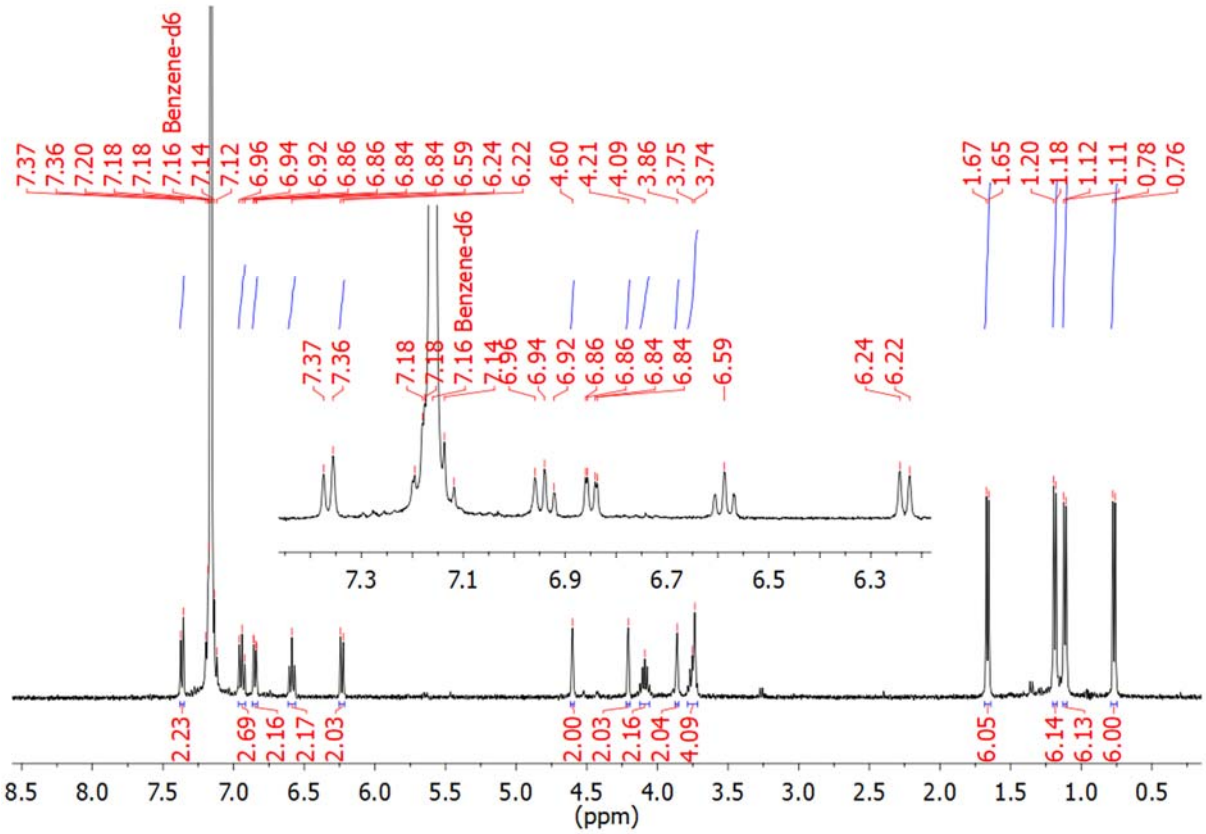


Fig. S25 ^{1}H NMR spectrum of **7** (C_6D_6, 499.7 MHz).

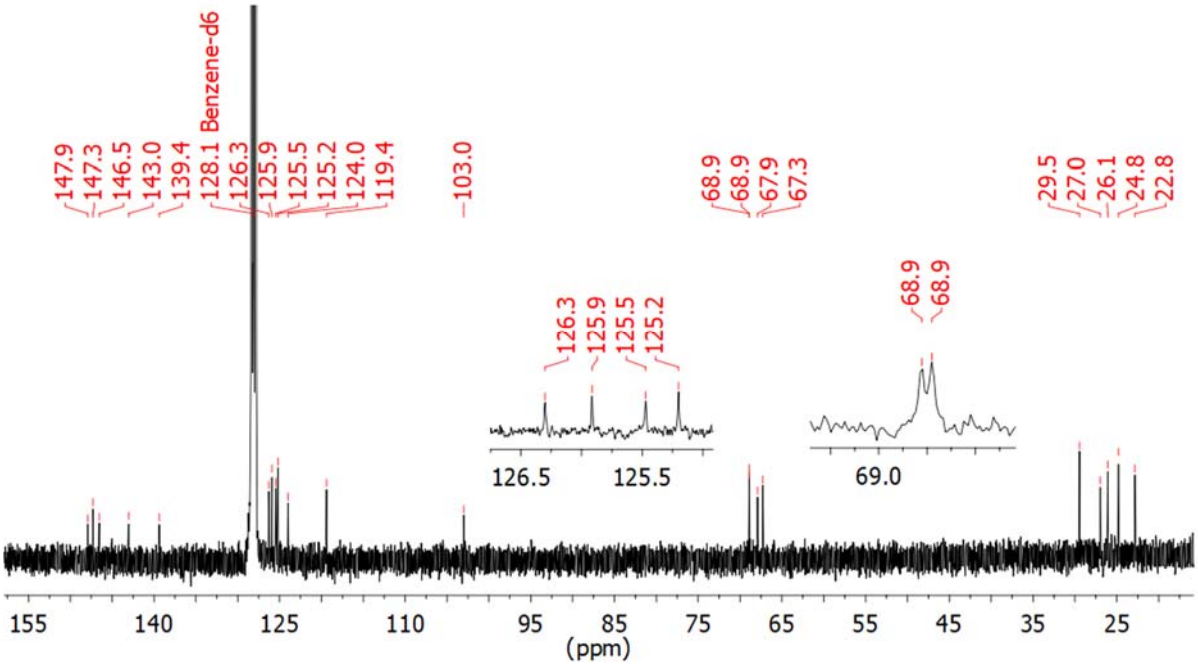


Fig. S26 $^{13}C\{^{1}H\}$ NMR spectrum of **7** (C_6D_6, 100.5 MHz).

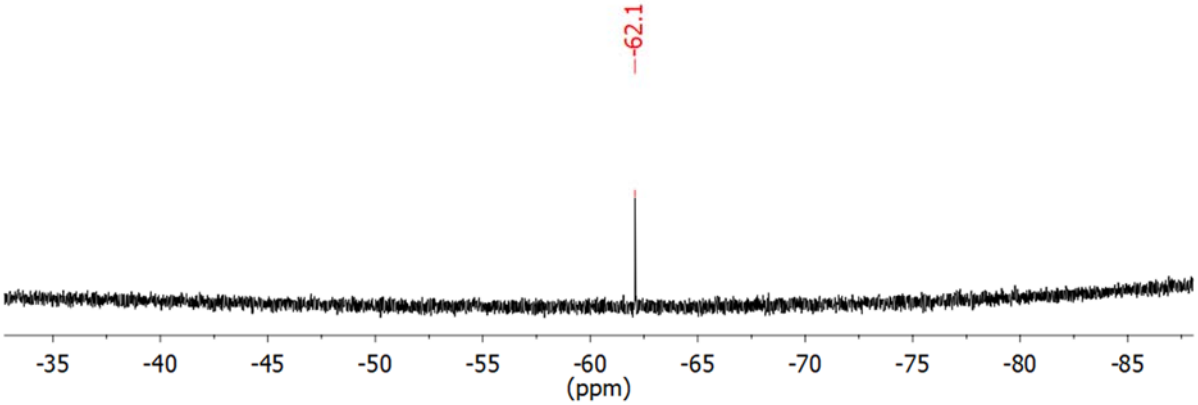


Fig. S27 $^{29}Si\{^{1}H\}$ NMR spectrum of **7** (C_6D_6, 99.3 MHz).

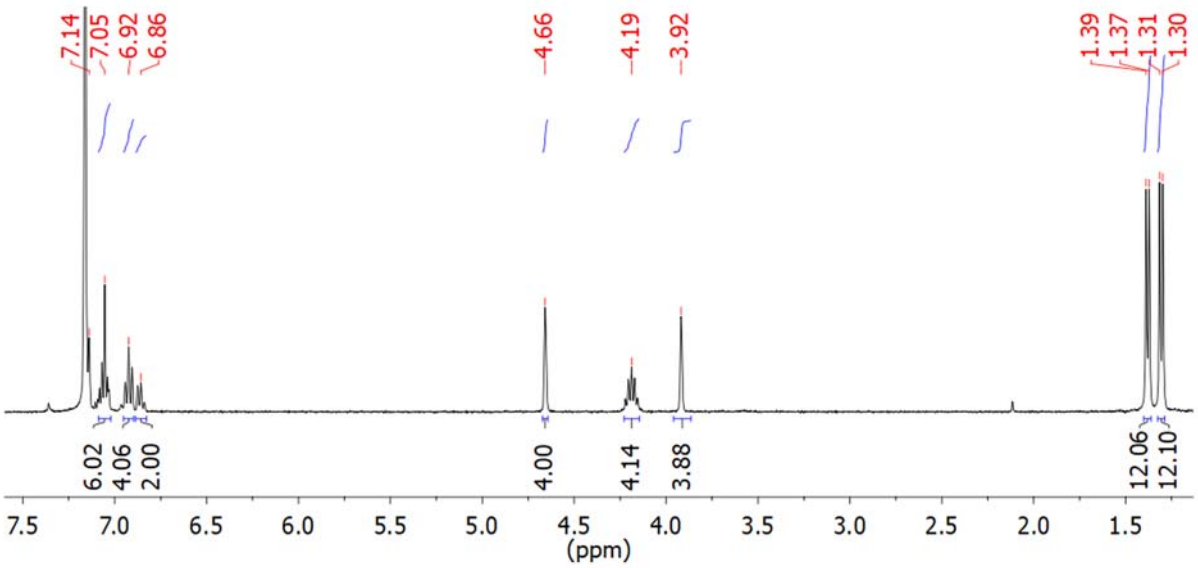


Fig. S28 ^{1}H NMR spectrum of **8** (C_6D_6, 499.7 MHz).

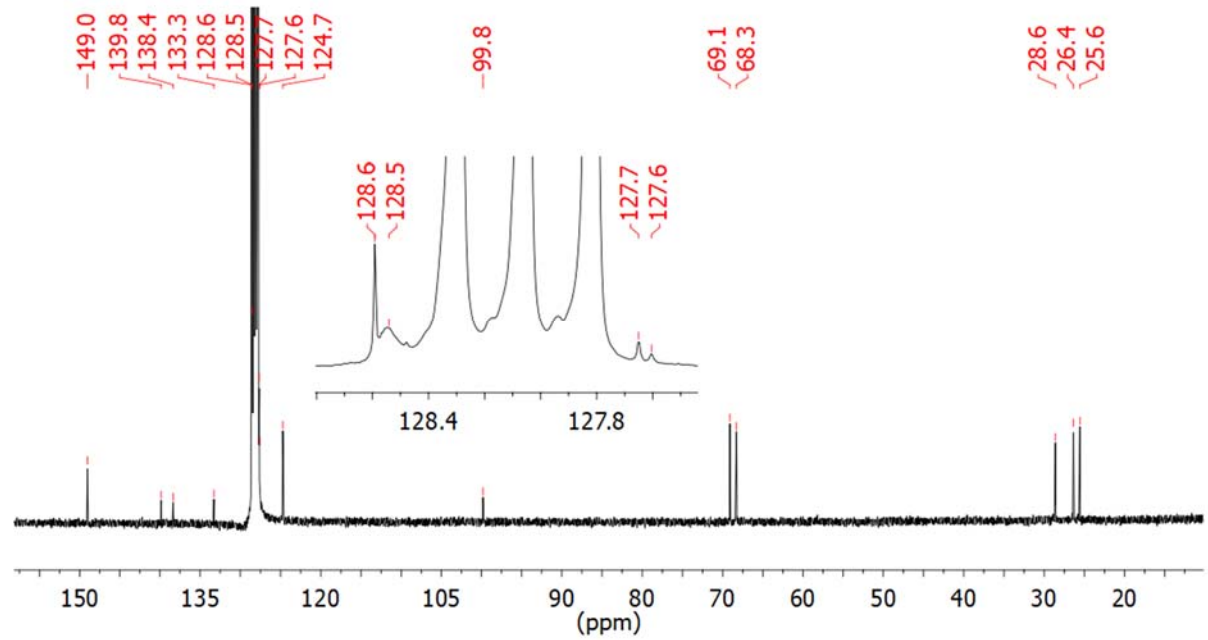


Fig. S29 $^{13}C\{^{1}H\}$ NMR spectrum of **8** (C_6D_6, 100.5 MHz).

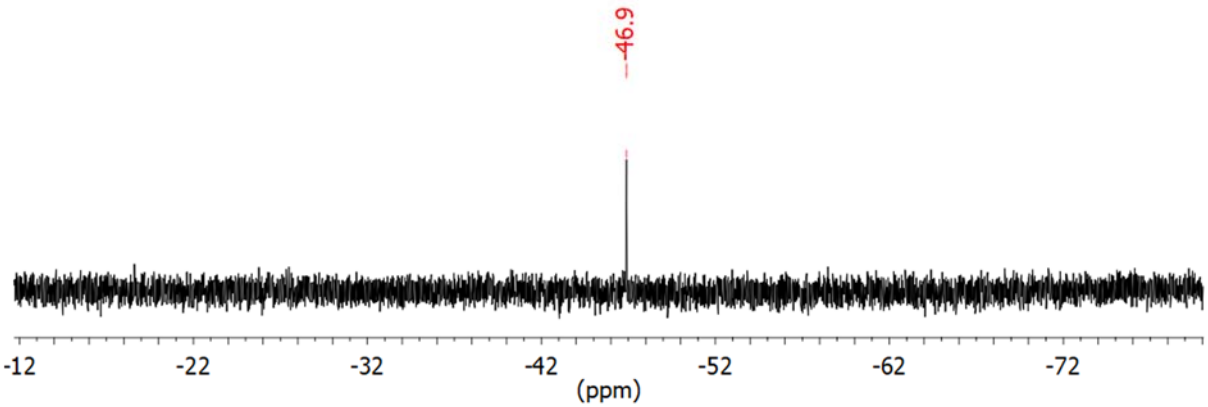


Fig. S30 $^{29}Si\{^{1}H\}$ NMR spectrum of **8** (C_6D_6, 99.3 MHz).

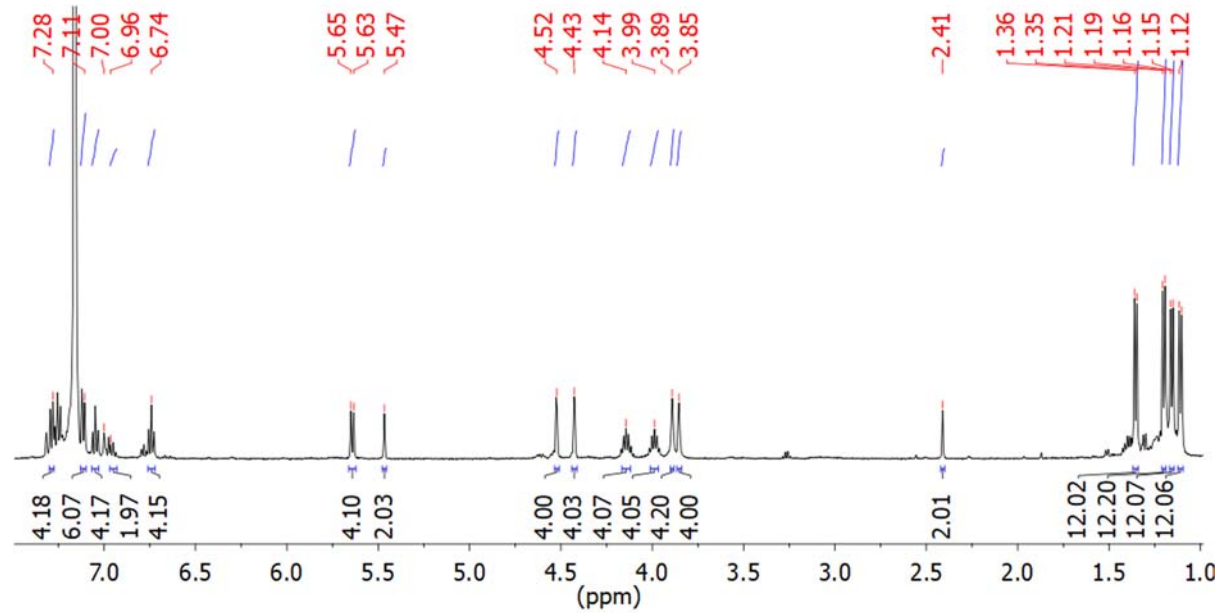


Fig. S31 ^{1}H NMR spectrum of **9** (C_6D_6, 499.7 MHz).

