Electronic Supplementary Information for

Organoborane-Catalysed Reductive Depolymerisation of Catechyl Lignin under Ambient Conditions

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1. General information

1.1 Chemicals

All manipulations were carried out in a nitrogen-filled glovebox or under an atmosphere of dry nitrogen using standard Schlenk techniques, unless otherwise stated. All commercially available chemical reagents were used without further purification unless especially noted. The castor (*Ricinus communis* L.) seeds were received from Shandong Province, China.

1.2 Methods

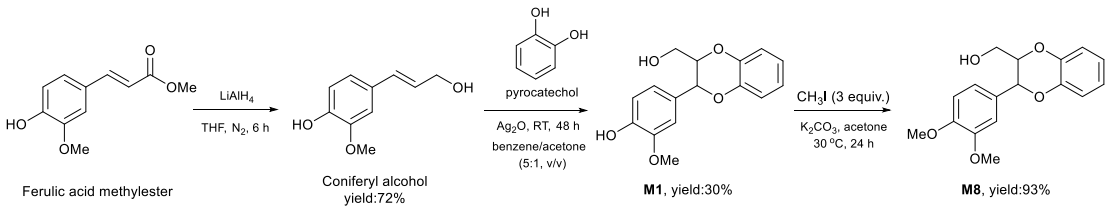
GC-MS/GC analysis. GC-MS (Shimadu GCMS-QP2010SE) analysis were carried out by using a HP-5 MS (30 m × 0.25 mm × 0.25 mm) capillary column. Helium was used as a carrier gas with a constant column flow of 1 mL min^{-1}. The GC (Shimadu GC-2010) was equipped with a HP5-column and an FID, and N_2 was used as a carrier gas. The injector temperature and the detection temperature were held constant at 250 and 290 °C, respectively. The identification and quantification of products were performed by comparison with corresponding authentic samples synthesized independently.[1,2]

NMR analysis. NMR spectra (^1H, ^{13}C and 2D HSQC) were acquired on a Bruker AVIII 600 MHz spectrometer at 25 °C. Samples were dissolved in DMSO-d_6, $CDCl_3$ and 1,2-$C_6D_4Cl_2$, respectively. As for ^1H NMR data are reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constant (Hz), and integration. As for 2D HSQC experiment, the solvent peak (deuterated 1,2-dichlorobenzene) at δ_C/δ_H = 132.6/7.4 ppm was used as an internal reference. The standard Bruker implementations of 2D HSQC NMR experiments were used for structural characterization and assignment authentication as previous reports.[3-5]

Computational Details. All calculations were carried out with Gaussian 16 program.[6] Geometrical optimizations and vibrational frequency analysis were performed at the M06-2X/6-31G (d) level.[7] Frequency calculations of optimized structures were performed to confirm that each stationary point was a transition state (one imaginary frequency) or a minimum (no imaginary frequency) and to obtain the thermodynamic corrections. Intrinsic reaction coordinate (IRC) calculations were conducted for each transition state to verify the direct connection between the corresponding reactant and product. Single-point calculations were carried out at the level of M06-2X/6-311+G (d, p) together with SMD implicit solvent model for considering the solvation effect of chlorobenzene.[8] Gibbs free energies in solution described in the text were obtained from such single-point energy calculations including gas-phase free energy corrections. The three-dimensional images of the optimized structures were prepared using CYL view software.[9]

2. Synthesis of benzodioxane mimics and molecular standards

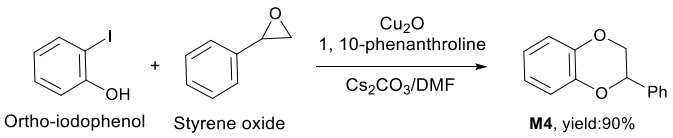
2.1 The synthesis of benzodioxane mimics



Coniferyl alcohol. In a typical step, ferulic acid methylester (500 mg, 2.4 mmol, 1.0 equiv.) dissolved in anhydrous THF (10 mL) was added slowly into a suspension of $LiAlH_4$ (273.2 mg, 7.2 mmol, 3.0 equiv.) in anhydrous THF (30 mL) at ice bath under N_2, and the mixture was allowed to stir at room temperature (RT) for 6 h. After reaction, the mixture was quenched and acidified with HCl to pH = 2. The organic phase was evaporated to afford a solid, which was purified by column chromatography with PE/EtOAc (2:1) to give coniferyl alcohol as white solid (311 mg, 72%).

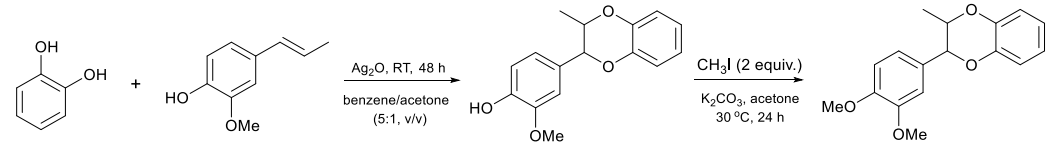
*Dimeric model compound **M1***. Silver oxide (282.7 mg, 1.2 mmol, 2.0 equiv.) was added to a solution of coniferyl alcohol (100 mg, 0.6 mmol, 1.0 equiv.) and pyrocatechol (66 mg, 0.6 mmol, 1.0 equiv.) in benzene/acetone (5:1, v/v, 25 mL), and the mixture was allowed to stir at room temperature (RT) for 48 h, then it was filtered. The organic phase was evaporated to afford a solid, which was purified by column chromatography with PE/EtOAc (4:1) to give **M1** as a while solid (51.9 mg, 30%).[10,11] **^{1}H NMR** (600 MHz, DMSO-d_6), δ: 6.98-6.77 (m, 7H), 4.88 (d, J = 11.4 Hz, 1H), 4.13-4.11 (m, 1H), 3.76 (s, 3H), 3.53 (d, J = 18 Hz, 1H), 3.33 (d, J = 17.4 Hz, 1H); **^{13}C NMR** (150 MHz, DMSO-d_6), δ: 148.05, 147.42, 144.15, 143.85, 128.07, 121.69, 121.41, 120.95, 117.30, 117.17, 115.76, 112.14, 78.46, 76.23, 60.67, 56.14.

*Dimeric model compound **M8***. Iodomethane (511 mg, 3.6 mmol, 3 equiv.) was added to a solution of **M1** (500 mg, 1.7 mmol, 1 equiv.) and K_2CO_3 (746.3 mg, 5.4 mmol, 3 equiv.) in acetone (25 mL), and was then stirred at 30 °C for 24 h. The organic phase was obtained by extraction with brine, drying with anhydrous $MgSO_4$. The solvent was removed via rotary evaporator and the mixture was purified by column chromatography with PE/EtOAc (5:1) to give **M8** as a white solid (477.5 mg, 93%). **^{1}H NMR** (600 MHz, $CDCl_3$), δ: 7.01-6.97 (m, 3H), 6.95-6.94 (m, 1H), 6.91-6.89 (m, 3H), 4.96 (d, J = 8.4 Hz, 1H); 4.06-4.04 (m, 1H), 3.90 (s, 6H), 3.80-3.77 (m, 1H), 3.56-3.52 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$), δ: 149.64, 149.40, 143.87, 143.23, 128.68, 121.64, 121.62, 120.13, 117.31, 117.00, 111.26, 110.08, 78.11, 76.22, 61.75, 55.98.



Ortho-iodophenol Styrene oxide **M4**, yield:90%

*Dimeric model compound **M4***. A Schlenk tube was charged with Cu_2O (22 mg, 0.2 mmol, 0.2 equiv.), 1,10-phenanthroline (57 mg, 0.3 mmol, 0.3 equiv.), Cs_2CO_3 (650 mg, 2.0 mmol, 2 equiv.), ortho-iodophenol (222 mg, 1.0 mmol, 1 equiv.), evacuated and backfilled with nitrogen. Styrene oxide (180 mg, 1.5 mmol, 1.5 equiv.) and DMF (2 mL) were successively added. The reaction tube was quickly sealed and the contents were stirred at 110 ºC for 48 h. Then the cooled reaction mixture was added wit H_2O and extracted with Et_2O. The combined organic layer was dried over $MgSO_4$. The product was further purified by column chromatography with PE/EtOAc (2:1) to give **M4** as a colorless oil (190.8 mg, 90%).[12] **^{1}H NMR** (600 MHz, $CDCl_3$), δ: 7.47-7.46 (m, 5H), 7.05-7.02 (m, 1H), 6.99-6.97 (m, 1H), 6.94-6.91 (m, 2H), 5.17 (dd, J = 2.4 Hz, 1H), 4.40 (dd, J = 2.4 Hz, 1H), 4.09 (dd, J = 9 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$), δ: 143.89, 143.05, 136.44, 128.77, 126.51, 121.57, 117.53, 117.11, 75.08, 69.34.

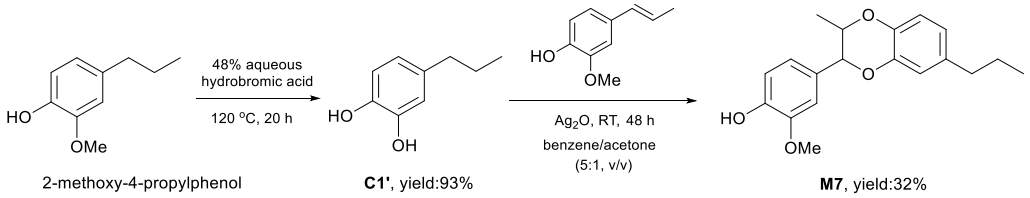


Pyrocatechol Isoeugenol **M5**, yield:35% **M6**, yield:95%

*Dimeric model compound **M5***. Silver oxide (278.1 mg, 1.2 mmol, 2 equiv.) was added to a solution of isoeugenol (100 mg, 0.6 mmol, 1 equiv.) and pyrocatechol (66.1 mg, 0.6 mmol, 1 equiv.) in benzene/acetone (5:1, v/v, 25 mL). The mixture was stirred for 48 h at RT, then it was filtered. The organic phase was evaporated to afford a solid, which was purified by column chromatography with PE/EtOAc (10:1) to give **M5** as a pale-yellow solid (57.1 mg, 35%). **^{1}H NMR** (600 MHz, $CDCl_3$), δ: 6.95-6.92 (m, 3H), 6.88-6.85 (m, 4H), 4.58 (d, J = 7.8 Hz, 1H), 4.13 (m, 1H), 3.91 (s, 3H), 1.18 (d, J = 6 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$), δ: 146.88, 146.26, 144.11, 143.53, 128.95, 121.49, 121.25, 121.02, 117.11, 116.91, 114.48, 109.42, 80.91, 74.12, 56.00, 17.28.

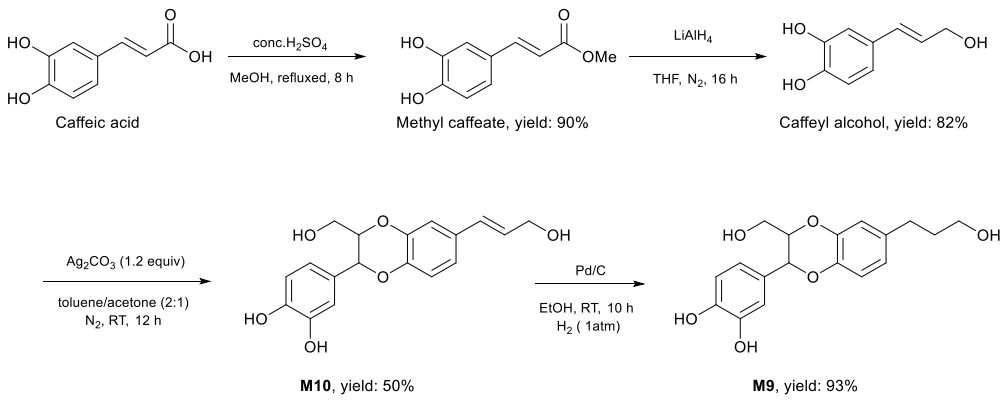
*Dimeric model compound **M6***. Iodomethane (510.9 mg, 3.6 mmol, 2 equiv.) was added to a mixture of **M5** (500 mg, 1.8 mmol, 1 equiv.) and K_2CO_3 (746.3 mg, 5.4 mmol, 3 equiv.) in acetone (25 mL). The mixture was stirred for 24 h at 30 ºC, then it was filtered. The organic phase was obtained by extraction with brine, drying with anhydrous $MgSO_4$. The solvent was removed via

rotary evaporator and the mixture was purified by column chromatography with PE/EtOAc (5:1) to give **M6** as a white solid (489.1 mg, 95%). **^{1}H NMR** (600 MHz, DMSO-d_6), δ: 6.97-6.88 (m, 5H), 6.84-6.81 (m, 2H), 4.69 (d, J = 12 HZ, 1H), 4.29 (m, 1H), 3.76 (s, 3H), 3.75 (s, 3H), 1.07 (d, J = 9.6 Hz, 3H); **^{13}C NMR** (150 MHz, DMSO-d_6), δ: 149.63, 149.31, 144.37, 143.71, 129.78, 121.52, 121.38, 120.80, 117.30, 117.11, 112.05, 111.63, 80.28, 73.70, 56.06, 55.97. 17.41.



*Molecular standards **C1'**.* The mixture of 2-methoxy-4-propylphenol (100 mg, 0.6 mmol, 1 equiv.) and hydrobromic acid (48% solution, 0.4 mL) was stirred at 120 °C for 20 h. After extraction with diethyl ether, the organic phase was washed with brine and dried over anhydrous $MgSO_4$. The solvent was removed via rotary evaporator and the product was purified by column chromatography with PE/EtOAc (2:1) to give **C1'** as a yellow oil (85.2 mg, 93%).

*Dimeric model compound **M7**.* Silver oxide (278.1 mg, 1.2 mmol, 2 equiv.) was added to a solution of isoeugenol (100 mg, 0.6 mmol, 1 equiv.) and **C1'** (91.2 mg, 0.6 mmol, 1 equiv.) in benzene/acetone (5:1, v/v, 25 mL). The mixture was stirred for 48 h at RT, then it was filtered. The organic phase was evaporated to afford a liquid, which was purified by column chromatography with PE/EtOAc (10:1) gave **M7** as a pale-yellow oil (60.3 mg, 32%). **^{1}H NMR** (600 MHz, $CDCl_3$), δ: 6.94-6.93 (m, 1H), 6.88-6.83 (m, 4H), 6.70-6.68 (m, 1H), 4.56 (d, J = 8.4 HZ, 1H), 4.10 (m, 1H), 3.91 (s, 3H), 2.51 (t, J = 7.8 Hz, 2H), 1.61-1.58 (m, 2H), 1.16 (d, J = 6.6 Hz, 3H), 0.94 (m, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$), δ:146.86, 146.21, 143.68, 141.37, 135.90, 129.11, 121.46, 121.02, 116.77, 116.45, 114.46, 109.43, 80.98, 74.04, 56.00, 37.33, 24.59, 17.30, 13.81.



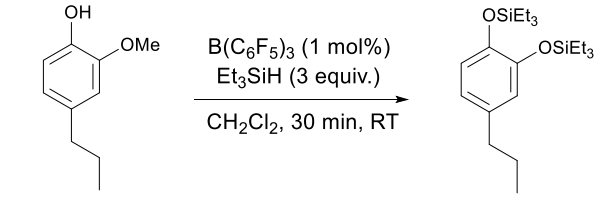
Methyl caffeate. A mixture containing caffeic acid (25 g) and *conc.* H_2SO_4 (1.3 mL) in MeOH (250 mL) was refluxed at 75 °C for 8 h. After the organic solvent was removed by rotary evaporator, the solid residue was extracted with EtOAc/water. Methyl caffeate was obtained the recrystallization of organic phase as a colorless solid (24 g, 90 %).

Caffeyl alcohol. Methyl caffeate (500 mg, 2.6 mmol) in anhydrous THF (10 mL) was added to a suspension of $LiAlH_4$ (296.4 mg, 7.8 mmol, 3.0 equiv) in anhydrous THF (30 mL) slowly at -78 °C under N_2, and the mixture was allowed to stir at RT overnight. After reaction, the mixture was quenched and acidified with HCl to pH = 2. THF was removed under low temperature by rotary evaporator and the remaining liquid was extracted with dichloromethane. The evaporation of dichloromethane and silica gel column chromatography with PE/EtOAc (1:1) to give caffeyl alcohol as a while solid (351 mg, 82%).

*Dimeric model compound **M10***. To a solution of caffeyl alcohol (1.0 g, 6.0 mmol) in anhydrous acetone/toluene (15 mL, 1:2, v/v) was added silver carbonate (2.0 g, 7.2 mmol, 1.2 equiv), and the mixture was stirred at RT for 12 h. After filtration, the liquid phase was concentrated and purified by column chromatography with PE/EtOAc (1:1) to give **M10** as a white solid (0.5 g, 50%).[4,13]

*Dimeric model compound **M9***. Compound **M10** (500 mg, 1.5 mmol), Pd/C (25 mg, 5 wt% on carbon)) and EtOH (30 mL) were added to a flask, and then the air was replaced by hydrogen (1atm). After the reaction mixture was stirred 10 h at RT, the mixture was filtered. The organic phase was dried over anhydrous $MgSO_4$ and evaporated under vacuum to give oily product, which was purified by column chromatography with PE/EtOAc (1:1) to give **M9** as white solid (467.8 mg, 93%).

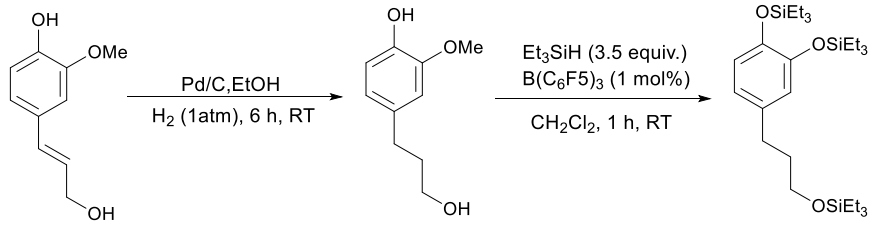
2.2 Synthesis of molecular standards



2-methoxy-4-propylphenol

C1, yield: 96%

*Molecular standards **C1***. A suspension of 2-methoxy-4-propylphenol (5.0 g, 30 mmol, 1.0 equiv.) and Et_3SiH (10.5 g, 90 mmol, 3 equiv.) in CH_2Cl_2 (20 mL) was stirred at RT. $B(C_6F_5)_3$ (153.6 mg, 0.3 mmol, 1 mol %) was added, and stirring was continued for 30 min. The organic phase was evaporated under vacuum to give oily product, which was purified by column chromatography with PE to give **C1** as colorless oil (10.9 g, 28.8 mmol, 96 %).[14] **^{1}H NMR** (600 MHz, $CDCl_3$), δ: 6.73 (d, J = 7.8 Hz, 1H), 6.65 (d, J = 1.8 Hz, 1H), 6.61 (dd, J = 2.4 Hz, 1H), 2.48 (t, J = 7.2 Hz, 2H), 1.61 (m, 2H), 1.01 (m, t = 3 Hz, 18H), 0.93(t, J = 7.2 Hz, 3H), 0.78(m, J = 3.6 Hz, 12H).



Coniferyl alcohol

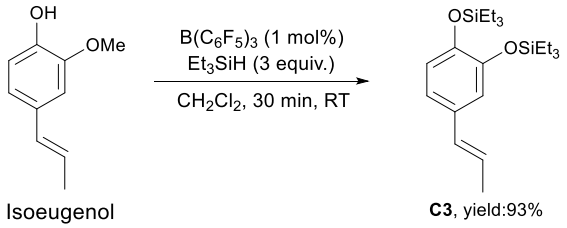
Dihydroconiferyl alcohol, yield: 95%

C2, yield: 61%

Dihydroconiferyl alcohol. The mixture containing coniferyl alcohol (1.0 g, 5.5 mmol), Pd/C (50 mg, 5 wt% on carbon) and EtOH (20 mL) was stirred under H_2 (1 atm) at RT for 6 h. After filtration, organic phase was evaporated under vacuum to give oily product, which was purified by column chromatography with PE/EtOAc (2:1) to afford dihydroconiferyl alcohol as a white solid (0.95 g, 95%).

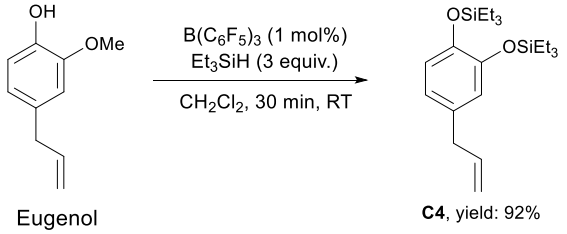
*Molecular standards **C2***. Compound **C2** was prepared using the same procedure with synthesis of compound **C1**. Starting from dihydroconiferyl alcohol (5.0 g, 27.4 mmol, 1 equiv.) and Et_3SiH (12.7 g, 115.5 mmol, 4 equiv.) in CH_2Cl_2 (20 mL) was stirred at RT. $B(C_6F_5)_3$ (140 mg, 0.27 mmol, 1 mol%) was added at RT, and stirring was continued for 30 min. The organic phase was evaporated under vacuum to give oily product, which was purified by column chromatography with PE to give **C2** as colorless oil (8.5 g, 61 %). **^{1}H NMR** (600 MHz, $CDCl_3$), δ: 6.72 (d, J = 8.4 Hz, 1H), 6.65 (d, J = 2.4 Hz, 1H), 6.61 (dd, J = 1.8 Hz, 1H), 3.62 (t, J = 6.6 Hz, 2H), 2.56 (t, J = 7.8 Hz, 2H), 1.82 (m,

2H), 1.00-0.95 (m, 27H), 0.77-0.72 (m, 12H), 0.62 (q, J = 7.8 Hz, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$), δ: 146.45, 144.67, 135.31, 121.19, 120.76, 120.20, 62.20, 34.55, 31.38, 6.80, 6.71, 5.15, 5.11, 4.48.



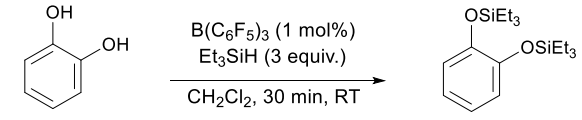
Isoeugenol — **C3**, yield:93%

*Molecular standards **C3***. A suspension of isoeugenol (5.0 g, 30 mmol, 1.0 equiv.) and Et_3SiH (10.5 g, 90 mmol, 3 equiv.) in CH_2Cl_2 (20 mL) was stirred. $B(C_6F_5)_3$ (153.8 mg, 0.3 mmol, 1 mol %) was added at RT, and stirring was continued for 30 min. The organic phase was evaporated under vacuum to give oily product, which was purified by column chromatography with PE to give **C3** as colorless oil (10.5 g, 93 %). **^{1}H NMR** (600 MHz, $CDCl_3$), δ: 6.82 (d, J = 1.8 Hz, 1H), 6.77 (dd, J = 2.4 Hz, 1H), 6.73 (d, J = 7.8 Hz, 1H), 6.28 (dd, J = 1.2 Hz, 1H), 6.06 (m, 1H), 1.85 (dd, J = 1.8 Hz, 3H), 0.99 (t, J = 7.8 Hz, 18 H), 0.76 (q, J = 8.4 Hz, 12H); **^{13}C NMR** (150 MHz, $CDCl_3$), δ: 146.77, 145.96, 131.70, 130.61, 123.46, 120.42, 119.15, 117.84, 18.37, 6.71, 6.69, 5.14, 5.11.



Eugenol — **C4**, yield: 92%

*Molecular standards **C4***. A suspension of eugenol (5.0 g, 30 mmol, 1.0 equiv.) and Et_3SiH (10.5 g, 95 mmol, 3 equiv.) in CH_2Cl_2 (20 mL) was stirred. $B(C_6F_5)_3$ (153.6 mg, 0.3 mmol, 1 mol %) was added at RT, and stirring was continued for 30 min. The organic phase was evaporated under vacuum to give oily product, which was purified by column chromatography with PE to give **C4** as colorless oil (10.4 g, 92 %). **^{1}H NMR** (600 MHz, $CDCl_3$), δ: 6.73 (d, J = 7.8Hz, 1H), 5.97 (d, J = 2.4 Hz, 1H), 6.65 (dd, J = 1.8 Hz, 1H), 5.97-5.90 (m, 1H), 5.04-5.01 (m, 2H), 3.26 (d, J = 6.6 Hz, 2H), 0.99 (t, J = 8.4 Hz, 18H), 0.76 (q, J = 7.8 Hz, 12H); **^{13}C NMR** (150 MHz, $CDCl_3$), δ: 146.59, 144.99, 137.86, 133.09, 121.32, 120.96, 120.27, 115.32, 39.48, 6.70, 5.14, 5.11.

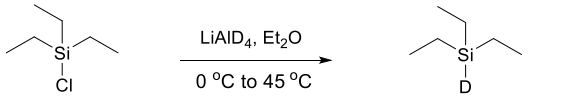


Pyrocatechol

C5, yield:96%

*Molecular standards **C5***. A suspension of catechol (5.0 g, 45 mmol, 1.0 equiv.) and Et_3SiH (15.8 g, 135 mmol, 3 equiv.) in CH_2Cl_2 (40 mL) was stirred. $B(C_6F_5)_3$ (230 mg, 0.45 mmol, 1 mol %) in CH_2Cl_2 (20 mL) was added at RT, and stirring was continued for 30 min. The organic phase was evaporated under vacuum to give oily product, which was purified by column chromatography with PE to give **C5** as colorless oil (14.6 g, 96 %). **^{1}H NMR** (600 MHz, $CDCl_3$), δ: 6.84-6.79 (m, 4H), 1.01 (t, J = 7.8 Hz, 18H), 0.78 (q, J = 7.8 Hz, 12H); **^{13}C NMR** (150 MHz, $CDCl_3$), δ: 146.92, 121.44, 120.65, 6.69, 5.12.

2.3 Preparation of deuterium-labeled Et_3SiD



Chlorotriethylsilane

Deuterated triethylsilane
yield: 58%

Deuterated triethylsilane. To a suspension of $LiAlD_4$ (1.9 g, 45.7 mmol, 0.8 equiv.) in anhydrous Et_2O (20 mL), a solution of chlorotriethylsilane (9.6 mL, 57.1 mmol, 1.0 equiv.) in dry Et_2O (20 mL) was added dropwise at 0 °C. After complete addition, the solution was heated to reflux for 18 h. The reaction mixture was quenched and acidified with HCl to pH = 2 at 0 °C. The organic phase was separated, and the aqueous layer was extrated with Et_2O (3 × 20 mL). The combined organic phases were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. Purification of the residue by vacuum distillation (360 mbar/100 °C) afforded deuterated triethylsilane as a colorless liquid (3.8 g, 58%).[15]

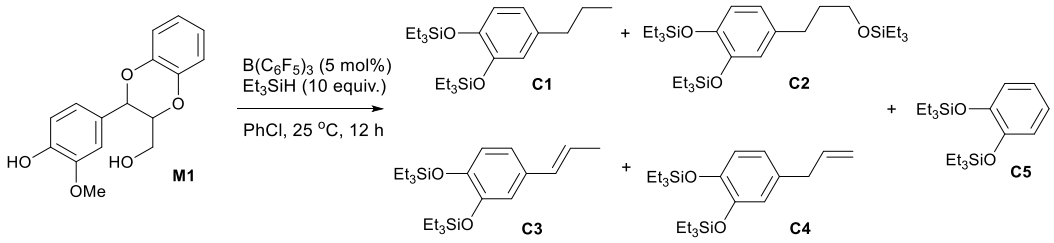
3. Organoborane-catalysed reductive depolymerisation of benzodioxane mimics

In a typical procedure, C-lignin model compound (0.1 mmol) and chlorobenzene (1 mL) were placed into a glass vial, followed by addition of a mixture of Et_3SiH (1 mmol) and $B(C_6F_5)_3$ (5 mol%) in chlorobenzene (1 mL). The reaction mixture was stirred for 12 h at 25 °C under N_2 (1 atm). Following the completion of the reaction, the resulted mixture was analyzed on GC and GC/MS after filtration with a PTFE filter (0.45 μm). The identification and quantification of products were assessed on GC and GC/MS by comparison with corresponding authentic samples synthesized independently.

For the reusability experiment: after the completion of the first reaction (monitored by thin-layer chromatography), an aliquot (*ca.* 50 μL) was collected for analysis. To the remained reaction mixture, **M1** (0.1 mmol) and Et_3SiH (1 mmol) were added. The mixture was then stirred at 25 °C for 12 h for the next run. The recycling experiments were repeated for 4 times. The yields and selectivity of each run were calculated based on the increment of catechol products and the newly added **M1**.

$$\text{Catechols yield (\%)} = \frac{\text{the increment of catechol products (mol)}}{\text{the newly added } \mathbf{M1} \text{ (mol)}} \times 100$$

Table S1 Organoborane-catalysed reductive depolymerisation of **M1** into silylated monocatechols under various conditions.



Entry	Conditions	Products yields (mol%)						
		C1	**C2**	**C3**	**C4**	**C5**	**C1-C4**	**Sel. to C2**
1	PhCl[a]	32	53	5	2	88	92	58
2	2.5 mol%[b]	6	43	5	1	53	55	78
3	6 h[c]	9	37	2	1	45	49	75
6	Mercury[d]	31	52	6	2	89	91	57
7	No $B(C_6F_5)_3$[e]	-	-	-	-	-	-	-
8	No Et_3SiH[f]	-	-	-	-	-	-	-
9	$B(C_6H_5)_3$[g]	-	-	-	-	-	-	-
10	2nd[h]	32	51	2	1	83	86	59
11	3rd[h]	31	50	2	2	82	85	59
12	4th[h]	29	49	2	2	80	82	60
13	5th[h]	29	48	2	1	78	80	60

[a] Reaction condition: **M1** (0.1 mmol), $B(C_6F_5)_3$ (5 mol%), Et_3SiH (1 mmol), PhCl (2 mL), 25 °C, 12 h, N_2 (1 atm);

[b] The amount of 5 mol% $B(C_6F_5)_3$ was reduced from 5 mol% to 2.5 mol%;

[c] The reaction time was reduced from 12 h to 6 h;

[d] Mercury was added to the reaction system;

[e&f] No catalyst and Et_3SiH were added to the reaction system, respectively;

[g] The $B(C_6F_5)_3$ was replaced by $B(C_6H_5)_3$;

[h] Reusability of $B(C_6F_5)_3$ condition: **M1** (0.1 mmol) and Et_3SiH (1 mmol) were constantly added in the reaction mixture every other 12 h under N_2 (1 atm) at 25 °C.