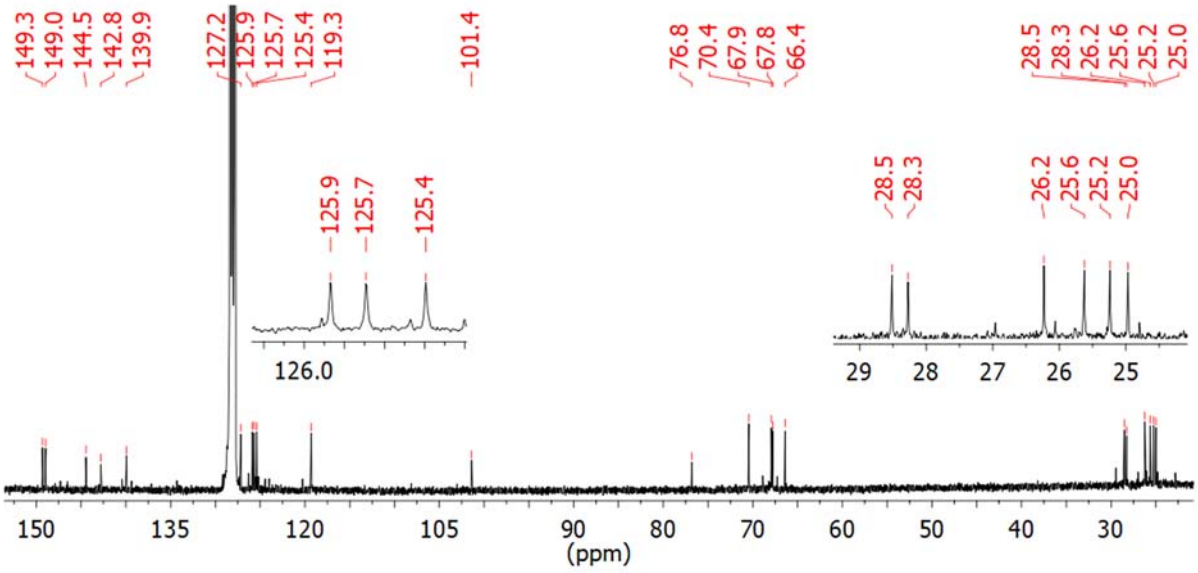


Fig. S32 $^{13}C\{^{1}H\}$ NMR spectrum of **9** (C_6D_6, 100.5 MHz).

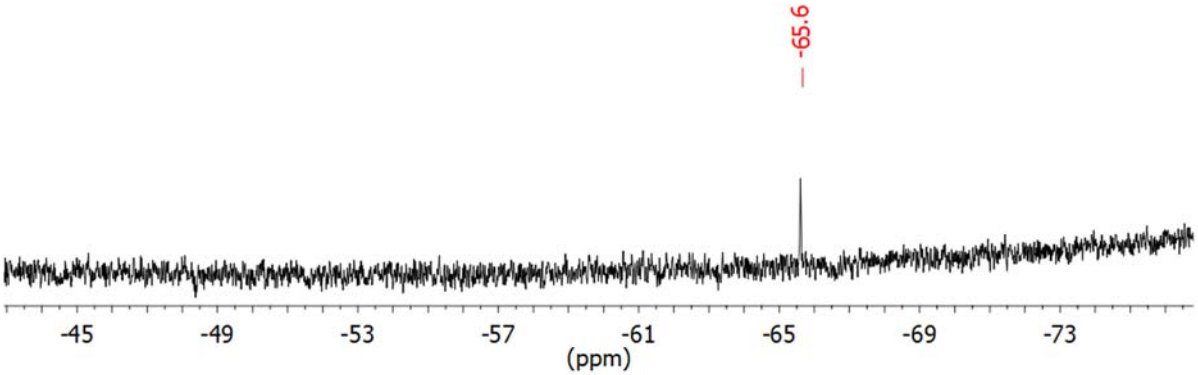


Fig. S33 $^{29}Si\{^{1}H\}$ NMR spectrum of **9** (C_6D_6, 99.3 MHz).

II Computational Details

Geometry optimizations and harmonic frequency calculations were performed using the ORCA program package[S6] (Version 4.1.2) employing the PBEh-3c density functional composite method[S7] combined with a higher integration grid (grid5) to avoid spurious imaginary frequencies. Optimised structures were characterised as minima or first order saddle points by eigenvalue analysis of the computed Hessians. Connectivities between minima and the corresponding transition states were validated by intrinsic reaction coordinate (IRC) calculations[S8] or by displacing the transition-state geometries along both directions of the transition mode, followed by unconstrained optimizations to the respective minima. Zero-point vibrational energies and thermal contributions to Gibbs free energies at 298.15 K were obtained at this level of theory.

A two-layer ONIOM(QM:QM) single-point approach was employed for improved energies. To this end, small molecular model systems are constructed from DFT-optimised real system structures by removing Dipp substituents and the ferrocene backbone and placing hydrogen atoms along the covalent bonds broken. The bond lengths of the newly introduced N–H bonds were reoptimised at the PBEh-3c level with all other model system coordinates fixed to their real system values. Single-point energy calculations on the model systems employing explicitly correlated F12 coupled-cluster theory (high level, HL) are combined with PBEh-3c single-point calculations (low level, LL) to give an improved extrapolated energy for the full systems according to Eq. 1 (Fig. S34).[S9–S11]

$$E_{ONIOM(HL:LL)} = E_{LL}^{real} - E_{LL}^{model} + E_{HL}^{model} \qquad (1)$$

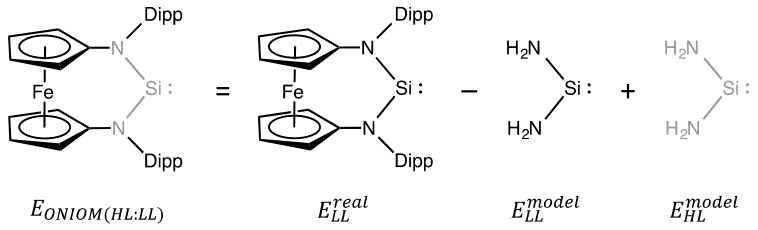


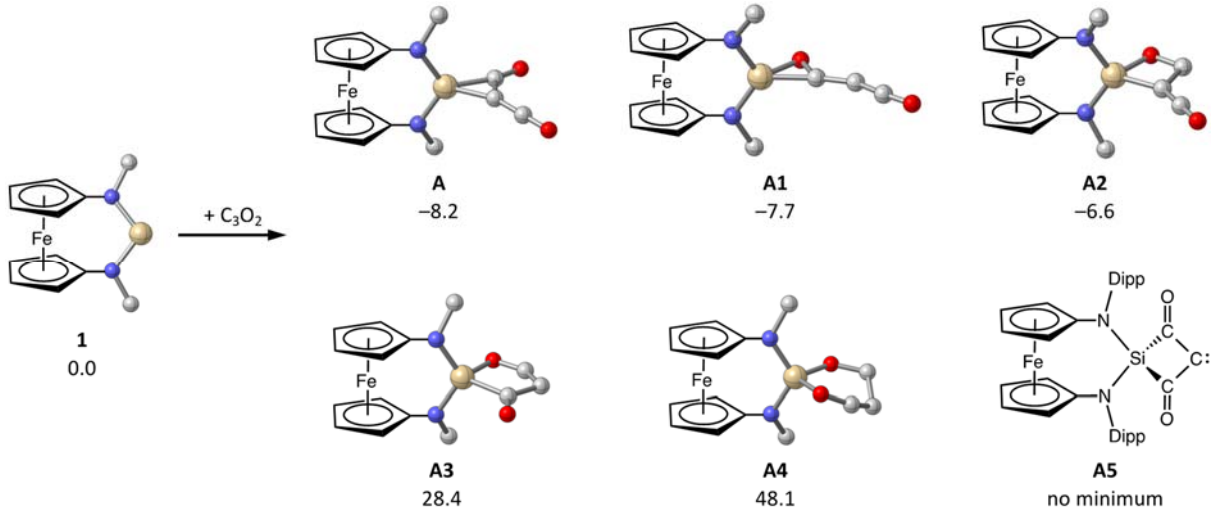
Fig. S34 Schematic presentation of the ONIOM(CC–F12:PBEh-3c) approach.

CCSD(T*)–F12b[S12] calculations were conducted using the MOLPRO 2015.1 program[S13] in combination with the F12-optimised correlation consistent polarised triple-zeta orbital[S14] and auxiliary[S15–S17] basis sets of the cc-pVTZ-F12 family. Pictures of molecular structures were

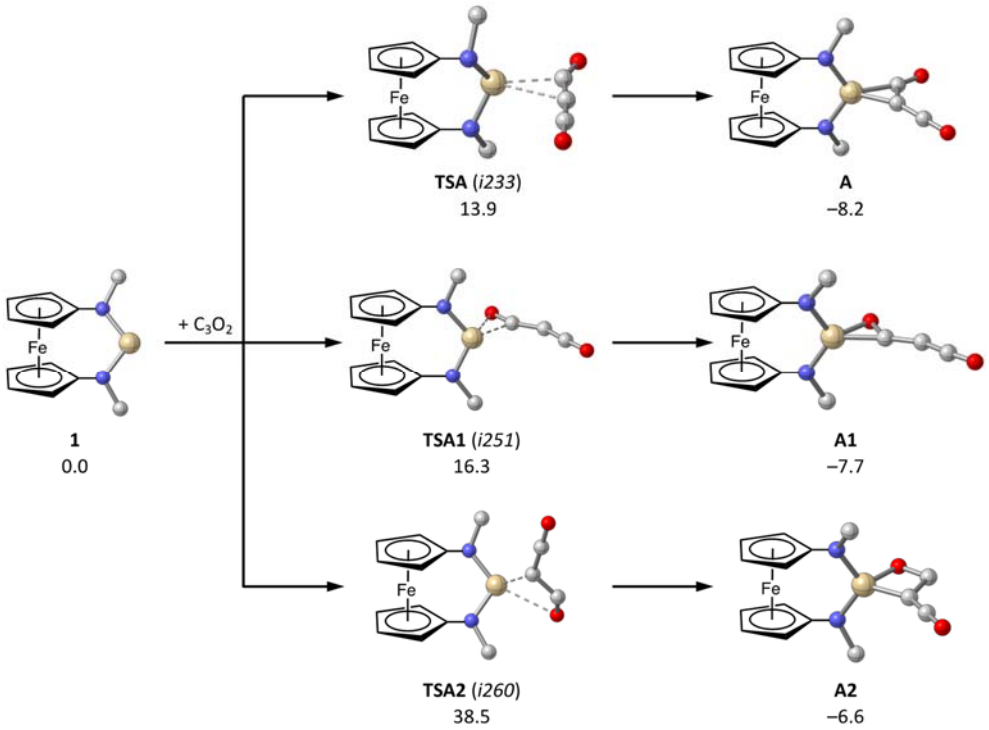
generated with the Cylview[S18] and ChemCraft[S19] programs. All energies given are relative free energies at 298.15 K and 1 atm (ΔG^{298}) in kcal mol^{-1}.

Additional information on reaction paths investigated

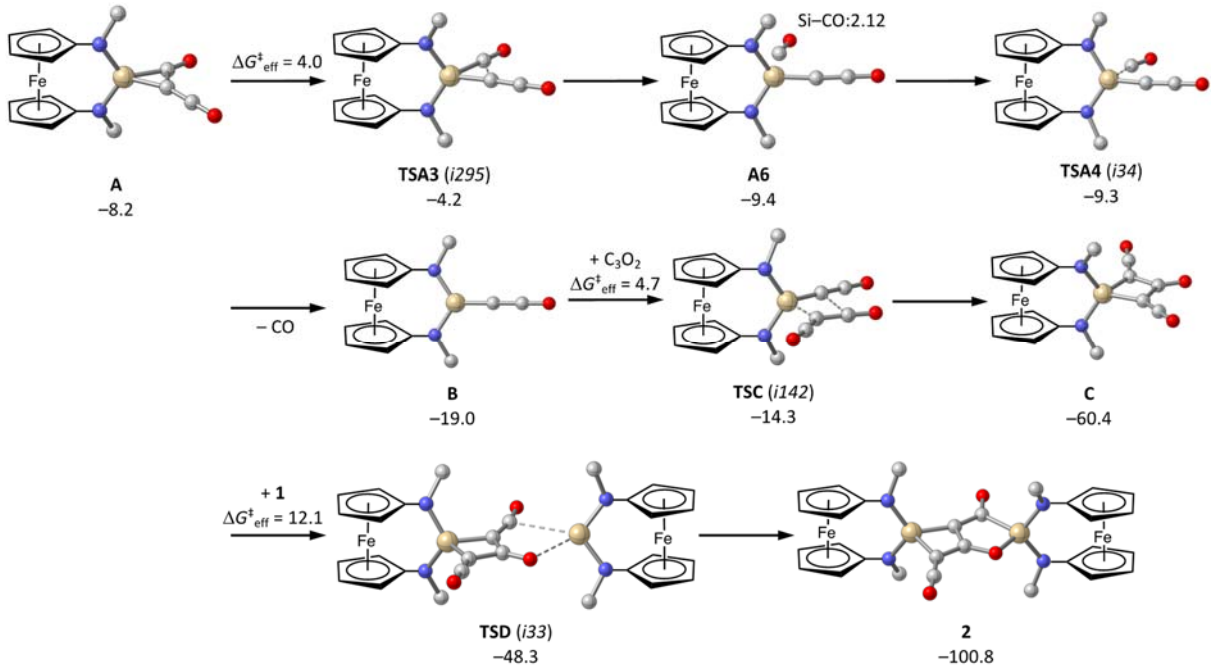
The PBEh-3c method has primarily been designed with an efficient assessment of molecular structures in mind,[S7] but, based on earlier benchmark calculations,[S1] this method is also expected to give reasonably accurate relative energies for the reactions investigated here. Unless stated otherwise, relative free energies ΔG^{298} obtained in PBEh-3c calculations are given in kcal mol^{-1} (imaginary wave numbers of transition modes in parentheses, cm^{-1}). Bonds formed or broken in transition states are shown dashed, unreactive H atoms are omitted and the orientation of Dipp substituents is indicated by showing the C_{ipso} atom only.



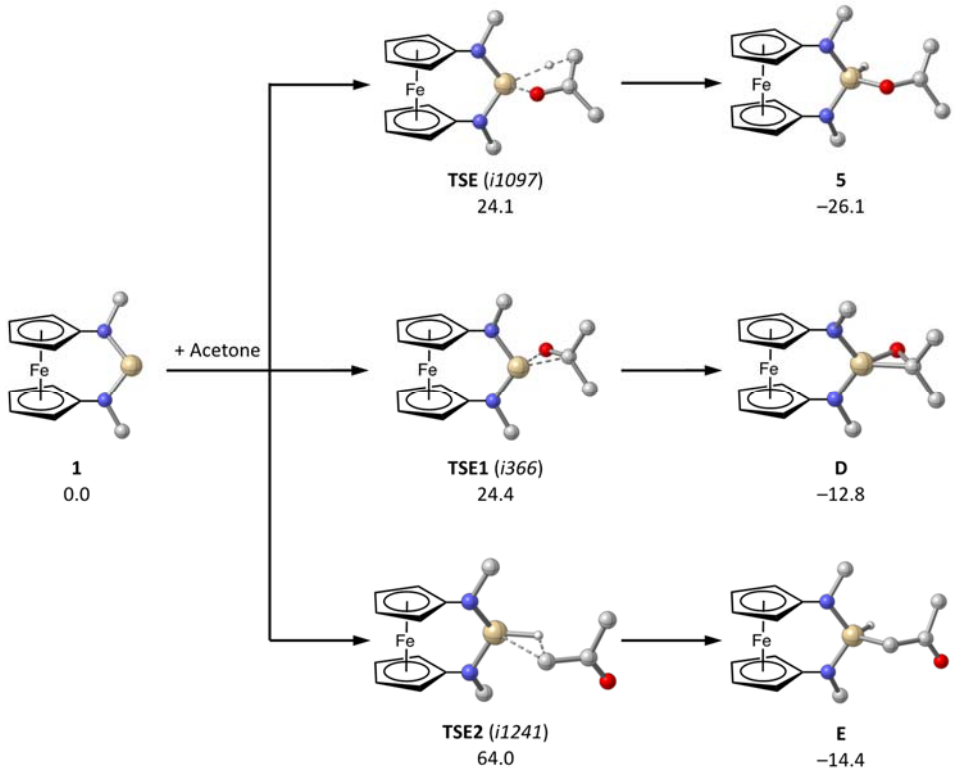
Scheme S2 Computed initial intermediates of the reaction of **1** with C_3O_2.



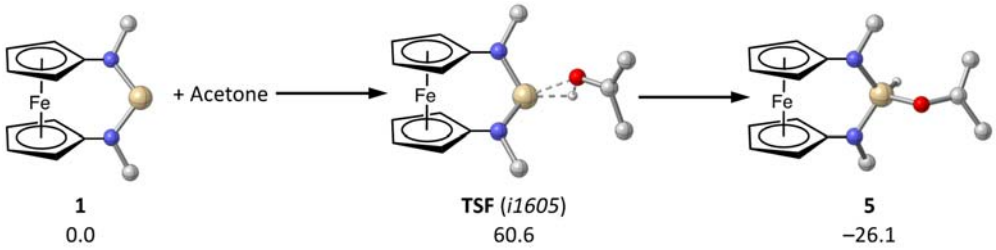
Scheme S3 Initial reaction steps of **1** with C_3O_2.



Scheme S4 Computed reaction path for the formation of the experimentally observed product **2** starting from **A**.



Scheme S5 Computed reaction paths for the reaction of **1** with acetone.



Scheme S6 Computed reaction path for the reaction of **1** with the enol tautomer of acetone.

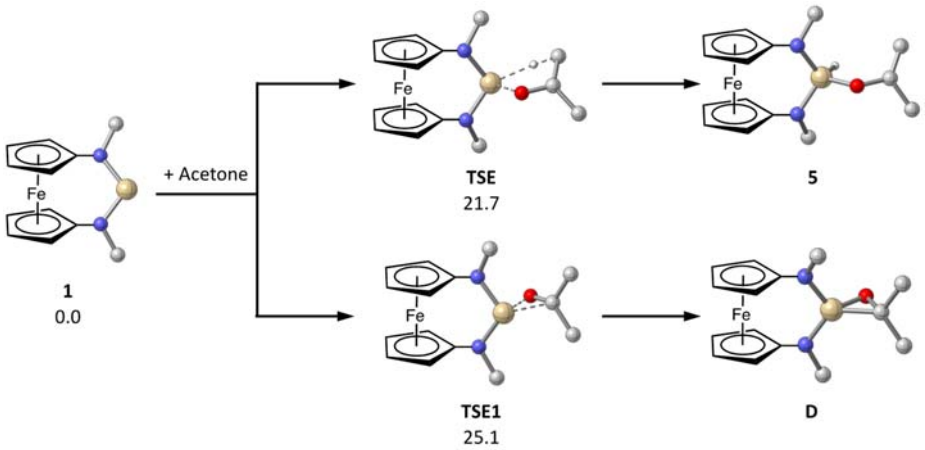
For the reaction of **1** with acetone we have further scrutinised the two routes commencing with **TSE** or **TSE1**. While ONIOM(CC–F12:PBEh-3c) results nicely confirm the overall suitability of the PBEh-3c approximation to assess the reactivity of the set of systems under study with pleasing accuracy, the order of activation energies $\Delta E^{\ddagger}$ is reversed. Owing to larger thermal contributions (obtained at the PBEh-3c level) **TSE1** is further destabilised and we arrive at a significantly favored free energy barrier for **TSE** (Scheme S7).

Table S2 Total energies from ONIOM component calculations

	PBEh-3c (real)	PBEh-3c (model)	CCSD(T)–F12 (model)	ONIOM(CC-F12:PBEh-3c)
1	-2979.40853	-400.82069	-400.90248	-2979.49032
Acetone	-192.73848	-192.73848	-192.91813	-192.91813
TSE	-3172.13153	-593.53220	-593.79753	-3172.39686
TSE1	-3172.13498	-593.53855	-593.79880	-3172.39522

Table S3 Computed reaction barriers for the competing paths shown in Scheme S7 ($\Delta E^{\ddagger}$ in kcal mol^{-1})

	TSE	TSE1	$\Delta E_{(\mathbf{TSE1-TSE})}$
ONIOM(CC-F12:PBEh-3c)	7.3	8.3	1.0
PBEh-3c	9.7	7.6	–2.1



Scheme S7 Computed reaction paths for the reaction of **1** with acetone. Relative energies at the ONIOM(CCSD(T*)–F12/cc-pVTZ-F12:PBEh-3c) level of theory (ΔG in kcal mol^{-1}).

Cartesian coordinates

Compound (point group): total energy/Hartree (PBEh-3c)

1 (C_2): E_{tot} = -2979.40853194

C	4.87836	17.81194	1.95428
C	3.99092	18.65654	1.22975
H	2.93130	18.76284	1.41570
C	4.74685	19.35782	0.25862
H	4.36163	20.08665	-0.43869
C	6.09282	18.92579	0.35392
H	6.91412	19.2703	-0.25638
C	6.17773	17.96968	1.39304
H	7.07257	17.45899	1.71659
C	4.95740	20.01912	4.07211
C	4.50328	21.12012	3.29029
H	3.47656	21.43371	3.17451
C	5.62899	21.71541	2.67521
H	5.60958	22.56533	2.00962
C	6.78342	20.99896	3.07638
H	7.79823	21.20806	2.77260
C	6.37553	19.9663	3.95557
H	7.02013	19.23931	4.42905
C	4.73190	15.59033	2.83797
C	3.76181	14.85549	2.14084
C	3.97823	13.49799	1.93618
H	3.24438	12.91525	1.39285
C	5.11062	12.87259	2.42510
H	5.25876	11.81296	2.26262
C	6.04945	13.60394	3.12814
H	6.92726	13.10191	3.51601
C	5.88583	14.96906	3.34042
C	2.49728	15.4906	1.60711
H	2.43347	16.50419	2.00338
C	2.54097	15.59044	0.08241
H	3.41135	16.15501	-0.25181
H	1.64904	16.09157	-0.29815
H	2.58616	14.60174	-0.3782
C	1.24463	14.75585	2.08296
H	1.18393	13.74147	1.68581
H	0.34834	15.28466	1.75467
H	1.21548	14.6898	3.17075
C	6.94184	15.72194	4.1243
H	6.74847	16.79103	4.01756
C	6.85817	15.38586	5.61413
H	5.86861	15.60486	6.01864
H	7.58944	15.96185	6.18492
H	7.05603	14.32735	5.79194
C	8.35183	15.46976	3.59103
H	8.67396	14.43973	3.74961
H	9.07062	16.11245	4.10174
H	8.42065	15.6718	2.52148
C	3.49673	19.70917	5.94153
C	2.16483	20.13695	5.83334
C	1.55822	20.70456	6.94891
H	0.52823	21.03414	6.89007
C	2.24733	20.85695	8.13762
H	1.76129	21.308	8.99287
C	3.55574	20.42054	8.23298
H	4.08424	20.53105	9.17221
C	4.19827	19.83247	7.14956
C	1.35417	19.96485	4.56519
H	2.03434	19.68344	3.75933
C	0.65959	21.25685	4.13645
H	-0.11666	21.55994	4.84037
H	0.17808	21.12462	3.16631
H	1.36438	22.08501	4.05278
C	0.34169	18.82934	4.72408
H	0.83429	17.89001	4.98034
H	-0.21843	18.67502	3.79977
H	-0.37685	19.04785	5.51599
C	5.61731	19.33663	7.32
H	5.91114	18.81908	6.40683
C	6.58768	20.49949	7.52317
H	6.5396	21.20369	6.69255
H	7.61446	20.13668	7.59832
H	6.36581	21.04888	8.43992
C	5.72192	18.31477	8.45188
H	5.49364	18.75288	9.42473
H	6.73437	17.9109	8.50704
H	5.03698	17.4813	8.2937
Fe	5.45522	19.71564	2.16061
N	4.53967	16.99393	3.0534
N	4.14424	19.12448	4.80349
Si	3.87163	17.40287	4.62251

2 (C_1): E_{tot} = -6374.24343413

C	3.76054	7.6275	8.54848
C	3.19658	8.04368	7.45147
C	3.73383	8.75064	6.33535
C	2.73454	8.98757	5.40663
C	3.23566	9.73192	4.27678
C	-0.87564	8.25246	7.88392
C	-0.94861	7.96989	9.28117
H	-0.18744	8.19198	10.01255
C	-2.17537	7.31843	9.53608
H	-2.51565	6.96376	10.49747
C	-2.87313	7.19616	8.30841
H	-3.83899	6.73342	8.1706
C	-2.08384	7.78495	7.29224
H	-2.33376	7.83271	6.24288
C	0.40901	5.63167	6.95092
C	0.79007	5.39949	8.30429
H	1.6529	5.80729	8.80997
C	-0.18166	4.55476	8.89363
H	-0.18145	4.21135	9.91727
C	-1.13821	4.22643	7.90289
H	-2.0008	3.59173	8.03933
C	-0.77671	4.88503	6.70476
H	-1.3095	4.8411	5.7674
C	0.05904	10.35401	7.38565
C	0.63635	10.99976	8.49293
C	0.33257	12.33804	8.72168
H	0.77798	12.84596	9.56808
C	-0.54349	13.0257	7.90656
H	-0.78993	14.05844	8.11669
C	-1.08302	12.39131	6.80588
H	-1.74623	12.94281	6.15089
C	-0.78106	11.0661	6.5117
C	1.57749	10.32107	9.46319
H	1.61311	9.26005	9.2192
C	2.9913	10.88446	9.32413
H	3.02967	11.92927	9.63249
H	3.35185	10.84949	8.2965
H	3.6951	10.33341	9.95137
C	1.10361	10.44547	10.91288
H	0.06685	10.13137	11.0337
H	1.17403	11.47213	11.27493
H	1.72476	9.83215	11.56805
C	-1.37674	10.47601	5.25249
H	-1.04553	9.44035	5.16477
C	-0.87038	11.22045	4.01583
H	0.20868	11.12613	3.90232
H	-1.11444	12.2831	4.06042
H	-1.33359	10.8211	3.11292
C	-2.90576	10.48213	5.29496
H	-3.31321	9.94142	4.4381
H	-3.30285	11.49779	5.25262
H	-3.28903	10.01886	6.20365
C	1.41129	5.80629	4.80731
C	0.62827	5.95255	3.6525
C	0.94273	5.18193	2.53761
H	0.34881	5.28048	1.63703
C	1.99886	4.29145	2.55458
H	2.22331	3.69835	1.67719
C	2.76883	4.16489	3.69544
H	3.59896	3.46919	3.70379
C	2.48828	4.90713	4.83628
C	-0.54891	6.89832	3.56611
H	-0.70478	7.33695	4.55362
C	-0.26847	8.03317	2.58268
H	-0.06293	7.6458	1.58299
H	0.58524	8.63959	2.88283
H	-1.1344	8.69197	2.5038
C	-1.84194	6.17712	3.18253
H	-2.05855	5.33843	3.84417
H	-1.80254	5.7856	2.16493
H	-2.6873	6.86595	3.23023
C	3.31668	4.67847	6.0798
H	3.01141	5.40242	6.83172
C	3.06563	3.28312	6.65198
H	3.39061	2.50432	5.95928
H	2.00843	3.12266	6.86347
H	3.61787	3.14672	7.58349
C	4.79987	4.91622	5.82574
H	5.36198	4.84073	6.75855
H	4.98037	5.90456	5.40256
H	5.22262	4.18826	5.13344
C	5.91771	12.50468	3.97459
C	6.98662	13.44014	4.04575
H	7.56691	13.66893	4.92692
C	7.1471	14.01219	2.76072
H	7.88221	14.75393	2.4871
C	6.18492	13.43484	1.8961
H	6.05523	13.66059	0.84828
C	5.40441	12.52304	2.64888
H	4.57433	11.92904	2.2859
C	7.40501	9.99021	3.06939
C	7.48229	10.21917	1.66327
H	6.76215	9.89329	0.93054
C	8.64185	10.98229	1.40419
H	8.96775	11.32819	0.43475
C	9.29051	11.2321	2.63899
H	10.19942	11.79863	2.77622
C	8.54405	10.60345	3.66445
H	8.77457	10.62715	4.71946
C	5.22905	12.33843	6.25809
C	6.06831	12.1516	7.36807
C	5.83047	12.90796	8.51178
H	6.471	12.78186	9.37616
C	4.80631	13.83352	8.56215
H	4.64735	14.41997	9.45803
C	3.98555	14.00408	7.46344
H	3.18037	14.72664	7.50884
C	4.17377	13.26531	6.3015
C	7.25382	11.21058	7.37147
H	7.24719	10.63821	6.44433
C	7.19277	10.21612	8.52908
H	6.26118	9.65374	8.52329
H	7.27725	10.71299	9.49665
H	8.01455	9.50233	8.46052
C	8.57251	11.98479	7.40439
H	8.6668	12.57839	8.31515
H	8.6618	12.66573	6.55814
H	9.42175	11.29911	7.36994
C	3.26361	13.52265	5.12036
H	3.43772	12.75868	4.36555
C	3.5611	14.88319	4.48837
H	4.60234	14.96963	4.18002
H	3.34954	15.69589	5.1865
H	2.93832	15.03508	3.60541
C	1.79551	13.40871	5.50615
H	1.48652	14.18367	6.20797
H	1.58187	12.444	5.96339
H	1.16648	13.50304	4.62024
C	6.462	7.85207	3.51947
C	5.7444	7.24065	2.47859
C	5.94062	5.88205	2.24481
H	5.38206	5.39468	1.45551
C	6.8477	5.14905	2.98217
H	7.00405	4.09968	2.76725
C	7.54908	5.76168	4.00302
H	8.25193	5.17893	4.5859
C	7.35999	7.10488	4.30344
C	4.77954	7.97656	1.57548
H	4.76633	9.03068	1.85576
C	3.36167	7.43147	1.72937
H	3.05511	7.36335	2.77185
H	3.28184	6.42865	1.31009
H	2.64556	8.06901	1.21082