Note: - represented the corresponding compounds were not detected.

Table S2 Organoborane-catalysed reductive depolymerisation of **M1** into corresponding silylated monocatechols under various hydrogen sources.[a]

Entry	Hydrogen source	Products yields (mol%)				
		C1''	**C2''**	**C5''**	**C1''+C2''**	**Sel. to C1''**
1	Ph_3SiH	3	1	4	4	75
2	$PhMeSiH_2$	39	2	40	41	95
3	$PhMe_2SiH$	29	1	28	30	96
4	$PhSiH_3$	21	1	21	22	95
5	PMHS	7	5	11	12	58
6	H_2 [b]	-	-	-	-	-
7	Hydrazine	-	-	-	-	-

[a] Reaction condition: **M1** (0.1 mmol), $B(C_6F_5)_3$ (5 mol%), hydrosilanes (1 mmol), PhCl (2 mL), 25 ^oC, 12 h, N_2 (1 atm);

[b&c] The hydrosilanes was replaced by H_2 (10 MPa) and hydrazine hydrate (1 mmol), respectively;

- represented the corresponding compounds were not detected.

Note 1. After reductive depolymerisation of **M1**, the as-obtained mixture of oily product was treated with *n*-Bu_4NF (80 mg in THF), and the solution was stirred for 1 h at RT. The mixture was eluted with PE/EtOAc (2:1) over column chromatography to remove other biopolymers. Evaporation of solvents and being treated with BSTFA (170 μL) at 65 °C for 1 h afforded trimethylsilylated products, which was then analyzed on GC-MS and GC.

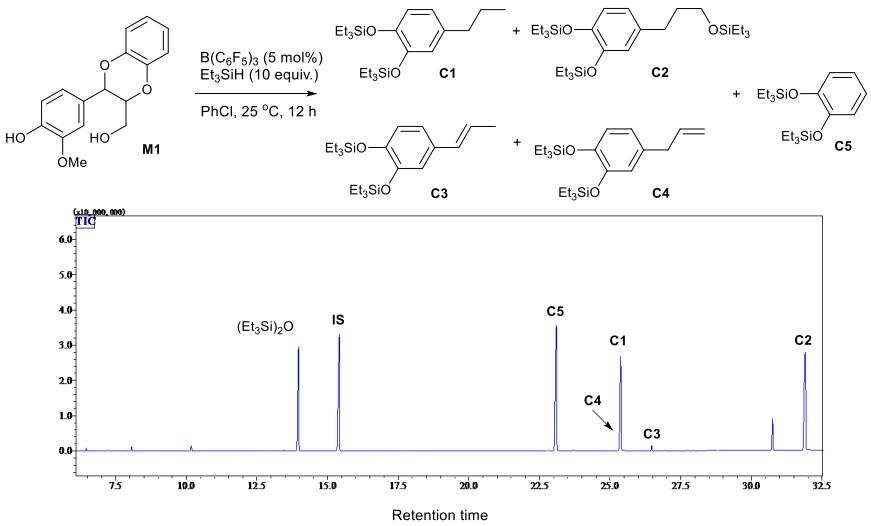


Figure S1. GC spectrum of the silylated monocatechols from organoborane-catalysed reductive depolymerisation of **M1**.

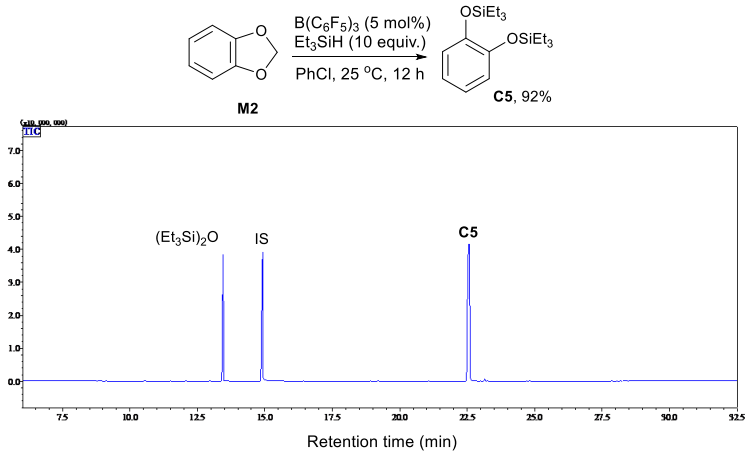


Figure S2. GC spectrum of the silylated monocatechols from organoborane-catalysed reductive depolymerisation of **M2**.

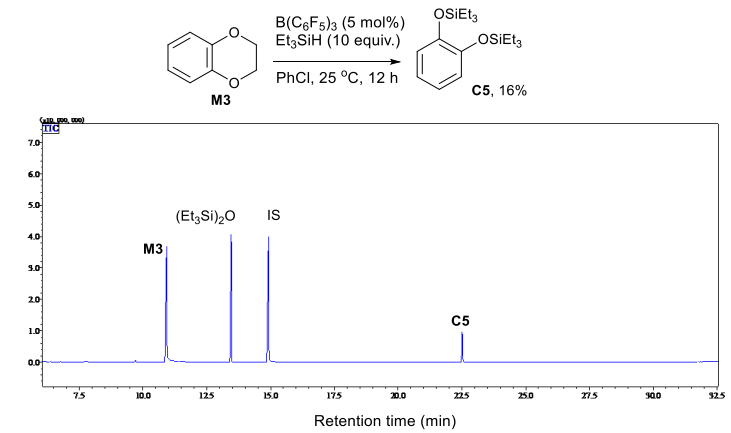


Figure S3. GC spectrum of the silylated monocatechols from organoborane-catalysed reductive depolymerisation of **M3**.

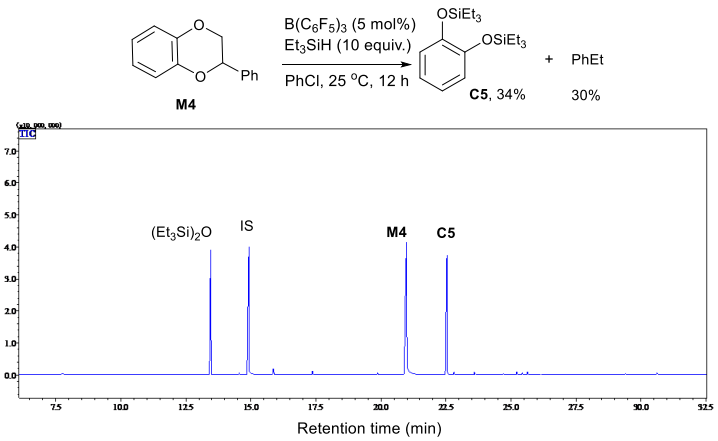


Figure S4. GC spectrum of the silylated monocatechols from organoborane-catalysed reductive depolymerisation of **M4**.

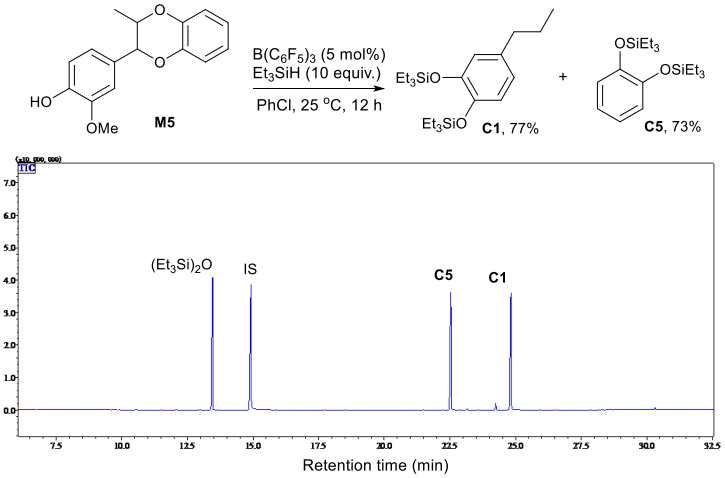


Figure S5. GC spectrum of the silylated monocatechols from organoborane-catalysed reductive depolymerisation of **M5**.

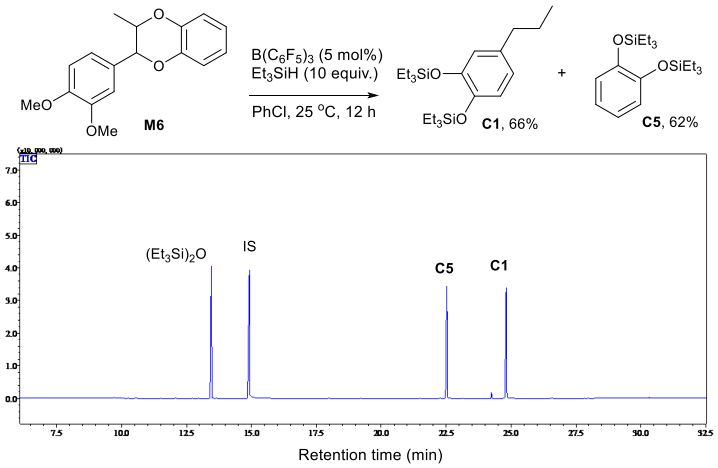


Figure S6. GC spectrum of the silylated monocatechols from organoborane-catalysed reductive depolymerisation of **M6**.

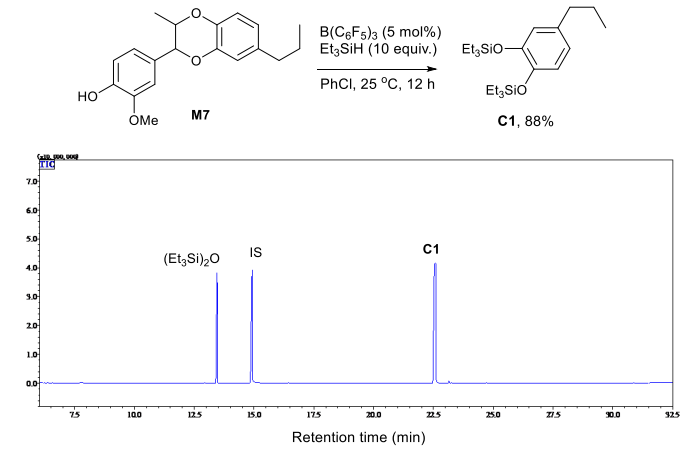


Figure S7. GC spectrum of the silylated monocatechols from organoborane-catalysed reductive depolymerisation of **M7**.

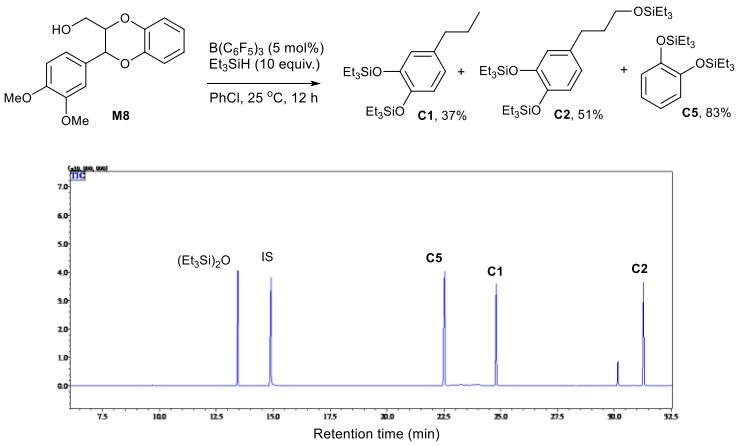


Figure S8. GC spectrum of the silylated monocatechols from organoborane-catalysed reductive depolymerisation of **M8**.

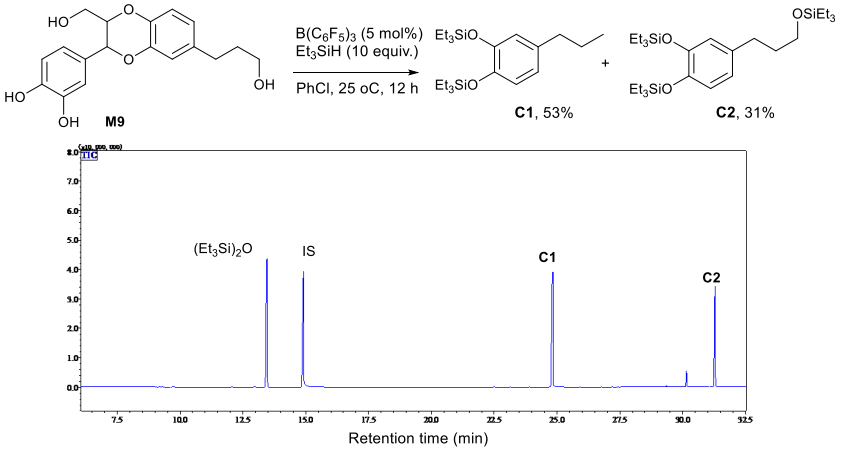


Figure S9. GC spectrum of the silylated monocatechols from organoborane-catalysed reductive depolymerisation of **M9**.

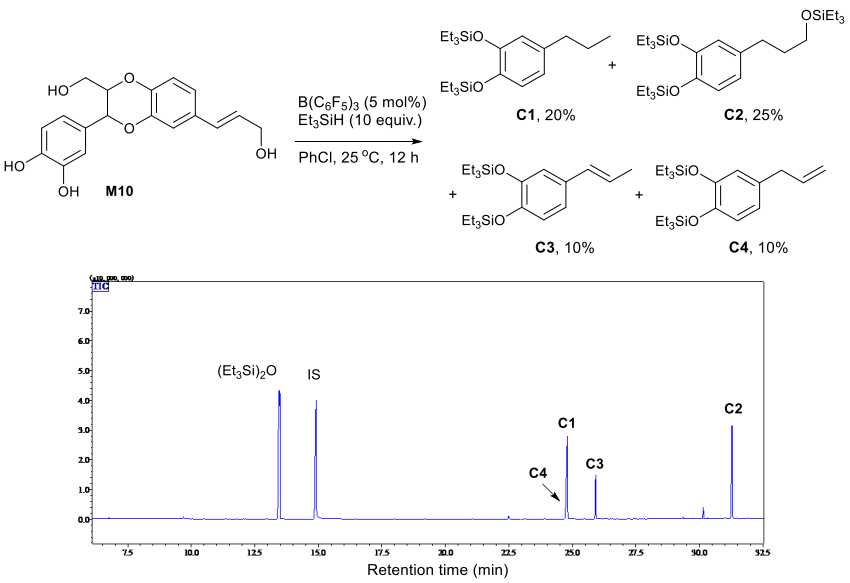


Figure S10. GC spectrum of the silylated monocatechols from organoborane-catalysed reductive depolymerisation of **M10**.

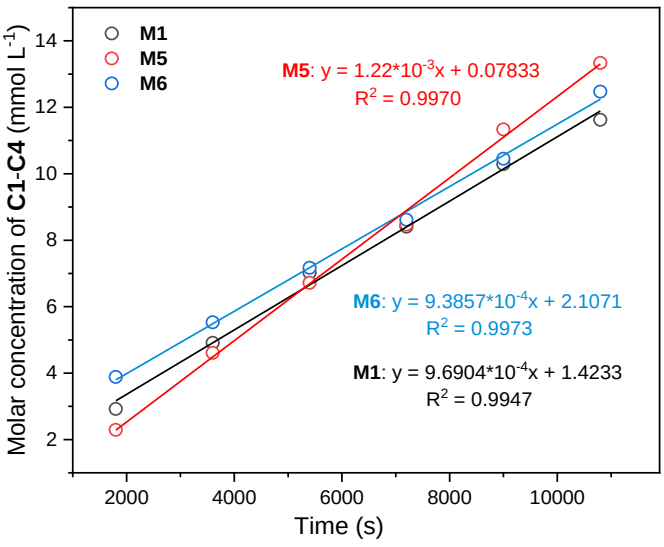


Figure S11. The initial rates of depolymerisation of **M1**, **M5**, and **M6** over $B(C_6F_5)_3/Et_3SiH$ into silylated monocatechols. Reaction condition: substrate (1 mmol), $B(C_6F_5)_3$ (5 mol%), Et_3SiH (10 mmol), PhCl (20 mL), 25 °C, N_2 (1 atm).

Table S3 The initial rates of depolymerisation of **M1**, **M5**, and **M6** over $B(C_6F_5)_3/Et_3SiH$ into silylated monocatechols.

Entry	Time (s)	The molar concentration of products (mmol L^{-1})					
		C1	**C2**	**C3**	**C4**	**C5**	**C1+C2+C3+C4**
M1	1800	0.515	1.89	0.31	0.205	2.83	2.92
	3600	0.61	3.195	0.91	0.195	4.785	4.91
	5400	1.205	4.71	0.89	0.215	7.005	7.02
	7200	1.69	5.795	0.755	0.165	8.495	8.405
	9000	2.36	6.925	0.76	0.245	10.305	10.29
	10800	3.09	7.645	0.63	0.26	11.3	11.625
M5	1800	2.29				2.005	2.29
	3600	4.61				4.26	4.61
	5400	6.72				6.465	6.72
	7200	8.47				8.22	8.47
	9000	11.335				11.34	11.335
	10800	13.335				12.005	13.335
M6	1800	3.885				3.56	3.885
	3600	5.53				5.555	5.53
	5400	7.17				6.97	7.17
	7200	8.615				8.835	8.615
	9000	10.45				9.955	10.45
	10800	12.47				12.31	12.47

Reaction condition: substrate (1 mmol), $B(C_6F_5)_3$ (5 mol%), Et_3SiH (10 mmol), PhCl (20 mL), 25 ^oC, N_2 (1 atm).

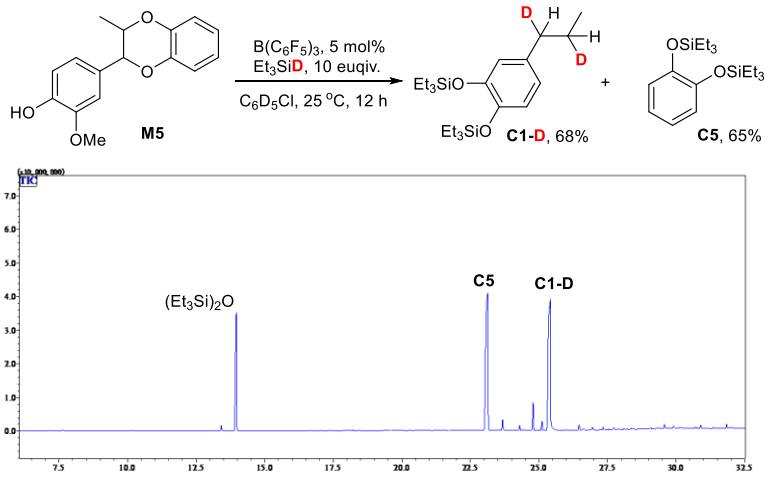


Figure S12. GC spectrum a of the deuterium silylated monocatechols from organoborane-catalysed reductive depolymerisation of **M5**.

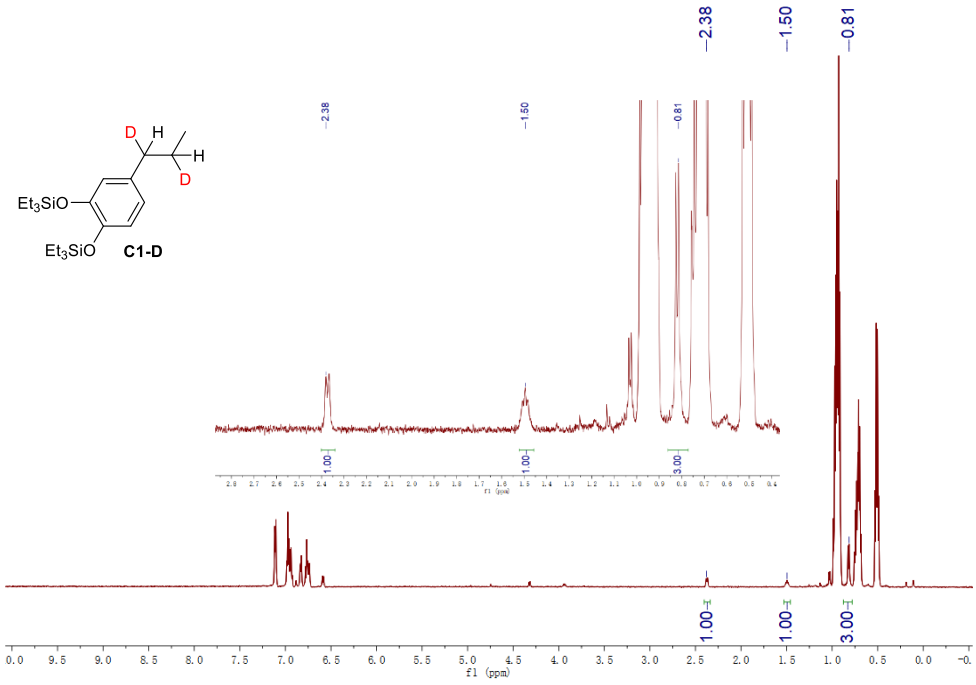


Figure S13. ^{1}**H NMR** spectrum of the as-formed **C1-D** (C_6D_5Cl).

4. DFT calculations

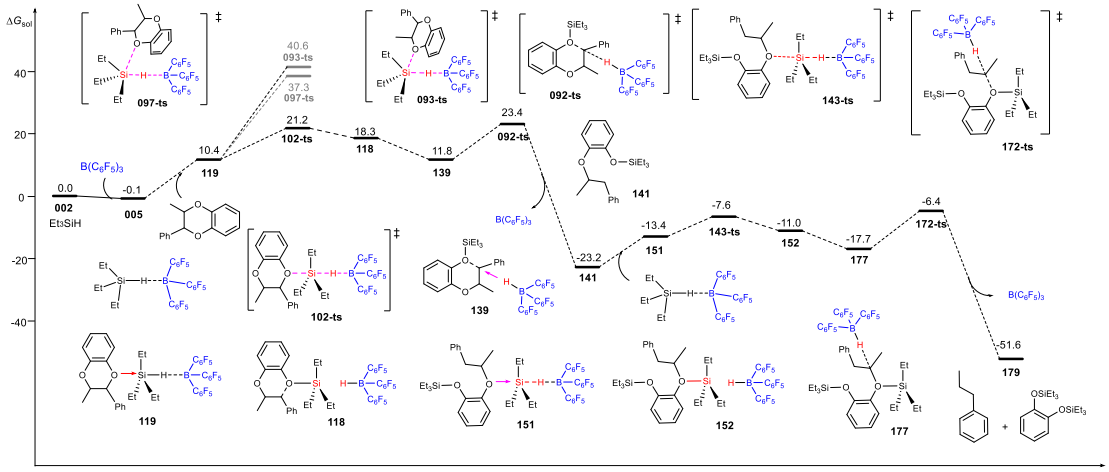


Figure S14. Energy profile of organoborane-catalysed reductive depolymerisation of benzodioxane model compounds.

Note 2. Optimized Coordinates Information. Optimized Cartesian coordinates and their corresponding single-point energies (*E*(SCRF), a.u.) calculated at the M06-2X/6-311+G(d, p) (SMD, PhCl)//M06-2X/6-31G (d) level as well as the imaginary frequency (IF, cm^{-1}) of transition states. The detailed data see below.

5. Depolymerising C-lignin biopolymer into catechols

5.1 Structural characterization of castor DL

Isolation of castor DL sample. Castor **DL** sample was prepared according to our previous reported protocol.[16] In a typical procedure, concentrated HCl (300 μL) was added to the suspension of castor seed coats (20~60 mesh, 20 g) in dioxane (200 mL), where [HCl] was estimated as 18 mmol L^{-1}. The mixture was heated at 90 °C under N_2 for 5 h, and solid residue was removed by centrifugation. The liquid phase was concentrated through evaporation to afford a thick solution, which was acidified to pH = 2.0 with 6 M HCl solution. The as-formed precipitate was collected by centrifugation and freeze-drying to give castor **DL** (2.5 g). The detailed structural characterization of castor **DL** were shown in Figure S15.

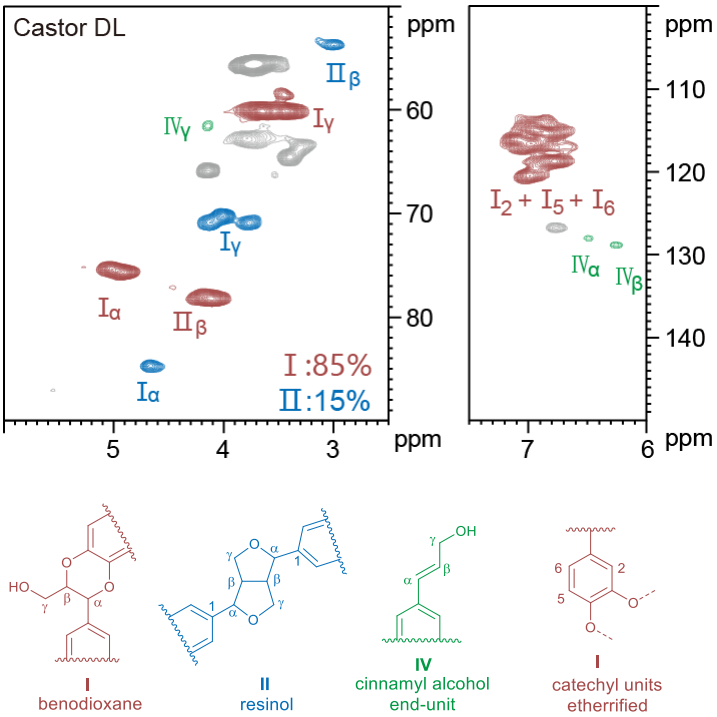


Figure S15. 2D NMR spectrum of castor **DL** (DMSO-d_6), and corresponding structural distributions of C-lignin.

Table S4. Quantitative ^{13}C NMR analysis of C-lignin content in the castor **DL**.

C_{IS} (μmol mL^{-1})	43.33
A_{IS}	1
$A_{C\beta}$	2.74
$C_{C\beta}$ (μmol mL^{-1})	356.40
ρC-lignin (mg mL^{-1})	120
Y_{CA} (μmol mL^{-1})	2.97
M_{WCA} (mg mmol^{-1})	166.18
$W_{C\text{-lignin}}$	49%

$$C_{C\beta} = \frac{C_{IS} \times 3}{A_{IS}} \, x \, A_{c\beta} \quad (1)$$

$$Y_{CA} = \frac{C_{c\beta}}{\rho \, AlCl_3 lignin} \quad (2)$$

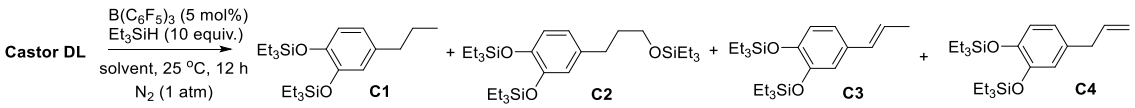
$$W_{C-\text{lignin}} = Y_{CA} \, x \, M_{WCA} \, x \, 100\% \quad (3)$$

C_{IS} (mmol mL^{-1}) is the molar concentration of internal standard (IS, 1,3,5-trioxane); A_{IS} is the peak integral of IS in the quantitative ^{13}C NMR spectrum; $A_{C\beta}$ is the peak integral of C_β in the quantitative ^{13}C NMR spectrum; $C_{C\beta}$ (mmol mL^{-1}) is the molar concentration of caffeyl alcohol (CA) unit in the **DL** sample; ρC-lignin (mg mL^{-1}) is the mass concentration of **DL** sample; Y_{CA} (mmol mg^{-1}) is the mole amount of caffeyl alcohol (CA) per mg of **DL** sample; M_{wCA} (mg mmol^{-1}) is the molecular weight of caffeyl alcohol (CA); W(C-lignin) is the weight percentage of C-lignin in **DL**.

5.2 Organoborane-catalysed reductive depolymerisation of castor DL

Typically, to a suspension of castor **DL** (300 mg, 0.9 mmol caffeyl alcohol units) in 1,2-$C_6H_4Cl_2$ (1 mL), a mixture of Et_3SiH (9 mmol) and $B(C_6F_5)_3$ (5 mol%) was added at 25 °C under N_2. A clear and brown homogeneous solution was formed in 5 min, which was then stirred at 25 °C for a desired time. The as-resulted mixture was analyzed on GC and GC/MS after filtration with a PTFE filter (0.45 μm). To isolate the catechol derivatives from C-lignin depolymerisation, the reaction mixture was treated with *n*-Bu_4NF (650 mg, 2.5 mmol) at room temperature for 1 h to afford catechol compounds, which was then purified over column chromatography with PE/EtOAc (2:1) to result in propylcatechol **C1'** as a colourless oil (isolated yield: 65 mol%, based on the mole of caffeyl alcohol in castor **DL**).

Table S5. Organoborane-catalysed reductive depolymerisation of castor **DL** with different solvents.



Entry	Solvents	Products yield (mol%)					
		C1	**C2**	**C3**	**C4**	**C1-**	**Sel. to C1**
1	PhCl	30	9	6	2	47	64
2	PhMe	25	6	4	1	36	69
3	Benzene	22	4	3	2	31	71
4	1,1,2,2-$C_2H_2Cl_4$	22	2	2	3	29	76
5	1,2-$C_2H_4Cl_2$	28	5	4	4	37	76
6	CH_2Cl_2	15	7	3	5	30	50
7	1,2-$C_6H_4F_2$	58	8	9	2	77	75
8	1,2-$C_6H_4Cl_2$	71	7	8	2	88	81

Reaction condition: castor **DL** (30 mg, 0.09 mmol caffeyl alcohol units), $B(C_6F_5)_3$ (10 mol%), Et_3SiH (0.9 mmol, 10 equiv.), solvents (2 mL), 25 °C, 12 h, N_2 (1 atm).

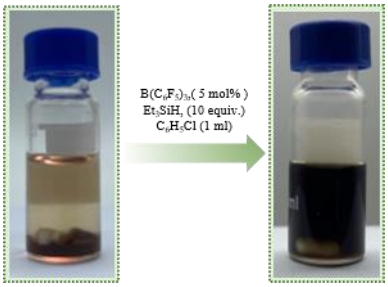
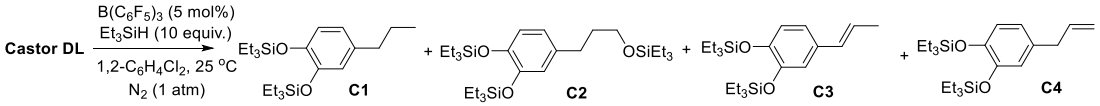


Figure S16. The comparison before and after the addition of Et_3SiH and $B(C_6F_5)_3$ in C_6H_5Cl to castor **DL**. After 5 min, the suspension of reaction mixture turned brown homogeneous phase.