C	5.20351	7.88538	0.10631	H	6.15365	-1.12393	5.02213	H	-0.25247	6.37738	7.54503
H	5.0894	6.87039	-0.27771	C	4.637	0.35218	4.69007	H	-0.64985	4.67485	7.72816
H	6.24478	8.16712	-0.04811	C	4.18474	2.38035	1.44457	H	-0.87842	5.48407	6.17288
H	4.57886	8.53497	-0.50888	H	3.30636	2.885	1.8488	C	2.9006	6.02073	1.90706
C	8.15459	7.69494	5.44804	C	5.19983	3.4508	1.04433	H	2.945	4.93113	1.85178
H	7.83732	8.72663	5.59366	H	6.07681	3.01322	0.56449	C	4.27185	6.53793	1.47439
C	7.88172	6.95929	6.75955	H	5.5439	4.02262	1.905	H	5.05825	6.20579	2.15033
H	8.172	5.90887	6.70909	H	4.75664	4.15087	0.33351	H	4.30399	7.62722	1.42553
H	6.82567	7.00136	7.02278	C	3.72618	1.60254	0.2095	H	4.51255	6.16791	0.47701
H	8.4473	7.41205	7.57528	H	3.25979	2.27287	-0.51467	C	1.81207	6.49307	0.94083
C	9.65015	7.70813	5.1297	H	3.00194	0.82865	0.46249	H	2.02029	6.14763	-0.07378
H	10.20749	8.21115	5.9226	H	4.56284	1.11228	-0.29058	H	1.76121	7.58308	0.91313
H	9.85436	8.22567	4.19286	C	3.97906	0.1025	6.03034	H	0.82805	6.12386	1.22899
H	10.04843	6.6956	5.04339	H	3.3734	0.97518	6.27801	Fe	0.11865	1.83397	3.13109
Fe	-1.03654	6.27927	8.16003	C	4.98245	-0.07835	7.16858	N	1.91383	4.1304	3.9332
Fe	7.35952	11.95113	2.7118	H	5.70203	0.73797	7.2101	C	1.83212	0.85654	3.49599
N	0.18698	8.92807	7.22223	H	5.5409	-1.0121	7.08554	C	1.19273	0.27814	2.36452
N	1.03904	6.4799	6.01424	H	4.45717	-0.10884	8.12417	H	1.60321	0.22267	1.36777
N	5.50021	11.66242	5.02733	C	3.05976	-1.11979	5.94923	C	-0.07215	-0.20096	2.77851
N	6.37274	9.27199	3.73049	H	2.53315	-1.26902	6.89358	H	-0.80095	-0.68751	2.14795
O	4.98684	9.14587	6.18289	H	3.63912	-2.02262	5.7449	C	-0.22323	0.08126	4.15837
O	4.19202	7.23127	9.5459	H	2.31157	-1.01913	5.16475	H	-1.08511	-0.15559	4.76407
O	2.64715	10.19365	3.3163	N	2.98441	2.07061	4.12161	C	0.9608	0.71388	4.61004
Si	1.50892	8.08939	6.47096	O	3.79916	3.87128	6.11246	H	1.16173	1.05343	5.61703
Si	5.12897	10.00208	4.68834	C	4.9338	4.52907	6.48598	C	4.21736	0.77454	3.05354
5 (C_1): E_{tot} = -3172.21510501				C	5.09661	5.838	6.31845	C	4.73071	0.97427	1.76337
C	0.60591	4.24722	3.68641	H	6.01116	6.31196	6.64248	C	5.84543	0.23836	1.37484
C	0.51631	3.85427	2.32069	H	4.33654	6.47227	5.88332	H	6.26356	0.38435	0.38639
H	1.33074	3.83787	1.61062	C	5.95198	3.63005	7.10511	C	6.42776	-0.68108	2.22546
C	-0.81126	3.43242	2.06681	H	6.81863	4.18941	7.45088	H	7.2911	-1.24814	1.90287
H	-1.1875	3.05875	1.12624	H	6.2909	2.88065	6.38543	C	5.90578	-0.87293	3.4918
C	-1.5604	3.60193	3.25662	H	5.52864	3.09154	7.95513	H	6.37034	-1.59549	4.15069
H	-2.60832	3.37548	3.38443	H	4.34021	4.27267	3.72067	C	4.80642	-0.14697	3.93349
C	-0.694	4.10228	4.25508	**C_3O_2** ($D_{\infty h}$): E_{tot} = -264.14709258				C	4.12426	1.94492	0.77306
H	-0.96298	4.30851	5.27863	C	0	0	1	H	3.23386	2.38524	1.22638
C	1.84609	6.03118	4.75401	C	0	0	-0.27177	C	5.08956	3.08122	0.43614
C	1.45973	6.43984	6.04174	C	0	0	2.27177	H	5.9769	2.70776	-0.07808
C	1.58608	7.78385	6.37786	O	0	0	-1.42657	H	5.42698	3.61078	1.32563
H	1.29885	8.11444	7.36855	O	0	0	3.42657	H	4.60994	3.8037	-0.22716
C	2.0736	8.7088	5.47444	**CO_2** ($D_{\infty h}$): E_{tot} = -188.19119100				C	3.67263	1.23441	-0.50401
H	2.16375	9.74972	5.75662	O	0	0	0.14466	H	3.15442	1.9307	-1.16544
C	2.44499	8.29728	4.20832	C	0	0	1.29999	H	2.99663	0.40532	-0.2938
H	2.8225	9.0279	3.5035	O	0	0	2.45533	H	4.51884	0.82805	-1.05992
C	2.34432	6.9637	3.8273	**CO** ($C_{\infty v}$): E_{tot} = -113.06606977				C	4.26161	-0.39696	5.3222
C	0.89657	5.49405	7.08051	C	0	0	0.08742	H	3.60102	0.43175	5.58139
H	0.89104	4.48856	6.65676	O	0	0	1.21257	C	5.36046	-0.43691	6.38329
C	1.75053	5.45491	8.34808	**Acetone** (C_1): E_{tot} = -192.73848350				H	6.00396	0.441	6.33083
H	2.78561	5.20474	8.12997	C	-0.00034	0	1.02366	H	5.99661	-1.31784	6.28558
H	1.36005	4.70928	9.04297	O	0	0	-0.1794	H	4.92022	-0.47209	7.3807
H	1.74279	6.41528	8.86668	C	-0.00839	-1.27639	1.83068	C	3.4352	-1.68439	5.34964
C	-0.54321	5.87533	7.43693	H	0.76552	-1.26102	2.59996	H	2.99769	-1.84214	6.33712
H	-0.58118	6.82695	7.96995	H	0.13396	-2.14467	1.19182	H	4.05811	-2.55113	5.12029
H	-0.99105	5.12183	8.08745	H	-0.96298	-1.37846	2.35203	H	2.62224	-1.65688	4.62467
H	-1.17325	5.98041	6.55364	C	0.00836	1.27639	1.83068	N	3.07326	1.52121	3.48041
C	2.75999	6.58195	2.4226	H	0.96302	1.37805	2.35198	Si	3.30673	3.12479	4.05867
H	2.76222	5.49495	2.34555	H	-0.76551	1.26136	2.60001	C	5.01643	3.79974	4.13485
C	4.17878	7.04684	2.09762	H	-0.13364	2.14473	1.19183	C	4.46106	3.37999	5.46421
H	4.89494	6.66936	2.82833	**A** (C_1): E_{tot} = -3243.57851454				C	5.01599	3.26062	6.63919
H	4.26357	8.13438	2.07875	C	0.6902	3.74679	3.33169	O	6.06149	4.27311	3.79155
H	4.4811	6.68287	1.11443	C	0.47179	3.46216	1.95395	O	5.51807	3.15475	7.67073
C	1.7519	7.10825	1.40091	H	1.21511	3.5148	1.17165	**A1** (C_1): E_{tot} = -3243.57744625			
H	2.02316	6.79047	0.39231	C	-0.87394	3.05504	1.79602	C	0.5789	3.82834	3.03669
H	1.71438	8.19914	1.40424	H	-1.34	2.75677	0.86886	C	0.30752	3.4691	1.68846
H	0.74796	6.7396	1.61127	C	-1.50405	3.11688	3.06333	H	1.01287	3.5079	0.86984
Fe	0.04252	2.32961	3.58988	H	-2.534	2.86933	3.27235	C	-1.03326	3.01979	1.62147
N	1.76685	4.6489	4.38511	C	-0.54622	3.5395	4.01203	H	-1.53736	2.66242	0.7361
Si	3.23745	3.7342	4.54648	H	-0.71608	3.65724	5.07014	C	-1.60226	3.13638	2.91359
C	1.74019	1.41391	4.14966	C	2.06622	5.51503	4.28369	H	-2.61524	2.88017	3.18508
C	1.15887	0.70545	3.06036	C	1.73932	5.94822	5.57896	C	-0.61138	3.63385	3.79127
H	1.621	0.54021	2.09885	C	1.89153	7.29549	5.8877	H	-0.73133	3.8268	4.84675
C	-0.12519	0.26525	3.46067	H	1.64267	7.64669	6.88162	C	1.9028	5.52989	4.17051
H	-0.8187	-0.29737	2.85404	C	2.3533	8.19831	4.94993	C	1.83974	5.63041	5.56786
C	-0.3462	0.70199	4.79006	H	2.46208	9.24353	5.20811	C	1.94213	6.89306	6.14043
H	-1.23736	0.52994	5.37504	C	2.67833	7.75919	3.68133	H	1.91044	6.99731	7.21791
C	0.81283	1.3913	5.22579	H	3.0406	8.47332	2.95295	C	2.08347	8.02297	5.35633
H	0.96101	1.8522	6.19288	C	2.55111	6.42106	3.32475	H	2.15749	8.99783	5.82005
C	4.12515	1.28466	3.76814	C	1.20752	5.02892	6.65682	C	2.13548	7.90531	3.97979
C	4.72532	1.44735	2.50826	H	1.20009	4.00957	6.2655	H	2.24972	8.79681	3.37596
C	5.85234	0.68932	2.20344	C	2.09544	5.03669	7.90103	C	2.05897	6.66273	3.36141
H	6.33111	0.80968	1.23907	H	3.13486	4.83489	7.65327	C	1.68221	4.42587	6.47225
C	6.36417	-0.2262	3.10099	H	1.76288	4.28197	8.61543	H	1.47585	3.55284	5.84895
H	7.23716	-0.81168	2.84347	H	2.06566	6.00045	8.41159	C	2.96793	4.14528	7.25061
C	5.7506	-0.39649	4.32921	C	-0.22493	5.40961	7.0416	H	3.8181	3.99084	6.58648

H	2.85785	3.25136	7.8679	H	1.14436	4.23823	6.51351	H	1.74092	8.97016	4.13087
H	3.22072	4.97448	7.91312	C	1.98072	5.41713	8.07164	C	1.67113	6.83335	4.01706
C	0.49754	4.58005	7.42659	H	3.03057	5.27696	7.82362	C	1.54858	4.44589	7.03879
H	0.66081	5.37702	8.15307	H	1.71599	4.67403	8.82511	H	1.51235	3.57045	6.38661
H	0.34001	3.65872	7.98945	H	1.87463	6.39937	8.53527	C	2.76105	4.30063	7.95678
H	-0.42541	4.81151	6.89363	C	-0.38139	5.54585	7.24086	H	3.69199	4.27263	7.39496
C	2.13082	6.5794	1.85299	H	-0.49138	6.53301	7.69261	H	2.68902	3.38058	8.53942
H	2.22516	5.53127	1.56985	H	-0.72446	4.81418	7.97484	H	2.82558	5.12681	8.66661
C	3.36239	7.29276	1.29775	H	-1.05248	5.50962	6.38261	C	0.26556	4.45302	7.87333
H	4.27744	6.90114	1.74095	C	2.4882	6.25844	1.99647	H	0.1517	3.50962	8.41006
H	3.3336	8.36853	1.47679	H	2.66793	5.18127	1.97919	H	-0.62399	4.60173	7.26189
H	3.42532	7.14752	0.21834	C	3.75009	6.93691	1.46406	H	0.27825	5.25109	8.61723
C	0.84113	7.1085	1.22512	H	4.60514	6.78676	2.1224	C	1.60293	6.85193	2.5065
H	0.87391	7.01205	0.13852	H	3.61709	8.01259	1.34316	H	1.72627	5.83762	2.13547
H	0.68899	8.16383	1.45863	H	4.00937	6.53785	0.48294	C	2.72044	7.68617	1.88264
H	-0.02894	6.55832	1.58456	C	1.30207	6.55519	1.07579	H	3.70227	7.36366	2.22904
Fe	0.05626	1.89357	2.96094	H	1.49434	6.19064	0.0644	H	2.61655	8.74876	2.1083
N	1.82478	4.23638	3.5571	H	1.1232	7.62995	1.00973	H	2.70268	7.58107	0.79758
C	1.8057	0.97395	3.30837	H	0.38441	6.09091	1.43477	C	0.22502	7.32945	2.04484
C	1.15255	0.3529	2.20489	Fe	0.22118	1.8394	3.40725	H	0.15596	7.30053	0.95628
H	1.52926	0.29441	1.19577	N	1.80109	4.33994	4.10149	H	0.03211	8.35576	2.3627
C	-0.08679	-0.1509	2.65931	Si	3.20099	3.39463	4.41397	H	-0.56885	6.69961	2.44736
H	-0.81859	-0.66672	2.05597	C	2.04156	1.03721	3.68229	Fe	-0.16719	2.0596	3.38771
C	-0.21068	0.15334	4.03726	C	1.42569	0.43653	2.54993	N	1.58281	4.38127	4.09707
H	-1.05112	-0.09284	4.66876	H	1.7982	0.46153	1.53757	Si	2.99981	3.49242	3.69653
C	0.96389	0.82811	4.44623	C	0.23345	-0.18801	2.98583	C	1.57665	1.12436	3.73865
H	1.17363	1.19603	5.44045	H	-0.46244	-0.72621	2.36001	C	0.94986	0.55991	2.58906
C	4.23366	0.82702	3.18683	C	0.10467	0.02515	4.37993	H	1.34801	0.55748	1.58678
C	4.80377	0.54082	1.93777	H	-0.70423	-0.3244	5.00382	C	-0.3	0.0355	2.9863
C	5.9374	-0.26393	1.9012	C	1.23227	0.76003	4.81895	H	-1.01651	-0.44857	2.33976
H	6.39628	-0.49612	0.94813	H	1.43597	1.07789	5.83259	C	-0.45885	0.27308	4.3741
C	6.49404	-0.77237	3.05892	C	4.41403	1.25709	3.19563	H	-1.31585	-0.0011	4.97091
H	7.37407	-1.39993	3.00803	C	4.82772	1.49575	1.87676	C	0.70212	0.93079	4.84486
C	5.92948	-0.46819	4.28292	C	6.03596	0.95321	1.45182	H	0.88093	1.25823	5.85849
H	6.37929	-0.86243	5.18549	H	6.3794	1.13731	0.44102	C	4.00546	0.95428	3.80568
C	4.80245	0.34048	4.37405	C	6.80381	0.17285	2.2951	C	4.63394	0.5405	2.61885
C	4.2521	1.06262	0.62803	H	7.74051	-0.24305	1.94776	C	5.74688	-0.29034	2.7117
H	3.36195	1.65842	0.83942	C	6.36504	-0.08301	3.58086	H	6.24286	-0.6151	1.80578
C	5.2547	1.97541	-0.07965	H	6.96543	-0.70818	4.22988	C	6.22988	-0.71409	3.93215
H	6.15533	1.43087	-0.36784	C	5.17321	0.45163	4.05731	H	7.09177	-1.36652	3.98113
H	5.55569	2.80769	0.55313	C	4.00466	2.29395	0.88811	C	5.60657	-0.2965	5.09171
H	4.81708	2.38447	-0.99207	H	3.06424	2.56621	1.37099	H	5.99093	-0.63285	6.04611
C	3.83694	-0.08656	-0.29358	C	4.70622	3.58601	0.47624	C	4.50078	0.5448	5.05691
H	3.33843	0.2976	-1.1852	H	5.65979	3.38738	-0.01518	C	4.17117	0.92199	1.22973
H	3.16143	-0.78554	0.20031	H	4.9095	4.22773	1.33195	H	3.34018	1.62339	1.31116
H	4.70183	-0.66057	-0.62953	H	4.08854	4.15542	-0.22101	C	5.28202	1.61255	0.43472
C	4.23789	0.64398	5.74513	C	3.66332	1.46569	-0.35237	H	6.07478	0.91095	0.16983
H	3.47335	1.41677	5.64449	H	2.96564	2.00688	-0.99366	H	5.74076	2.42902	0.98996
C	5.3005	1.2024	6.69047	H	3.21015	0.50892	-0.0926	H	4.88559	2.02416	-0.49336
H	5.79561	2.07228	6.25995	H	4.55028	1.2485	-0.94934	C	3.67251	-0.30929	0.46763
H	6.06888	0.4656	6.92786	C	4.72733	0.10663	5.46161	H	3.2401	-0.01713	-0.49098
H	4.84558	1.50862	7.63351	H	3.86867	0.72315	5.71939	H	2.91997	-0.86318	1.02857
C	3.56565	-0.59411	6.33967	C	5.80384	0.4019	6.50419	H	4.48973	-1.00126	0.25782
H	3.10951	-0.36054	7.30363	H	6.11098	1.44764	6.47623	C	3.87468	0.93778	6.37764
H	4.28981	-1.39386	6.50435	H	6.69312	-0.21574	6.36874	H	3.13864	1.72363	6.19939
H	2.78781	-0.98238	5.68224	H	5.41967	0.20061	7.50493	C	4.90725	1.50311	7.3525
N	3.05288	1.64326	3.25892	C	4.26965	-1.35148	5.52374	H	5.43418	2.35469	6.92457
Si	3.25973	3.32204	3.47285	H	3.90485	-1.59643	6.52263	H	5.65112	0.75919	7.63956
C	5.85968	4.60562	4.56098	H	5.08632	-2.03767	5.29172	H	4.42	1.83563	8.26915
C	6.45748	4.93454	5.64037	H	3.46177	-1.54166	4.81645	C	3.14658	-0.25617	6.9989
O	4.57358	3.99588	2.60492	N	3.19611	1.84733	3.66485	H	2.62806	0.03971	7.91321
O	7.09164	5.28077	6.55715	O	3.56824	3.31158	6.1086	H	3.84879	-1.04905	7.2623
C	4.8197	4.08526	3.94588	C	4.75877	3.90873	6.01248	H	2.41266	-0.68234	6.31551
A2 (C_1): E_{tot} = -3243.57673861				C	4.82994	4.1973	4.55649	N	2.83059	1.78858	3.75837
C	0.58991	3.80997	3.58792	C	5.83413	4.75283	3.92916	O	4.30209	4.0088	4.84372
C	0.3127	3.49943	2.227	O	6.71585	5.24526	3.38004	C	5.06238	4.59857	4.00981
H	0.99075	3.63716	1.39755	**A3** (C_1): E_{tot} = -3243.57744625				C	5.20582	4.86726	2.80716
C	-0.98755	2.94554	2.15722	C	0.33892	3.99445	3.55103	C	3.99063	4.28758	2.15827
H	-1.4796	2.59641	1.26176	C	0.08569	3.69106	2.1839	O	3.61075	4.33559	1.02969
C	-1.53179	2.93496	3.46533	H	0.80014	3.77659	1.37516	**A4** (C_1): E_{tot} = -3243.52081453			
H	-2.51065	2.57278	3.74193	C	-1.24957	3.23289	2.08374	C	0.79318	4.10688	3.76747
C	-0.56484	3.46225	4.34984	H	-1.74056	2.91029	1.1779	C	0.57677	3.72192	2.41478
H	-0.67423	3.56306	5.41781	C	-1.8332	3.28906	3.37328	H	1.30471	3.77374	1.61829
C	1.81807	5.74329	4.42061	H	-2.84654	3.01256	3.62284	C	-0.74088	3.21887	2.30806
C	1.49596	6.18505	5.71512	C	-0.85596	3.75649	4.28299	H	-1.19882	2.83113	1.41045
C	1.53122	7.55203	5.97707	H	-0.98725	3.89712	5.34444	C	-1.3563	3.32051	3.58
H	1.28966	7.9077	6.97085	C	1.64207	5.6486	4.76924	H	-2.36452	3.01987	3.82254
C	1.86166	8.46633	4.99838	C	1.64333	5.68361	6.17258	C	-0.4166	3.86488	4.48301
H	1.87771	9.5246	5.22376	C	1.70256	6.92195	6.80283	H	-0.58121	4.04144	5.53374
C	2.17108	8.02067	3.72776	H	1.71008	6.97043	7.88487	C	2.06574	6.03178	4.55598
H	2.42466	8.74399	2.96334	C	1.7435	8.09591	6.07554	C	1.68171	6.55504	5.8023
C	2.16487	6.66628	3.41728	H	1.78792	9.04961	6.58497	C	1.7442	7.93237	5.99021
C	1.07413	5.27304	6.84818	C	1.71947	8.04632	4.6951	H	1.45486	8.3523	6.94547