Table S6. Organoborane-catalysed reductive depolymerisation of castor **DL** with different times.



Entry	Time (h)	Products yield (mol%)					
		C1	**C2**	**C3**	**C4**	**C1-C4**	**Sel. to C1**
1	8	25	6	3	2	36	69
2	12	39	5	3	7	54	72
3	24	52	8	1	8	69	75
4	36	63	8	1	6	78	81
5	48	77	3	1	4	85	91

Reaction condition: castor **DL** (300 mg, 0.9 mmol caffeyl alcohol units), $B(C_6F_5)_3$ (5 mol%), Et_3SiH (9 mmol, 10 equiv.), 1,2-$C_6H_4Cl_2$ (1 mL), 25 °C, N_2 (1 atm).

Note 3. To isolate catechol compound derived from the C-lignin depolymerisation (300 mg), the as-resulted lignin oil was initially eluted with petroleum ether over silica gel column chromatography to remove the 1,2-$C_6H_4Cl_2$ and other biopolymers. Evaporation of petroleum ether gave a crude product, which was then dissolved in THF (5 mL). This solution was treated with n-Bu_4NF (650 mg, 2.5 mmol) at room temperature for 1 hour. After the removal of volatiles under vacuum, purification over column chromatography with PE/EtOAc (2:1) afforded propylcatechol **C1'** as a colorless oil (isolated yield: 65 mol%, based on the mole of caffeyl alcohol in castor **DL**).

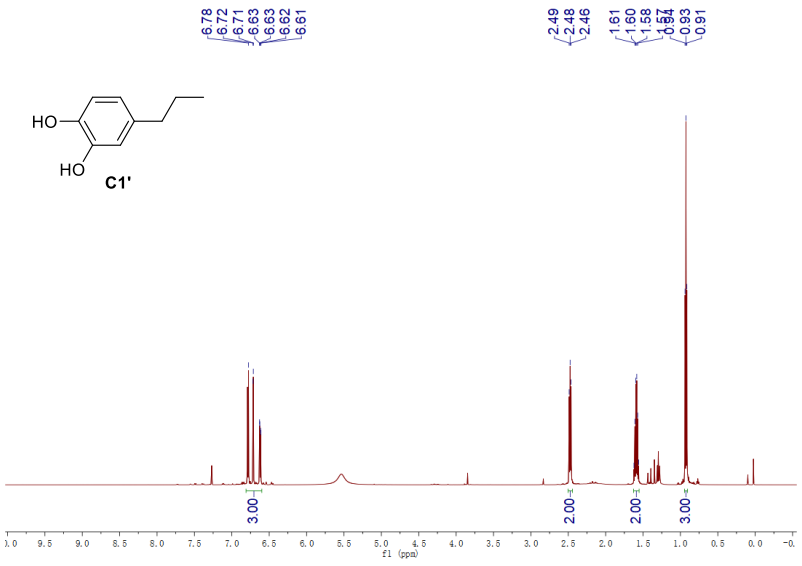
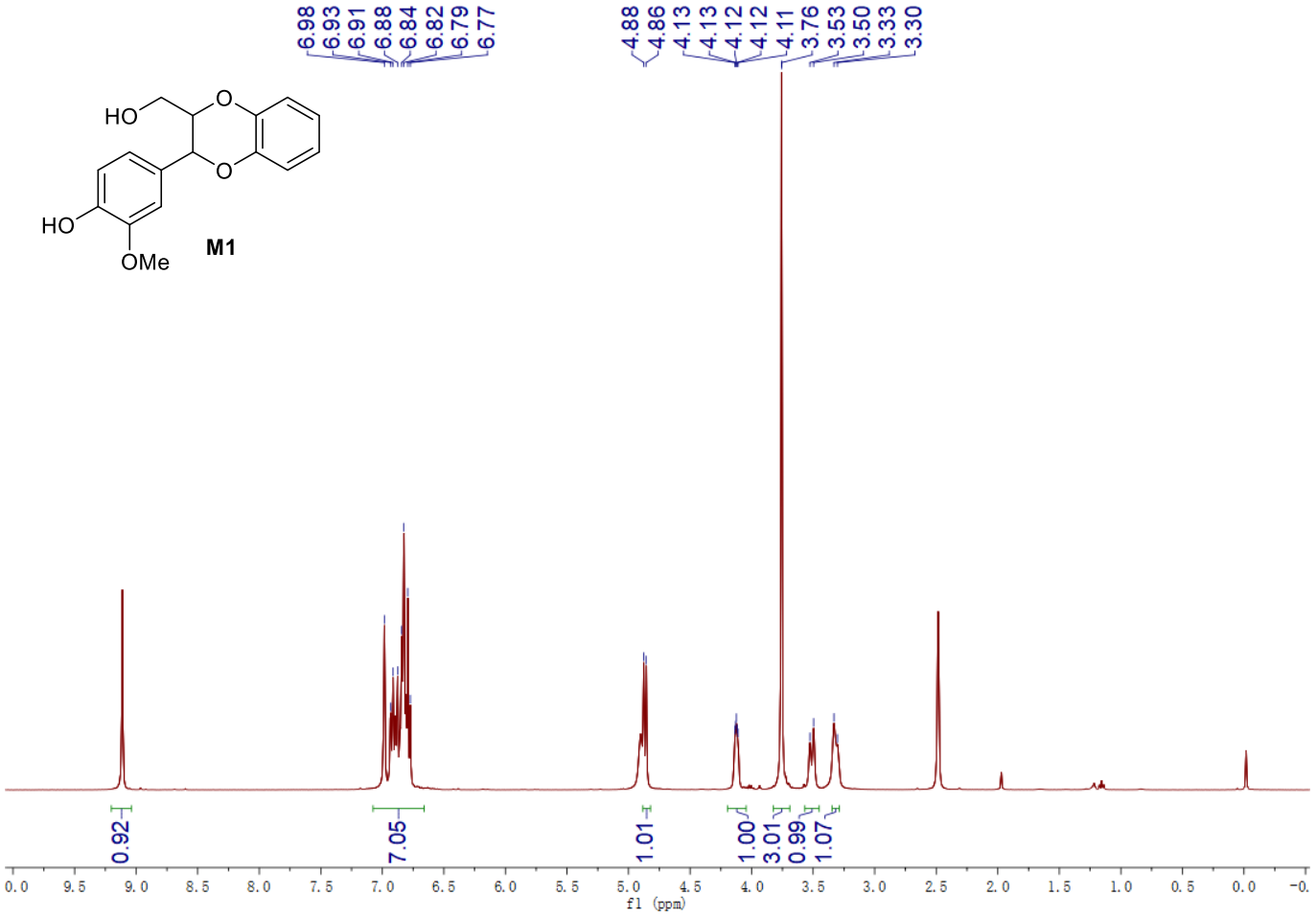


Figure S17. **^{1}H NMR** spectra of isolated **C1'** from C-lignin depolymerisation ($CDCl_3$).

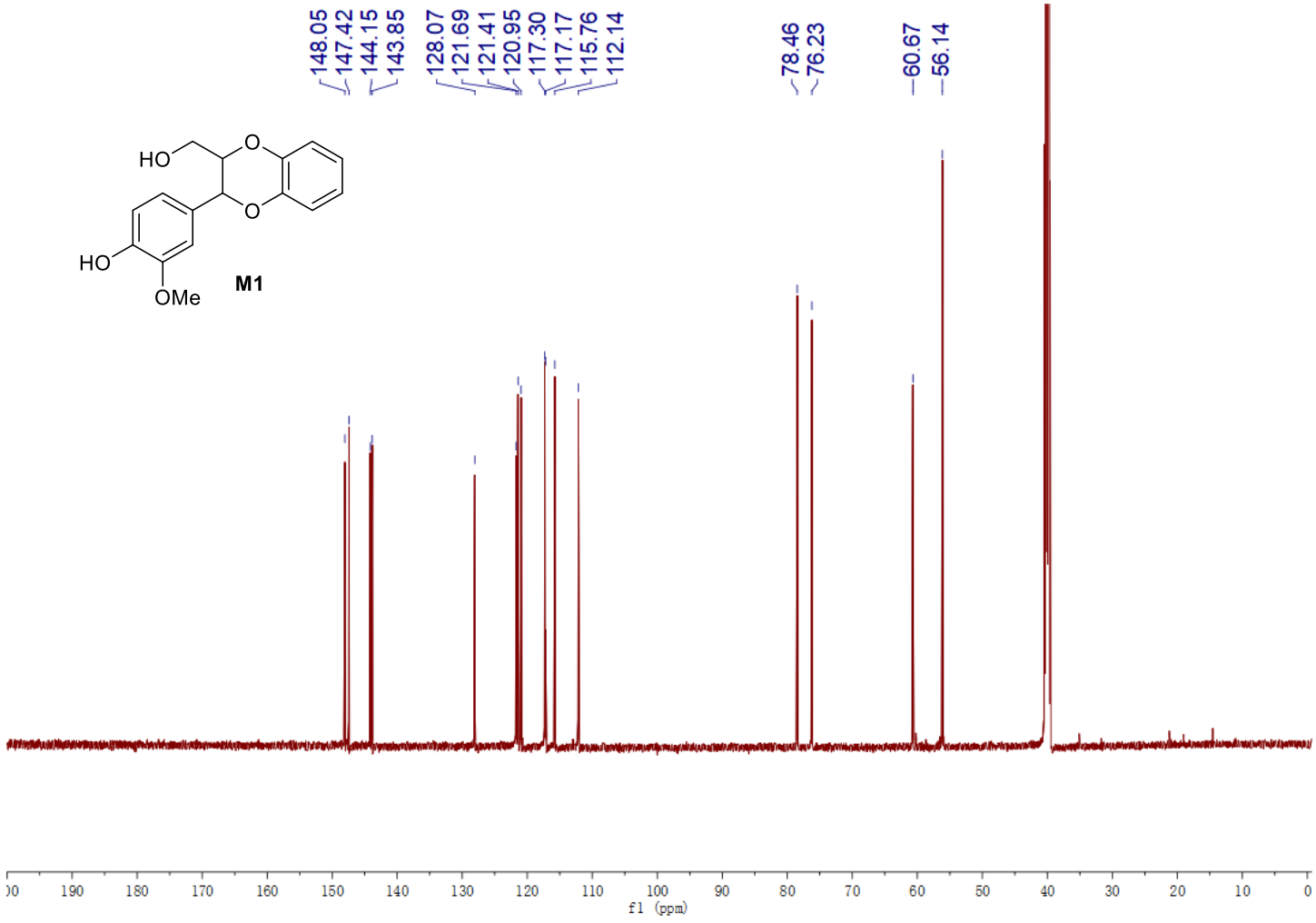
Table S7. NMR data for the signal assignments in lignin oily products in 1,2-$C_6D_4Cl_2$.

Lable	δ_C/δ_H (ppm)	Assignment
I_α	75.4/4.8	C_α-H_α in benzodioxane substructures (I)
I_β	77.8/4.1	C_β-H_β inbenzodioxane substructures (I)
I_γ	59.9/3.3-3.6	C_γ-H_γ in benzodioxane substructures (I)
II_α	84.5/4.62	C_α-H_α in β-β resinol substructures (II)
II_β	53.4/3.04	C_β-H_β in β-β resinol substructures (II)
II_γ	70.7/3.74-4.09	C_γ-H_γ in β-β resinol substructures (II)
IV_α	127.9/6.42	C_α-H_α in cinnamyl alcohol end-units (IV)
IV_β	128.7/6.20	C_β-H_β in cinnamyl alcohol end-units (IV)
IV_γ	61.4/4.10	C_γ-H_γ in cinnamyl alcohol end-units (IV)
$C1_\alpha$	37.9/2.5	C_α-H_α in **C1**
$C1_\beta$	24.1/1.6	C_β-H_β in **C1**
$C1_\gamma$	13.6/0.9	C_γ-H_γ in **C1**
$C1_2$	120.0/6.8	C_2-H_2 in **C1**
$C1_{5/6}$	121.0-122.0/6.54-6.63	$C_{5/6}$-$H_{5/6}$ in **C1**

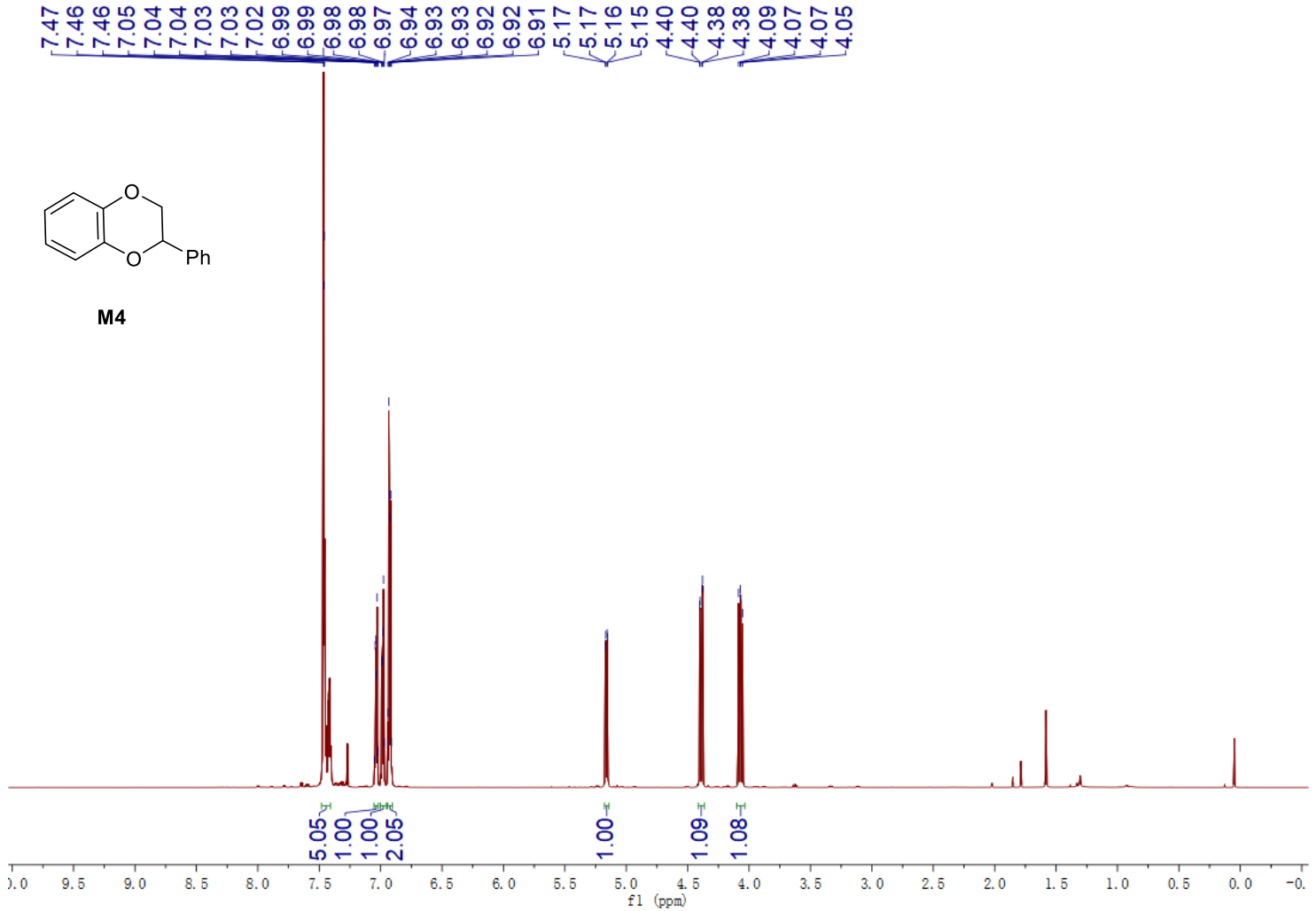
Supplementary Data Files: NMR spectra



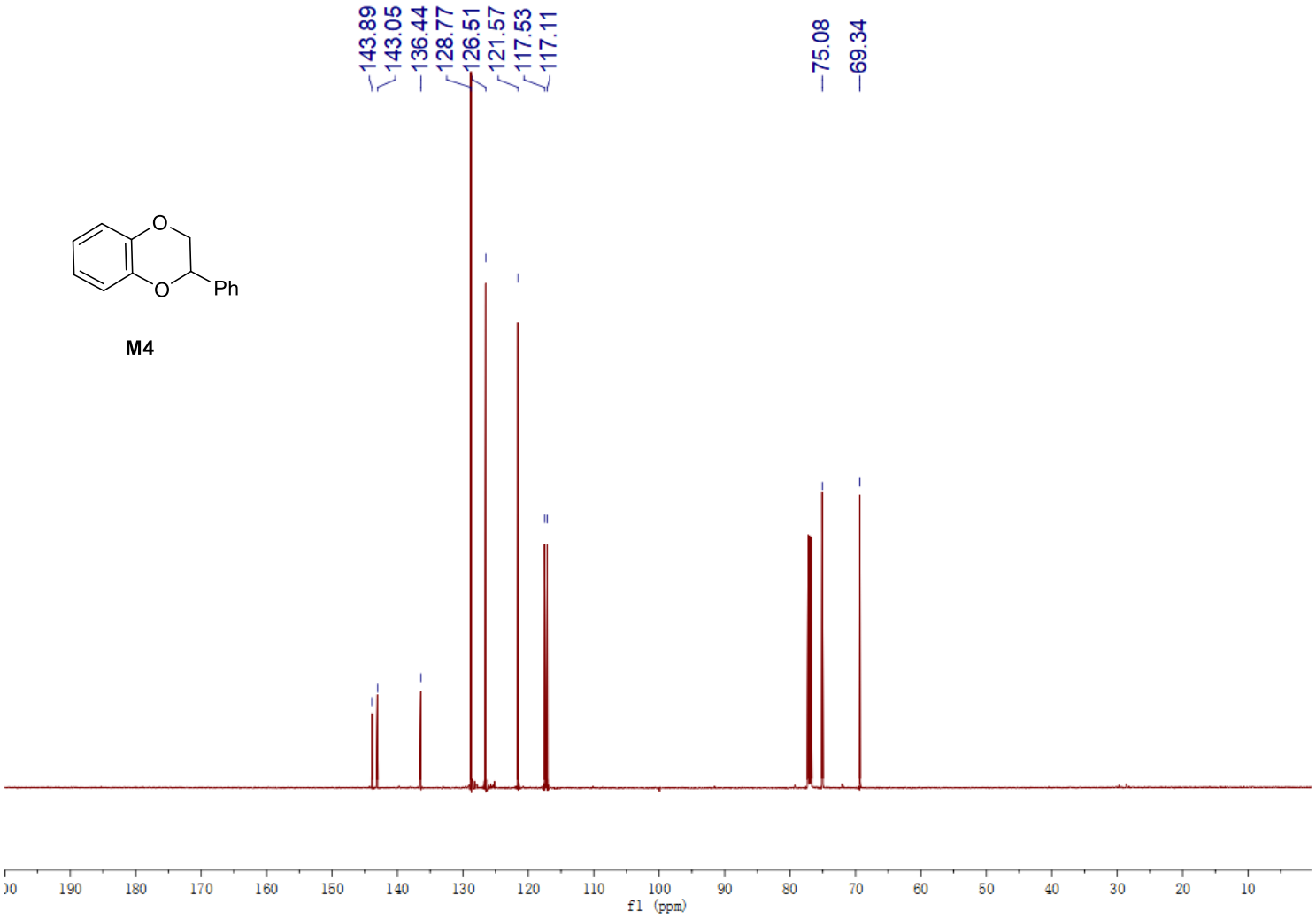
^{1}H NMR spectrum of **M1** (DMSO-d_6).



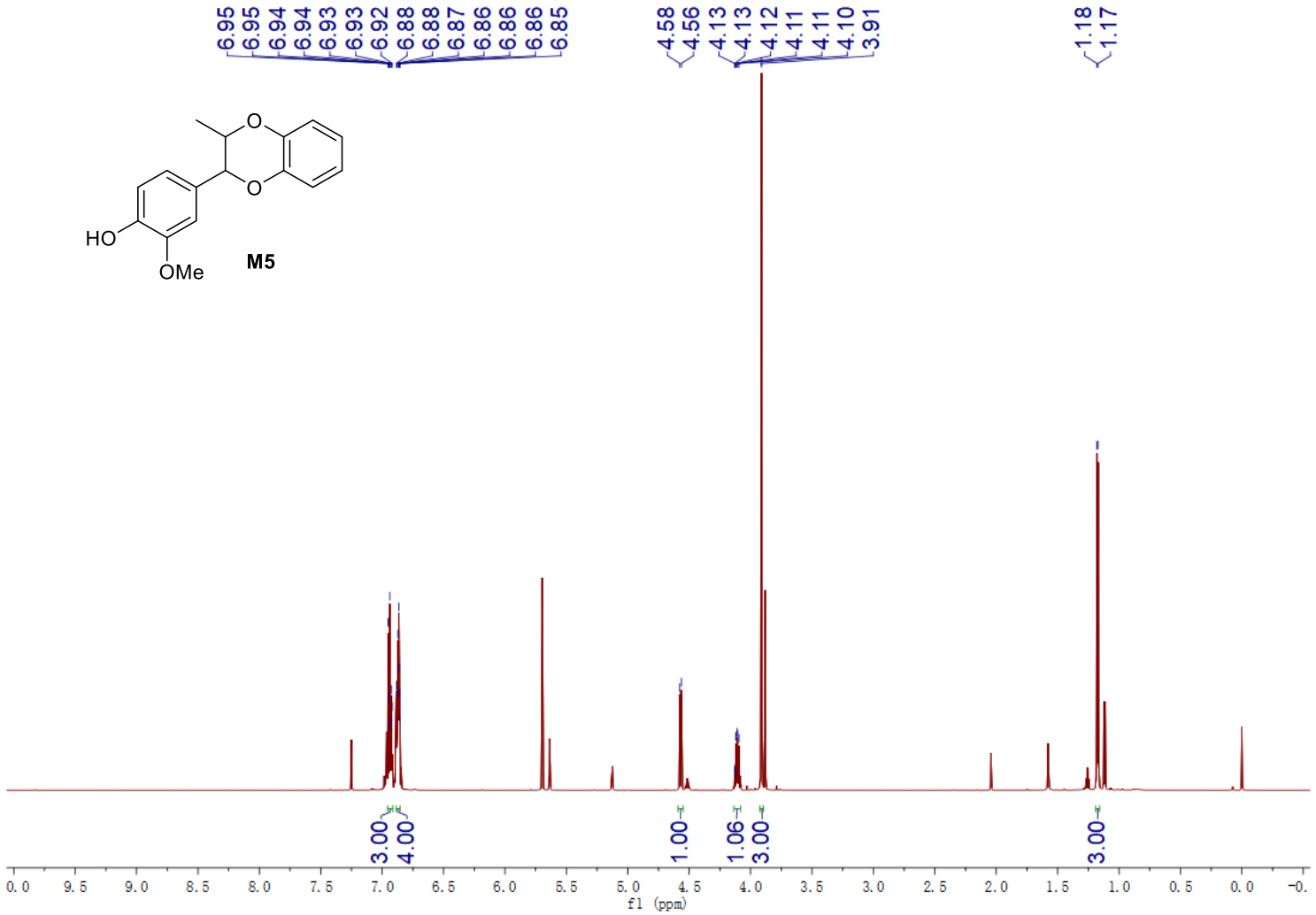
^{13}C NMR spectrum of **M1** (DMSO-d_6).



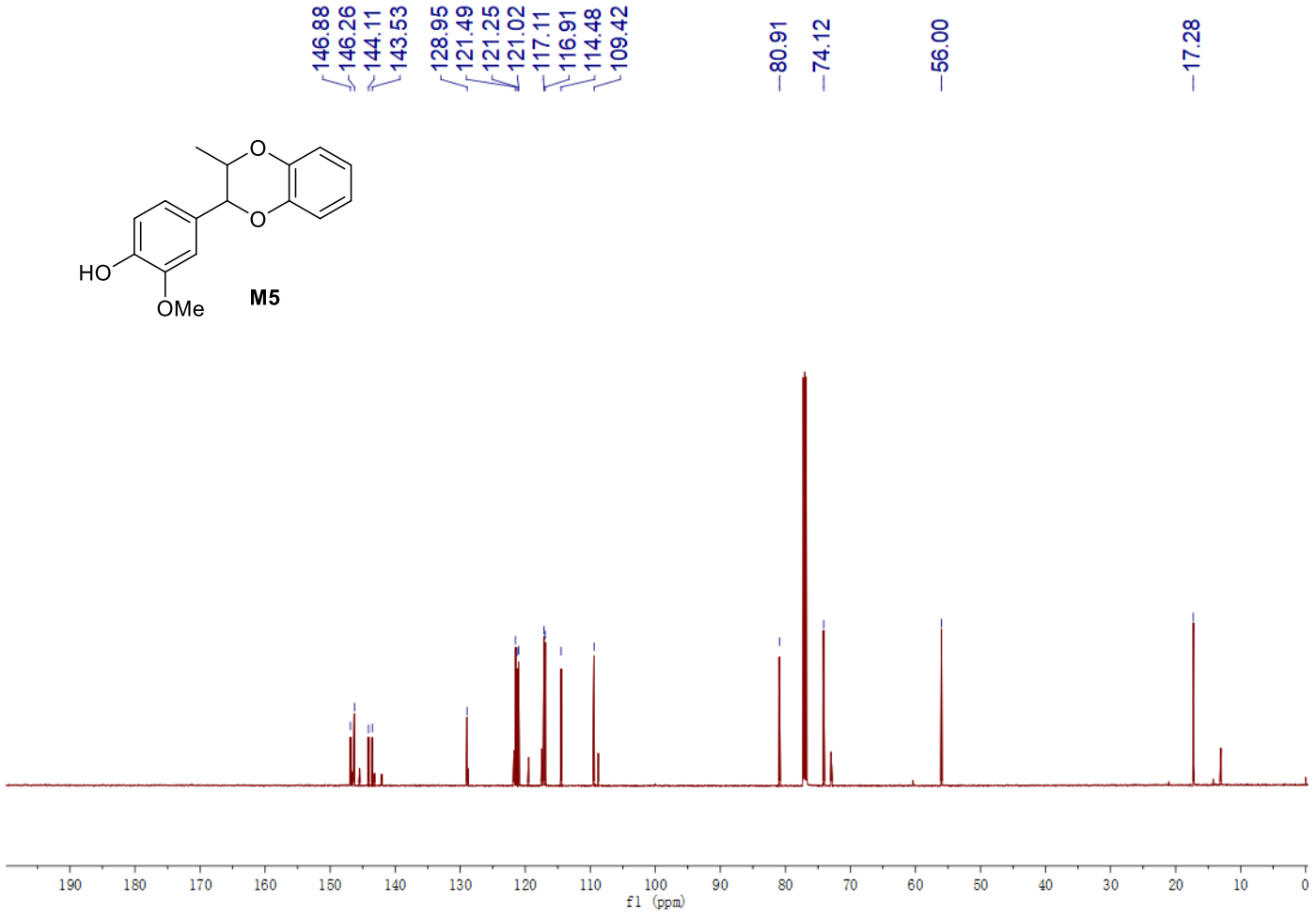
^{1}H NMR spectrum of **M4** ($CDCl_3$).



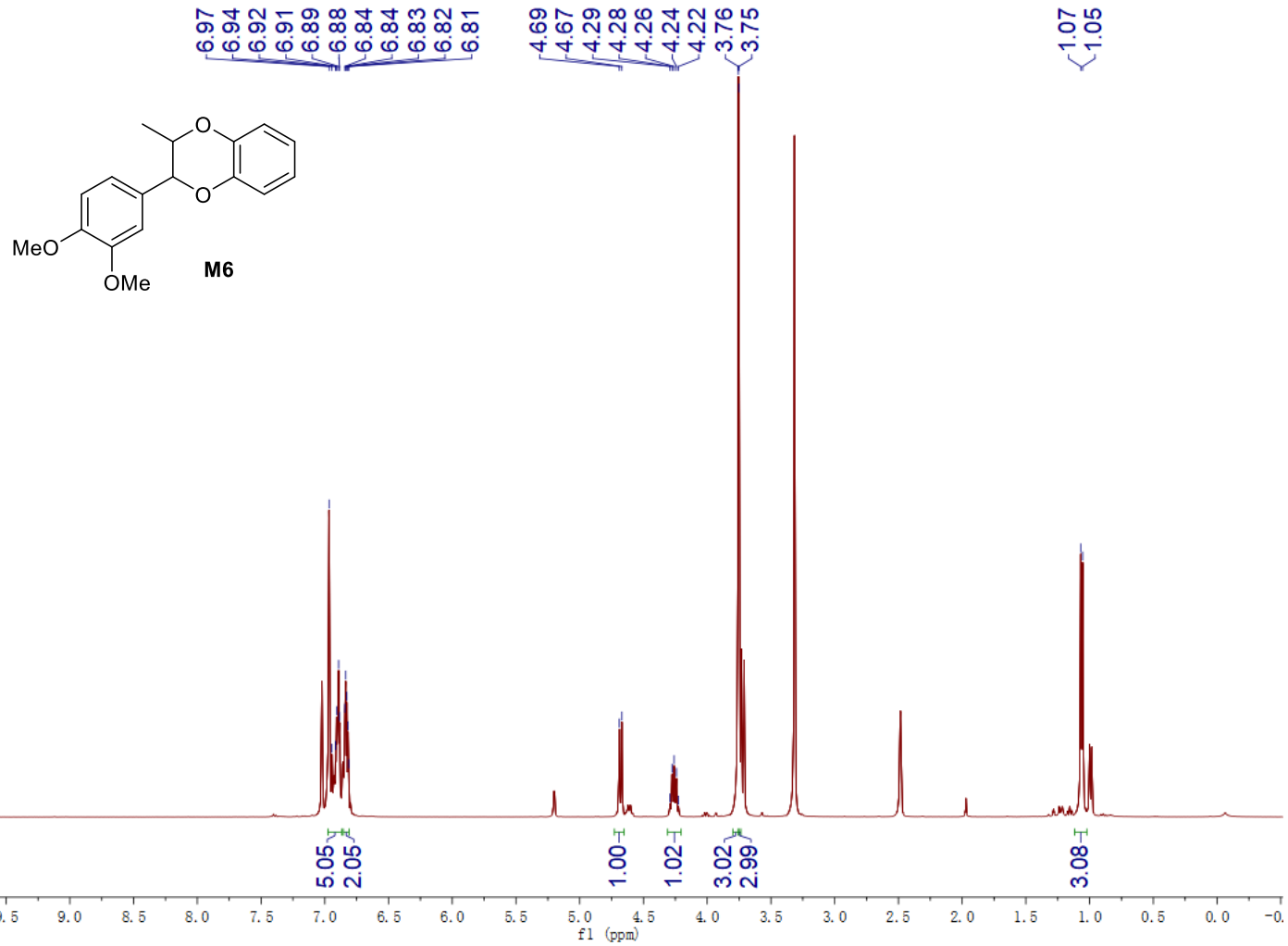
^{13}C NMR spectrum of **M4** ($CDCl_3$).