C	2.16215	8.77768	4.98273
H	2.19909	9.84637	5.14831
C	2.53405	8.25016	3.76193
H	2.86029	8.9193	2.97623
C	2.50329	6.88071	3.52481
C	1.174	5.71939	6.95862
H	1.20831	4.66744	6.67527
C	2.04417	5.88587	8.20564
H	1.72849	5.19076	8.98507
H	1.96407	6.89268	8.61835
H	3.09554	5.70034	7.99685
C	-0.28001	6.0719	7.28632
H	-0.36201	7.08233	7.68957
H	-0.68093	5.39002	8.0387
H	-0.92174	6.02568	6.40656
C	2.91258	6.39247	2.15177
H	3.00426	5.30627	2.17536
C	4.27414	6.94472	1.73119
H	5.0454	6.70672	2.46252
H	4.25442	8.02765	1.60155
H	4.5746	6.51655	0.77444
C	1.8387	6.74412	1.12007
H	2.09828	6.33725	0.1406
H	1.73724	7.82515	1.00921
H	0.86276	6.34925	1.4027
Fe	0.3479	2.15207	3.70045
N	2.00124	4.61148	4.3157
Si	3.36836	3.64065	4.62648
C	2.11762	1.29616	4.10846
C	1.51247	0.62518	3.01179
H	1.92323	0.54229	2.01793
C	0.2788	0.09484	3.45634
H	-0.42058	-0.46564	2.85459
C	0.11444	0.43793	4.82031
H	-0.72994	0.18218	5.44264
C	1.26016	1.16	5.23425
H	1.44486	1.55465	6.22399
C	4.49357	1.3337	3.60382
C	4.96966	1.53839	2.30053
C	6.10265	0.83841	1.89649
H	6.49439	0.98961	0.8982
C	6.73531	-0.05217	2.74044
H	7.61365	-0.58796	2.40535
C	6.24002	-0.25878	4.01439
H	6.73899	-0.96315	4.6673
C	5.12338	0.42836	4.47298
C	4.30556	2.45466	1.29447
H	3.44386	2.92698	1.77058
C	5.2463	3.56034	0.81691
H	6.09643	3.15058	0.26935
H	5.63607	4.15061	1.64283
H	4.72129	4.235	0.13832
C	3.78308	1.66729	0.09024
H	3.22545	2.32176	-0.58194
H	3.12508	0.84966	0.38303
H	4.60063	1.23039	-0.48503
C	4.6042	0.1333	5.86345
H	3.90581	0.92037	6.14805
C	5.71215	0.12054	6.91618
H	6.30957	1.0309	6.8802
H	6.38548	-0.72926	6.79443
H	5.27763	0.0392	7.91366
C	3.83357	-1.18932	5.87018
H	3.41182	-1.38404	6.85778
H	4.4911	-2.02389	5.61955
H	3.01385	-1.18348	5.1521
N	3.32202	2.03296	4.056
O	3.61087	3.64947	6.39283
C	4.88306	3.64965	6.4438
C	6.0003	3.7469	5.92675
C	5.93793	4.65184	4.73747
O	4.7844	4.41333	4.09985

A6 (C_1): E_{tot} = -3243.57786710

C	0.79737	4.05836	2.97392
C	0.56131	3.9688	1.57235
H	1.29455	4.10329	0.78968
C	-0.80225	3.64048	1.37945
H	-1.28691	3.48643	0.427
C	-1.4202	3.56449	2.65145
H	-2.45893	3.33743	2.83869
C	-0.43961	3.82368	3.63616
H	-0.59372	3.83	4.70423
C	2.07471	5.48217	4.42866
C	1.93444	5.37649	5.81951
C	1.95309	6.54264	6.57804
H	1.85883	6.47908	7.6551
C	2.08554	7.78322	5.98636
H	2.09433	8.67834	6.59421
C	2.20528	7.87352	4.61271
H	2.30491	8.84883	4.15233
C	2.20785	6.73605	3.81486
C	1.7648	4.05967	6.54473
H	1.68721	3.26083	5.80328
C	2.97629	3.76454	7.4262
H	3.89266	3.72941	6.83847
H	2.85627	2.80577	7.93341
H	3.10141	4.52767	8.19608
C	0.48089	4.02802	7.37624
H	0.52164	4.73067	8.20967
H	0.327	3.03402	7.79935
H	-0.39958	4.28179	6.78525
C	2.33678	6.90855	2.3188
H	2.41029	5.9206	1.86618
C	3.60316	7.67736	1.94383
H	4.49028	7.22662	2.38919
H	3.56157	8.71501	2.2776
H	3.73567	7.69301	0.86076
C	1.08707	7.56472	1.73223
H	1.16765	7.64684	0.64686
H	0.94161	8.57092	2.12894
H	0.19379	6.983	1.96014
Fe	0.14857	2.21969	2.52849
N	2.03323	4.30009	3.61287
C	1.7901	1.12118	2.86558
C	1.23861	0.78125	1.59528
H	1.72465	0.89452	0.63893
C	-0.07336	0.29897	1.80188
H	-0.75621	-0.02606	1.03121
C	-0.34265	0.33178	3.19264
H	-1.26588	0.03418	3.66695
C	0.80844	0.82199	3.85247
H	0.91693	0.97723	4.91599
C	4.11927	0.64938	3.19312
C	4.77971	0.22974	2.02712
C	5.70194	-0.80739	2.11307
H	6.21595	-1.13989	1.2196
C	5.97936	-1.42178	3.31725
H	6.69385	-2.2329	3.36561
C	5.3477	-0.98019	4.46212
H	5.58301	-1.45241	5.40761
C	4.42331	0.05872	4.42981
C	4.57746	0.86594	0.66987
H	3.81164	1.63916	0.76277
C	5.87031	1.53226	0.19227
H	6.63427	0.78748	-0.03501
H	6.28956	2.19491	0.94914
H	5.70055	2.10957	-0.71825
C	4.08371	-0.14129	-0.36996
H	3.84783	0.36013	-1.31045
H	3.1932	-0.67064	-0.03197
H	4.84304	-0.89347	-0.588
C	3.81359	0.4874	5.74621
H	3.18348	1.36238	5.57611
C	4.90125	0.90367	6.7364
H	5.50053	1.72089	6.3368
H	5.57278	0.07728	6.9725
H	4.45884	1.23608	7.67547
C	2.93278	-0.61641	6.33429
H	2.42823	-0.26528	7.2367
H	3.52387	-1.49059	6.61254
H	2.17318	-0.94892	5.62678
N	3.08299	1.6492	3.1103
Si	3.42602	3.30002	3.44343
C	4.1147	4.04876	1.5861
C	4.89687	3.75587	4.12091
C	6.02588	4.17492	4.51423
O	4.71584	4.58936	0.802
O	7.07281	4.55591	4.88145

B (C_1): E_{tot} = -3172.19597629

C	0.2334	3.81503	3.71072
C	-0.02508	3.48933	2.34993
H	0.68676	3.54767	1.53872
C	-1.36302	3.03767	2.25804
H	-1.85614	2.69934	1.35912
C	-1.94502	3.11793	3.54717
H	-2.95882	2.84864	3.80253
C	-0.96655	3.59933	4.44601
H	-1.10073	3.763	5.50451
C	1.51781	5.61787	4.68258
C	1.29582	5.91791	6.0327
C	1.32221	7.25284	6.42019
H	1.16165	7.51266	7.45917
C	1.55813	8.25918	5.50198
H	1.57	9.29277	5.82202
C	1.7953	7.94109	4.17781
H	1.9996	8.73488	3.46975
C	1.79279	6.62026	3.74507
C	1.08332	4.85186	7.0871
H	0.94327	3.89137	6.58629
C	2.32055	4.72467	7.9784
H	3.21379	4.5137	7.39029
H	2.19225	3.92013	8.70507
H	2.50263	5.64604	8.53401
C	-0.16932	5.10581	7.92517
H	-0.34889	4.27	8.60312
H	-1.05575	5.23278	7.30227
H	-0.07417	6.00176	8.53988
C	2.1098	6.32279	2.29617
H	2.14752	5.24078	2.16435
C	3.48949	6.85513	1.91042
H	4.25901	6.45828	2.57243
H	3.53592	7.94413	1.9567
H	3.7381	6.56169	0.88902
C	1.01843	6.85563	1.36873
H	1.23481	6.59649	0.33074
H	0.94162	7.94282	1.42501
H	0.043	6.44058	1.62393
Fe	-0.27795	1.88498	3.58153
N	1.46769	4.24924	4.2491
Si	2.90453	3.33792	4.33391
C	1.47199	0.98748	3.95588
C	0.8686	0.37921	2.81957
H	1.28507	0.34054	1.8242
C	-0.37568	-0.15535	3.22498
H	-1.07804	-0.67229	2.58863
C	-0.54707	0.1147	4.60513
H	-1.40086	-0.16287	5.20485
C	0.60266	0.79974	5.06573
H	0.78106	1.14672	6.074
C	3.87329	0.9113	3.67929
C	4.38794	0.91067	2.37585
C	5.51283	0.1361	2.11664
H	5.93794	0.12332	1.1208
C	6.1045	-0.61948	3.11229
H	6.9763	-1.22063	2.88985
C	5.58868	-0.59541	4.39462
H	6.0692	-1.17817	5.17085
C	4.4756	0.17662	4.70625
C	3.79748	1.7508	1.26197
H	2.82703	2.12905	1.59168
C	4.68746	2.96079	0.96893
H	5.6656	2.6484	0.59954
H	4.85409	3.56276	1.86272
H	4.23449	3.59978	0.2081
C	3.54587	0.94123	-0.00959
H	3.02382	1.55001	-0.7493
H	2.94021	0.05541	0.18621
H	4.47485	0.60416	-0.47096
C	3.9749	0.20838	6.13275
H	3.16688	0.93737	6.19802
C	5.0654	0.68149	7.0932
H	5.45153	1.65544	6.79309
H	5.90475	-0.0141	7.1367
H	4.66668	0.77289	8.10487
C	3.4021	-1.146	6.54788
H	3.00547	-1.10102	7.56366
H	4.16523	-1.92603	6.52851
H	2.59373	-1.4547	5.88452
N	2.69989	1.68663	3.96672
C	4.37578	4.00453	4.72271
C	5.49945	4.51452	5.01224
O	6.53743	4.98503	5.28066

C (C_1): E_{tot} = -3394.73295615

C	0.98834	4.09487	3.28292
C	0.67667	3.94269	1.90148
H	1.33517	4.1494	1.06936
C	-0.64624	3.4485	1.80302
H	-1.16788	3.21715	0.88647
C	-1.1697	3.33243	3.11296

H	-2.16058	2.99056	3.37164
C	-0.16598	3.72757	4.02813
H	-0.25416	3.73472	5.10296
C	2.30603	5.61423	4.64624
C	2.30818	5.47624	6.04275
C	2.43106	6.62075	6.82458
H	2.44826	6.53167	7.90411
C	2.51842	7.8739	6.2501
H	2.61545	8.75281	6.87381
C	2.46201	8.00016	4.8746
H	2.50449	8.98747	4.43204
C	2.35453	6.88522	4.05167
C	2.12661	4.14579	6.74145
H	2.01373	3.37344	5.97788
C	3.32932	3.77649	7.60473
H	4.24669	3.71819	7.0232
H	3.17715	2.80454	8.0779
H	3.49446	4.50456	8.40022
C	0.85891	4.14634	7.60013
H	0.95777	4.81466	8.45691
H	0.6584	3.14653	7.98913
H	-0.01756	4.47413	7.04142
C	2.22689	7.09114	2.5588
H	2.3322	6.125	2.07091
C	3.31739	7.99568	1.98876
H	4.31485	7.63751	2.24329
H	3.23232	9.02259	2.34768
H	3.24432	8.03135	0.90064
C	0.83205	7.6192	2.21967
H	0.7138	7.72625	1.14002
H	0.65592	8.59711	2.67166
H	0.05581	6.94139	2.57568
Fe	0.53534	2.17462	2.91412
N	2.24324	4.44299	3.82309
Si	3.68139	3.6741	3.23526
C	2.32295	1.26475	3.12442
C	1.68517	0.81675	1.92813
H	2.06016	0.93744	0.9243
C	0.45963	0.21025	2.28197
H	-0.25463	-0.21954	1.59567
C	0.32264	0.28074	3.69061
H	-0.51298	-0.08848	4.26625
C	1.47268	0.91848	4.21269
H	1.66141	1.1356	5.25361
C	4.75051	1.13147	3.16526
C	5.36627	0.82546	1.9385
C	6.50859	0.02978	1.94127
H	6.99167	-0.20832	1.00194
C	7.03678	-0.47067	3.11236
H	7.92305	-1.09109	3.09161
C	6.41979	-0.17555	4.31164
H	6.83255	-0.57921	5.22704
C	5.28454	0.62476	4.36542
C	4.84657	1.26661	0.58754
H	4.00332	1.9396	0.74404
C	5.90603	2.02681	-0.21253
H	6.72181	1.37169	-0.52167
H	6.34292	2.84219	0.36188
H	5.47181	2.4445	-1.1222
C	4.34945	0.06214	-0.21718
H	3.87423	0.3877	-1.14466
H	3.63183	-0.53574	0.34392
H	5.17497	-0.59735	-0.48944
C	4.65463	0.85704	5.72123
H	3.93329	1.67255	5.63202
C	5.67923	1.25944	6.78236
H	6.27746	2.11619	6.4751
H	6.36943	0.44692	7.01167
H	5.17825	1.51836	7.71515
C	3.90404	-0.39748	6.17684
H	3.36684	-0.21163	7.1095
H	4.60027	-1.21865	6.35683
H	3.18538	-0.73619	5.432
N	3.56393	1.94677	3.2121
C	5.26026	4.41995	3.85489
C	5.94023	4.64907	4.95131
O	6.54246	4.85441	5.90902
C	5.62468	4.95036	2.50973
C	4.45779	4.4867	1.7224
C	4.17289	4.74914	0.47652
O	3.87101	4.9554	-0.61822
O	6.58564	5.58361	2.1692

D (C_1): E_{tot} = -3172.19706117

C	0.7865	4.54782	4.32821
C	0.63346	4.14945	2.96996
H	1.41051	4.13492	2.21967
C	-0.70437	3.72623	2.78181
H	-1.12433	3.34927	1.86124
C	-1.39621	3.89627	4.00628
H	-2.43599	3.6669	4.18508
C	-0.48429	4.40103	4.95974
H	-0.70278	4.61513	5.9939
C	1.96859	6.38859	5.322
C	1.64334	6.79268	6.62702
C	1.6825	8.15146	6.92762
H	1.44667	8.48023	7.93228
C	2.0061	9.09289	5.97102
H	2.02359	10.1445	6.22596
C	2.30389	8.6839	4.68452
H	2.55048	9.42821	3.93772
C	2.30217	7.33793	4.33969
C	1.22379	5.84016	7.72728
H	1.23671	4.82385	7.32976
C	2.17977	5.88151	8.91976
H	3.19619	5.64106	8.61996
H	1.87088	5.15706	9.67561
H	2.18184	6.86387	9.39572
C	-0.20328	6.1459	8.19309
H	-0.25472	7.10126	8.7179
H	-0.55202	5.37793	8.88571
H	-0.90807	6.20098	7.36314
C	2.64279	6.95551	2.91536
H	2.81096	5.878	2.88187
C	3.92897	7.61712	2.42182
H	4.7706	7.39631	3.07757
H	3.83628	8.70166	2.35172
H	4.17945	7.25452	1.42369
C	1.47722	7.28402	1.98045
H	1.689	6.94757	0.96346
H	1.30108	8.36073	1.94154
H	0.55349	6.80785	2.3069
Fe	0.22419	2.62957	4.26062
N	1.96646	4.99749	4.97082
Si	3.37135	4.04102	5.31306
C	1.9388	1.73407	4.77934
C	1.36069	1.0412	3.67939
H	1.8186	0.9077	2.71042
C	0.08975	0.56734	4.08357
H	-0.60028	0.00719	3.47078
C	-0.12431	0.96683	5.42579
H	-1.00428	0.7614	6.01678
C	1.0271	1.66571	5.86681
H	1.17883	2.09964	6.84607
C	4.27842	1.66512	4.26261
C	4.83702	1.97109	3.01348
C	5.9121	1.21053	2.56304
H	6.36106	1.43687	1.60324
C	6.40952	0.16025	3.30956
H	7.23879	-0.42692	2.93727
C	5.84445	-0.13452	4.53771
H	6.2448	-0.95454	5.12069
C	4.78945	0.61442	5.04327
C	4.31673	3.08001	2.12478
H	3.4707	3.55174	2.62577
C	5.36789	4.16292	1.88931
H	6.24788	3.76903	1.37842
H	5.6967	4.60549	2.82922
H	4.96107	4.96384	1.26991
C	3.79179	2.53321	0.79689
H	3.3577	3.33503	0.19653
H	3.02099	1.77792	0.95164
H	4.5853	2.07521	0.20451
C	4.23229	0.28161	6.4109
H	3.5952	1.10686	6.72874
C	5.32964	0.15445	7.46732
H	5.94477	1.05323	7.51253
H	5.98857	-0.69588	7.28518
H	4.88367	0.00956	8.45223
C	3.37763	-0.98538	6.35525
H	2.93792	-1.19606	7.3316
H	3.9779	-1.8512	6.06822
H	2.5635	-0.88987	5.63717
N	3.16928	2.41705	4.75209
H	5.94831	6.45513	4.90041
C	5.36749	6.16425	5.77755
H	4.49737	6.81398	5.82965