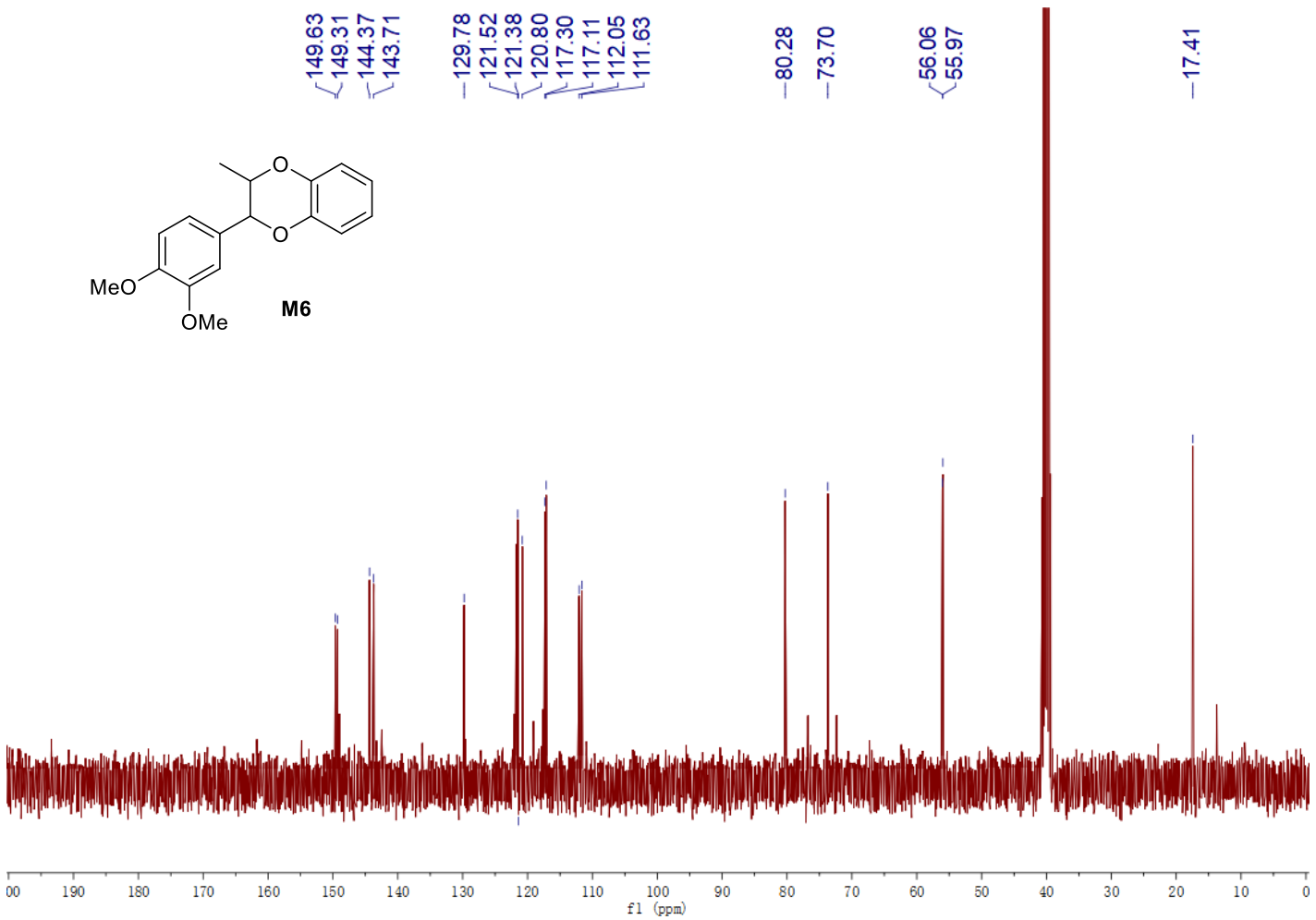
^{1}H NMR spectrum of **M5** ($CDCl_3$).



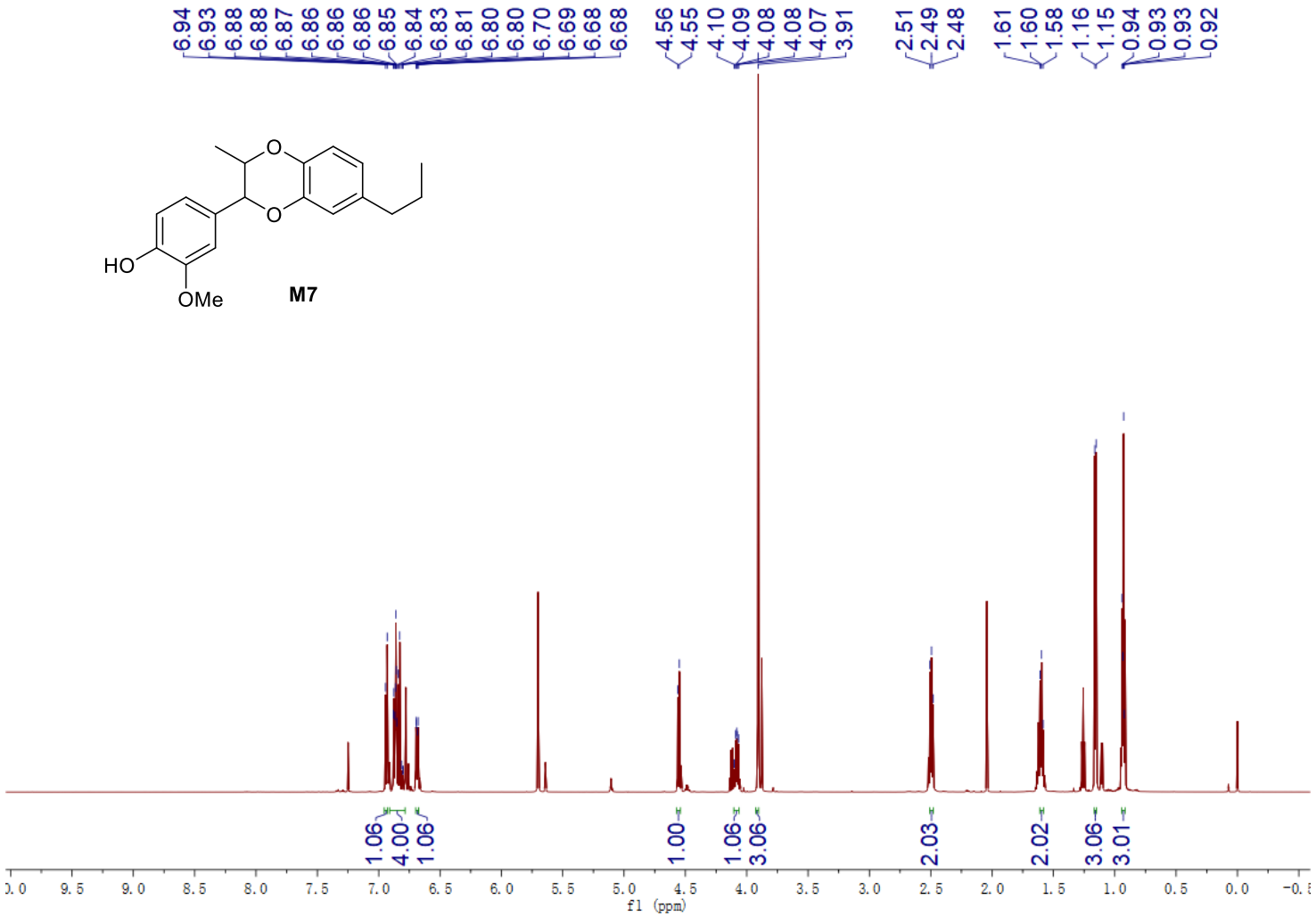
^{13}C NMR spectrum of **M5** ($CDCl_3$).



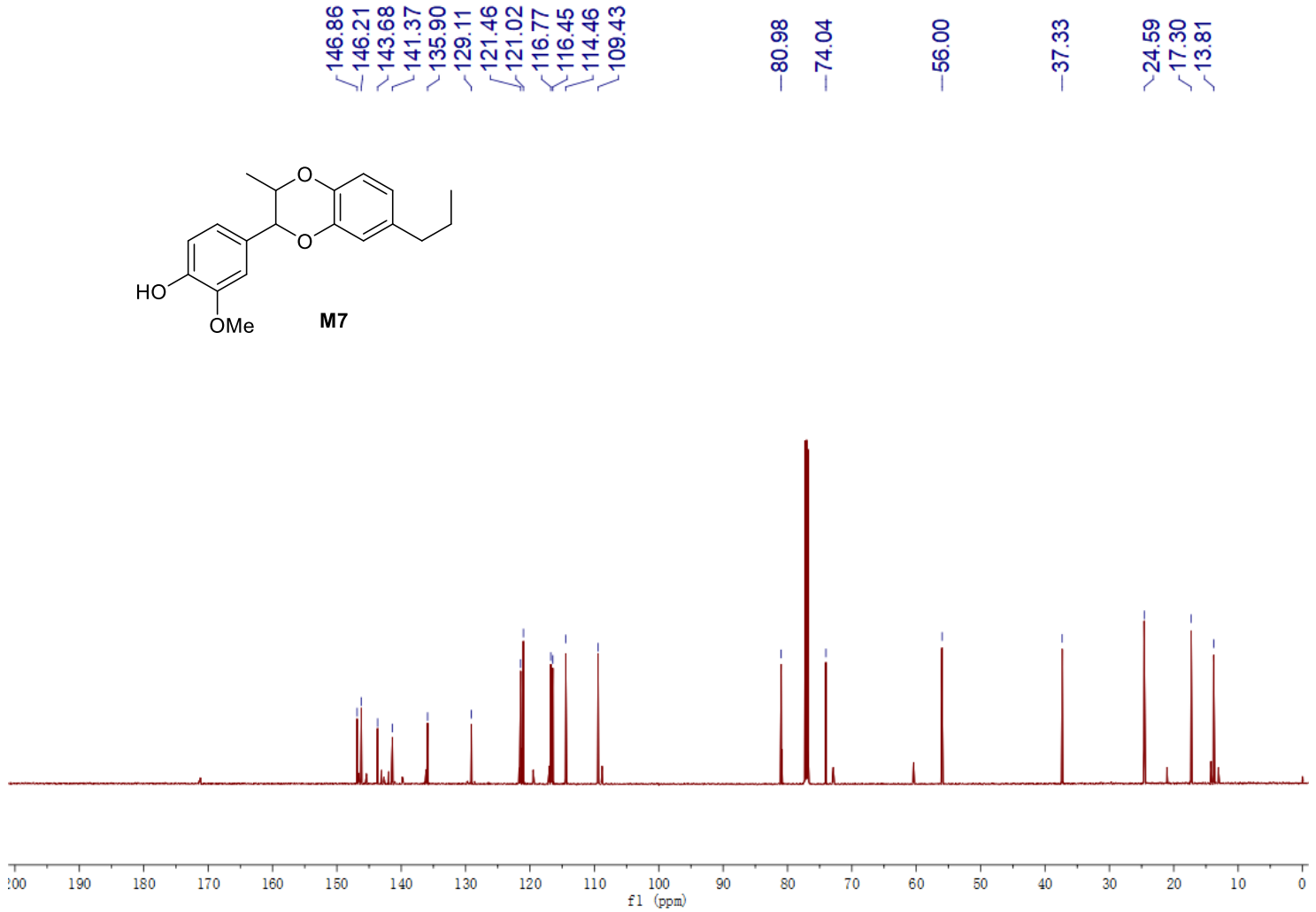
^{1}H NMR spectrum of **M6** (DMSO-d_6).



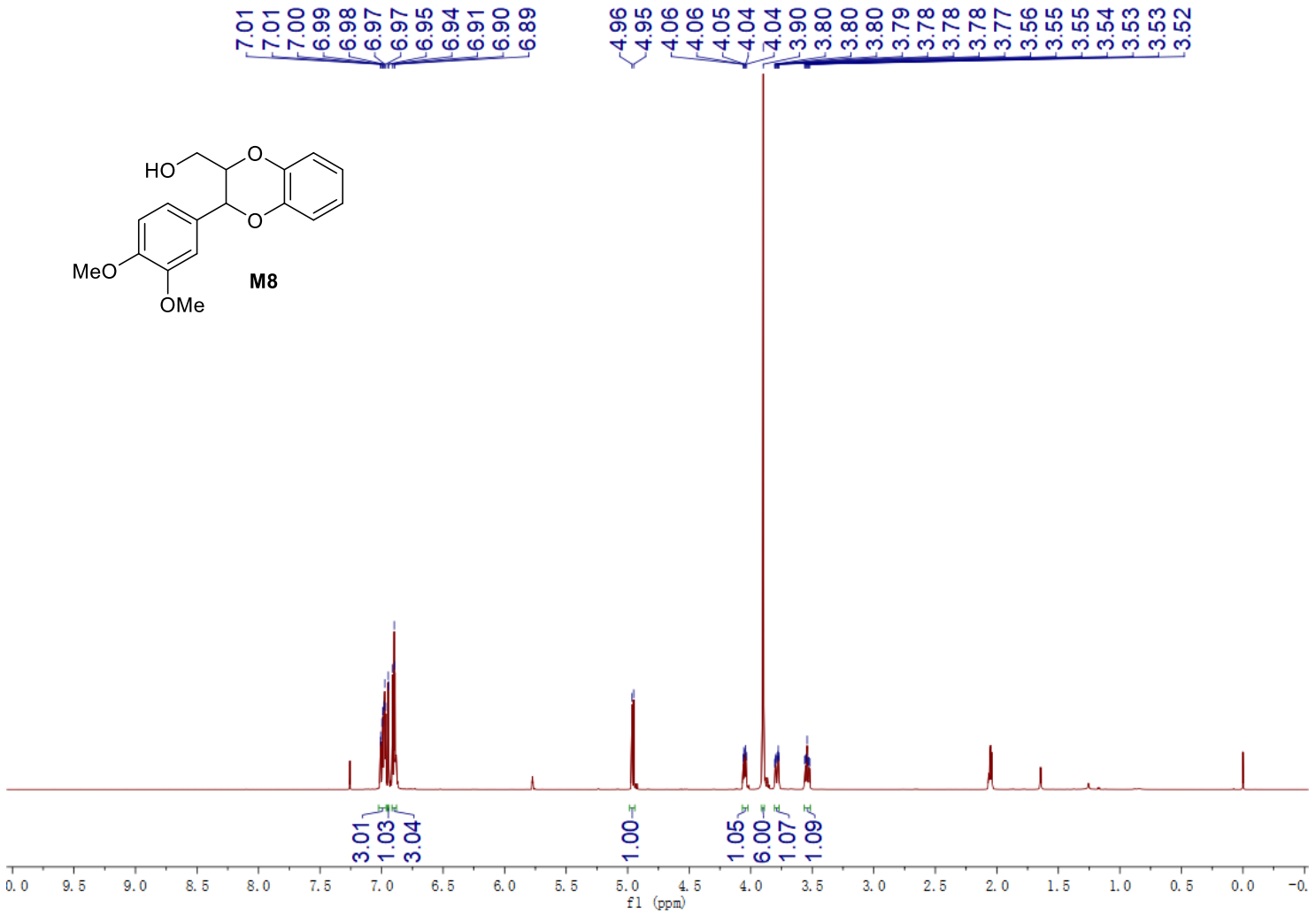
^{13}C NMR spectrum of **M6** (DMSO-d_6).



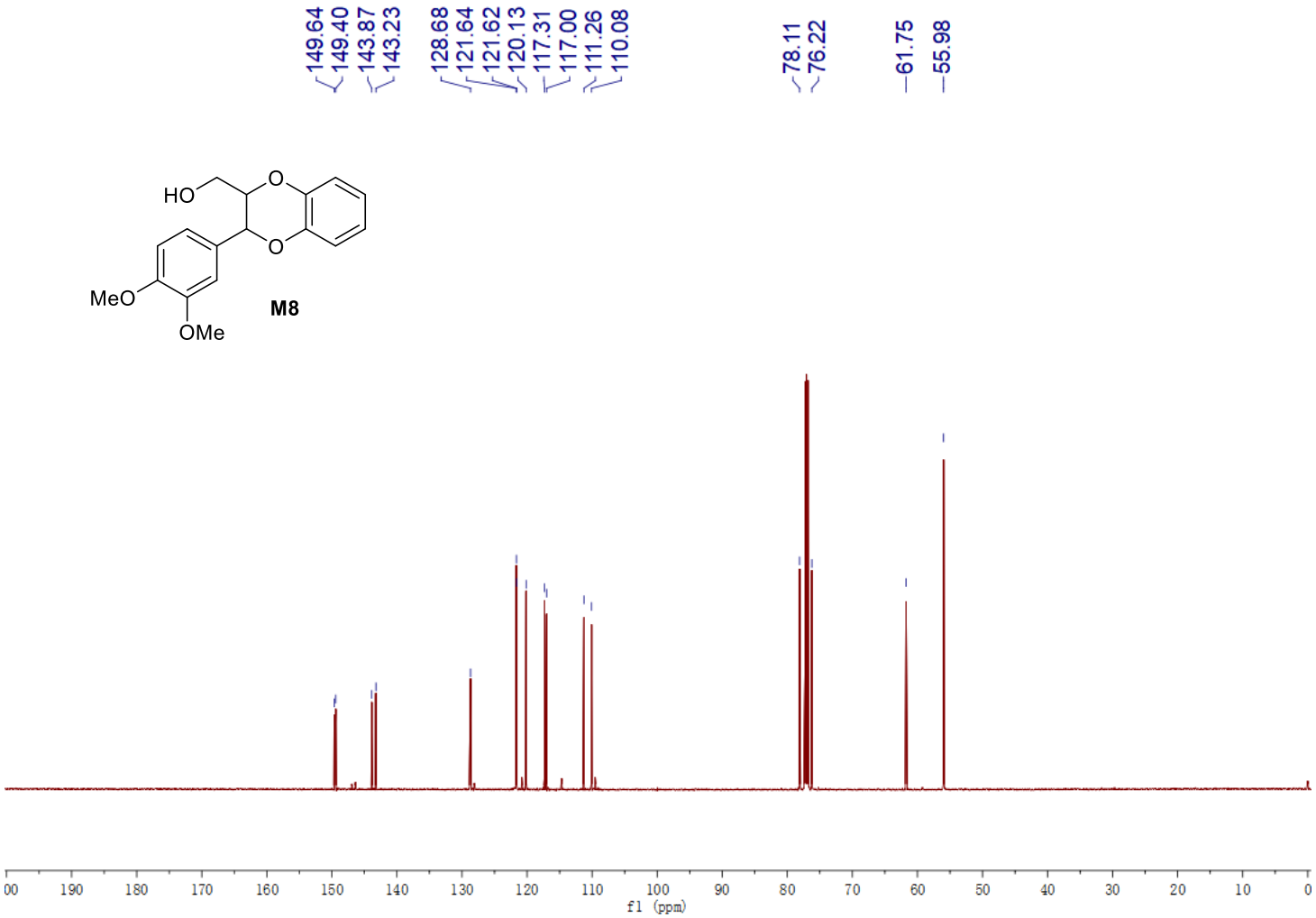
^{1}H NMR spectrum of **M7** ($CDCl_3$).



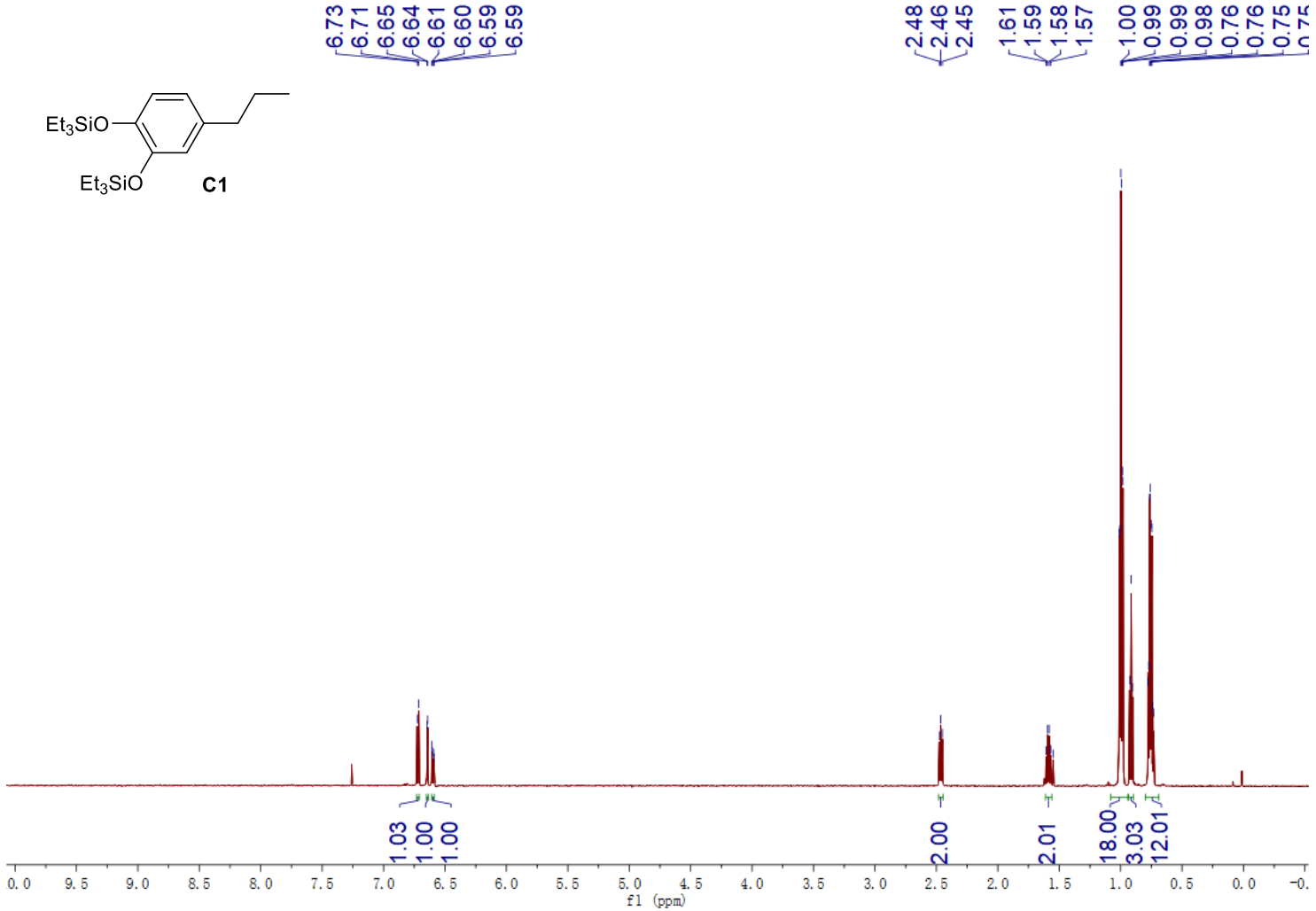
^{13}C NMR spectrum of **M7** ($CDCl_3$).



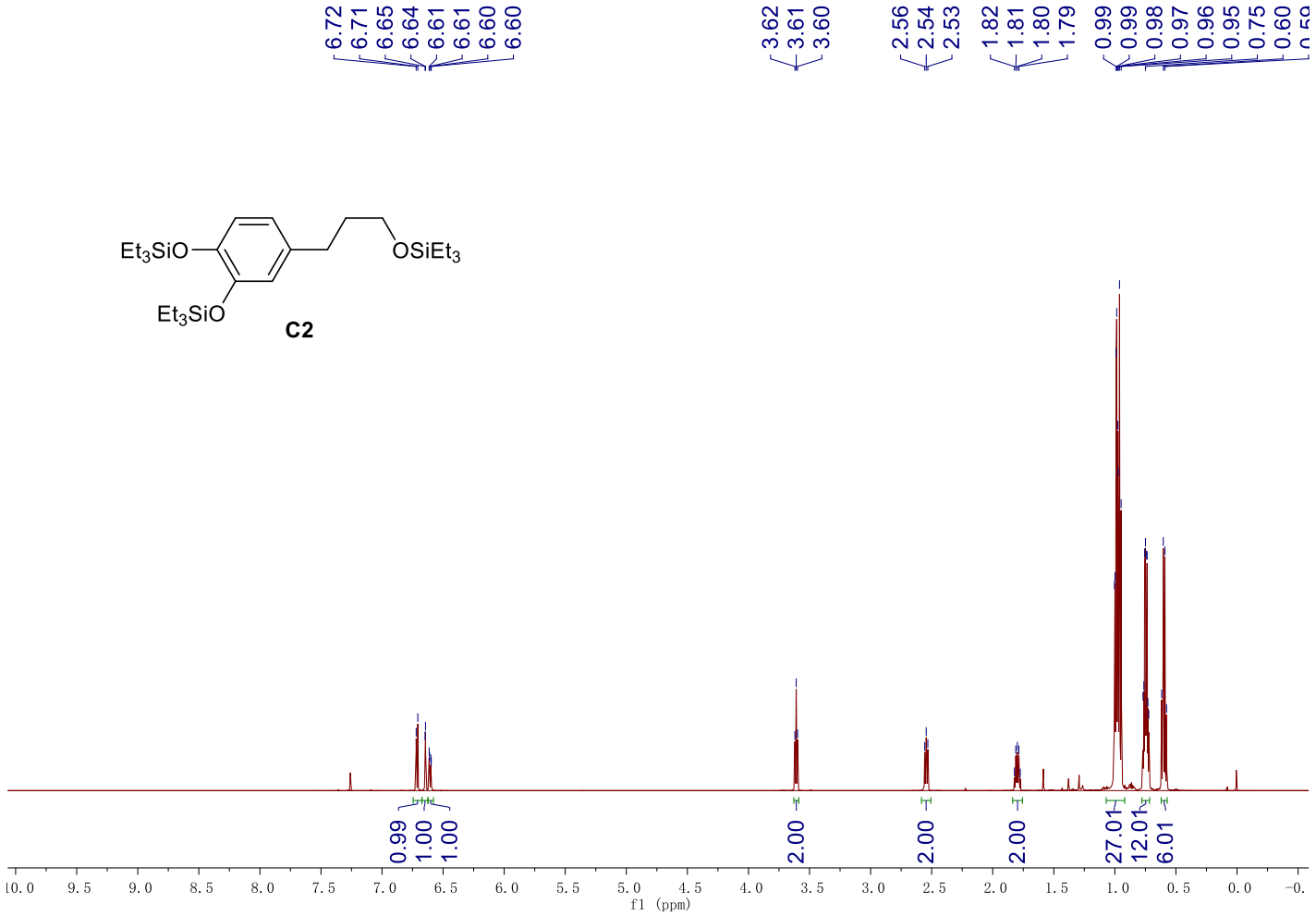
^{1}H NMR spectrum of **M8** ($CDCl_3$).



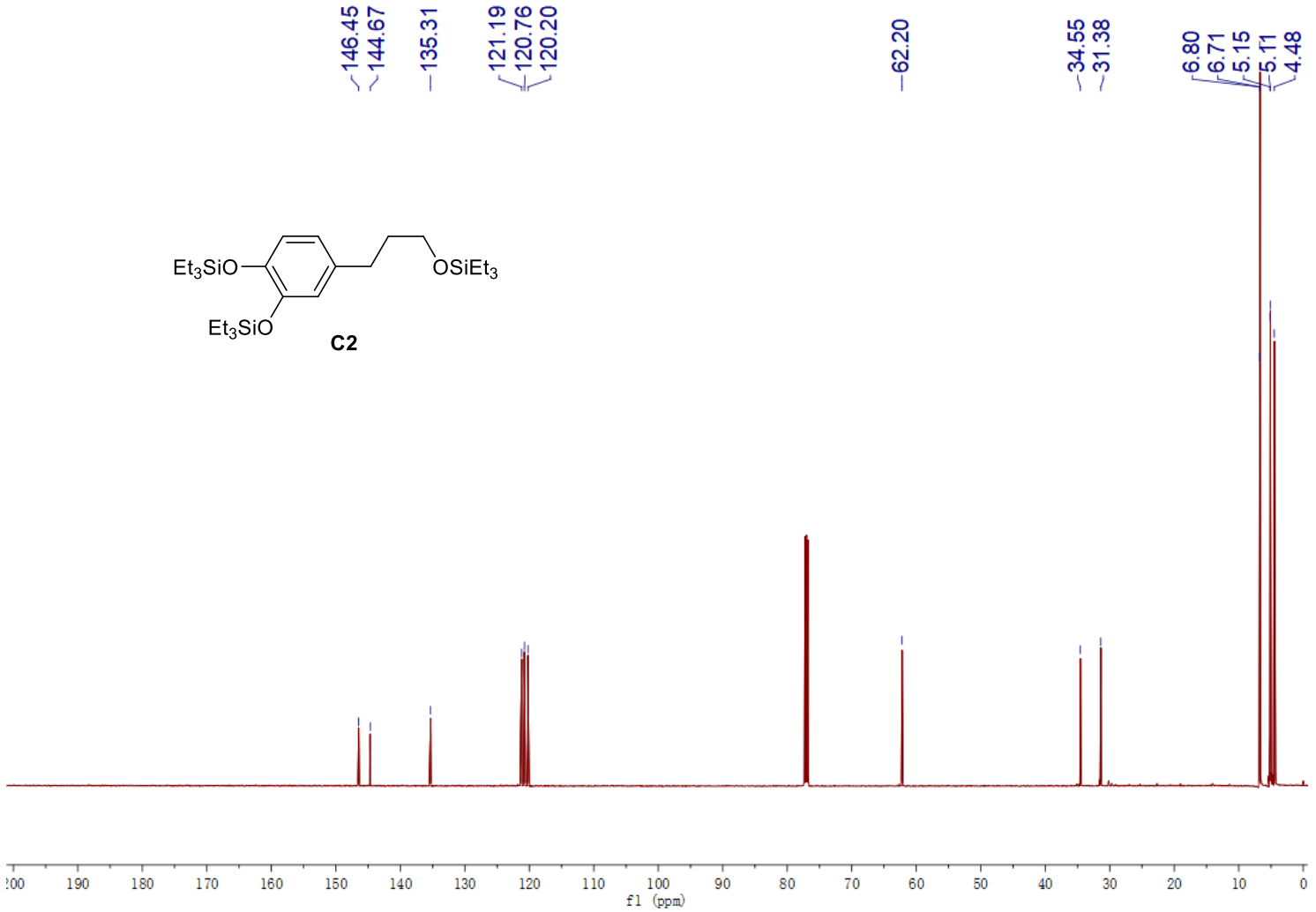
^{13}C NMR spectrum of **M8** ($CDCl_3$).



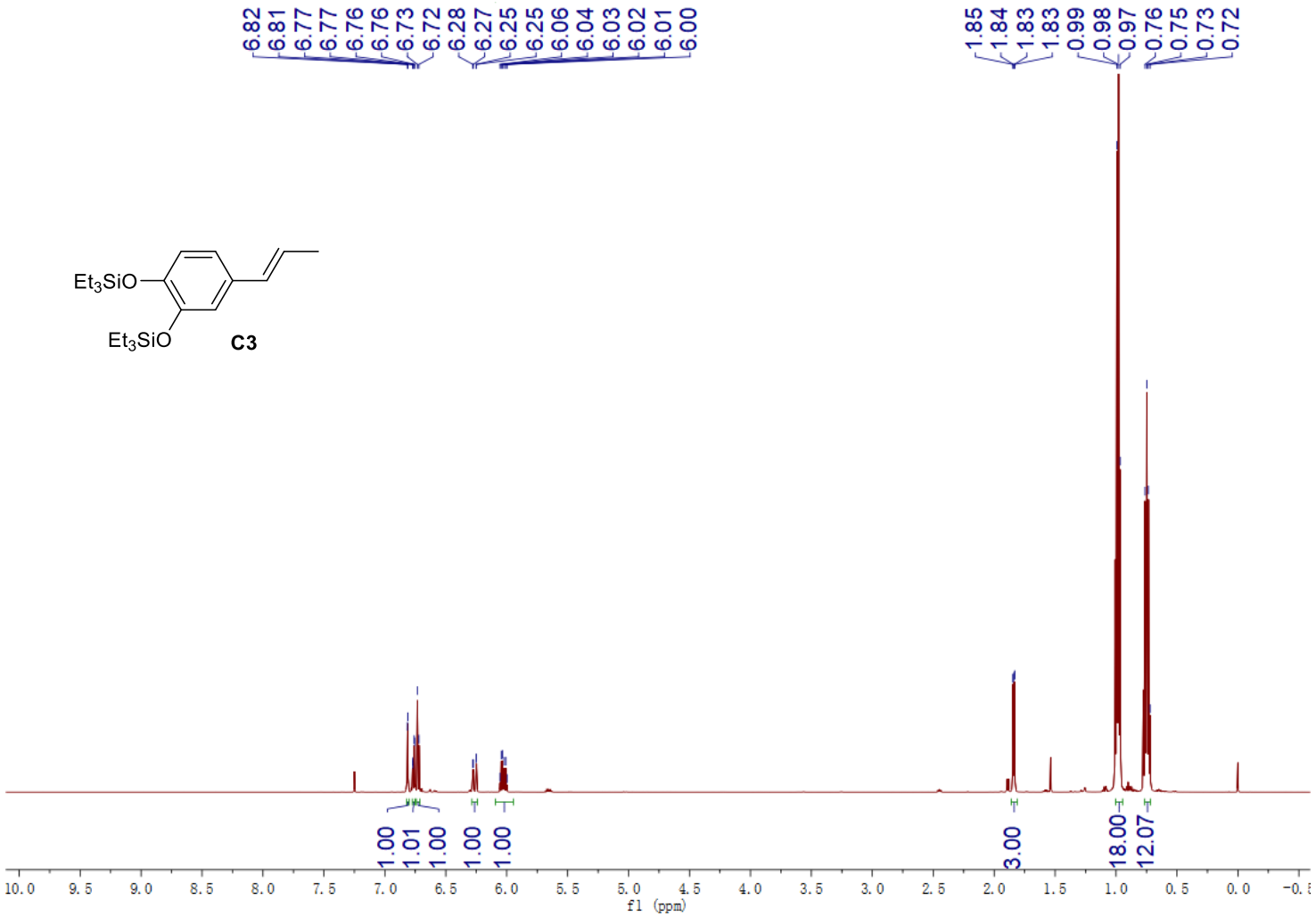
^{1}H NMR spectrum of **C1** ($CDCl_3$).



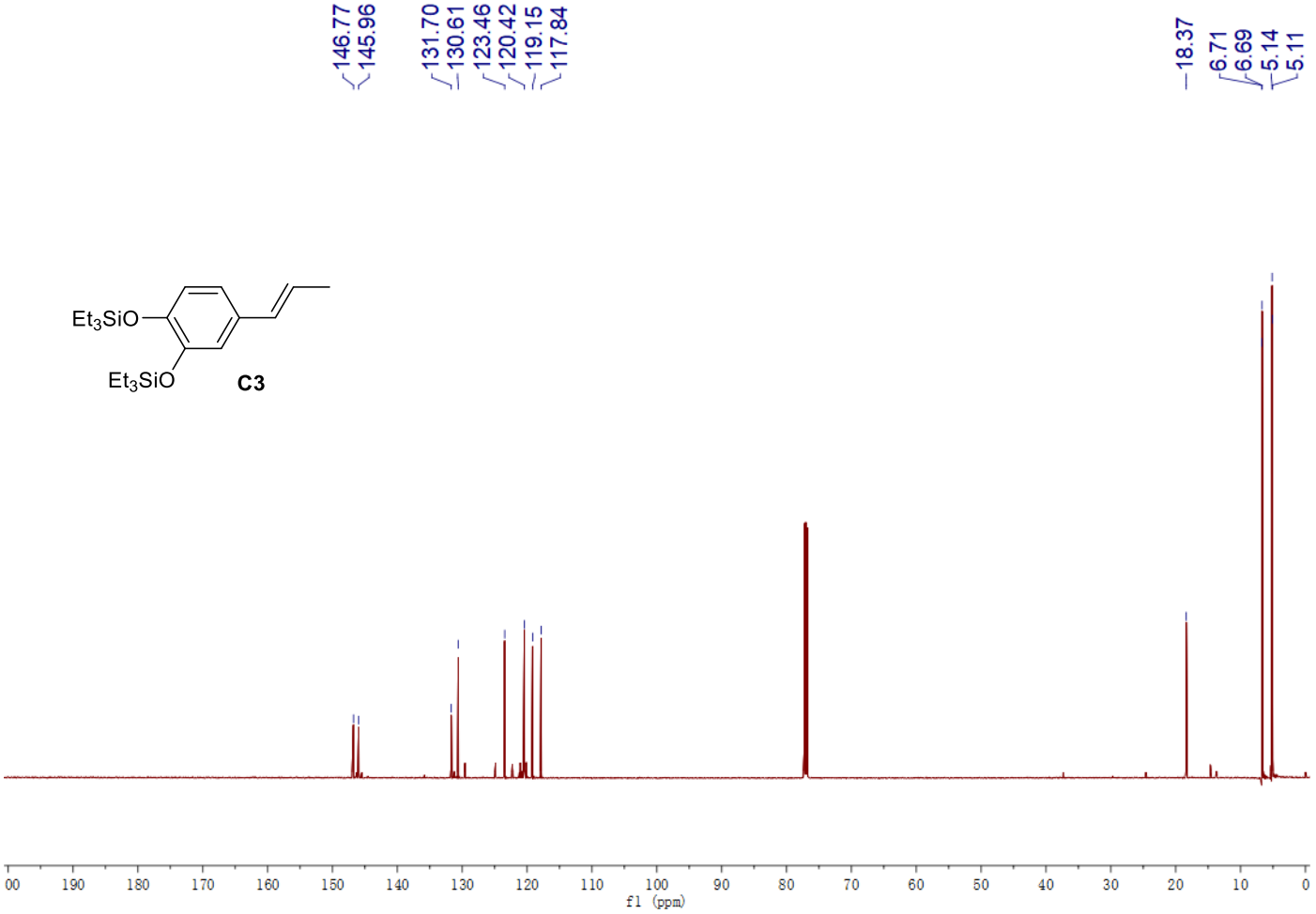
^{1}H NMR spectrum of **C2** ($CDCl_3$).



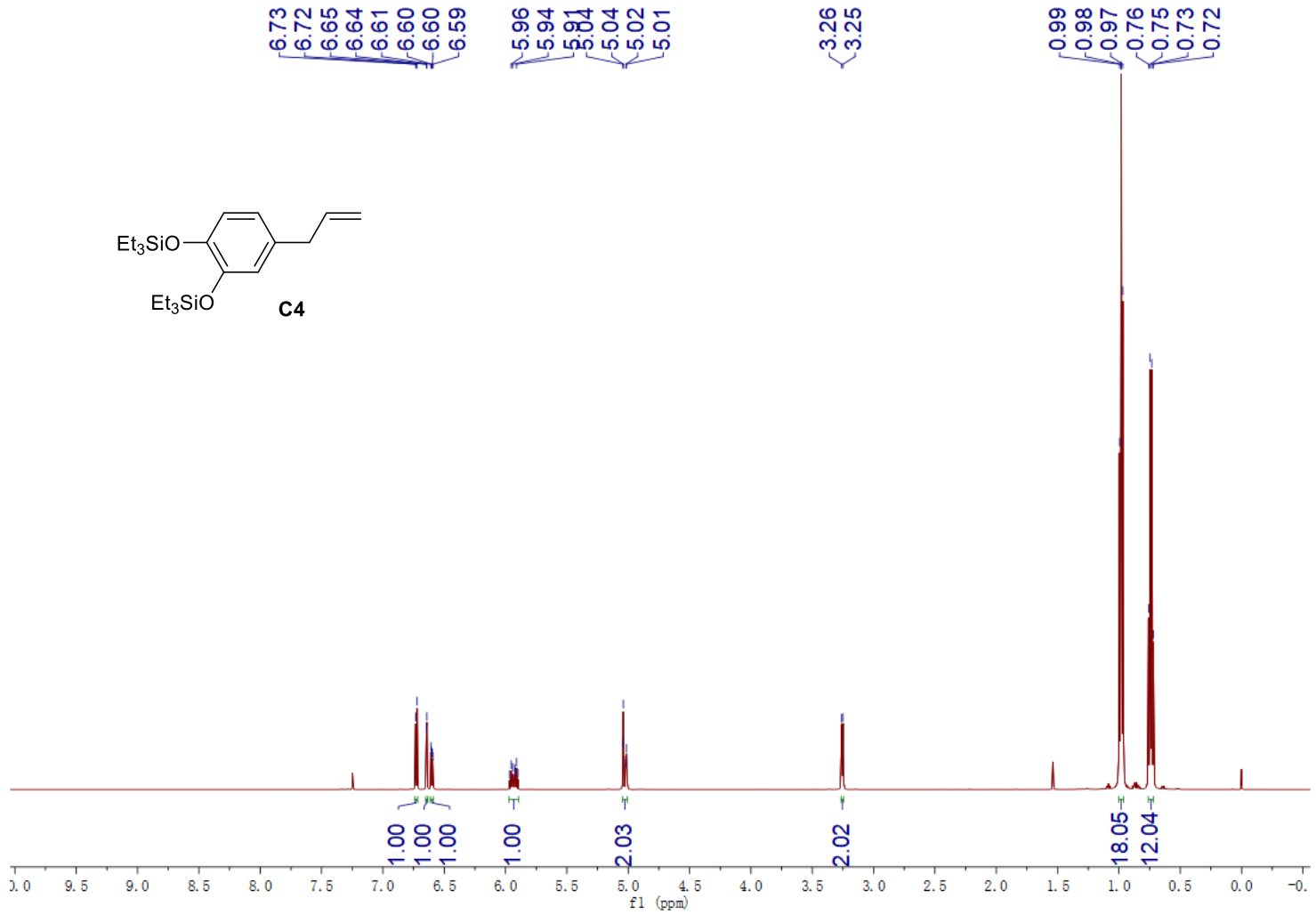
^{13}C NMR spectrum of **C2** ($CDCl_3$).



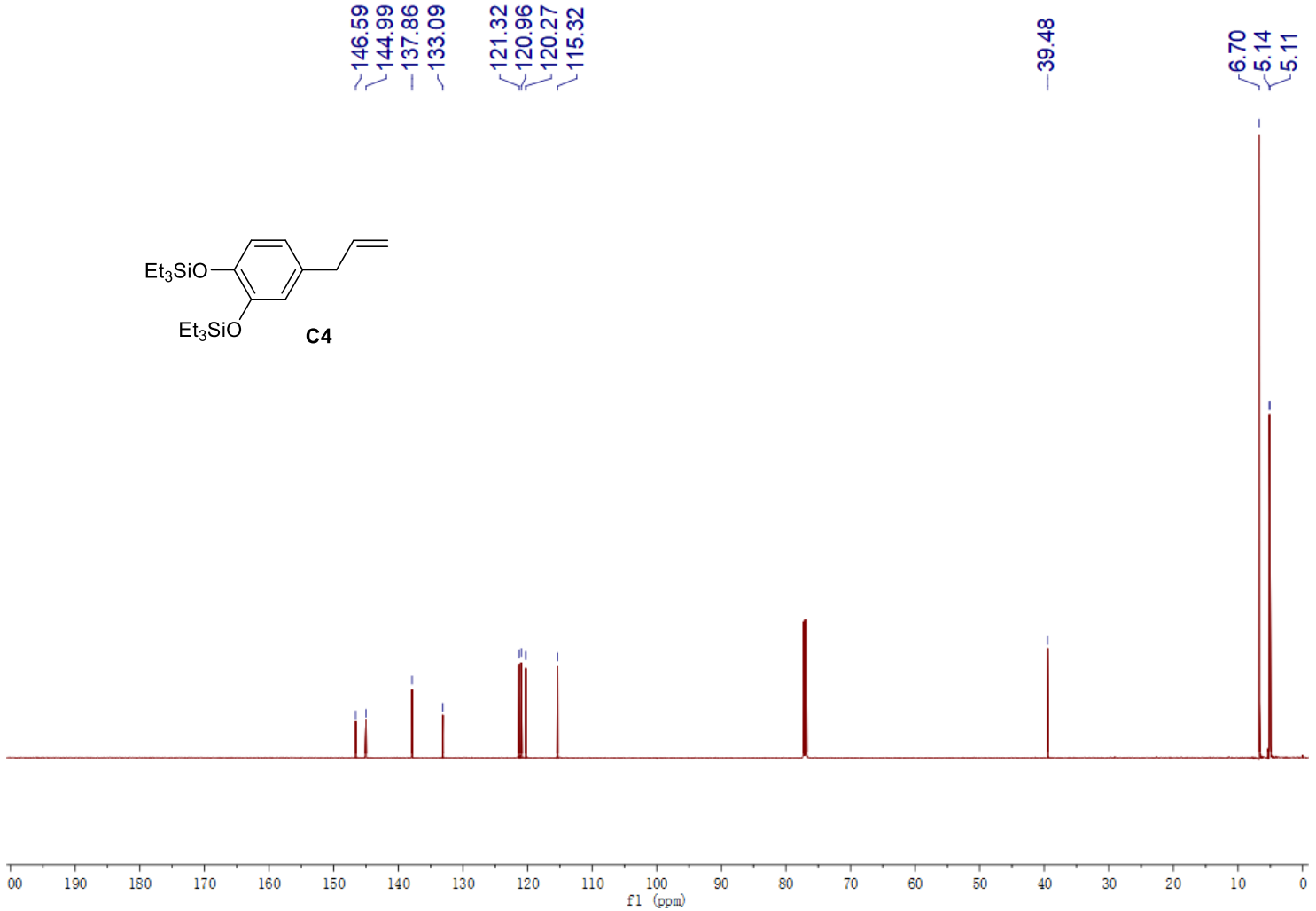
^{1}H NMR spectrum of **C3** ($CDCl_3$).



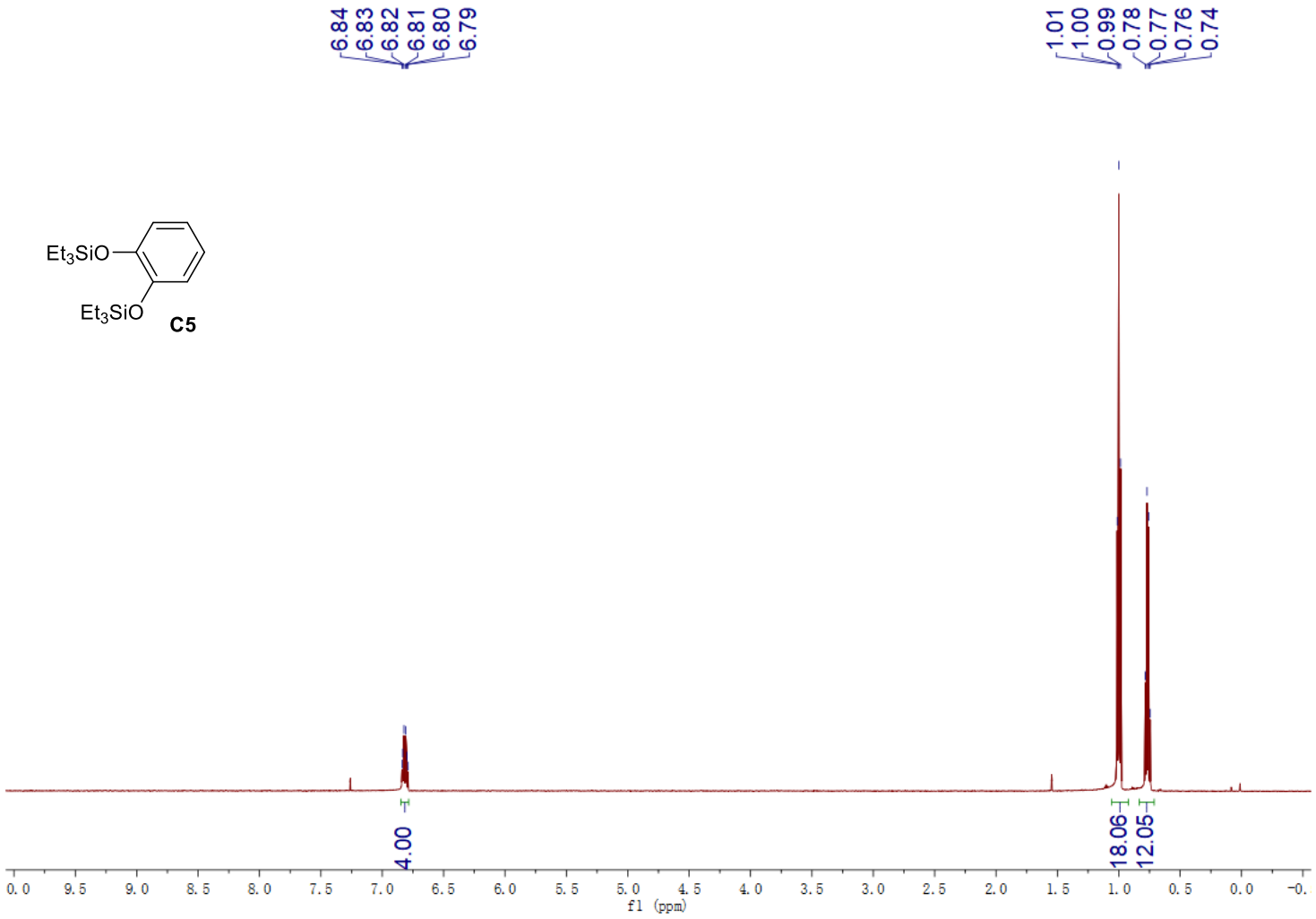
^{13}C NMR spectrum of **C3** ($CDCl_3$).



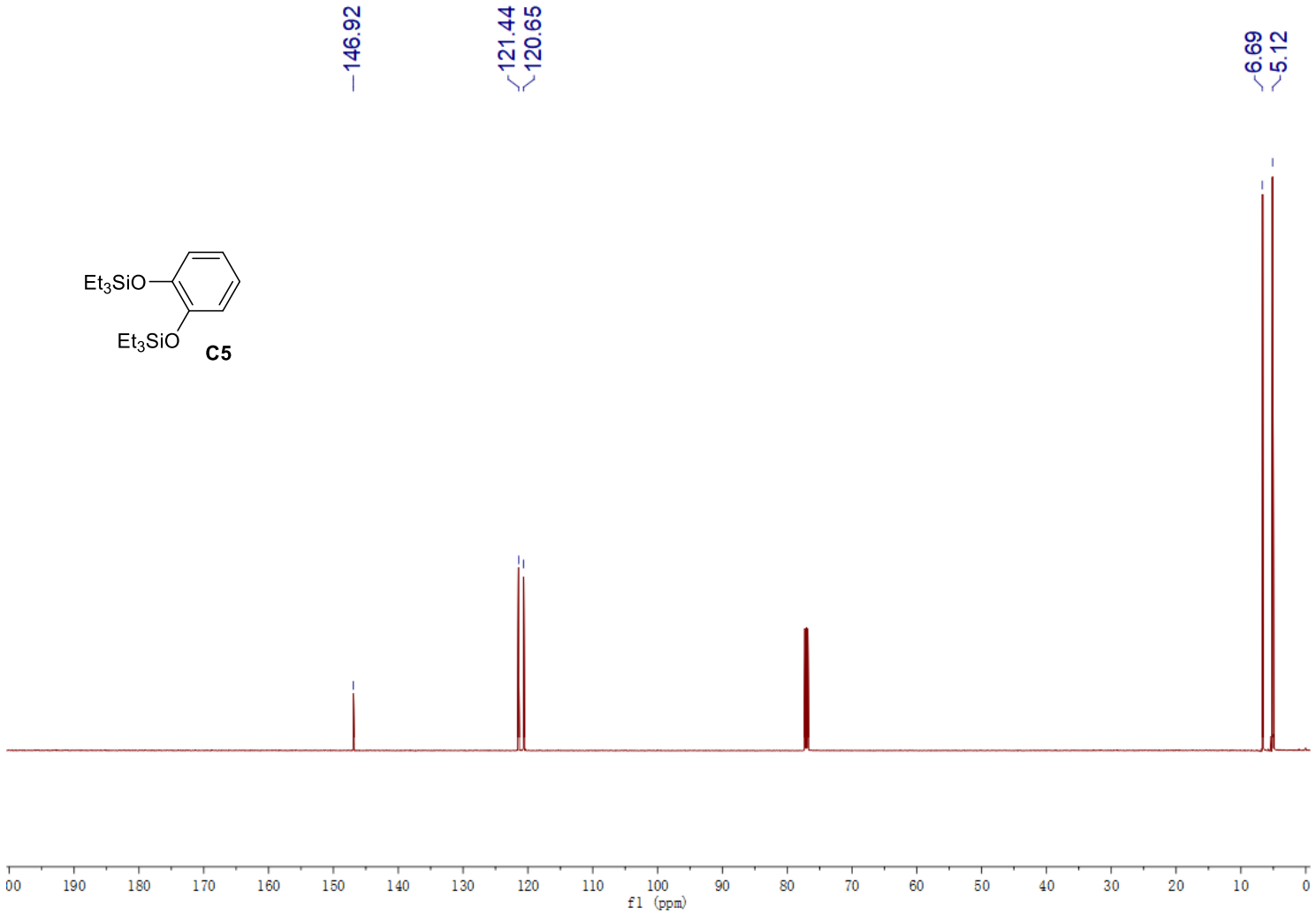
^{1}H NMR spectrum of **C4** ($CDCl_3$).



^{13}C NMR spectrum of **C4** ($CDCl_3$).



^{1}H NMR spectrum of **C5** ($CDCl_3$).



^{13}C NMR spectrum of **C5** ($CDCl_3$).

Standard curves

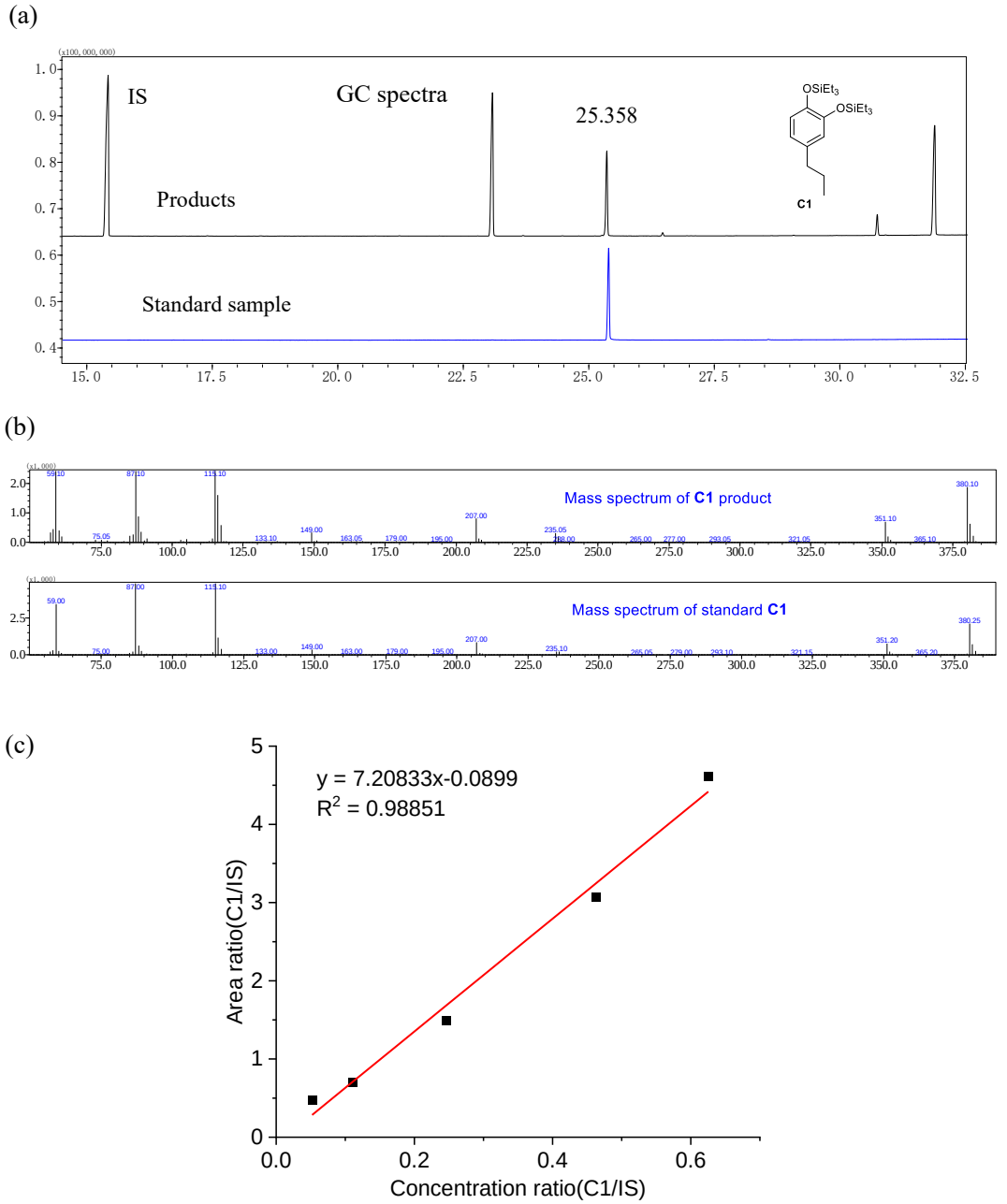
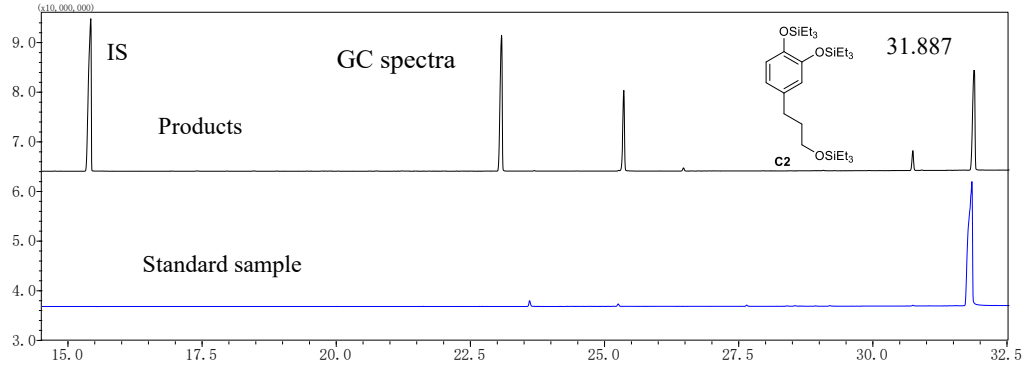
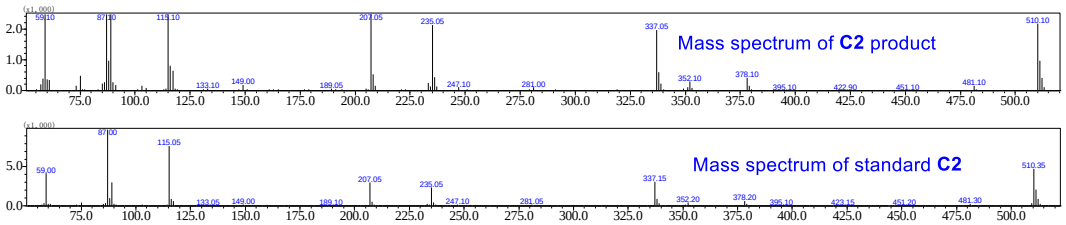


Figure S18. The identification and quantification of **C1** products derived from **M1** depolymerisation. (a) GC spectra, (b) mass spectra of **C1** product and standard sample **C1**, respectively. (c) Standard curve of **C1**.