H	5.98558	6.36402	6.65813
C	5.03085	4.69243	5.71412
C	6.28606	3.85239	5.73204
H	6.8891	4.04316	4.84315
H	6.09513	2.78283	5.76742
H	6.89203	4.11465	6.60485
O	4.07625	4.28995	6.79511

E (C_1): E_{tot} = -3172.19597629

C	1.01128	4.78139	4.68895
C	0.86678	4.39122	3.32693
H	1.63344	4.44864	2.56784
C	-0.43558	3.86629	3.14813
H	-0.83816	3.47317	2.22659
C	-1.1194	3.95892	4.38456
H	-2.13481	3.64433	4.57387
C	-0.23405	4.51515	5.3357
H	-0.45627	4.67414	6.37808
C	2.24577	6.68138	5.59558
C	1.85271	7.17825	6.85456
C	2.00673	8.53503	7.1201
H	1.70956	8.92659	8.08507
C	2.52028	9.4004	6.17462
H	2.63222	10.4526	6.40122
C	2.87558	8.91396	4.93209
H	3.25615	9.60141	4.18747
C	2.74941	7.56406	4.61963
C	1.19406	6.32813	7.92072
H	1.27713	5.2811	7.62039
C	1.84009	6.47267	9.3008
H	2.91503	6.29438	9.28457
H	1.39879	5.76058	9.99947
H	1.68513	7.4677	9.71982
C	-0.29154	6.69183	8.02602
H	-0.41486	7.69492	8.43803
H	-0.8169	5.99973	8.68734
H	-0.78625	6.68182	7.05606
C	3.10961	7.12567	3.21571
H	3.16551	6.03746	3.19221
C	4.4746	7.64853	2.7723
H	5.26156	7.34541	3.4637
H	4.49825	8.73616	2.69474
H	4.72819	7.25428	1.78817
C	2.01392	7.55102	2.23649
H	2.23525	7.18981	1.23023
H	1.92916	8.63811	2.18636
H	1.04235	7.15439	2.53039
Fe	0.59262	2.81682	4.60055
N	2.18116	5.27667	5.31266
Si	3.71154	4.42266	5.4542
C	2.38132	2.01193	5.04268
C	1.78308	1.27958	3.97949
H	2.19699	1.15675	2.9905
C	0.55747	0.74943	4.44732
H	-0.13216	0.14908	3.87332
C	0.38808	1.15264	5.79411
H	-0.45206	0.91268	6.42859
C	1.52412	1.91148	6.17192
H	1.69451	2.36715	7.13803
C	4.71932	2.05709	4.47383
C	5.18255	2.25117	3.16224
C	6.29793	1.53664	2.73719
H	6.67064	1.67912	1.72992
C	6.93516	0.63761	3.57013
H	7.79754	0.08653	3.2185
C	6.46354	0.44622	4.85507
H	6.96569	-0.2607	5.50387
C	5.36468	1.15094	5.33128
C	4.51697	3.18785	2.17774
H	3.66375	3.65239	2.67449
C	5.46546	4.29946	1.73133
H	6.31802	3.90094	1.17913
H	5.85511	4.85893	2.58079
H	4.95088	5.00085	1.07194
C	3.97847	2.4364	0.95914
H	3.434	3.11492	0.29987
H	3.30005	1.6321	1.24207
H	4.78385	1.98974	0.37409
C	4.89145	0.88934	6.74406
H	4.12055	1.61987	6.98695
C	6.01521	1.06816	7.76469
H	6.48069	2.04987	7.67464
H	6.7978	0.31661	7.64974
H	5.62337	0.96807	8.77864

C	4.24721	-0.49271	6.85282
H	3.87023	-0.66292	7.86284
H	4.96517	-1.28434	6.63029
H	3.41008	-0.59501	6.16186
N	3.56593	2.76142	4.94272
H	4.7512	5.03656	4.58881
C	5.68567	5.32633	7.24778
C	5.61256	6.83314	7.27159
H	6.60592	7.27316	7.22658
H	5.10937	7.17502	8.17853
H	5.01407	7.20878	6.43749
C	4.36579	4.60871	7.2356
H	4.49058	3.61206	7.66167
H	3.62299	5.1406	7.82727
O	6.73659	4.73535	7.20352

TSA (C_1): E_{tot} = -3243.54167339

C	0.6961	3.73559	3.54104
C	0.2758	3.54052	2.19383
H	0.88631	3.68804	1.3146
C	-1.06316	3.08357	2.21343
H	-1.65887	2.83096	1.34909
C	-1.48616	3.02	3.56383
H	-2.45915	2.70448	3.90964
C	-0.40747	3.42045	4.38564
H	-0.41107	3.4426	5.46346
C	2.10513	5.5749	4.20191
C	1.80757	6.08588	5.47739
C	1.86684	7.46132	5.67471
H	1.63448	7.86802	6.65091
C	2.21598	8.32188	4.65368
H	2.25023	9.38946	4.82654
C	2.53211	7.80708	3.41303
H	2.81836	8.48531	2.61897
C	2.49158	6.43925	3.16289
C	1.41311	5.23032	6.66134
H	1.48134	4.18085	6.36915
C	2.35682	5.44087	7.84746
H	3.39959	5.30687	7.56538
H	2.12869	4.73131	8.64388
H	2.25439	6.44255	8.26769
C	-0.02747	5.52179	7.09224
H	-0.11278	6.52196	7.52032
H	-0.35033	4.81375	7.85774
H	-0.72702	5.46895	6.25885
C	2.87859	5.98032	1.77282
H	2.88008	4.88778	1.74094
C	4.29484	6.43844	1.42344
H	5.02046	6.06705	2.14792
H	4.37576	7.52568	1.40306
H	4.58551	6.0755	0.43738
C	1.86861	6.46045	0.72999
H	2.11612	6.06378	-0.25647
H	1.86381	7.5488	0.65217
H	0.85536	6.14556	0.97951
Fe	0.17048	1.82223	3.28425
N	1.98818	4.15831	3.94839
C	1.93568	0.9041	3.46995
C	1.2701	0.40503	2.3151
H	1.63287	0.46701	1.30009
C	0.04828	-0.17008	2.73429
H	-0.68993	-0.62523	2.09127
C	-0.04319	-0.03688	4.1423
H	-0.86305	-0.37282	4.75941
C	1.12805	0.6101	4.60362
H	1.35935	0.86098	5.62971
C	4.29652	0.82144	3.01061
C	4.78903	1.01858	1.71094
C	5.88737	0.27119	1.29614
H	6.29045	0.42082	0.30206
C	6.46977	-0.66698	2.12456
H	7.31999	-1.2421	1.78216
C	5.95669	-0.87101	3.39188
H	6.41181	-1.61493	4.03338
C	4.87489	-0.13571	3.86028
C	4.18809	1.99948	0.72616
H	3.27949	2.42456	1.16052
C	5.15348	3.14845	0.44205
H	6.07417	2.78798	-0.0193
H	5.43136	3.67474	1.35612
H	4.70424	3.87087	-0.24129
C	3.77044	1.3135	-0.57558
H	3.24809	2.01717	-1.22561
H	3.10739	0.46753	-0.39317
H	4.63014	0.93676	-1.13108
C	4.34106	-0.42786	5.24349
H	3.6396	0.3602	5.50864
C	5.43763	-0.42679	6.30725
H	6.01499	0.49712	6.28623
H	6.13221	-1.25911	6.18354
H	4.99519	-0.5223	7.2996
C	3.57258	-1.7505	5.25054
H	3.13108	-1.93109	6.23197
H	4.2323	-2.59014	5.02322
H	2.76739	-1.75026	4.51611
N	3.17073	1.59095	3.46838
Si	3.4661	3.25624	3.84747
C	5.14831	3.71786	5.35449
C	4.46441	3.09847	6.3003
C	3.71577	2.48302	7.1075
O	6.08651	4.31993	4.99259
O	3.00986	1.91233	7.84794

TSA1 (C_1): E_{tot} = -3243.53636676

C	0.61279	3.86808	3.14613
C	0.24124	3.67215	1.78692
H	0.88192	3.82302	0.93004
C	-1.09928	3.21968	1.76609
H	-1.66782	2.96697	0.8836
C	-1.56669	3.15831	3.10284
H	-2.5527	2.84931	3.41581
C	-0.5157	3.56301	3.95764
H	-0.55377	3.61991	5.03534
C	1.92962	5.57623	4.23127
C	1.93919	5.67821	5.63114
C	1.99718	6.94557	6.20254
H	2.02064	7.04568	7.28062
C	2.01923	8.08247	5.41936
H	2.05835	9.06003	5.88164
C	1.9925	7.96614	4.04208
H	2.00892	8.86293	3.43595
C	1.95731	6.72304	3.42182
C	1.8995	4.48041	6.55798
H	1.7278	3.5788	5.96416
C	3.23236	4.31124	7.28614
H	4.06274	4.19355	6.58762
H	3.21338	3.4337	7.93375
H	3.45685	5.17764	7.90991
C	0.74448	4.57011	7.55631
H	0.87773	5.39092	8.26196
H	0.67448	3.65092	8.13989
H	-0.21106	4.72572	7.05449
C	1.91633	6.66195	1.91132
H	2.11634	5.6367	1.60453
C	2.9951	7.52833	1.26273
H	3.98643	7.284	1.6404
H	2.8234	8.59349	1.42566
H	3.00328	7.36613	0.18429
C	0.52686	7.05274	1.40361
H	0.47172	6.95319	0.31799
H	0.29668	8.09079	1.65145
H	-0.25291	6.42702	1.83741
Fe	0.09902	1.95558	2.86195
N	1.8807	4.27402	3.62066
C	1.85408	1.02359	3.1175
C	1.2763	0.62826	1.87724
H	1.69957	0.79316	0.89907
C	0.02946	0.02028	2.15104
H	-0.65595	-0.37285	1.4152
C	-0.17207	0.03258	3.55319
H	-1.03555	-0.35363	4.07376
C	0.95635	0.63846	4.15448
H	1.10051	0.8056	5.21158
C	4.26156	0.85043	3.34464
C	4.95856	0.55335	2.16155
C	6.06473	-0.28641	2.23728
H	6.61203	-0.52666	1.33452
C	6.48465	-0.81745	3.44016
H	7.34713	-1.46973	3.47679
C	5.80308	-0.50114	4.59834
H	6.14515	-0.91202	5.53972
C	4.69258	0.33579	4.57945
C	4.57073	1.08128	0.79707
H	3.75799	1.79926	0.91773
C	5.72909	1.81585	0.11843
H	6.52395	1.12705	-0.17188
H	6.17005	2.57431	0.76128
H	5.38135	2.3098	-0.78944
C	4.0803	-0.05833	-0.10078
H	3.69558	0.33211	-1.04491
H	3.29469	-0.6467	0.37236
H	4.89443	-0.74398	-0.34152
C	4.01071	0.62406	5.90032
H	3.24991	1.39342	5.74702
C	4.99203	1.16807	6.93886
H	5.5172	2.05243	6.57939
H	5.74586	0.42931	7.2127
H	4.46428	1.43953	7.85403
C	3.30605	-0.6267	6.4295
H	2.74578	-0.39975	7.33862
H	4.02777	-1.40692	6.67681
H	2.61435	-1.04192	5.69712
N	3.09063	1.6958	3.29412
Si	3.34277	3.3621	3.65349
C	6.27474	4.43942	3.39194
C	6.84027	4.20813	4.51145
O	4.55541	4.50994	1.70773
O	7.42451	4.02871	5.50352
C	5.12719	4.32757	2.74624

TSA2 (C_1): E_{tot} = -3243.50141933

C	0.69884	3.90667	3.3697
C	0.60894	3.56094	1.99398
H	1.41316	3.62636	1.27649
C	-0.70336	3.09524	1.73757
H	-1.07592	2.74567	0.78634
C	-1.44503	3.19002	2.94039
H	-2.48218	2.9194	3.07011
C	-0.58782	3.68756	3.94778
H	-0.85849	3.85725	4.97766
C	1.80081	5.69389	4.55033
C	1.40022	5.95936	5.86899
C	1.40783	7.27942	6.30699
H	1.1143	7.50457	7.32509
C	1.7828	8.3132	5.47086
H	1.77775	9.33326	5.83222
C	2.16619	8.03838	4.17156
H	2.45684	8.85433	3.52153
C	2.19341	6.734	3.69263
C	0.95458	4.8863	6.8415
H	0.94481	3.9284	6.3179
C	1.91678	4.7451	8.0212
H	2.91913	4.48752	7.68687
H	1.57179	3.96262	8.70006
H	1.98314	5.67071	8.59538
C	-0.46516	5.15399	7.34849
H	-0.50203	6.03516	7.99084
H	-0.82609	4.30983	7.9386
H	-1.1684	5.32386	6.53264
C	2.60977	6.48477	2.25925
H	2.78687	5.41482	2.14106
C	3.91232	7.19314	1.891
H	4.71336	6.94867	2.58862
H	3.80368	8.27866	1.87743
H	4.23408	6.89205	0.89235
C	1.48703	6.88052	1.29873
H	1.75855	6.64525	0.26752
H	1.28601	7.95226	1.3514
H	0.55999	6.35686	1.53039
Fe	0.20592	1.96464	3.20837
N	1.85232	4.3473	4.06152
Si	3.27619	3.41307	4.49285
C	1.95458	1.09597	3.67514
C	1.36091	0.39967	2.5829
H	1.78137	0.27457	1.59773
C	0.10872	-0.10124	3.01239
H	-0.58178	-0.67087	2.40895
C	-0.0816	0.277	4.3623
H	-0.94137	0.04614	4.97316
C	1.06787	0.99027	4.7827
H	1.23283	1.414	5.76477
C	4.33974	1.22664	3.22769
C	4.71722	1.29747	1.87452
C	5.92811	0.731	1.49252
H	6.24087	0.78371	0.45695
C	6.74878	0.10776	2.41392
H	7.6927	-0.3179	2.0997
C	6.35619	0.02421	3.73697
H	6.99915	-0.47819	4.4495
C	5.15103	0.5687	4.16724
C	3.84731	1.94699	0.81715
H	2.88107	2.16025	1.26946

C	4.41057	3.27849	0.319
H	5.42598	3.17261	-0.06592
H	4.42292	4.03507	1.10426
H	3.79207	3.67175	-0.49031
C	3.6052	1.0057	-0.36459
H	2.84895	1.42212	-1.0318
H	3.2629	0.02291	-0.03901
H	4.50782	0.85254	-0.95806
C	4.75552	0.41201	5.61961
H	3.80511	0.92139	5.78004
C	5.77193	1.0598	6.5581
H	5.88627	2.12231	6.3416
H	6.7554	0.5929	6.48256
H	5.44518	0.96776	7.59483
C	4.53282	-1.0616	5.9609
H	4.19278	-1.16701	6.99228
H	5.44869	-1.64577	5.85541
H	3.77735	-1.5044	5.31181
N	3.13625	1.86429	3.65362
O	4.60072	5.31826	5.8611
C	5.28284	5.18734	4.90036
C	5.08121	4.25692	3.91097
C	6.12854	3.8793	3.18176
O	7.01784	3.53197	2.55013

TSA3 (C_1): E_{tot} = -3243.57093004

C	0.78949	4.05843	2.95264
C	0.61816	3.89975	1.5499
H	1.39703	3.98151	0.80406
C	-0.74141	3.58399	1.31149
H	-1.18575	3.38828	0.34708
C	-1.41826	3.58477	2.55587
H	-2.46885	3.38639	2.70568
C	-0.47815	3.87678	3.57136
H	-0.67989	3.94205	4.62963
C	2.07154	5.48031	4.42325
C	1.91086	5.39437	5.81286
C	1.97135	6.56623	6.5602
H	1.86087	6.51992	7.63673
C	2.16473	7.79231	5.95428
H	2.20432	8.69367	6.5517
C	2.30646	7.86286	4.58078
H	2.45413	8.82839	4.11351
C	2.27187	6.71801	3.79391
C	1.67139	4.08829	6.53846
H	1.56447	3.29646	5.79405
C	2.85471	3.73006	7.43514
H	3.77962	3.65916	6.86434
H	2.68673	2.77134	7.92934
H	3.00474	4.47861	8.21479
C	0.37682	4.11964	7.35254
H	0.43683	4.82568	8.18196
H	0.17092	3.13652	7.77899
H	-0.4813	4.40858	6.74516
C	2.41656	6.85653	2.29436
H	2.57068	5.86427	1.86882
C	3.62793	7.70128	1.90163
H	4.54156	7.33727	2.3704
H	3.50573	8.74868	2.18107
H	3.77232	7.67235	0.82092
C	1.13283	7.42011	1.68234
H	1.21488	7.47417	0.59534
H	0.93341	8.42838	2.05007
H	0.26935	6.80031	1.92319
Fe	0.12844	2.20667	2.57195
N	2.00521	4.28861	3.62913
C	1.76206	1.1004	2.94172
C	1.17583	0.70048	1.70455
H	1.63893	0.75943	0.73296
C	-0.13711	0.24907	1.96683
H	-0.84111	-0.10906	1.23065
C	-0.37623	0.36783	3.35825
H	-1.29252	0.11212	3.869
C	0.79702	0.87546	3.9641
H	0.93109	1.08679	5.01507
C	4.14145	0.68769	3.15633
C	4.8004	0.3291	1.96842
C	5.81622	-0.61994	2.03028
H	6.3321	-0.90754	1.12262
C	6.18006	-1.20678	3.22503
H	6.96866	-1.94723	3.25134
C	5.53363	-0.83679	4.38808
H	5.82784	-1.29644	5.32309
C	4.51984	0.11417	4.38204
C	4.46032	0.89694	0.60666
H	3.6997	1.67075	0.73216
C	5.67438	1.54577	-0.06205
H	6.4192	0.80028	-0.34431
H	6.16743	2.26656	0.58604
H	5.37538	2.06403	-0.97425
C	3.89221	-0.19166	-0.30921
H	3.52961	0.23916	-1.24453
H	3.07333	-0.73723	0.15803
H	4.65883	-0.92435	-0.56621
C	3.86664	0.45904	5.70266
H	3.21934	1.32585	5.55697
C	4.89762	0.8464	6.76185
H	5.52497	1.67034	6.42357
H	5.55324	0.014	7.02022
H	4.40025	1.15823	7.68061
C	2.99525	-0.69938	6.19212
H	2.46437	-0.42446	7.10591
H	3.60141	-1.57868	6.41717
H	2.25729	-0.99206	5.44547
N	3.06103	1.6384	3.12598
Si	3.39565	3.30064	3.40975
C	4.6685	4.09268	2.27239
C	4.87219	3.79815	4.16372
C	5.90842	4.12475	4.83954
O	5.43298	4.61733	1.58229
O	6.88008	4.4411	5.39954

TSA4 (C_1): E_{tot} = -3243.57722292

C	0.79675	4.04477	2.98965
C	0.55218	3.96385	1.5896
H	1.28512	4.09506	0.8069
C	-0.81351	3.64164	1.40463
H	-1.3051	3.49333	0.45481
C	-1.42354	3.55879	2.68042
H	-2.46159	3.33334	2.87316
C	-0.43603	3.80998	3.66006
H	-0.58347	3.81183	4.72914
C	2.08181	5.48074	4.42744
C	1.9419	5.38386	5.81937
C	1.96179	6.55518	6.56965
H	1.86864	6.49945	7.6472
C	2.09325	7.79148	5.96878
H	2.10221	8.69085	6.57028
C	2.21211	7.87213	4.59454
H	2.31116	8.84409	4.12726
C	2.2155	6.72927	3.80434
C	1.77327	4.07272	6.55608
H	1.68479	3.26679	5.82304
C	2.99078	3.77982	7.4305
H	3.90395	3.73931	6.83796
H	2.87249	2.82436	7.9442
H	3.12247	4.54756	8.19455
C	0.49545	4.05097	7.39715
H	0.54473	4.75856	8.2258
H	0.34126	3.06023	7.8276
H	-0.388	4.30432	6.8105
C	2.3439	6.8886	2.30728
H	2.43526	5.89573	1.86882
C	3.59873	7.67263	1.92598
H	4.49228	7.2354	2.37159
H	3.54354	8.71184	2.25289
H	3.72888	7.68375	0.84264
C	1.08557	7.52233	1.7143
H	1.164	7.59193	0.62788
H	0.92962	8.53188	2.09854
H	0.19853	6.93441	1.95037
Fe	0.14204	2.21177	2.5386
N	2.03686	4.29085	3.62072
C	1.78235	1.11414	2.86519
C	1.2382	0.78936	1.58872
H	1.7286	0.91859	0.6366
C	-0.07306	0.30044	1.78444
H	-0.75217	-0.01585	1.00689
C	-0.34762	0.31289	3.17447
H	-1.27142	0.0054	3.64122
C	0.79933	0.79751	3.84552
H	0.90349	0.93689	4.91168
C	4.10802	0.63788	3.20037
C	4.77207	0.22824	2.03415
C	5.68426	-0.81799	2.11473
H	6.202	-1.14416	1.22114
C	5.9485	-1.4481	3.31388
H	6.65556	-2.26595	3.35761
C	5.31491	-1.01295	4.46018
H	5.54173	-1.4962	5.4022
C	4.39894	0.03353	4.43322
C	4.58811	0.89077	0.68749
H	3.82441	1.66416	0.78741
C	5.88915	1.56733	0.24976
H	6.66685	0.82969	0.04676
H	6.27451	2.23403	1.02112
H	5.74315	2.14306	-0.6659
C	4.11184	-0.09475	-0.38049
H	3.88876	0.42702	-1.31297
H	3.21678	-0.63217	-0.06753
H	4.87467	-0.84147	-0.60518
C	3.79139	0.45765	5.75243
H	3.15264	1.32785	5.58788
C	4.88272	0.88257	6.73515
H	5.47458	1.70241	6.32973
H	5.56058	0.06009	6.96665
H	4.44474	1.21358	7.6769
C	2.91979	-0.64993	6.34657
H	2.41871	-0.30017	7.25135
H	3.51642	-1.52084	6.62279
H	2.15798	-0.98696	5.64356
N	3.07386	1.64174	3.12006
Si	3.41186	3.27107	3.52035
C	4.13405	4.16997	1.26023
C	4.91189	3.73976	4.08435
C	6.03859	4.19006	4.44759
O	4.81268	4.7511	0.57734
O	7.08405	4.59852	4.78634

TSC (C_1): E_{tot} = -3394.65490980

C	1.00004	4.01518	3.51215
C	0.37084	4.14915	2.23869
H	0.79113	4.60788	1.35676
C	-0.9107	3.55645	2.316
H	-1.62303	3.48432	1.50769
C	-1.09459	3.07503	3.63532
H	-1.972	2.56844	4.00877
C	0.07506	3.36011	4.37539
H	0.25294	3.10048	5.40718
C	2.32623	5.66957	4.64502
C	2.39311	5.62242	6.04684
C	2.39242	6.82019	6.75477
H	2.44924	6.79736	7.83588
C	2.31761	8.0401	6.11384
H	2.31771	8.95859	6.6858
C	2.23979	8.07526	4.73607
H	2.1748	9.03244	4.23311
C	2.24537	6.90634	3.98431
C	2.43679	4.34265	6.85272
H	2.45758	3.49365	6.16606
C	3.69416	4.2662	7.71593
H	4.59522	4.31874	7.10925
H	3.7138	3.33022	8.27536
H	3.73138	5.07719	8.44465
C	1.18931	4.20879	7.73159
H	1.1839	4.95618	8.52654
H	1.1604	3.22804	8.20998
H	0.26761	4.3401	7.16471
C	2.14421	7.03846	2.48261
H	2.24718	6.04428	2.05583
C	3.27119	7.89878	1.91119
H	4.2484	7.56942	2.26497
H	3.16726	8.94622	2.19738
H	3.26791	7.86615	0.8194
C	0.77716	7.57914	2.06362
H	0.69	7.61319	0.97562
H	0.61889	8.59235	2.43653
H	-0.02981	6.95565	2.44763
Fe	0.56668	2.2003	2.78455
N	2.29519	4.44688	3.8822
Si	3.77439	3.62809	3.51754
C	2.37836	1.34426	2.70527
C	1.78265	1.33234	1.40829
H	2.16644	1.80556	0.51742
C	0.57364	0.60317	1.48605
H	-0.11276	0.42947	0.67075
C	0.41925	0.1457	2.81793
H	-0.40779	-0.43627	3.19639
C	1.52959	0.59397	3.56868
H	1.69581	0.42803	4.62185
C	4.72283	1.06947	3.15558
C	5.40389	0.72239	1.97637

C	6.45443	-0.18519	2.04259
H	6.98003	-0.4595	1.136
C	6.8423	-0.74448	3.24309
H	7.66248	-1.44927	3.27981
C	6.17269	-0.39325	4.39724
H	6.48149	-0.83333	5.33703
C	5.11272	0.50817	4.38305
C	5.04928	1.27679	0.61617
H	4.2638	2.01464	0.75542
C	6.23687	1.99078	-0.02981
H	7.02618	1.29179	-0.30916
H	6.68501	2.71976	0.64557
H	5.93011	2.50565	-0.94304
C	4.50131	0.18771	-0.30588
H	4.18236	0.61163	-1.26044
H	3.64657	-0.3179	0.14238
H	5.25755	-0.56877	-0.52115
C	4.44024	0.79845	5.70727
H	3.67338	1.56139	5.55653
C	5.43747	1.34495	6.72774
H	5.91448	2.25315	6.36656
H	6.22078	0.62001	6.95309
H	4.93486	1.57542	7.66712
C	3.75821	-0.45632	6.26034
H	3.17161	-0.21441	7.14856
H	4.49278	-1.20851	6.5525
H	3.09729	-0.92361	5.53052
N	3.59148	1.96193	3.09305
C	5.21086	4.15026	4.23983
C	6.22962	4.56362	4.86145
O	7.18781	4.94943	5.42502
C	5.51078	5.0728	1.72457
C	4.31743	4.51947	1.55476
C	3.64101	4.51313	0.4344
O	2.95132	4.43778	-0.48023
O	6.53233	5.57354	1.78244

TSD (C_1): E_{tot} = -6374.15257802

C	3.64888	6.70313	8.48805
C	3.11507	7.3568	7.49408
C	3.80287	8.23911	6.52965
C	2.65365	8.72278	5.73459
C	2.50278	9.68018	4.83634
C	-0.42616	7.94593	8.64677
C	0.09849	7.04569	9.61904
H	1.14143	6.81743	9.78335
C	-0.98794	6.48741	10.33311
H	-0.91469	5.75985	11.12749
C	-2.18108	7.06546	9.83795
H	-3.18105	6.85109	10.18424
C	-1.84062	7.96246	8.79862
H	-2.53556	8.53928	8.21077
C	-0.32619	5.60241	6.54447
C	-0.16532	4.53989	7.48602
H	0.77098	4.14184	7.84409
C	-1.44841	4.10849	7.88872
H	-1.65746	3.32273	8.59927
C	-2.41158	4.89645	7.2106
H	-3.4835	4.81572	7.31335
C	-1.72467	5.81043	6.37754
H	-2.17731	6.56052	5.74632
C	0.30112	10.04605	7.65379
C	1.17975	10.74579	8.4975
C	1.18374	12.13428	8.4553
H	1.86948	12.68487	9.08602
C	0.33658	12.82774	7.61265
H	0.3631	13.90911	7.58249
C	-0.55137	12.1325	6.81683
H	-1.22798	12.68339	6.17482
C	-0.59526	10.74118	6.8265
C	2.08504	10.05096	9.48843
H	2.10367	8.99016	9.25036
C	3.52724	10.5458	9.40983
H	3.63263	11.57454	9.75837
H	3.90953	10.51152	8.39039
H	4.17442	9.92571	10.0324
C	1.52353	10.19012	10.90417
H	0.51509	9.78107	10.97191
H	1.48187	11.23627	11.21333
H	2.15061	9.65668	11.62097
C	-1.65021	10.06147	5.9807
H	-1.54103	8.98103	6.09964
C	-1.49638	10.3851	4.49726
H	-0.51454	10.11128	4.12038
H	-1.63382	11.44978	4.30163
H	-2.24433	9.8481	3.9107
C	-3.05619	10.45677	6.44319
H	-3.81239	9.8551	5.93565
H	-3.26644	11.5028	6.21454
H	-3.19013	10.33642	7.51792
C	1.24871	5.74545	4.70436
C	0.68956	6.09012	3.45919
C	1.1789	5.48029	2.30914
H	0.74075	5.72372	1.34967
C	2.2141	4.56902	2.35974
H	2.58323	4.10898	1.45201
C	2.76602	4.24591	3.58104
H	3.57706	3.52972	3.62139
C	2.29473	4.80603	4.76448
C	-0.46638	7.05282	3.29408
H	-0.61949	7.57717	4.24007
C	-0.19129	8.10512	2.21949
H	-0.06608	7.65735	1.23308
H	0.70749	8.68115	2.43382
H	-1.02567	8.8023	2.14629
C	-1.74927	6.28812	2.9562
H	-1.95037	5.49165	3.67152
H	-1.6781	5.82772	1.96905
H	-2.60974	6.96067	2.94239
C	2.92349	4.30892	6.04728
H	2.50066	4.8727	6.87591
C	2.59695	2.82982	6.27
H	3.07087	2.20109	5.51448
H	1.52484	2.63893	6.22528
H	2.9626	2.49806	7.24395
C	4.43681	4.52597	6.06966
H	4.84175	4.27789	7.05251
H	4.71363	5.55246	5.83474
H	4.94411	3.88654	5.34571
C	6.39088	12.91091	3.40446
C	7.49225	13.78017	3.64348
H	7.90461	14.02689	4.61004
C	7.95919	14.24813	2.39168
H	8.79205	14.91785	2.23848
C	7.15127	13.67888	1.37644
H	7.25711	13.84229	0.3144
C	6.16854	12.87147	1.99981
H	5.39415	12.30288	1.50341
C	7.88062	10.25744	3.04118
C	8.1655	10.33494	1.6468
H	7.53669	9.95932	0.85441
C	9.39507	11.01289	1.48338
H	9.87293	11.23813	0.54174
C	9.88262	11.35602	2.76859
H	10.80012	11.88421	2.98089
C	8.96179	10.87441	3.73086
H	9.05212	10.97808	4.80202
C	5.12287	12.92588	5.45395
C	5.76645	12.8973	6.70278
C	5.20033	13.60206	7.76195
H	5.67848	13.57999	8.73387
C	4.04872	14.34304	7.59114
H	3.6286	14.89529	8.42237
C	3.43928	14.38693	6.34964
H	2.54029	14.97645	6.22479
C	3.95122	13.68242	5.26793
C	7.0816	12.18218	6.94018
H	7.41855	11.76996	5.98866
C	6.94495	11.02216	7.92444
H	6.23585	10.2737	7.57671
H	6.60936	11.36732	8.90442
H	7.90676	10.5242	8.06424
C	8.16304	13.15449	7.41632
H	7.9492	13.54233	8.41348
H	8.26447	14.01192	6.75072
H	9.1307	12.65205	7.46566
C	3.26635	13.78703	3.92357
H	3.55988	12.92002	3.32846
C	3.72723	15.0508	3.191
H	4.80905	15.08712	3.07308
H	3.42104	15.94408	3.73953
H	3.28144	15.1029	2.1959
C	1.74124	13.77123	4.02676
H	1.35105	14.70256	4.44216
H	1.3806	12.95168	4.64588
H	1.30365	13.66118	3.03365
C	6.65137	8.24987	3.46534
C	5.86485	7.67993	2.45201
C	5.81581	6.29238	2.34429
H	5.19521	5.83849	1.58161
C	6.54469	5.48312	3.19018
H	6.50223	4.4065	3.08539
C	7.32829	6.05545	4.17546
H	7.89673	5.41326	4.83636
C	7.39008	7.43283	4.34129
C	5.06007	8.48892	1.45648
H	5.23425	9.55053	1.64444
C	3.56422	8.22306	1.61643
H	3.25083	8.32608	2.65312
H	3.30436	7.20836	1.31294
H	2.97658	8.91241	1.00765
C	5.49325	8.20469	0.01663
H	5.257	7.18085	-0.27711
H	6.56599	8.3381	-0.12335
H	4.97544	8.86913	-0.67726
C	8.28989	7.99147	5.42219
H	8.02513	9.03861	5.57692
C	8.11642	7.29081	6.76958
H	8.46509	6.25694	6.74478
H	7.07719	7.29449	7.08892
H	8.70531	7.80449	7.53177
C	9.75337	7.91699	4.97749
H	10.40609	8.39566	5.71048
H	9.91561	8.40226	4.01623
H	10.07303	6.87721	4.88188
Fe	-1.16685	6.10746	8.31322
Fe	8.01492	12.17916	2.49456
N	0.31232	8.61113	7.64548
N	0.70993	6.33202	5.90533
N	5.67466	12.17565	4.36657
N	6.71714	9.67952	3.60653
O	4.98587	8.46868	6.45379
O	4.07156	6.11002	9.38457
O	2.06446	10.4365	4.07975
Si	1.4388	7.69766	6.69073
Si	5.33882	10.44356	4.38022