(a)



(b)



(c)

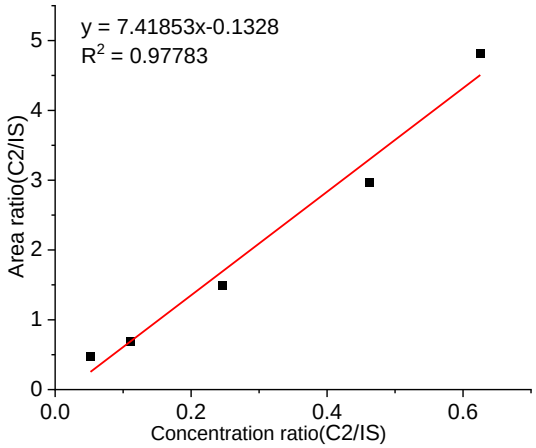
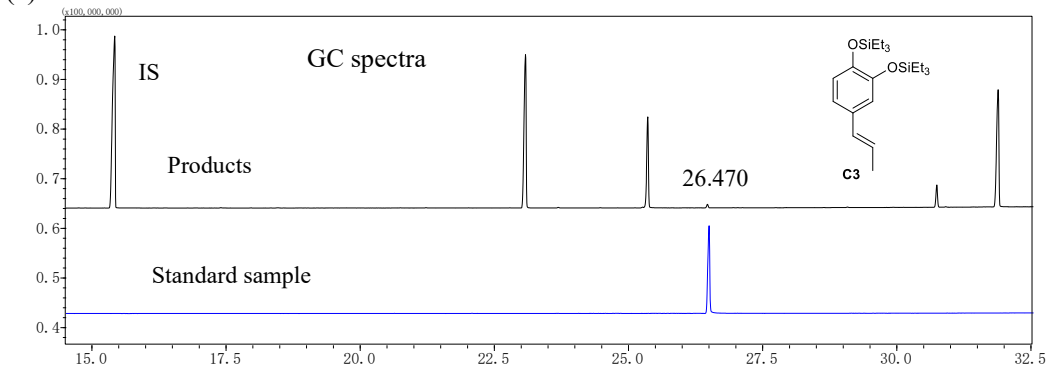
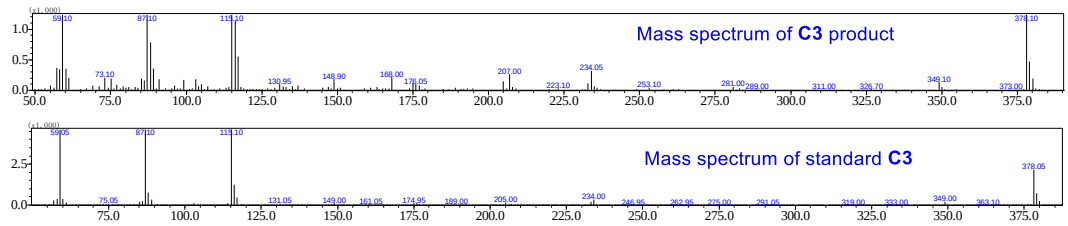


Figure S19. The identification and quantification of **C2** products derived from **M1** depolymerisation. (a) GC spectra, (b) mass spectra of **C2** product and standard sample **C2**, respectively. (c) Standard curve of **C2**.

(a)



(b)



(c)

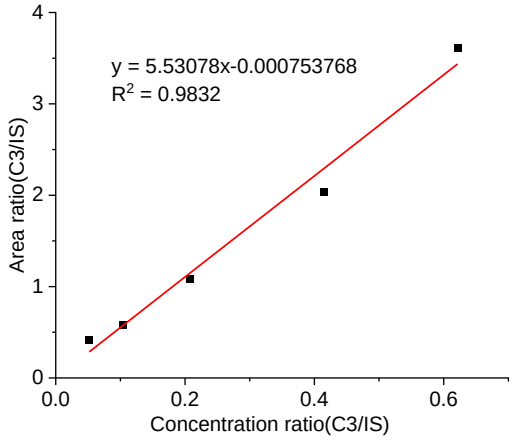


Figure S20. The identification and quantification of **C3** products derived from **M1** depolymerisation. (a) GC spectra, (b) mass spectra of **C3** product and standard sample **C3**, respectively. (c) Standard curve of **C3**.

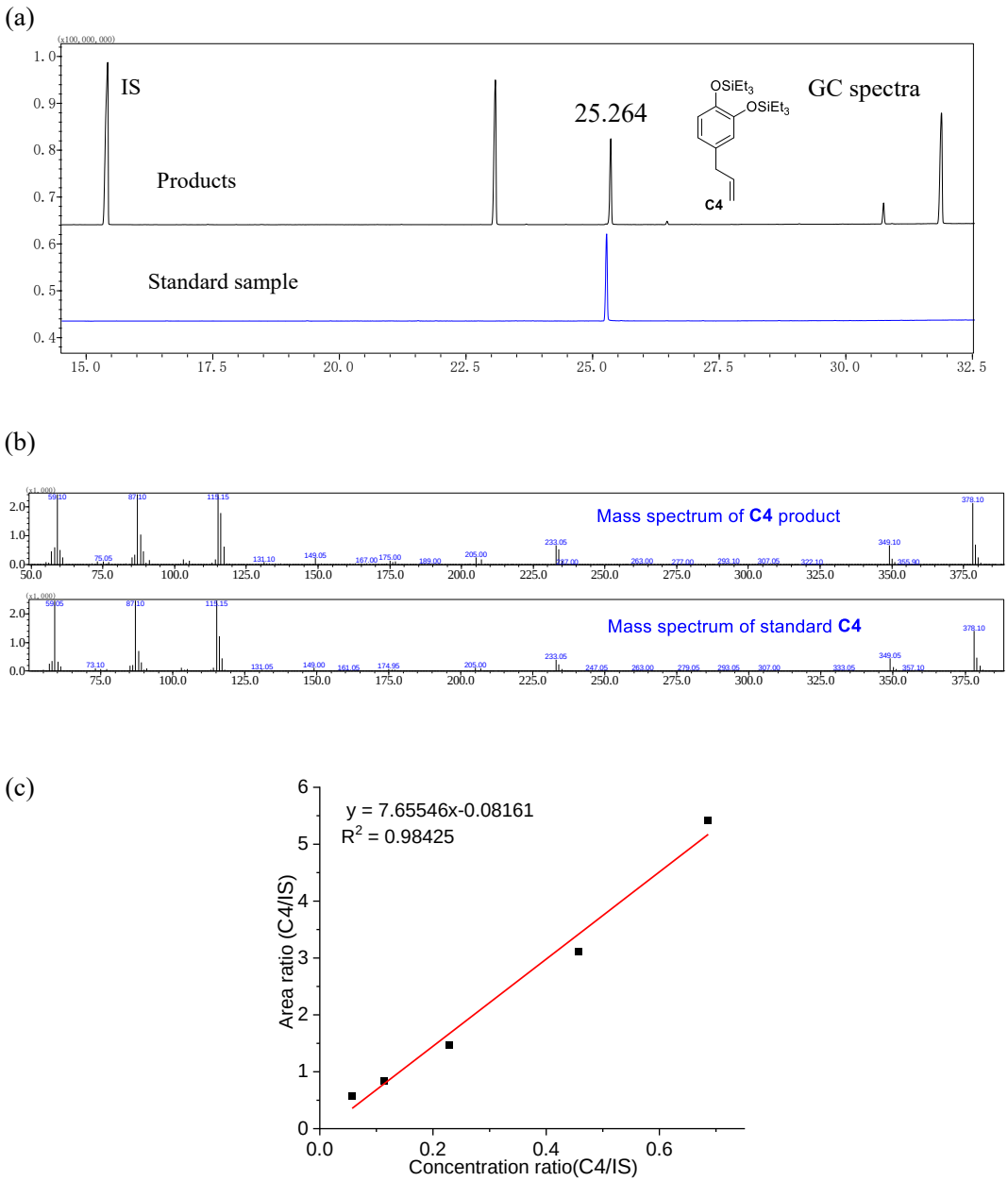
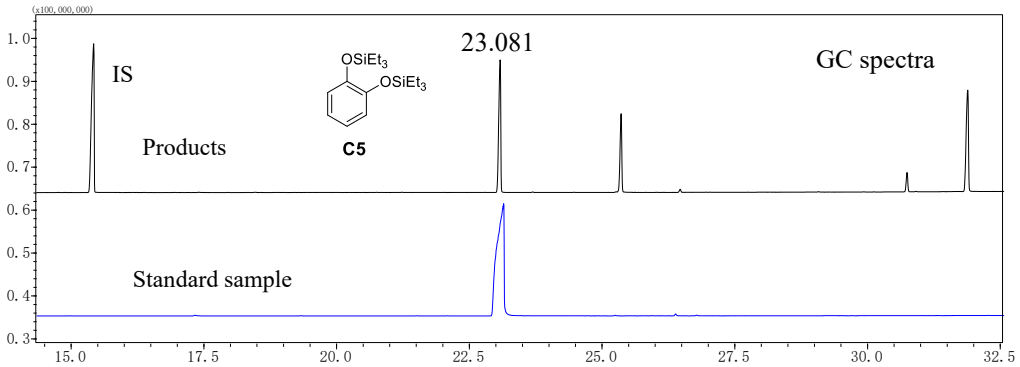
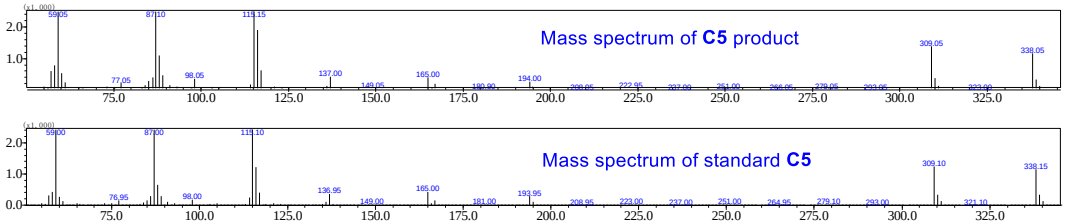


Figure S21. The identification and quantification of **C4** products derived from **M1** depolymerisation. (a) GC spectra, (b) mass spectra of **C4** product and standard sample **C4**, respectively. (c) Standard curve of **C4**.

(a)



(b)



(c)

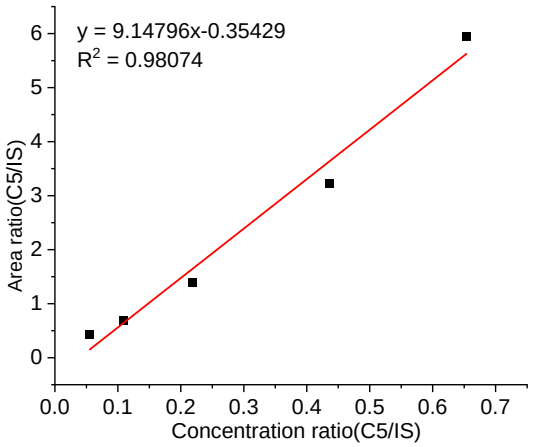


Figure S22. The identification and quantification of **C5** products derived from **M1** depolymerisation. (a) GC spectra, (b) mass spectra of **C5** product and standard sample **C5**, respectively. (c) Standard curve of **C5**.

DFT data

34 (the number of atoms involved in the molecule)

$B(C_6F_5)_3$, *E*(SCRF) = -2208.224117 a.u.

B	-0.000226000	0.000272000	0.000212000
C	-1.514118000	0.407319000	0.000033000
C	-1.976439000	1.564415000	0.635567000
C	-2.494105000	-0.362107000	-0.635627000
C	-3.311711000	1.935772000	0.653474000
C	-3.835592000	-0.013765000	-0.654155000
C	-4.244916000	1.141531000	-0.000613000
C	0.404152000	-1.514267000	0.000486000
C	-0.366295000	-2.492910000	0.636965000
C	1.559981000	-1.978467000	-0.635891000
C	-0.020469000	-3.835028000	0.654873000
C	1.928932000	-3.314421000	-0.654266000
C	1.133424000	-4.246353000	0.000060000
C	1.109465000	1.107495000	0.000418000
C	0.933779000	2.341098000	-0.635051000
C	2.342604000	0.928573000	0.635917000
C	1.906664000	3.328252000	-0.653146000
C	3.332424000	1.898705000	0.653963000
C	3.111758000	3.104280000	0.000252000
F	4.483156000	1.686824000	1.283509000
F	2.610026000	-0.206974000	1.282623000
F	4.049076000	4.038551000	-0.000326000
F	1.697989000	4.479332000	-1.283108000
F	-0.201036000	2.611736000	-1.281738000
F	-1.127133000	2.364428000	1.282044000
F	-3.704090000	3.037935000	1.283243000
F	-5.522836000	1.485535000	-0.001459000
F	-4.727397000	-0.770220000	-1.284893000
F	-2.160257000	-1.480096000	-1.282099000
F	2.360719000	-1.130543000	-1.283318000
F	3.029606000	-3.708737000	-1.285427000
F	1.474214000	-5.525140000	-0.000845000
F	-0.778406000	-4.725801000	1.285287000
F	-1.483196000	-2.157061000	1.284219000

23

Et_3SiH, *E*(SCRF) = -527.710229 a.u.

Si	-0.583020000	0.075037000	0.000000000
H	-1.906385000	-0.617261000	0.000000000
C	0.343425000	-0.417820000	1.574412000
H	1.375634000	-0.049465000	1.507580000

H	-0.115185000	0.130349000	2.408449000
C	0.343425000	-1.919916000	1.886114000
H	0.882121000	-2.488219000	1.122151000
H	0.821728000	-2.132484000	2.847694000
H	-0.676551000	-2.315338000	1.928454000
C	0.343425000	-0.417820000	-1.574412000
H	-0.115185000	0.130349000	-2.408449000
H	1.375634000	-0.049465000	-1.507580000
C	0.343425000	-1.919916000	-1.886114000
H	0.821728000	-2.132484000	-2.847694000
H	0.882121000	-2.488219000	-1.122151000
H	-0.676551000	-2.315338000	-1.928454000
C	-0.849649000	1.946067000	0.000000000
H	-1.449255000	2.220969000	-0.876726000
H	-1.449255000	2.220969000	0.876726000
C	0.467874000	2.733500000	0.000000000
H	0.296071000	3.814555000	0.000000000
H	1.072030000	2.497995000	0.882811000
H	1.072030000	2.497995000	-0.882811000

57

A, *E*(SCRF) = -2735.957592 a.u.

B	-0.073704000	0.018440000	-0.511309000
C	-1.664676000	-0.006736000	-0.646531000
C	-2.434404000	0.944282000	0.017841000
C	-2.384033000	-0.959245000	-1.361713000
C	-3.818389000	0.957039000	0.012750000
C	-3.773806000	-0.973915000	-1.411812000
C	-4.494117000	-0.011669000	-0.719505000
C	0.735050000	-1.330248000	-0.799618000
C	0.326215000	-2.519753000	-0.200729000
C	1.913944000	-1.407982000	-1.533876000
C	1.029884000	-3.708470000	-0.287486000
C	2.647023000	-2.583881000	-1.660082000
C	2.203671000	-3.738409000	-1.031711000
C	0.668148000	1.418306000	-0.726694000
C	0.130845000	2.511038000	-1.400016000
C	1.916891000	1.633470000	-0.150087000
C	0.783156000	3.736549000	-1.489376000
C	2.593434000	2.840025000	-0.194653000
C	2.018055000	3.903405000	-0.879880000
F	3.770542000	2.985640000	0.409995000
F	2.501695000	0.632799000	0.530948000
F	2.645275000	5.070652000	-0.948312000
F	0.228595000	4.750607000	-2.147342000

F	-1.060692000	2.427417000	-1.998432000
F	-1.820999000	1.887295000	0.755910000
F	-4.496546000	1.871111000	0.702426000
F	-5.820719000	-0.020142000	-0.748507000
F	-4.415593000	-1.903962000	-2.113308000
F	-1.754987000	-1.921004000	-2.042985000
F	2.404851000	-0.331732000	-2.154596000
F	3.767131000	-2.608910000	-2.376253000
F	2.895815000	-4.865356000	-1.138500000
F	0.602927000	-4.804428000	0.334642000
F	-0.786796000	-2.526852000	0.554819000
Si	0.006288000	-0.078900000	2.491844000
H	0.045294000	-0.032192000	0.939091000
C	1.076835000	-1.542951000	2.986786000
H	1.102076000	-1.528722000	4.086961000
H	0.517212000	-2.448858000	2.718743000
C	2.508678000	-1.624557000	2.439577000
H	3.099573000	-0.748141000	2.717160000
H	3.016659000	-2.510029000	2.833046000
H	2.518620000	-1.689477000	1.348486000
C	0.572989000	1.628145000	3.044622000
H	0.308438000	2.336056000	2.248401000
H	-0.079444000	1.888909000	3.890309000
C	2.042354000	1.796439000	3.452338000
H	2.218373000	2.797571000	3.856759000
H	2.328189000	1.074863000	4.224875000
H	2.716611000	1.659551000	2.603694000
C	-1.797036000	-0.390265000	2.915531000
H	-2.362021000	0.538494000	2.774953000
H	-2.210408000	-1.124523000	2.214127000
C	-1.950946000	-0.891467000	4.361197000
H	-3.005296000	-1.015841000	4.623269000
H	-1.459246000	-1.858864000	4.502288000
H	-1.517225000	-0.189497000	5.082784000

31

m, *E*(SCRF) = -730.380753 a.u.

C	-0.402252000	0.211851000	0.461361000
C	1.739793000	-0.693786000	0.138787000
C	2.234699000	0.597993000	-0.070648000
C	0.045114000	1.329616000	-0.490683000
H	2.203812000	-2.753205000	0.414634000
C	2.621127000	-1.764329000	0.255386000
C	3.608694000	0.810150000	-0.136817000
C	4.486741000	-0.259785000	-0.010609000

C	3.992137000	-1.550176000	0.176189000
H	3.960539000	1.824346000	-0.294860000
H	5.556221000	-0.085987000	-0.065834000
H	4.673018000	-2.389677000	0.268967000
C	-1.843551000	-0.171764000	0.255819000
C	-2.198055000	-1.012298000	-0.800599000
C	-2.839718000	0.351307000	1.080109000
C	-3.535282000	-1.322436000	-1.029013000
H	-1.417505000	-1.434851000	-1.425969000
C	-4.177829000	0.045659000	0.848423000
H	-2.564751000	0.998518000	1.909633000
C	-4.527566000	-0.792101000	-0.207479000
H	-3.803348000	-1.981737000	-1.848835000
H	-4.945753000	0.454907000	1.497450000
H	-5.570200000	-1.035902000	-0.386149000
O	1.398194000	1.669821000	-0.205857000
O	0.397440000	-0.942566000	0.231892000
H	-0.016404000	0.933513000	-1.516206000
H	-0.240828000	0.567644000	1.490769000
C	-0.760727000	2.604496000	-0.353157000
H	-1.791159000	2.450798000	-0.679886000
H	-0.764071000	2.939982000	0.689028000
H	-0.304591000	3.387225000	-0.963424000

88

TS1, *E*(SCRF) = -3466.333829 a.u., IF= -79.43 cm^{-1}

B	1.804163000	-0.186812000	0.069706000
H	0.606228000	-0.470807000	0.164229000
Si	-1.751844000	-0.592351000	-0.041501000
O	-3.858429000	-0.421560000	-0.266953000
C	1.066607000	3.562891000	-0.918242000
C	2.964665000	2.875744000	-2.197752000
C	2.051055000	3.857669000	-1.848476000
C	2.493204000	-1.391389000	-0.792556000
C	1.792337000	-2.056157000	-1.791439000
C	3.803901000	-1.832805000	-0.625588000
C	2.305777000	-3.097625000	-2.552579000
C	4.366635000	-2.868049000	-1.361901000
C	3.611406000	-3.507457000	-2.334741000
C	2.381494000	-0.061436000	1.593993000
C	3.484553000	0.723510000	1.927843000
C	1.803608000	-0.720580000	2.671669000
C	3.959405000	0.874646000	3.223656000
C	2.237827000	-0.599411000	3.986679000
C	3.327768000	0.208569000	4.265046000

F	1.619154000	-1.253118000	4.973567000
F	0.745233000	-1.537126000	2.483947000
F	3.767248000	0.341969000	5.515201000
F	5.017968000	1.644327000	3.478757000
F	4.164988000	1.370768000	0.973693000
F	0.015978000	2.069300000	0.520072000
F	0.194665000	4.516984000	-0.560724000
F	2.117135000	5.071597000	-2.393254000
F	3.923594000	3.150239000	-3.081541000
F	3.827931000	0.747801000	-1.965418000
F	4.608605000	-1.245372000	0.267319000
F	5.627390000	-3.246743000	-1.152258000
F	4.134593000	-4.501274000	-3.050222000
F	1.559459000	-3.698174000	-3.483656000
F	0.509645000	-1.716590000	-2.062233000
C	1.012784000	2.290636000	-0.366060000
C	1.899241000	1.265944000	-0.682715000
C	-1.681329000	-2.460483000	-0.220342000
H	-2.609929000	-2.871227000	0.188500000
H	-1.687417000	-2.682133000	-1.293635000
C	-0.507735000	-3.199181000	0.445907000
H	-0.491531000	-4.234574000	0.092946000
H	0.459555000	-2.749249000	0.227776000
H	-0.616306000	-3.220486000	1.531215000
C	-1.701815000	0.029328000	1.718792000
H	-0.650745000	0.188401000	1.969012000
H	-2.158802000	1.019568000	1.760938000
C	-2.343921000	-0.942412000	2.718233000
H	-1.755744000	-1.859306000	2.795667000
H	-2.380813000	-0.497758000	3.717419000
H	-3.367914000	-1.221994000	2.444834000
C	-1.405407000	0.440366000	-1.560094000
H	-1.663932000	1.484215000	-1.361057000
H	-0.323136000	0.414023000	-1.704691000
C	-2.089613000	-0.079674000	-2.829320000
H	-1.885353000	0.588947000	-3.671089000
H	-1.708448000	-1.069526000	-3.100320000
H	-3.176996000	-0.146144000	-2.719304000
C	-4.717352000	0.769055000	-0.006978000
C	-4.697891000	-1.546946000	-0.229857000
C	-5.629961000	-1.596422000	0.803653000
C	-5.171636000	0.686006000	1.442715000
H	-3.955127000	-2.395958000	-2.047230000
C	-4.665912000	-2.502563000	-1.233796000

C	-6.493822000	-2.687847000	0.879405000
C	-6.426059000	-3.684783000	-0.086236000
C	-5.525302000	-3.592427000	-1.148399000
H	-7.209241000	-2.724314000	1.693546000
H	-7.096915000	-4.534677000	-0.019506000
H	-5.495253000	-4.361864000	-1.911360000
C	-4.040971000	2.033367000	-0.448394000
C	-3.313513000	2.857702000	0.413542000
C	-4.121983000	2.367219000	-1.803276000
C	-2.610317000	3.947880000	-0.086276000
H	-3.280565000	2.656485000	1.479425000
C	-3.426950000	3.461999000	-2.304320000
H	-4.714500000	1.747716000	-2.471964000
C	-2.649621000	4.239285000	-1.448213000
H	-2.013709000	4.556830000	0.582658000
H	-3.482833000	3.701194000	-3.361290000
H	-2.076073000	5.074624000	-1.835490000
C	2.879358000	1.619485000	-1.607482000
O	-5.724848000	-0.610324000	1.731899000
H	-4.309185000	0.810334000	2.105765000
H	-5.582947000	0.595706000	-0.656485000
C	-6.245929000	1.711956000	1.761663000
H	-5.854121000	2.728758000	1.685211000
H	-7.089256000	1.603916000	1.072895000
H	-6.607558000	1.546376000	2.778456000

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B, *E*(SCRF) = -3466.346487 a.u.

B	-1.589688000	-0.088013000	0.123627000
H	-0.483528000	0.215993000	-0.269914000
C	2.191651000	-0.309249000	-1.043480000
O	2.802992000	0.741607000	-0.115987000
C	-3.056473000	3.211693000	-1.349855000
C	-3.702564000	3.192707000	0.951926000
C	-3.689369000	3.829393000	-0.279221000
C	-1.437523000	-0.764610000	1.596628000
C	-0.223247000	-0.953597000	2.231428000
C	-2.528852000	-1.311525000	2.267373000
C	-0.062628000	-1.633563000	3.432308000
C	-2.429995000	-1.987186000	3.475222000
C	-1.180097000	-2.153452000	4.063128000
C	-2.159826000	-1.227866000	-0.901496000
C	-3.467659000	-1.322210000	-1.367448000
C	-1.306691000	-2.216074000	-1.376471000
C	-3.889328000	-2.297826000	-2.265813000

C	-1.673218000	-3.200613000	-2.281778000
C	-2.985610000	-3.242666000	-2.729236000
F	-0.782552000	-4.095281000	-2.721989000
F	-0.014448000	-2.244836000	-0.966844000
F	-3.372066000	-4.179140000	-3.595294000
F	-5.153897000	-2.335809000	-2.687502000
F	-4.398023000	-0.446748000	-0.969791000
F	-1.822444000	1.453551000	-2.223597000
F	-2.979014000	3.832842000	-2.532432000
F	-4.261223000	5.025113000	-0.430515000
F	-4.300510000	3.778804000	1.991979000
F	-3.131463000	1.422086000	2.327010000
F	-3.747884000	-1.187490000	1.732148000
F	-3.508658000	-2.487452000	4.077350000
F	-1.060682000	-2.808157000	5.217625000
F	1.156797000	-1.791213000	3.965220000
F	0.930896000	-0.483164000	1.682433000
C	-2.465711000	1.973280000	-1.159123000
C	-2.443157000	1.293522000	0.054817000
C	4.644737000	2.638626000	1.138355000
H	4.104213000	3.423746000	0.598545000
H	4.146266000	2.533481000	2.107438000
C	6.113301000	3.050907000	1.350299000
H	6.174399000	3.982609000	1.918339000
H	6.671903000	2.292046000	1.908737000
H	6.630506000	3.213715000	0.398778000
C	5.423277000	1.239534000	-1.471353000
H	6.498959000	1.277699000	-1.244038000
H	5.295864000	0.344070000	-2.086199000
C	5.004154000	2.504992000	-2.235472000
H	5.211102000	3.407390000	-1.651091000
H	5.553814000	2.591765000	-3.176691000
H	3.935370000	2.502583000	-2.472430000
C	5.162387000	-0.412916000	1.219986000
H	5.183675000	-1.330298000	0.622299000
H	6.208919000	-0.199157000	1.481245000
C	4.333079000	-0.604692000	2.499977000
H	4.660240000	-1.493479000	3.046306000
H	4.442542000	0.252323000	3.173236000
H	3.266650000	-0.725878000	2.287060000
Si	4.587435000	1.029060000	0.187441000
C	1.866898000	1.808335000	0.026095000
C	1.302082000	2.252435000	-1.161367000
C	2.042078000	0.334091000	-2.417899000

H	1.875267000	1.808894000	2.168268000
C	1.468441000	2.260180000	1.269986000
C	0.351930000	3.268304000	-1.107640000
C	-0.022557000	3.778145000	0.130483000
C	0.518782000	3.275360000	1.314827000
H	-0.113339000	3.600439000	-2.029955000
H	-0.782454000	4.552073000	0.174895000
H	0.180811000	3.653008000	2.273074000
C	2.982042000	-1.584006000	-0.968974000
C	3.942953000	-1.950150000	-1.916995000
C	2.733571000	-2.438322000	0.112336000
C	4.678070000	-3.121974000	-1.758141000
H	4.119555000	-1.341605000	-2.797747000
C	3.471596000	-3.604656000	0.273322000
H	1.961168000	-2.177609000	0.826688000
C	4.453484000	-3.943031000	-0.656131000
H	5.419563000	-3.396100000	-2.501415000
H	3.271744000	-4.254196000	1.119196000
H	5.028771000	-4.855218000	-0.533178000
C	-3.088386000	1.950203000	1.094365000
O	1.693715000	1.728838000	-2.350726000
H	2.999647000	0.325175000	-2.948483000
H	1.213264000	-0.446652000	-0.583639000
C	0.962792000	-0.393960000	-3.207193000
H	1.153295000	-1.470946000	-3.242109000
H	-0.006698000	-0.219547000	-2.729907000
H	0.929243000	-0.000022000	-4.224766000

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TS2, *E*(SCRF) = -3466.323185 a.u., IF= -233.05 cm^{-1}

B	1.820601000	0.135828000	0.014230000
H	0.655671000	-0.014336000	0.391826000
C	-1.558504000	-0.259173000	0.575812000
O	-3.536161000	0.213826000	0.154918000
C	1.201823000	4.025287000	-0.279380000
C	3.270574000	3.524198000	-1.381600000
C	2.305049000	4.449885000	-1.002452000
C	1.887985000	-0.719010000	-1.370249000
C	0.949271000	-0.436312000	-2.354966000
C	2.739554000	-1.776912000	-1.674088000
C	0.798510000	-1.162090000	-3.526344000
C	2.639384000	-2.525233000	-2.843508000
C	1.655508000	-2.223140000	-3.774131000
C	2.747474000	-0.461895000	1.207688000
C	3.877187000	0.128035000	1.763248000

C	2.401486000	-1.685769000	1.772699000
C	4.602491000	-0.441424000	2.807638000
C	3.085142000	-2.290379000	2.814117000
C	4.205719000	-1.658428000	3.336930000
F	2.681214000	-3.460840000	3.316907000
F	1.317435000	-2.346016000	1.307823000
F	4.884712000	-2.214422000	4.339102000
F	5.675601000	0.175809000	3.303098000
F	4.334736000	1.304965000	1.317014000
F	-0.013056000	2.335680000	0.749461000
F	0.260271000	4.899897000	0.092070000
F	2.441406000	5.734048000	-1.330625000
F	4.333835000	3.929958000	-2.076604000
F	4.064483000	1.336355000	-1.414884000
F	3.707973000	-2.145518000	-0.827780000
F	3.473100000	-3.539139000	-3.075737000
F	1.521138000	-2.954237000	-4.880804000
F	-0.209485000	-0.897120000	-4.366714000
F	0.045484000	0.551960000	-2.152962000
C	1.090777000	2.679771000	0.047446000
C	2.021052000	1.716106000	-0.305082000
C	-6.458494000	0.313432000	0.089923000
H	-6.378848000	1.254867000	0.646487000
H	-6.491830000	0.591036000	-0.970075000
C	-7.750742000	-0.425516000	0.475014000
H	-8.633383000	0.177647000	0.245659000
H	-7.852376000	-1.371906000	-0.067746000
H	-7.779209000	-0.653743000	1.545667000
C	-4.963086000	-1.324915000	2.211660000
H	-5.810820000	-2.015532000	2.321250000
H	-4.073198000	-1.934631000	2.415435000
C	-5.091511000	-0.173521000	3.220853000
H	-6.029559000	0.372234000	3.073613000
H	-5.084548000	-0.540401000	4.251235000
H	-4.276554000	0.552338000	3.121162000
C	-4.819531000	-2.182282000	-0.779980000
H	-3.957260000	-2.805457000	-0.512198000
H	-5.702158000	-2.821427000	-0.641408000
C	-4.722495000	-1.726567000	-2.242049000
H	-4.556933000	-2.572659000	-2.915427000
H	-5.641654000	-1.224726000	-2.562665000
H	-3.895411000	-1.023196000	-2.385323000
Si	-4.954880000	-0.757190000	0.424164000
C	-3.504547000	1.597551000	0.173744000

C	-2.765337000	2.202623000	1.189988000
C	-1.702018000	0.156563000	2.007657000
H	-4.585149000	1.848005000	-1.655291000
C	-4.066819000	2.356351000	-0.847879000
C	-2.628915000	3.589135000	1.202847000
C	-3.230166000	4.352441000	0.211654000
C	-3.948891000	3.740450000	-0.816195000
H	-2.017421000	4.036162000	1.978394000
H	-3.110142000	5.430343000	0.224317000
H	-4.394651000	4.336983000	-1.604431000
C	-1.490564000	-1.633658000	0.155297000
C	-1.527394000	-2.711831000	1.060779000
C	-1.419340000	-1.891505000	-1.225790000
C	-1.466212000	-4.012098000	0.587847000
H	-1.573279000	-2.533510000	2.130624000
C	-1.361623000	-3.195710000	-1.695065000
H	-1.431427000	-1.058152000	-1.919585000
C	-1.378521000	-4.253149000	-0.786984000
H	-1.472730000	-4.842421000	1.285322000
H	-1.296915000	-3.382316000	-2.762483000
H	-1.322245000	-5.275214000	-1.148590000
C	3.108341000	2.191065000	-1.031704000
O	-2.160497000	1.494930000	2.187816000
H	-2.451653000	-0.508586000	2.452235000
H	-1.312709000	0.502253000	-0.159099000
C	-0.406524000	0.031104000	2.814633000
H	0.020575000	-0.968353000	2.715214000
H	0.317408000	0.762898000	2.458940000
H	-0.649181000	0.229968000	3.861133000

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C, *E*(SCRF) = -1258.1524178 a.u.

H	-1.201590000	-3.437387000	-0.259694000
C	-0.899488000	-2.381693000	-0.240292000
O	0.412856000	0.252414000	-0.363093000
C	1.613190000	2.886256000	0.078137000
H	2.578364000	2.379361000	0.202517000
H	1.552625000	3.160120000	-0.982901000
C	1.563253000	4.152268000	0.945999000
H	2.340078000	4.868391000	0.661496000
H	0.597895000	4.663670000	0.854672000
H	1.708903000	3.913726000	2.004855000
C	0.206855000	1.345739000	2.337856000
H	0.047502000	2.298705000	2.861159000
H	-0.667097000	0.727435000	2.581939000

C	1.495763000	0.677025000	2.836330000
H	2.373015000	1.295399000	2.614006000
H	1.476121000	0.514159000	3.918634000
H	1.653017000	-0.295963000	2.357671000
C	-1.454222000	2.328464000	-0.080633000
H	-2.184398000	1.532244000	0.118326000
H	-1.757979000	3.185476000	0.534765000
C	-1.479769000	2.697469000	-1.568332000
H	-2.492256000	2.944190000	-1.904596000
H	-0.840002000	3.562330000	-1.776830000
H	-1.124583000	1.861217000	-2.180536000
Si	0.211665000	1.698907000	0.490747000
C	1.574967000	-0.353341000	-0.741559000
C	1.963794000	-1.574770000	-0.164387000
C	-0.103682000	-2.113575000	1.051392000
H	2.001942000	1.116134000	-2.222812000
C	2.348173000	0.192259000	-1.768365000
C	3.138934000	-2.187276000	-0.604741000
C	3.920916000	-1.616385000	-1.600216000
C	3.520836000	-0.421202000	-2.192216000
H	3.414557000	-3.125932000	-0.135211000
H	4.832136000	-2.111526000	-1.919534000
H	4.110917000	0.029011000	-2.983617000
C	-2.115537000	-1.498481000	-0.415555000
C	-3.032025000	-1.287080000	0.619580000
C	-2.353756000	-0.873911000	-1.642786000
C	-4.157110000	-0.487087000	0.429751000
H	-2.873518000	-1.754047000	1.587968000
C	-3.481515000	-0.082949000	-1.842184000
H	-1.636318000	-1.006102000	-2.449009000
C	-4.389714000	0.114129000	-0.804652000
H	-4.854735000	-0.337569000	1.248465000
H	-3.643614000	0.390546000	-2.806192000
H	-5.267786000	0.734647000	-0.954734000
O	1.314398000	-2.216877000	0.849639000
H	-0.339623000	-1.109287000	1.410536000
H	-0.240858000	-2.234723000	-1.101795000
C	-0.381007000	-3.128396000	2.149158000
H	-1.443354000	-3.149593000	2.406228000
H	-0.086835000	-4.126697000	1.811344000
H	0.193010000	-2.881708000	3.046344000

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TS3, *E*(SCRF) = -3994.116249 a.u., IF= -91.90 cm^{-1}

O	2.317551000	-0.693004000	1.173991000

Si	0.378554000	-0.072737000	0.670063000
B	-2.917824000	-0.030423000	-0.150337000
H	-1.759445000	0.306392000	0.155997000
H	4.180635000	3.984569000	-0.176900000
H	5.832882000	4.035589000	0.417152000
C	5.657058000	4.499936000	-1.687244000
H	5.639611000	5.579468000	-1.513846000
H	6.677028000	4.233762000	-1.987596000
H	4.999455000	4.291004000	-2.536722000
C	4.885530000	1.352037000	-2.415524000
H	5.509870000	1.915418000	-3.121313000
H	5.163391000	0.298336000	-2.546461000
C	3.399477000	1.551989000	-2.731724000
H	3.091624000	2.596025000	-2.597796000
H	3.154670000	1.263177000	-3.758331000
H	2.781693000	0.949106000	-2.057908000
C	7.055675000	1.198811000	-0.242748000
H	7.155378000	0.206995000	-0.703338000
H	7.788961000	1.841557000	-0.751111000
C	7.389764000	1.111062000	1.251076000
H	8.385204000	0.684351000	1.409316000
H	7.372401000	2.095864000	1.731088000
H	6.673154000	0.475274000	1.783057000
Si	5.352815000	1.859571000	-0.674603000
C	3.827318000	1.162145000	1.572766000
C	2.937075000	0.196404000	2.065307000
C	3.190377000	-1.576830000	0.342114000
H	5.003548000	2.874873000	2.107899000
C	4.323667000	2.110203000	2.467644000
C	2.603822000	0.125066000	3.407160000
C	3.108208000	1.077697000	4.289868000
C	3.954592000	2.072380000	3.810745000
H	1.939300000	-0.665278000	3.741348000
H	2.838863000	1.039857000	5.339199000
H	4.346843000	2.824163000	4.487510000
C	5.677468000	-2.138145000	0.080999000
C	5.557221000	-2.216923000	-1.307397000
C	6.950777000	-2.289278000	0.644495000
C	6.681393000	-2.416829000	-2.111342000
H	4.589107000	-2.121761000	-1.790848000
C	8.070954000	-2.491695000	-0.151224000
H	7.060577000	-2.233149000	1.725415000
C	7.940491000	-2.549780000	-1.538983000
H	6.563165000	-2.470156000	-3.189261000

H	9.047651000	-2.599655000	0.310285000
H	8.813225000	-2.703535000	-2.165294000
H	4.400577000	-2.705582000	1.717206000
H	3.361439000	-1.004624000	-0.570056000
H	4.831206000	-1.014177000	1.650128000
C	2.454779000	-2.876491000	0.073888000
H	3.060642000	-3.468958000	-0.619490000
H	2.344473000	-3.452326000	0.994548000
H	1.469613000	-2.740030000	-0.373128000
O	4.160404000	1.076185000	0.269087000
C	5.215422000	3.724515000	-0.435740000
C	4.525276000	-1.858889000	1.030057000
C	-5.556686000	-1.179199000	2.580889000
C	-5.268854000	-0.321553000	3.633118000
C	-2.731798000	-1.402310000	-1.017195000
C	-2.460340000	-2.624384000	-0.402626000
C	-2.622544000	-1.434224000	-2.405750000
C	-2.042297000	-3.763921000	-1.076256000
C	-2.218035000	-2.554069000	-3.126867000
C	-1.914688000	-3.729217000	-2.457819000
C	-3.585348000	1.211622000	-0.960911000
C	-4.829081000	1.069164000	-1.569357000
C	-3.040250000	2.484540000	-1.031761000
C	-5.490543000	2.101584000	-2.216192000
C	-3.663439000	3.552629000	-1.669132000
C	-4.899817000	3.358800000	-2.262923000
F	-3.083316000	4.754539000	-1.713252000
F	-1.833838000	2.746208000	-0.488511000
F	-5.516103000	4.367341000	-2.877717000
F	-6.679216000	1.908122000	-2.788463000
F	-5.431451000	-0.127425000	-1.547410000
F	-2.517391000	1.534093000	2.250084000
F	-3.938076000	1.415339000	4.511637000
F	-5.974759000	-0.380110000	4.761307000
F	-6.545055000	-2.065621000	2.704580000
F	-5.128622000	-1.975184000	0.447194000
F	-2.853612000	-0.338048000	-3.143974000
F	-2.100130000	-2.498212000	-4.454187000
F	-1.512095000	-4.807736000	-3.127553000
F	-1.753027000	-4.881849000	-0.405332000
F	-2.557033000	-2.755999000	0.933599000
C	-3.515765000	0.630606000	2.314858000
C	-3.760803000	-0.206640000	1.232380000
C	0.453915000	-0.575215000	-1.146781000

H	1.490740000	-0.812044000	-1.406664000
H	-0.108433000	-1.510295000	-1.257355000
C	-0.069829000	0.464492000	-2.149574000
H	-0.133337000	0.016120000	-3.146154000
H	-1.063716000	0.829686000	-1.890414000
H	0.599659000	1.325303000	-2.211757000
C	0.497133000	1.742936000	1.111860000
H	-0.545350000	2.052101000	1.237998000
H	0.943484000	1.803860000	2.110426000
C	1.204088000	2.702398000	0.145644000
H	0.575602000	2.904807000	-0.723560000
H	1.395627000	3.659614000	0.641330000
H	2.163451000	2.311324000	-0.206126000
C	-0.391771000	-1.061376000	2.068403000
H	-0.214243000	-0.452717000	2.966164000
H	-1.471762000	-1.036534000	1.914111000
C	0.037858000	-2.509158000	2.313652000
H	-0.550580000	-2.939765000	3.128702000
H	-0.132413000	-3.137941000	1.434537000
H	1.095263000	-2.580092000	2.587104000
C	-4.808327000	-1.105676000	1.412080000
C	-4.232607000	0.591104000	3.503316000

111

D, *E*(SCRF) = -3994.128570 a.u.

O	-2.603766000	-1.006903000	1.542633000
C	-1.080645000	-0.739457000	1.587988000
H	1.125510000	-0.084365000	0.295128000
B	2.257661000	-0.212787000	-0.118052000
H	-5.224398000	0.482970000	-2.178771000
H	-5.358430000	2.191353000	-1.820718000
C	-5.020660000	1.768931000	-3.918821000
H	-6.082175000	1.759059000	-4.182829000
H	-4.626021000	2.755678000	-4.185371000
H	-4.516364000	1.031995000	-4.553323000
C	-2.031654000	0.241492000	-3.042477000
H	-1.974815000	0.612007000	-4.073793000
H	-1.000912000	0.202282000	-2.673121000
C	-2.656373000	-1.156248000	-3.005178000
H	-3.666884000	-1.159051000	-3.433069000
H	-2.055294000	-1.889896000	-3.547817000
H	-2.731554000	-1.503582000	-1.969739000
C	-2.233107000	3.188862000	-2.209718000
H	-1.190395000	3.162960000	-1.878047000
H	-2.176707000	3.311678000	-3.302286000

C	-2.974390000	4.386865000	-1.607046000
H	-2.542825000	5.330515000	-1.954834000
H	-4.035212000	4.391254000	-1.887307000
H	-2.909173000	4.384992000	-0.515133000
Si	-2.968201000	1.478088000	-2.000384000
C	-3.502986000	1.067720000	0.694964000
C	-3.418556000	0.135857000	1.737240000
Si	-3.522972000	-2.486402000	0.931360000
H	-4.372526000	2.951984000	0.145514000
C	-4.304469000	2.189956000	0.914131000
C	-4.106899000	0.263909000	2.928738000
C	-4.918522000	1.379470000	3.118786000
C	-5.001007000	2.336596000	2.111311000
H	-3.986952000	-0.496799000	3.694806000
H	-5.463697000	1.504335000	4.047389000
H	-5.613891000	3.220362000	2.256015000
C	-1.024661000	1.743277000	2.392816000
C	-0.514806000	2.315939000	1.225481000
C	-1.698326000	2.553831000	3.305992000
C	-0.693693000	3.670637000	0.966348000
H	0.022735000	1.694290000	0.518340000
C	-1.879889000	3.910952000	3.049706000
H	-2.090549000	2.119349000	4.222512000
C	-1.381983000	4.472249000	1.877243000
H	-0.282964000	4.102095000	0.056208000
H	-2.410000000	4.528690000	3.768568000
H	-1.517678000	5.531014000	1.677172000
H	0.297527000	0.163512000	2.867656000
H	-0.866653000	-0.365149000	0.588047000
H	-1.285509000	-0.029870000	3.607654000
C	-4.803866000	1.466299000	-2.427730000
C	2.722604000	1.274923000	-0.603910000
C	1.814170000	2.083457000	-1.275071000
C	3.959332000	1.867369000	-0.371922000
C	2.054532000	3.401021000	-1.631333000
C	4.258381000	3.178401000	-0.731646000
C	3.295834000	3.956282000	-1.358093000
C	2.203209000	-1.215214000	-1.396937000
C	1.041329000	-1.834265000	-1.823066000
C	3.325493000	-1.486788000	-2.174058000
C	0.973863000	-2.702974000	-2.905277000
C	3.311034000	-2.331977000	-3.274372000
C	2.120295000	-2.949724000	-3.642061000
C	3.122998000	-0.755651000	1.154563000

C	3.057240000	-0.023199000	2.339012000
C	3.896028000	-1.908468000	1.237096000
C	3.690340000	-0.382545000	3.518994000
C	4.554799000	-2.309193000	2.397222000
C	4.454210000	-1.541519000	3.545684000
F	5.276353000	-3.431657000	2.413758000
F	4.040615000	-2.725909000	0.183260000
F	5.071903000	-1.915481000	4.666204000
F	3.570479000	0.362199000	4.620771000
F	2.321110000	1.106422000	2.376641000
F	0.586596000	1.599139000	-1.583860000
F	1.096445000	4.142971000	-2.206463000
F	3.557928000	5.219064000	-1.693895000
F	5.458294000	3.699518000	-0.473366000
F	4.935394000	1.188232000	0.242013000
F	4.495628000	-0.931230000	-1.842015000
F	4.416874000	-2.566880000	-3.980622000
F	2.084595000	-3.774422000	-4.688209000
F	-0.181924000	-3.302188000	-3.232616000
F	-0.132460000	-1.618462000	-1.174681000
C	-0.777664000	0.278987000	2.685069000
O	-2.804346000	0.814194000	-0.420186000
C	-3.950684000	-3.352037000	2.539345000
H	-3.088202000	-3.271990000	3.213534000
H	-4.776390000	-2.820318000	3.029142000
C	-4.315855000	-4.833189000	2.341372000
H	-5.189993000	-4.954616000	1.694266000
H	-3.489142000	-5.390055000	1.889300000
H	-4.547873000	-5.309298000	3.297788000
C	-5.028669000	-1.801346000	0.041931000
H	-5.377683000	-0.881205000	0.518905000
H	-4.737613000	-1.531517000	-0.980513000
C	-6.187889000	-2.815144000	0.020372000
H	-5.911571000	-3.759509000	-0.457467000
H	-6.534717000	-3.040564000	1.034077000
H	-7.038315000	-2.407041000	-0.532609000
C	-2.455216000	-3.541188000	-0.192980000
H	-1.713830000	-2.929926000	-0.713651000
H	-1.894107000	-4.256196000	0.420127000
C	-3.283911000	-4.310643000	-1.237595000
H	-2.613719000	-4.858841000	-1.905047000
H	-3.960990000	-5.035753000	-0.774032000
H	-3.881165000	-3.635509000	-1.858915000
C	-0.390389000	-2.053284000	1.870937000

H	0.685202000	-1.849069000	1.887539000
H	-0.683641000	-2.449345000	2.849147000
H	-0.551415000	-2.798104000	1.096014000

111

TS4, *E*(SCRF) = -3994.108201 a.u., IF= -435.45 cm^{-1}

O	-2.543161000	-1.157449000	1.515647000
C	-0.551914000	-0.710724000	1.328480000
H	1.054988000	-0.090123000	0.335683000
B	2.196071000	-0.217542000	-0.129570000
H	-5.462878000	0.714763000	-1.696966000
H	-5.465578000	2.400533000	-1.226927000
C	-5.425695000	2.099122000	-3.373033000
H	-6.511054000	2.175907000	-3.486321000
H	-4.998625000	3.071454000	-3.644349000
H	-5.068649000	1.368783000	-4.106877000
C	-2.422626000	0.458347000	-3.042299000
H	-2.578580000	0.913719000	-4.029302000
H	-1.338700000	0.423208000	-2.892459000
C	-3.000668000	-0.958876000	-3.010483000
H	-4.076155000	-0.960201000	-3.228569000
H	-2.507567000	-1.617194000	-3.730771000
H	-2.860646000	-1.399558000	-2.018944000
C	-2.359645000	3.293001000	-1.929381000
H	-1.306044000	3.204497000	-1.641241000
H	-2.334810000	3.466013000	-3.015773000
C	-3.020090000	4.494644000	-1.245022000
H	-2.571322000	5.435231000	-1.580000000
H	-4.092661000	4.548183000	-1.467886000
H	-2.902041000	4.450380000	-0.158514000
Si	-3.159531000	1.601702000	-1.757159000
C	-3.394132000	1.007153000	0.937186000
C	-3.261219000	-0.028577000	1.877700000
Si	-3.465449000	-2.528351000	0.924716000
H	-4.176013000	2.980502000	0.624186000
C	-4.083251000	2.155813000	1.322517000
C	-3.809972000	0.067796000	3.147677000
C	-4.510192000	1.216105000	3.513515000
C	-4.636564000	2.254810000	2.598214000
H	-3.673898000	-0.761356000	3.837055000
H	-4.940732000	1.297829000	4.505541000
H	-5.163548000	3.162261000	2.874880000
C	-0.690775000	1.642084000	2.394425000
C	-0.384227000	2.354867000	1.234640000
C	-1.247876000	2.318508000	3.479552000

C	-0.631658000	3.721977000	1.163629000
H	0.037521000	1.838051000	0.381203000
C	-1.501415000	3.685262000	3.408186000
H	-1.496058000	1.769503000	4.384704000
C	-1.193078000	4.391864000	2.249245000
H	-0.375085000	4.266550000	0.258325000
H	-1.942185000	4.195913000	4.258994000
H	-1.383394000	5.459351000	2.191990000
H	0.697361000	0.060101000	2.789464000
H	-0.855219000	-0.297047000	0.375335000
H	-0.917145000	-0.284500000	3.352078000
C	-5.031878000	1.694131000	-1.944054000
C	2.596938000	1.255099000	-0.699064000
C	1.674394000	1.946557000	-1.475574000
C	3.808755000	1.912123000	-0.516652000
C	1.882294000	3.215515000	-1.992706000
C	4.072928000	3.178670000	-1.029048000
C	3.102701000	3.837383000	-1.769645000
C	2.106167000	-1.229061000	-1.399609000
C	0.925828000	-1.647119000	-1.991675000
C	3.262904000	-1.650689000	-2.050676000
C	0.865364000	-2.475577000	-3.105898000
C	3.259739000	-2.468045000	-3.171114000
C	2.045093000	-2.888482000	-3.702603000
C	3.084771000	-0.719001000	1.134014000
C	3.229170000	0.138828000	2.225327000
C	3.674123000	-1.968898000	1.303903000
C	3.927421000	-0.177764000	3.380580000
C	4.387749000	-2.331299000	2.443655000
C	4.518519000	-1.429941000	3.487535000
F	4.929050000	-3.545367000	2.545609000
F	3.562702000	-2.921833000	0.366762000
F	5.186834000	-1.765606000	4.588443000
F	4.024289000	0.691761000	4.386509000
F	2.651840000	1.353185000	2.185746000
F	0.467583000	1.384684000	-1.724400000
F	0.926781000	3.839929000	-2.689631000
F	3.336320000	5.053275000	-2.259089000
F	5.249380000	3.766513000	-0.815549000
F	4.793257000	1.345423000	0.190251000
F	4.452243000	-1.264777000	-1.574174000
F	4.397718000	-2.853973000	-3.745830000
F	2.018059000	-3.680165000	-4.772468000
F	-0.315154000	-2.873333000	-3.594688000

F	-0.274641000	-1.265027000	-1.489369000
C	-0.364044000	0.172212000	2.519046000
O	-2.814227000	0.824095000	-0.268974000
C	-3.834739000	-3.551457000	2.461096000
H	-2.954341000	-3.498719000	3.116452000
H	-4.655422000	-3.082194000	3.019689000
C	-4.166511000	-5.022785000	2.166161000
H	-5.059050000	-5.120513000	1.540242000
H	-3.341880000	-5.517406000	1.642376000
H	-4.351010000	-5.580924000	3.088580000
C	-5.032591000	-1.860503000	0.126705000
H	-5.366667000	-0.972153000	0.675201000
H	-4.792911000	-1.521361000	-0.888523000
C	-6.176945000	-2.886945000	0.089081000
H	-5.902368000	-3.793214000	-0.459968000
H	-6.472242000	-3.187500000	1.099788000
H	-7.061332000	-2.465931000	-0.397925000
C	-2.393891000	-3.478713000	-0.291469000
H	-1.741187000	-2.778925000	-0.822856000
H	-1.734973000	-4.163292000	0.257399000
C	-3.214724000	-4.269987000	-1.323863000
H	-2.552650000	-4.758604000	-2.044289000
H	-3.827378000	-5.046612000	-0.853643000
H	-3.883475000	-3.612659000	-1.889874000
C	-0.008893000	-2.096003000	1.432638000
H	1.013363000	-2.040567000	1.822009000
H	-0.598326000	-2.667366000	2.157881000
H	0.008826000	-2.607936000	0.473458000

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P1, *E*(SCRF) = -1435.803828 a.u.

O	1.488962000	1.040237000	-0.620684000
C	1.836475000	-1.841355000	-0.314852000
H	0.826232000	-2.047668000	0.053345000
H	1.768342000	-1.831791000	-1.410663000
C	2.812351000	-2.928764000	0.154210000
H	2.474977000	-3.929576000	-0.133511000
H	3.809780000	-2.780858000	-0.273801000
H	2.924764000	-2.924307000	1.245191000
C	1.993088000	0.093854000	2.125385000
H	2.943780000	-0.089888000	2.644147000
H	1.757629000	1.151535000	2.304780000
C	0.896141000	-0.796888000	2.725689000
H	1.133224000	-1.858995000	2.592612000
H	0.781727000	-0.619274000	3.799828000

H	-0.069574000	-0.614959000	2.245564000
C	4.127267000	0.190895000	-0.117445000
H	4.388208000	1.195388000	0.240174000
H	4.753543000	-0.507981000	0.453137000
C	4.427254000	0.071776000	-1.617382000
H	5.474283000	0.295779000	-1.844703000
H	4.220589000	-0.940665000	-1.982716000
H	3.803038000	0.761380000	-2.194102000
O	-0.914747000	-0.022435000	0.118392000
C	-3.717266000	-0.730952000	0.579503000
H	-4.326416000	0.162412000	0.390101000
H	-4.365830000	-1.585881000	0.342631000
C	-3.307396000	-0.783197000	2.059963000
H	-4.181079000	-0.766302000	2.718920000
H	-2.738468000	-1.689922000	2.287389000
H	-2.669655000	0.065882000	2.326885000
C	-1.715457000	-2.539426000	-0.928811000
H	-2.448968000	-2.995131000	-1.608496000
H	-0.768090000	-2.515078000	-1.480385000
C	-1.573384000	-3.402316000	0.332788000
H	-2.542917000	-3.547021000	0.821175000
H	-1.170093000	-4.393063000	0.100376000
H	-0.905224000	-2.937273000	1.066993000
C	-2.576322000	0.141599000	-2.219642000
H	-3.430594000	-0.313750000	-2.737140000
H	-2.870795000	1.173223000	-1.989345000
C	-1.333283000	0.140865000	-3.123001000
H	-1.490570000	0.737713000	-4.026386000
H	-0.462155000	0.549176000	-2.598264000
H	-1.077155000	-0.875853000	-3.439709000
Si	-2.253771000	-0.770580000	-0.612096000
C	-0.752696000	1.332003000	0.183277000
C	0.503278000	1.856966000	-0.167709000
Si	2.318798000	-0.130319000	0.280656000
H	-2.731548000	1.787626000	0.871861000
C	-1.764270000	2.197939000	0.596660000
C	0.720123000	3.230002000	-0.094771000
C	-0.296205000	4.088909000	0.316269000
C	-1.539856000	3.571972000	0.660633000
H	1.698352000	3.604096000	-0.380150000
H	-0.112938000	5.157296000	0.364921000
H	-2.339550000	4.230603000	0.983257000

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P2, *E*(SCRF) = -350.123579 a.u.

H	1.529188000	-1.295455000	0.874538000
C	1.333187000	-0.659672000	-0.000040000
H	2.157016000	1.129670000	0.879260000
C	2.329173000	0.496822000	-0.000001000
H	1.529173000	-1.295378000	-0.874678000
H	2.157068000	1.129686000	-0.879261000
C	-0.133542000	-0.277495000	-0.000009000
C	-1.098547000	-1.291667000	0.000004000
C	-0.570814000	1.047216000	-0.000012000
C	-2.455477000	-0.994624000	0.000014000
H	-0.772914000	-2.329847000	0.000005000
C	-1.932401000	1.351143000	-0.000001000
H	0.151239000	1.857788000	-0.000019000
C	-2.879093000	0.333918000	0.000013000
H	-3.184842000	-1.799223000	0.000028000
H	-2.249642000	2.389761000	-0.000002000
H	-3.938523000	0.570750000	0.000022000
C	3.772644000	0.000416000	0.000031000
H	3.974977000	-0.613491000	-0.883929000
H	4.481557000	0.832929000	0.000069000
H	3.974926000	-0.613528000	0.883977000

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TS1', *E*(SCRF) = -3466.335667 a.u., IF= -71.60 cm^{-1}

B	2.123762000	0.191714000	0.029409000
H	0.916590000	-0.083925000	0.089455000
Si	-1.364365000	-0.387218000	-0.252596000
O	-3.363669000	-0.601984000	-0.744453000
C	1.190209000	3.757086000	-1.396333000
C	3.387348000	3.235383000	-2.182156000
C	2.307401000	4.106423000	-2.137572000
C	2.875862000	-1.022933000	-0.775533000
C	2.255644000	-1.807154000	-1.738874000
C	4.207711000	-1.367469000	-0.538314000
C	2.858953000	-2.870752000	-2.398766000
C	4.858449000	-2.417703000	-1.172558000
C	4.176919000	-3.181288000	-2.110059000
C	2.648935000	0.234667000	1.571304000
C	3.433577000	1.228187000	2.146172000
C	2.333451000	-0.819053000	2.421659000
C	3.849248000	1.199833000	3.473687000
C	2.716967000	-0.890212000	3.752129000
C	3.489492000	0.133297000	4.282976000
F	2.350755000	-1.919208000	4.519665000
F	1.565992000	-1.834656000	1.968007000

F	3.875655000	0.093150000	5.557204000
F	4.596483000	2.184826000	3.973541000
F	3.841943000	2.283146000	1.427950000
F	0.060532000	2.291170000	-0.003636000
F	0.134691000	4.575528000	-1.341121000
F	2.343776000	5.261663000	-2.798646000
F	4.471187000	3.566378000	-2.883122000
F	4.415227000	1.257610000	-1.561238000
F	4.946127000	-0.662557000	0.325724000
F	6.132713000	-2.695327000	-0.897906000
F	4.784124000	-4.192156000	-2.728339000
F	2.182644000	-3.583085000	-3.304563000
F	0.975709000	-1.560248000	-2.102900000
C	1.185435000	2.547698000	-0.714685000
C	2.221710000	1.623151000	-0.747261000
C	-0.897840000	-2.186104000	0.004427000
H	-1.091574000	-2.771388000	-0.900131000
C	-1.743954000	0.489848000	1.365520000
H	-2.103136000	1.506365000	1.171771000
C	-0.996574000	0.438811000	-1.896900000
H	-1.357878000	1.470347000	-1.872265000
H	0.090163000	0.506354000	-1.971287000
C	-1.539056000	-0.315933000	-3.117282000
H	-1.206080000	0.166905000	-4.040393000
H	-1.167072000	-1.344980000	-3.142445000
H	-2.633521000	-0.349283000	-3.135080000
C	-4.423180000	0.423996000	-0.739751000
C	-3.978055000	-1.848049000	-0.548305000
C	-4.896568000	-1.911185000	0.494506000
C	-5.047843000	0.481493000	0.662070000
H	-3.030500000	-2.810333000	-2.207757000
C	-3.718401000	-2.925032000	-1.376286000
C	-5.524014000	-3.123016000	0.767583000
C	-5.223436000	-4.234284000	-0.015719000
C	-4.337168000	-4.139309000	-1.089153000
H	-6.227159000	-3.172034000	1.591880000
H	-5.701273000	-5.182824000	0.205044000
H	-4.130777000	-5.006223000	-1.706362000
C	3.326665000	2.031480000	-1.491369000
O	-5.150278000	-0.818696000	1.261932000
H	-4.396024000	1.066891000	1.317462000
H	-5.162405000	0.035139000	-1.448750000
C	-6.413660000	1.126273000	0.595605000
C	-6.583750000	2.458736000	0.967590000

C	-7.506620000	0.394519000	0.126403000
C	-7.834741000	3.062123000	0.861959000
H	-5.736588000	3.025024000	1.347978000
C	-8.756666000	0.995063000	0.027103000
H	-7.380405000	-0.651254000	-0.145233000
C	-8.921276000	2.330642000	0.391624000
H	-7.960558000	4.099004000	1.156313000
H	-9.604698000	0.420868000	-0.332052000
H	-9.897795000	2.797763000	0.314436000
C	-3.919511000	1.764931000	-1.221327000
H	-4.768203000	2.454524000	-1.232612000
H	-3.149476000	2.182462000	-0.568277000
H	-3.529475000	1.688891000	-2.237605000
C	-0.621235000	0.539262000	2.408682000
H	-1.012758000	0.906833000	3.361752000
H	-0.189341000	-0.448968000	2.578645000
H	0.182975000	1.200894000	2.086561000
H	-2.588949000	-0.081160000	1.778742000
C	-1.457225000	-2.882160000	1.253810000
H	-0.956435000	-3.844302000	1.392279000
H	-1.272511000	-2.293791000	2.156757000
H	-2.531035000	-3.075522000	1.189951000
H	0.192554000	-2.148038000	0.095476000

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B', *E*(SCRF) = -3466.346202 a.u.