TSE (C_1): E_{tot} = -3172.13153272

C	1.30765	3.57784	4.00411
C	1.02068	3.18085	2.66555
H	1.71557	3.19736	1.83809
C	-0.31256	2.70747	2.61654
H	-0.81511	2.31921	1.74322
C	-0.87417	2.8454	3.90948
H	-1.87951	2.57582	4.19677
C	0.11645	3.37997	4.76487
H	0.00104	3.56842	5.82003
C	2.61364	5.44585	4.77805
C	2.39105	5.91671	6.08502
C	2.50887	7.28068	6.33543
H	2.34054	7.6553	7.33785
C	2.83266	8.17056	5.32972
H	2.91818	9.22803	5.54371
C	3.0426	7.70085	4.0469
H	3.28911	8.40461	3.26144
C	2.9426	6.34619	3.74762
C	2.00001	5.01498	7.23646
H	2.00827	3.98467	6.87727
C	2.97997	5.10616	8.40657
H	4.00288	4.90232	8.09854
H	2.71392	4.38366	9.17996
H	2.96442	6.09449	8.86935
C	0.58794	5.35066	7.72651
H	0.5597	6.33072	8.2062
H	0.25037	4.61902	8.46311
H	-0.136	5.37396	6.91255
C	3.17233	5.91183	2.31584
H	3.23534	4.82365	2.28963
C	4.49375	6.43637	1.75703
H	5.33471	6.12773	2.37851
H	4.51096	7.52467	1.68277
H	4.66226	6.04302	0.75365
C	1.99506	6.33101	1.43447
H	2.13134	5.973	0.41206
H	1.89873	7.41767	1.39332
H	1.05523	5.92726	1.81038
Fe	0.80892	1.64171	3.98329
N	2.54477	4.04227	4.50459
Si	4.11113	3.2248	4.41379
C	2.60339	0.81029	4.30862
C	1.92275	0.07703	3.29496

H	2.26638	-0.06095	2.2804
C	0.72205	-0.42607	3.8497
H	-0.01649	-1.01765	3.32984
C	0.6528	-0.00879	5.20234
H	-0.14772	-0.22758	5.89331
C	1.82194	0.73713	5.49379
H	2.0698	1.20321	6.43735
C	4.91455	0.75148	3.65932
C	5.35204	0.89984	2.33282
C	6.45856	0.16922	1.90827
H	6.81544	0.28386	0.89172
C	7.10218	-0.71286	2.75304
H	7.95563	-1.27868	2.40259
C	6.64356	-0.8755	4.0483
H	7.14601	-1.57868	4.70057
C	5.55974	-0.14956	4.52664
C	4.66152	1.79889	1.32856
H	3.77462	2.22231	1.80315
C	5.55819	2.95953	0.901
H	6.46197	2.60478	0.40216
H	5.85887	3.55701	1.76132
H	5.03372	3.6147	0.20245
C	4.17887	1.0108	0.10982
H	3.60093	1.65436	-0.55572
H	3.54521	0.17132	0.39704
H	5.01009	0.60721	-0.47028
C	5.07901	-0.38565	5.9422
H	4.45601	0.4601	6.23297
C	6.21988	-0.46123	6.95569
H	6.87631	0.40553	6.8882
H	6.834	-1.35398	6.82744
H	5.8167	-0.49684	7.96889
C	4.22964	-1.65757	6.00868
H	3.8257	-1.80066	7.01269
H	4.82985	-2.53616	5.76278
H	3.39053	-1.62176	5.31547
N	3.80636	1.5183	4.13483
H	5.56823	4.52634	4.37705
C	5.85872	4.00725	6.2684
C	5.96711	5.16607	5.47965
H	5.14001	5.87134	5.47273
H	6.93417	5.65679	5.44135
O	4.79385	3.29321	6.11191
C	7.02854	3.34898	6.91228
H	7.81563	4.06148	7.14667
H	7.43693	2.59109	6.23329
H	6.73674	2.83238	7.82649

TSE1 (C_1): E_{tot} = -3172.13497694

C	0.66446	4.53307	4.43992
C	0.42	4.18812	3.0786
H	1.13913	4.24685	2.27374
C	-0.90613	3.70577	2.97251
H	-1.37993	3.34763	2.07081
C	-1.50544	3.78943	4.25277
H	-2.51579	3.5003	4.50071
C	-0.54605	4.29797	5.15819
H	-0.69864	4.44029	6.21497
C	1.94429	6.39025	5.28579
C	1.59201	6.83065	6.5751
C	1.67244	8.19037	6.85948
H	1.40449	8.54316	7.84789
C	2.08826	9.10277	5.90933
H	2.14414	10.15599	6.15188
C	2.42763	8.66061	4.64571
H	2.74402	9.38156	3.90206
C	2.36329	7.31213	4.31022
C	1.10575	5.90969	7.67527
H	1.1462	4.88431	7.30594
C	1.98707	5.9683	8.92336
H	3.00619	5.66049	8.70639
H	1.59708	5.29247	9.68648
H	2.01019	6.96881	9.35888
C	-0.34012	6.24947	8.05319
H	-0.39696	7.20956	8.56938
H	-0.74867	5.49589	8.72936
H	-0.99211	6.31709	7.18262
C	2.72355	6.91856	2.89311
H	2.76622	5.82991	2.82917
C	4.10379	7.43376	2.49012
H	4.87086	7.07563	3.17758
H	4.1501	8.52341	2.47375
H	4.36364	7.08555	1.48971
C	1.64628	7.38787	1.91453
H	1.87631	7.05737	0.89971
H	1.57161	8.47667	1.89773
H	0.66732	6.99226	2.18497
Fe	0.18661	2.59969	4.33484
N	1.89631	4.99125	4.96824
Si	3.45418	4.18269	4.868
C	1.97375	1.77222	4.68847
C	1.32851	1.06213	3.63615
H	1.70356	0.95269	2.62905
C	0.11757	0.53612	4.14543
H	-0.60249	-0.04677	3.59107
C	0.00999	0.91746	5.50649
H	-0.80765	0.67625	6.16935
C	1.16422	1.66406	5.85023
H	1.38681	2.10937	6.80992
C	4.28637	1.70643	4.08143
C	4.78485	1.91658	2.78623
C	5.87907	1.16692	2.36179
H	6.28457	1.32939	1.37033
C	6.44619	0.20461	3.17239
H	7.28978	-0.3754	2.82154
C	5.92357	-0.01926	4.43407
H	6.36708	-0.78285	5.0604
C	4.85372	0.72382	4.9164
C	4.17623	2.90159	1.81034
H	3.28227	3.33193	2.26646
C	5.13757	4.04623	1.49615
H	6.04869	3.68305	1.01752
H	5.42527	4.57827	2.4035
H	4.67458	4.76513	0.8176
C	3.71645	2.20856	0.52683
H	3.20205	2.91644	-0.12534
H	3.02954	1.38878	0.73836
H	4.55376	1.79581	-0.03761
C	4.31882	0.43141	6.30338
H	3.71336	1.27984	6.61996
C	5.42028	0.27613	7.35201
H	6.07843	1.14364	7.38282
H	6.03741	-0.60801	7.1845
H	4.97316	0.17017	8.34115
C	3.43995	-0.8218	6.27877
H	2.99253	-0.99631	7.25886
H	4.0308	-1.70356	6.02136
H	2.63071	-0.74004	5.55471
N	3.1833	2.483	4.55623
H	5.66075	6.50484	5.81687
C	5.12176	6.08075	6.66148
H	4.18646	6.61673	6.79211
H	5.72914	6.23933	7.55978
C	4.93302	4.58768	6.50948
C	6.21349	3.86413	6.158
H	6.75175	4.36644	5.35716
H	6.0485	2.82829	5.87737
H	6.84846	3.87477	7.0512
O	3.99573	3.98591	7.10785

TSE2 (C_1): E_{tot} = -3172.06661014

C	0.23428	3.89759	3.67007
C	0.18085	3.61694	2.27395
H	0.9859	3.76773	1.56859
C	-1.09146	3.07373	1.97894
H	-1.43079	2.74728	1.00735
C	-1.84371	3.04329	3.17818
H	-2.85606	2.68283	3.28322
C	-1.03227	3.54233	4.22276
H	-1.31827	3.60448	5.2595
C	1.39916	5.80639	4.65989
C	0.81721	6.29811	5.84492
C	0.90426	7.65912	6.11782
H	0.46106	8.04843	7.02547
C	1.5367	8.52967	5.25345
H	1.59357	9.58497	5.48549
C	2.08564	8.04318	4.08495
H	2.56294	8.73399	3.40205
C	2.03109	6.69023	3.76461
C	0.02182	5.4478	6.8127
H	0.1846	4.39758	6.56064
C	0.43635	5.63932	8.27349
H	1.50507	5.50208	8.42656
H	-0.08378	4.91889	8.9061
H	0.17691	6.63252	8.64202
C	-1.47094	5.76981	6.67194
H	-1.68089	6.77617	7.03816
H	-2.07662	5.0768	7.25983
H	-1.8086	5.72763	5.63756
C	2.61208	6.27175	2.42957
H	2.66718	5.18111	2.38524
C	4.0356	6.78931	2.23282
H	4.69185	6.45698	3.03746
H	4.07707	7.8782	2.1966
H	4.44644	6.42403	1.29176
C	1.69792	6.72348	1.28894
H	2.07745	6.36998	0.3282
H	1.63804	7.81199	1.23924
H	0.68421	6.34303	1.4143
Fe	-0.11405	1.93812	3.40209
N	1.36424	4.39584	4.36922
Si	2.88872	3.56432	4.45649
C	1.62596	1.12178	3.97115
C	1.18246	0.49067	2.77545
H	1.71317	0.47405	1.83555
C	-0.0736	-0.10236	3.03991
H	-0.67568	-0.65092	2.33135
C	-0.40963	0.15728	4.39169
H	-1.31248	-0.15887	4.89254
C	0.64718	0.8965	4.97597
H	0.69481	1.25649	5.9943
C	4.03446	1.19559	3.80409
C	4.67423	1.40566	2.57257
C	5.87326	0.74433	2.3273
H	6.38999	0.90577	1.38916
C	6.41345	-0.12537	3.25418
H	7.34575	-0.6331	3.04467
C	5.75271	-0.35059	4.44707
H	6.17545	-1.04337	5.16335
C	4.56299	0.30132	4.74834
C	4.12182	2.30417	1.48653
H	3.13776	2.66411	1.79778
C	5.01967	3.52007	1.26905
H	6.00973	3.22474	0.91824
H	5.15298	4.08466	2.19194
H	4.59186	4.18886	0.51976
C	3.91718	1.54688	0.17343
H	3.42555	2.18551	-0.56221
H	3.30307	0.65626	0.30891
H	4.86431	1.22308	-0.25983
C	3.86329	-0.02372	6.04889
H	3.06608	0.70351	6.19847
C	4.79043	0.07813	7.25898
H	5.2488	1.06367	7.33849
H	5.58685	-0.66724	7.23072
H	4.22414	-0.09777	8.17515
C	3.2097	-1.40448	5.96288
H	2.65666	-1.62382	6.87778
H	3.959	-2.18781	5.83371
H	2.51232	-1.46774	5.12703
N	2.80738	1.8804	4.09806
C	4.46047	4.21759	7.61689
C	3.28823	3.59819	7.02602
C	4.35518	5.70885	7.88601
O	5.4979	3.61886	7.84971
H	3.70771	6.21623	7.16792
H	5.34051	6.1711	7.87267
H	3.9261	5.87356	8.87752
H	2.34401	4.10714	7.1748
H	3.90096	4.05303	5.44013
H	3.23644	2.51937	7.12247

TSF (C_1): E_{tot} = -3172.07055291

C	0.72987	4.70321	4.20541
C	0.62376	4.39054	2.82213
H	1.42764	4.42412	2.10202
C	-0.70947	3.99255	2.56034
H	-1.09905	3.68051	1.60283
C	-1.44377	4.08722	3.76857
H	-2.49099	3.85633	3.8945
C	-0.5633	4.52219	4.78332
H	-0.81835	4.67999	5.82023
C	1.93452	6.44705	5.3624
C	1.58975	6.79196	6.68047
C	1.70315	8.12477	7.06841
H	1.45604	8.40563	8.08503
C	2.10514	9.10234	6.18006
H	2.17311	10.13391	6.50009
C	2.41736	8.75493	4.87824
H	2.7279	9.52647	4.18483
C	2.35731	7.43390	4.45235
C	1.07681	5.80154	7.70629

H	1.00314	4.81809	7.23761
C	2.03245	5.66549	8.89067
H	3.01662	5.33550	8.56027
H	1.65641	4.93000	9.60393
H	2.15009	6.60997	9.42446
C	-0.32572	6.18328	8.18584
H	-0.31848	7.11187	8.75853
H	-0.73188	5.40564	8.83487
H	-1.01457	6.32417	7.35249
C	2.73033	7.10918	3.02245
H	2.843	6.02727	2.94259
C	4.06733	7.72192	2.60749
H	4.87488	7.41402	3.27135
H	4.03734	8.81253	2.59211
H	4.33019	7.39454	1.60038
C	1.61759	7.54801	2.06869
H	1.848	7.25158	1.04339
H	1.49993	8.63347	2.0791
H	0.65837	7.10749	2.3383
Fe	0.15255	2.78567	3.99133
N	1.88839	5.08732	4.92385
Si	3.05632	3.9807	5.61795
C	1.8297	1.80624	4.52482
C	1.30419	1.2386	3.33018
H	1.8061	1.19258	2.3763
C	0.00318	0.75584	3.6094
H	-0.65518	0.27272	2.90314
C	-0.28877	1.02593	4.9679
H	-1.20508	0.77974	5.4832
C	0.84704	1.64788	5.54329
H	0.94667	1.96609	6.57297
C	4.24791	1.83293	4.30600
C	4.80294	2.03086	3.03310
C	6.00563	1.40342	2.72796
H	6.45420	1.55136	1.75273
C	6.63742	0.58420	3.64562
H	7.57179	0.10131	3.39037
C	6.06608	0.37762	4.88749
H	6.56184	-0.27442	5.59627
C	4.87319	0.99783	5.24226
C	4.12494	2.87408	1.97472
H	3.15500	3.17652	2.36890
C	4.90366	4.14895	1.66000
H	5.90203	3.92618	1.27803
H	5.02166	4.77790	2.54004
H	4.38588	4.73511	0.89721
C	3.88121	2.07516	0.69296
H	3.26974	2.64968	-0.00514
H	3.37181	1.13101	0.88840
H	4.81488	1.83531	0.18163
C	4.28220	0.73152	6.60937
H	3.45818	1.42719	6.77133
C	5.28870	0.98196	7.73051
H	5.69949	1.99003	7.66958
H	6.12344	0.27989	7.70306
H	4.80705	0.87293	8.70343
C	3.70348	-0.68184	6.67751
H	3.24335	-0.86508	7.65020
H	4.47780	-1.43697	6.52914
H	2.94074	-0.83082	5.91285
N	3.04052	2.50948	4.65368
H	4.55752	7.15741	5.94269
C	5.54714	6.73809	6.13028
H	5.57905	6.45365	7.18541
H	6.28242	7.52526	5.97682
C	5.83498	5.56098	5.25280
C	6.86825	5.48550	4.42038
H	7.54945	6.31814	4.31909
H	4.40130	4.35361	6.47786
H	7.06332	4.59724	3.83690
O	4.98853	4.49515	5.39034

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