B	1.550761000	-0.316099000	0.104568000
H	0.541118000	0.338354000	0.024362000
C	-1.946117000	1.105060000	0.333578000
O	-3.231122000	0.318920000	0.153230000
C	0.570805000	-2.354773000	-3.140018000
C	2.659528000	-3.206955000	-2.330001000
C	1.616748000	-3.256333000	-3.248733000
C	1.401978000	-1.242719000	1.441420000
C	0.185801000	-1.855887000	1.715683000
C	2.417590000	-1.537419000	2.344594000
C	-0.040546000	-2.686720000	2.802772000
C	2.239063000	-2.360172000	3.453112000
C	1.000848000	-2.940405000	3.683844000
C	2.732999000	0.793690000	0.199851000
C	3.776252000	0.991899000	-0.695671000
C	2.640065000	1.758847000	1.198517000
C	4.656207000	2.069059000	-0.620580000
C	3.486414000	2.848504000	1.314006000
C	4.509873000	3.005002000	0.389689000

F	3.299851000	3.770448000	2.263755000
F	1.646570000	1.678999000	2.109257000
F	5.316879000	4.066624000	0.452272000
F	5.627618000	2.218472000	-1.524744000
F	3.973459000	0.156672000	-1.727395000
F	-0.473075000	-0.578548000	-2.071918000
F	-0.443262000	-2.397318000	-4.015559000
F	1.624056000	-4.163553000	-4.225871000
F	3.666098000	-4.076086000	-2.430379000
F	3.638396000	-2.251627000	-0.445289000
F	3.639955000	-1.020699000	2.183725000
F	3.244727000	-2.602040000	4.294126000
F	0.809140000	-3.733618000	4.738019000
F	-1.240852000	-3.246129000	3.011603000
F	-0.877192000	-1.646504000	0.891908000
C	0.587332000	-1.420069000	-2.110458000
C	1.601506000	-1.325660000	-1.171430000
C	-6.064480000	-0.344600000	0.060493000
H	-6.089389000	0.110768000	-0.936289000
H	-5.811324000	-1.398993000	-0.091775000
C	-7.441850000	-0.227241000	0.738951000
H	-8.214352000	-0.704117000	0.130645000
H	-7.451718000	-0.714576000	1.719485000
H	-7.737742000	0.817675000	0.882263000
C	-5.149816000	2.323909000	1.291588000
H	-5.948881000	2.376238000	2.045907000
H	-4.304177000	2.856026000	1.741518000
C	-5.611583000	3.009362000	-0.004221000
H	-6.530724000	2.551819000	-0.383756000
H	-5.819793000	4.068586000	0.168286000
H	-4.859227000	2.941554000	-0.796716000
C	-4.437675000	-0.399357000	2.710920000
H	-3.746869000	0.175156000	3.336848000
H	-5.388860000	-0.421369000	3.261429000
C	-3.917841000	-1.827193000	2.487172000
H	-3.730760000	-2.333574000	3.436706000
H	-4.645360000	-2.428595000	1.930467000
H	-2.976907000	-1.831469000	1.930533000
Si	-4.775892000	0.500298000	1.115239000
C	-3.267297000	-0.095406000	-1.206843000
C	-2.986713000	0.907542000	-2.124391000
C	-2.117911000	2.404685000	-0.445129000
H	-3.514981000	-2.176999000	-0.769288000
C	-3.396240000	-1.428401000	-1.546825000

C	-2.930515000	0.568783000	-3.473836000
C	-3.110907000	-0.757899000	-3.847544000
C	-3.331019000	-1.756463000	-2.896567000
H	-2.708650000	1.345911000	-4.196860000
H	-3.037703000	-1.027039000	-4.895668000
H	-3.416573000	-2.792039000	-3.204454000
C	2.624124000	-2.258235000	-1.318867000
O	-2.763905000	2.185032000	-1.717179000
H	-2.779597000	3.079917000	0.110343000
H	-1.217951000	0.452986000	-0.149473000
C	-0.773749000	3.068387000	-0.646220000
C	-0.390321000	4.129712000	0.172414000
C	0.100351000	2.594055000	-1.625660000
C	0.859262000	4.722652000	0.010798000
H	-1.071249000	4.497135000	0.937436000
C	1.341835000	3.197524000	-1.797099000
H	-0.183271000	1.744380000	-2.240488000
C	1.719772000	4.265198000	-0.983956000
H	1.158906000	5.541126000	0.657214000
H	2.020497000	2.824623000	-2.557823000
H	2.691297000	4.732084000	-1.116028000
C	-1.606939000	1.261711000	1.789986000
H	-2.265781000	1.962854000	2.312697000
H	-1.624895000	0.285513000	2.280717000
H	-0.578494000	1.632900000	1.843563000

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TS2', *E*(SCRF) = -3466.314007 a.u., IF= -537.13 cm^{-1}

B	1.474296000	-0.395622000	0.160408000
H	0.461756000	0.323904000	-0.022655000
C	-1.405421000	0.783911000	0.170450000
O	-3.398453000	0.389671000	0.026635000
C	0.585718000	-2.537774000	-3.045751000
C	2.355386000	-3.643438000	-1.864841000
C	1.465078000	-3.602678000	-2.932224000
C	1.252648000	-1.117964000	1.609933000
C	0.102217000	-1.869942000	1.831832000
C	2.134286000	-1.096873000	2.687457000
C	-0.198152000	-2.521100000	3.018110000
C	1.883031000	-1.738976000	3.897282000
C	0.708556000	-2.455383000	4.066902000
C	2.700001000	0.662238000	0.085583000
C	3.731193000	0.659962000	-0.848124000
C	2.720565000	1.742209000	0.962421000
C	4.707295000	1.651836000	-0.910790000

C	3.668993000	2.747940000	0.943716000
C	4.671672000	2.706946000	-0.015112000
F	3.587773000	3.786278000	1.779166000
F	1.762267000	1.846565000	1.907616000
F	5.566319000	3.691927000	-0.091356000
F	5.661801000	1.604494000	-1.841489000
F	3.841379000	-0.312706000	-1.763370000
F	-0.260182000	-0.521546000	-2.258629000
F	-0.276386000	-2.479777000	-4.064175000
F	1.460422000	-4.578563000	-3.838291000
F	3.208286000	-4.661841000	-1.757528000
F	3.229127000	-2.686780000	0.070403000
F	3.296530000	-0.441411000	2.612582000
F	2.763749000	-1.673030000	4.894358000
F	0.449864000	-3.068837000	5.219064000
F	-1.343116000	-3.195894000	3.160417000
F	-0.838846000	-1.962706000	0.860326000
C	0.617791000	-1.535684000	-2.083766000
C	1.472972000	-1.533248000	-0.995907000
C	-6.343949000	0.309683000	0.279711000
H	-6.354900000	0.483532000	-0.802553000
H	-6.437843000	-0.774082000	0.415753000
C	-7.537512000	1.016774000	0.944601000
H	-8.485445000	0.627321000	0.563753000
H	-7.540877000	0.874706000	2.031060000
H	-7.524581000	2.094492000	0.752817000
C	-4.693581000	2.784605000	0.999362000
H	-5.459292000	3.150412000	1.696261000
H	-3.741289000	3.162124000	1.393953000
C	-4.952086000	3.344613000	-0.409582000
H	-5.947430000	3.062935000	-0.768674000
H	-4.893186000	4.436389000	-0.424662000
H	-4.228329000	2.964823000	-1.140617000
C	-4.410197000	0.114312000	2.690982000
H	-3.654589000	0.676531000	3.251009000
H	-5.334886000	0.197719000	3.278001000
C	-4.003114000	-1.363355000	2.565117000
H	-3.812496000	-1.811836000	3.543629000
H	-4.795088000	-1.950007000	2.085793000
H	-3.097484000	-1.492588000	1.963559000
Si	-4.727788000	0.908184000	1.023991000
C	-3.508362000	-0.099605000	-1.266190000
C	-2.789958000	0.552993000	-2.268435000
C	-1.526846000	1.970361000	-0.751299000

H	-4.691530000	-1.797174000	-0.727683000
C	-4.207171000	-1.270611000	-1.544035000
C	-2.844016000	0.064878000	-3.572592000
C	-3.588098000	-1.069632000	-3.861894000
C	-4.264797000	-1.747187000	-2.847324000
H	-2.265012000	0.578811000	-4.332024000
H	-3.613894000	-1.445490000	-4.878926000
H	-4.817470000	-2.654155000	-3.065364000
C	2.340956000	-2.618917000	-0.929983000
O	-1.998570000	1.644013000	-2.048643000
H	-2.259537000	2.629729000	-0.266598000
H	-1.318408000	-0.211929000	-0.235151000
C	-0.238700000	2.767088000	-0.892740000
C	0.029696000	3.794600000	0.010874000
C	0.647765000	2.504535000	-1.936259000
C	1.179420000	4.566702000	-0.129268000
H	-0.668743000	4.006422000	0.818043000
C	1.788725000	3.287419000	-2.082364000
H	0.436526000	1.695075000	-2.625981000
C	2.053912000	4.320061000	-1.184853000
H	1.389832000	5.359180000	0.581198000
H	2.476362000	3.085859000	-2.897960000
H	2.951892000	4.921220000	-1.296308000
C	-1.302256000	1.031408000	1.633272000
H	-1.928091000	1.880919000	1.921550000
H	-1.588614000	0.144433000	2.198915000
H	-0.266444000	1.282977000	1.880515000

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C', *E*(SCRF) = -1258.153436 a.u.

H	-2.610680000	2.752245000	-0.096182000
C	-2.057565000	2.388520000	0.779112000
O	1.390039000	0.140340000	0.943384000
C	2.582266000	-1.219888000	-1.333965000
H	1.863635000	-0.817494000	-2.059674000
H	3.381855000	-0.472565000	-1.257501000
C	3.151590000	-2.557375000	-1.829059000
H	3.582914000	-2.468997000	-2.830715000
H	3.940374000	-2.922127000	-1.162022000
H	2.378455000	-3.333411000	-1.873300000
C	0.124136000	-2.385596000	0.177991000
H	0.330667000	-3.433620000	0.433954000
H	-0.554446000	-2.018279000	0.959577000
C	-0.567193000	-2.302638000	-1.189933000
H	0.023986000	-2.810054000	-1.960542000

H	-1.558112000	-2.769304000	-1.163461000
H	-0.704061000	-1.263820000	-1.502244000
C	2.858205000	-2.207487000	1.589218000
H	2.307858000	-2.324473000	2.531668000
H	3.092668000	-3.225608000	1.250272000
C	4.147300000	-1.413584000	1.828693000
H	4.808431000	-1.910133000	2.545843000
H	4.711818000	-1.279156000	0.898542000
H	3.917908000	-0.418401000	2.222788000
Si	1.722062000	-1.406994000	0.325064000
C	1.542868000	1.298770000	0.242500000
C	0.497304000	1.776863000	-0.562084000
C	-1.511964000	0.995458000	0.452355000
H	3.522093000	1.644326000	0.959123000
C	2.725726000	2.030391000	0.329637000
C	0.654491000	2.962545000	-1.273082000
C	1.842834000	3.683108000	-1.189909000
C	2.876978000	3.217077000	-0.382763000
H	-0.172656000	3.297962000	-1.891158000
H	1.956297000	4.605436000	-1.750040000
H	3.805935000	3.773268000	-0.308175000
O	-0.658399000	1.051020000	-0.705572000
H	-0.929274000	0.620652000	1.304647000
H	-1.209307000	3.065501000	0.931446000
C	-2.616080000	0.018105000	0.127509000
C	-3.057928000	-0.899270000	1.079973000
C	-3.231012000	0.046349000	-1.126459000
C	-4.092341000	-1.785228000	0.784833000
H	-2.583045000	-0.923914000	2.058614000
C	-4.260073000	-0.839915000	-1.425236000
H	-2.874891000	0.750024000	-1.873285000
C	-4.693021000	-1.759138000	-0.470397000
H	-4.423055000	-2.498462000	1.533619000
H	-4.723870000	-0.817719000	-2.406776000
H	-5.494548000	-2.452633000	-0.705468000
C	-2.951990000	2.392084000	2.016009000
H	-2.419321000	1.989217000	2.884772000
H	-3.268612000	3.408999000	2.261878000
H	-3.848199000	1.784675000	1.860751000

111

TS3', *E*(SCRF) = -3994.114998 a.u., IF= -117.21 cm^{-1}

B	2.633908000	-0.117482000	-0.078924000
H	1.484569000	-0.525705000	0.134032000
Si	-0.745277000	-0.225800000	0.646995000

O	-2.748539000	0.294952000	1.227651000
C	5.232125000	0.437262000	2.865090000
C	4.950043000	-0.636097000	3.698513000
C	2.419924000	1.409082000	-0.621191000
C	2.096021000	2.443923000	0.254962000
C	2.299648000	1.749899000	-1.966059000
C	1.604413000	3.677960000	-0.144421000
C	1.813418000	2.974997000	-2.415899000
C	1.453392000	3.946083000	-1.496776000
C	3.321784000	-1.140950000	-1.136904000
C	4.550851000	-0.846214000	-1.718414000
C	2.802720000	-2.387121000	-1.454314000
C	5.223249000	-1.710160000	-2.568942000
C	3.438460000	-3.288628000	-2.301962000
C	4.659606000	-2.946930000	-2.859994000
F	2.885949000	-4.472111000	-2.580460000
F	1.613067000	-2.781157000	-0.957617000
F	5.288227000	-3.794949000	-3.673287000
F	6.397186000	-1.376275000	-3.106736000
F	5.125154000	0.337037000	-1.461701000
F	2.243987000	-2.184255000	1.905572000
F	3.644378000	-2.544550000	4.157319000
F	5.646558000	-0.817927000	4.819836000
F	6.205240000	1.288393000	3.192960000
F	4.805105000	1.676594000	0.951878000
F	2.586894000	0.865863000	-2.932252000
F	1.666610000	3.210105000	-3.720718000
F	0.948369000	5.116048000	-1.900896000
F	1.234719000	4.592985000	0.761917000
F	2.202875000	2.271202000	1.585232000
C	3.222688000	-1.300211000	2.183225000
C	3.463167000	-0.240118000	1.316583000
C	-0.759557000	0.622340000	-1.020152000
H	-1.808792000	0.824023000	-1.237332000
H	-0.283847000	1.605512000	-0.926183000
C	-0.171819000	-0.171661000	-2.196351000
H	-0.076773000	0.485807000	-3.066835000
H	0.815425000	-0.584997000	-1.987090000
H	-0.831703000	-0.997559000	-2.473834000
C	-0.866013000	-2.093621000	0.691090000
H	0.178568000	-2.398733000	0.833173000
H	-1.378022000	-2.375696000	1.617407000
C	-1.459478000	-2.843448000	-0.509529000
H	-0.745124000	-2.867963000	-1.333895000

H	-1.675677000	-3.880405000	-0.233083000
H	-2.388720000	-2.391637000	-0.868917000
C	-0.013358000	0.375126000	2.267527000
H	-0.271941000	-0.415348000	2.986272000
H	1.072117000	0.317356000	2.150512000
C	-0.380053000	1.743886000	2.837814000
H	0.137812000	1.906815000	3.787486000
H	-0.077124000	2.552156000	2.168410000
H	-1.454958000	1.825623000	3.024765000
C	4.494067000	0.611938000	1.700928000
H	-3.383931000	2.549075000	2.772740000
C	-4.202808000	2.015351000	2.280993000
O	-4.361477000	-1.300253000	-0.266245000
C	-6.510074000	-3.034452000	-1.297681000
H	-6.964842000	-3.338415000	-0.347253000
H	-7.340004000	-2.989342000	-2.016640000
C	-5.473532000	-4.066907000	-1.767410000
H	-5.896959000	-5.074179000	-1.814122000
H	-5.102765000	-3.820200000	-2.767892000
H	-4.603458000	-4.099243000	-1.101561000
C	-5.223818000	-0.747636000	-2.901214000
H	-5.803260000	-1.314030000	-3.642671000
H	-5.502249000	0.302927000	-3.056079000
C	-3.721795000	-0.933901000	-3.160942000
H	-3.422325000	-1.982348000	-3.059871000
H	-3.446088000	-0.603024000	-4.166611000
H	-3.126708000	-0.362038000	-2.442790000
C	-7.006475000	-0.086951000	-0.424563000
H	-6.648557000	0.937762000	-0.599630000
H	-7.943419000	-0.167961000	-0.993360000
C	-7.288963000	-0.297005000	1.070678000
H	-8.068886000	0.381936000	1.428936000
H	-7.620543000	-1.319987000	1.278823000
H	-6.394089000	-0.122714000	1.679566000
Si	-5.792529000	-1.301698000	-1.194759000
C	-4.188962000	-1.628811000	1.037000000
C	-3.383321000	-0.798739000	1.828050000
C	-3.729431000	1.406871000	0.967445000
H	-5.313506000	-3.455211000	1.022365000
C	-4.724734000	-2.775384000	1.627384000
C	-3.158997000	-1.062966000	3.171083000
C	-3.712805000	-2.200714000	3.750697000
C	-4.485692000	-3.055948000	2.969975000
H	-2.538548000	-0.376165000	3.739907000

H	-3.533476000	-2.418904000	4.797364000
H	-4.907922000	-3.955431000	3.405664000
C	3.930884000	-1.513297000	3.358815000
H	-4.570561000	0.898163000	0.489960000
H	-4.523106000	1.215516000	2.956095000
C	-3.167220000	2.404982000	-0.004656000
C	-3.621644000	2.388232000	-1.325255000
C	-2.210243000	3.349085000	0.372898000
C	-3.076601000	3.248018000	-2.273916000
H	-4.381623000	1.665355000	-1.615710000
C	-1.661314000	4.209934000	-0.573393000
H	-1.878973000	3.410383000	1.403540000
C	-2.077591000	4.145727000	-1.902027000
H	-3.421377000	3.208100000	-3.302388000
H	-0.901653000	4.924107000	-0.274653000
H	-1.623200000	4.800128000	-2.639016000
C	-5.371398000	2.969012000	2.025355000
H	-6.191593000	2.453479000	1.512207000
H	-5.759443000	3.357546000	2.969639000
H	-5.064319000	3.816196000	1.406354000

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D', *E*(SCRF) = -3994.125107 a.u.

B	-2.192986000	-0.020478000	0.108372000
H	-0.995039000	0.173903000	0.226772000
C	1.452933000	1.045017000	0.677240000
O	2.978860000	0.829485000	0.975530000
C	-4.370127000	3.286588000	-0.471006000
C	-3.711738000	3.848085000	-1.553971000
C	-2.709301000	-0.487020000	1.584969000
C	-2.655377000	0.420544000	2.639108000
C	-3.081517000	-1.770779000	1.970624000
C	-2.919060000	0.111018000	3.962569000
C	-3.370390000	-2.131703000	3.284911000
C	-3.285950000	-1.185998000	4.292739000
C	-2.401581000	-1.124686000	-1.068168000
C	-3.657896000	-1.631089000	-1.385028000
C	-1.375393000	-1.554870000	-1.891738000
C	-3.889419000	-2.524159000	-2.421220000
C	-1.553750000	-2.451251000	-2.938693000
C	-2.820836000	-2.942452000	-3.205549000
F	-0.506291000	-2.862886000	-3.671867000
F	-0.108330000	-1.119769000	-1.699557000
F	-3.012366000	-3.807812000	-4.201764000
F	-5.113639000	-2.989527000	-2.674297000

F	-4.712057000	-1.261654000	-0.647342000
F	-1.184705000	1.362349000	-2.145315000
F	-1.987179000	3.707272000	-3.159097000
F	-4.119215000	5.010940000	-2.066043000
F	-5.423948000	3.913386000	0.057011000
F	-4.630184000	1.596866000	1.087625000
F	-3.157715000	-2.774828000	1.078917000
F	-3.713392000	-3.387365000	3.582435000
F	-3.538190000	-1.517475000	5.559609000
F	-2.781590000	1.036111000	4.918810000
F	-2.276277000	1.693999000	2.402012000
C	-2.222912000	1.975410000	-1.550941000
C	-2.826831000	1.384530000	-0.442741000
C	4.378681000	2.753595000	-1.003193000
H	4.341817000	1.946899000	-1.741632000
H	3.511947000	3.392138000	-1.201392000
C	5.686101000	3.554536000	-1.160557000
H	5.701781000	4.071982000	-2.123336000
H	5.804740000	4.317198000	-0.381647000
H	6.566336000	2.904908000	-1.122278000
C	5.865761000	1.010376000	0.980286000
H	6.706512000	1.718074000	0.992732000
H	5.872502000	0.521196000	1.958030000
C	6.062331000	-0.017064000	-0.145776000
H	6.250804000	0.479002000	-1.103972000
H	6.911949000	-0.674462000	0.059559000
H	5.178102000	-0.650296000	-0.276806000
C	4.077657000	3.376279000	2.035059000
H	3.550266000	2.952062000	2.898018000
H	5.078839000	3.639145000	2.403684000
C	3.358445000	4.643434000	1.548955000
H	3.260392000	5.372077000	2.357969000
H	3.905839000	5.124425000	0.732716000
H	2.355120000	4.422328000	1.174450000
C	-3.928326000	2.074140000	0.051327000
H	-0.213202000	1.987775000	1.481040000
C	0.765256000	1.683947000	1.866759000
O	2.845396000	-1.612136000	-0.191844000
C	3.980156000	-4.192078000	-1.038998000
H	3.765347000	-4.966675000	-0.291889000
H	4.016263000	-4.725226000	-2.000088000
C	5.351745000	-3.562166000	-0.755601000
H	6.146495000	-4.314159000	-0.780392000
H	5.603818000	-2.791572000	-1.490328000

H	5.377697000	-3.088463000	0.231262000
C	2.487608000	-2.277285000	-2.913861000
H	2.255471000	-3.108690000	-3.593582000
H	1.636339000	-1.596644000	-3.001090000
C	3.788347000	-1.592158000	-3.353558000
H	4.612112000	-2.308616000	-3.433262000
H	3.676587000	-1.117868000	-4.333929000
H	4.096995000	-0.815065000	-2.642529000
C	0.897796000	-3.776953000	-0.642790000
H	0.240926000	-3.742803000	-1.519937000
H	1.070257000	-4.842388000	-0.443092000
C	0.183712000	-3.132390000	0.559776000
H	-0.836207000	-3.514074000	0.658071000
H	0.709120000	-3.336921000	1.497737000
H	0.101551000	-2.045874000	0.449726000
Si	2.522844000	-2.991705000	-1.182007000
C	3.132568000	-1.579386000	1.117917000
C	3.249294000	-0.332731000	1.744380000
Si	4.330230000	2.050311000	0.726238000
H	3.233994000	-3.697981000	1.465866000
C	3.345761000	-2.715109000	1.912565000
C	3.618526000	-0.204358000	3.075166000
C	3.860193000	-1.340231000	3.836075000
C	3.705144000	-2.594468000	3.248154000
H	3.702999000	0.787282000	3.509799000
H	4.146619000	-1.246331000	4.877069000
H	3.868097000	-3.492376000	3.834829000
C	-2.626393000	3.181948000	-2.105004000
H	1.131842000	0.011816000	0.530384000
H	1.290679000	2.603954000	2.154592000
C	1.367093000	1.786651000	-0.623567000
C	1.779619000	1.123779000	-1.782115000
C	0.845485000	3.079133000	-0.720245000
C	1.694970000	1.747681000	-3.019240000
H	2.165280000	0.112670000	-1.693381000
C	0.761631000	3.705935000	-1.961061000
H	0.469738000	3.592250000	0.159196000
C	1.185912000	3.042037000	-3.109244000
H	2.007336000	1.217058000	-3.914001000
H	0.332536000	4.699609000	-2.035686000
H	1.093789000	3.526043000	-4.076359000
C	0.502522000	0.782982000	3.073596000
H	1.387445000	0.596424000	3.681348000
H	-0.250605000	1.252066000	3.711414000

H	0.101616000	-0.182712000	2.743679000

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TS4', *E*(SCRF) = -3994.116164 a.u., IF= -251.68 cm^{-1}

B	-2.225761000	-0.031264000	0.101319000
H	-1.024430000	0.162460000	0.266346000
C	1.239561000	0.923162000	0.711605000
O	3.214584000	0.755703000	1.050135000
C	-4.410256000	3.321115000	-0.058639000
C	-3.763071000	4.007862000	-1.074354000
C	-2.769511000	-0.695144000	1.489665000
C	-2.732590000	0.058214000	2.660053000
C	-3.163762000	-2.015012000	1.685811000
C	-3.047899000	-0.421120000	3.919471000
C	-3.502559000	-2.544829000	2.929255000
C	-3.445113000	-1.744146000	4.056995000
C	-2.397328000	-0.975989000	-1.211870000
C	-3.646245000	-1.435624000	-1.617525000
C	-1.352662000	-1.310707000	-2.055598000
C	-3.852371000	-2.201723000	-2.755497000
C	-1.503816000	-2.081191000	-3.202101000
C	-2.764713000	-2.532176000	-3.555524000
F	-0.439361000	-2.404764000	-3.952688000
F	-0.091532000	-0.896040000	-1.788295000
F	-2.932887000	-3.274500000	-4.649595000
F	-5.070304000	-2.628046000	-3.091537000
F	-4.717941000	-1.150601000	-0.867626000
F	-1.243471000	1.612533000	-1.979192000
F	-2.050089000	4.056531000	-2.699170000
F	-4.173892000	5.222848000	-1.439803000
F	-5.458272000	3.879506000	0.549655000
F	-4.660503000	1.460734000	1.290192000
F	-3.214216000	-2.890588000	0.667295000
F	-3.867872000	-3.823392000	3.042508000
F	-3.747960000	-2.237879000	5.257204000
F	-2.931992000	0.360496000	4.997390000
F	-2.311189000	1.339924000	2.609232000
C	-2.277729000	2.148216000	-1.305921000
C	-2.867217000	1.429114000	-0.268686000
C	4.371647000	2.798892000	-0.782786000
H	4.331676000	2.050351000	-1.582051000
H	3.449172000	3.384290000	-0.863508000
C	5.592474000	3.714955000	-0.978535000
H	5.523535000	4.262717000	-1.922390000
H	5.676938000	4.457784000	-0.176603000

H	6.526617000	3.143706000	-0.997955000
C	6.089160000	0.964026000	0.951168000
H	6.922120000	1.679161000	0.968503000
H	6.153892000	0.400946000	1.888078000
C	6.223994000	0.018888000	-0.252482000
H	6.321512000	0.582066000	-1.187433000
H	7.102667000	-0.626598000	-0.161410000
H	5.346134000	-0.629477000	-0.353698000
C	4.344071000	3.209247000	2.267412000
H	4.123728000	2.705727000	3.216455000
H	5.342317000	3.649733000	2.397694000
C	3.321910000	4.325780000	2.013478000
H	3.300859000	5.042858000	2.838894000
H	3.553868000	4.878711000	1.097375000
H	2.309166000	3.926779000	1.898453000
C	-3.964375000	2.055787000	0.313663000
H	-0.208307000	1.811617000	1.917841000
C	0.723971000	1.256778000	2.074696000
O	2.927119000	-1.558086000	-0.285198000
C	4.027559000	-4.076640000	-1.342212000
H	3.793097000	-4.895702000	-0.650652000
H	4.050031000	-4.541448000	-2.338475000
C	5.413061000	-3.501454000	-1.014974000
H	6.188517000	-4.270562000	-1.085256000
H	5.688143000	-2.692803000	-1.698621000
H	5.445176000	-3.091931000	-0.000102000
C	2.580963000	-1.955186000	-3.046564000
H	2.426827000	-2.722131000	-3.817992000
H	1.688139000	-1.325007000	-3.096549000
C	3.843698000	-1.141447000	-3.359937000
H	4.717712000	-1.788349000	-3.484673000
H	3.730966000	-0.568924000	-4.286567000
H	4.075344000	-0.433633000	-2.554267000
C	0.951498000	-3.644752000	-0.965444000
H	0.313972000	-3.522010000	-1.849770000
H	1.108101000	-4.726091000	-0.860337000
C	0.214910000	-3.106992000	0.274743000
H	-0.794308000	-3.523929000	0.340291000
H	0.743024000	-3.356147000	1.200495000
H	0.101483000	-2.018760000	0.236500000
Si	2.601491000	-2.834595000	-1.389912000
C	3.249487000	-1.638045000	1.023405000
C	3.453408000	-0.435963000	1.720203000
Si	4.493774000	1.947089000	0.879235000

H	3.211676000	-3.778121000	1.213052000
C	3.390127000	-2.838574000	1.727406000
C	3.822328000	-0.439072000	3.060871000
C	3.987620000	-1.641158000	3.739908000
C	3.757198000	-2.839055000	3.068907000
H	3.952098000	0.510766000	3.571476000
H	4.273635000	-1.639082000	4.785683000
H	3.861745000	-3.784859000	3.589885000
C	-2.684647000	3.411190000	-1.710727000
H	1.274278000	-0.126146000	0.428193000
H	1.421318000	1.953737000	2.558811000
C	1.206569000	1.843167000	-0.400642000
C	1.641853000	1.368079000	-1.648357000
C	0.710232000	3.153073000	-0.283511000
C	1.579444000	2.184668000	-2.765842000
H	2.035522000	0.357757000	-1.708396000
C	0.647236000	3.965964000	-1.405093000
H	0.336936000	3.516231000	0.668964000
C	1.073879000	3.478474000	-2.643144000
H	1.906928000	1.812177000	-3.731202000
H	0.232288000	4.965326000	-1.330984000
H	0.993949000	4.112795000	-3.520535000
C	0.416975000	0.047887000	2.958442000
H	1.316870000	-0.456397000	3.311476000
H	-0.162638000	0.371927000	3.827054000
H	-0.191322000	-0.673139000	2.404031000

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