Supporting Information

For

Studies of Iron-Mediated Pauson-Khand Reactions of 1,1-Disubstituted-Allenylsilanes: Mechanistic Implications for a Reactive Three-Membered Iron Metallacycle

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Table of Contents Page

I. Experimental Information

General information.....S-2

Reaction profile and initial rate kinetics.....S-3

Experimental procedures and characterization data for products **7**, **8**, **12-22** and **25**.....S-7

Experimental procedures and characterization data for iron metallacycles.....S-16

Experimental procedures and characterization data for 1,1-disubstituted allenes.....S-19

^{1}H, ^{13}C NMR and 2D NOESY spectra.....S-23

II. Computational Information

General information.....S-67

Studies of regioselective complexation of $FeCO_4$ with 1,1-disubstituted allenes.....S-69

Other Structural isomers of **41**, **42** and their energetic data.....S-69

Energetics of mechanistic pathway following the insertion of alkyne.....S-70

Exploration of the triplet potential energy surface.....S-71

Computed energy components of the optimized structures.....S-72

Cartesian coordinates of the optimized geometries.....S-73

Computed vibrational frequencies (cm^{-1}) of the optimized structures.....S-101

III. X-ray Information

X-ray crystal structure data for **18**.....S-113

X-ray crystal structure data for **24**.....S-128

General Information:

Unless otherwise noted, all reactions were performed in flame-dried or oven-dried glassware under argon atmosphere. Non-aqueous reagents were transferred using syringe techniques under argon atmosphere. Bulk grade hexanes, pentane, diethylether and ethyl acetate for chromatography were distilled prior to use. Tetrahydrofuran (THF) and dimethylformamide (DMF) were obtained anhydrous by degassing with argon and then passing through activated alumina columns to remove water and oxygen.[1] Diiron nonacarbonyl was obtained from Strem Chemicals, Inc. and stored in the freezer under argon atmosphere.

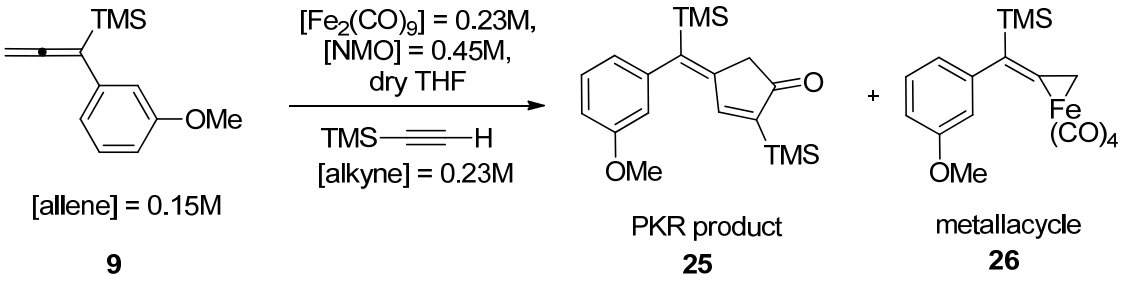
Reactions were monitored by standard thin-layer chromatography (TLC) techniques using EMD silica gel 60 F_{254} pre-coated plates (0.25 mm thickness). Developed TLC plates were visualized under UV light and/or by appropriate stains (*p*-anisaldehyde or cerric ammonium nitrate or potassium permanganate). Preparative TLC separations were performed using Merck silica gel 60 F_{254} pre-coated plates (0.50 mm thick). Flash column chromatography was performed with Silica-P Flash Silica Gel (ultra-pure 40-63 μm) from Silicycle Chemical Division (Quebec QC, Canada).

Proton nuclear magnetic resonance (^{1}H NMR) spectra were recorded on Varian VXR 400 (400 MHz), Varian INOVA 400 (400 MHz) or Varian Gemini 2000 (300 MHz) instruments. Carbon nuclear magnetic resonance (^{13}C NMR) spectra were measured using Varian VXR 400 (101 MHz), Varian INOVA 400 (101 MHz) or Varian Gemini 2000 (75.5 MHz) instruments. NMR coupling constants and signal patterns are reported as *J* values in Hz and δ values in parts per million (ppm). ^{1}H NMR Chemical shifts (δ) are reported in ppm relative to $CDCl_3$ (δ 7.26). ^{13}C NMR Chemical shifts (δ) are reported in ppm relative to $CDCl_3$ (δ 77.23). The following abbreviations were used to indicate the multiplicities: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. High resolution mass measurements (HRMS) were obtained on Thermo Electron Corporation MAT 95XP (EI/CI) or Agilent 1200 HPLC-6130 MSD (ESI). The analyses of kinetic

experiments were performed on the Agilent 6890N Gas Chromatograph equipped with a 5973 Inert Mass Selective Detector.

Reaction Profile:

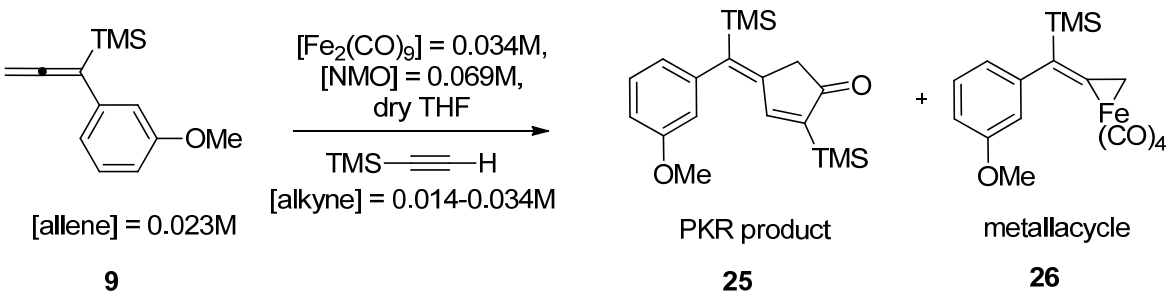
A small vial was charged with N-methylmorpholine N-oxide (64.4 mg, 0.55 mmol) followed by dry THF (1.0 mL) under N_2 atmosphere. To this solution, $Fe_2(CO)_9$ (99.8 mg, 0.28 mmol) was added at -50 °C. The allene **9** (40.0 mg, 0.18 mmol) was then added at -50 °C immediately followed by alkyne (38.9 µL, 0.28 mmol) addition. A small amount of 1,3,5-trimethoxybenzene was added as an internal standard in a THF solution (220 µL, 0.83M) which established a reaction concentration of 0.15M with respect to allene **9**. After stirring the reaction mixture at -50 °C for 5 min, it was then allowed to warm to rt by removal of the dry ice bath. Aliquots (~150 µL) were then removed periodically and immediately passed through a pipette plug of Florisil® with diethyl ether elution. These samples were then analyzed by ^{1}H NMR spectroscopy and amounts of allene **9**, PKR product **25** and iron metallacycle **26** were measured relative to the internal standard. The readings were plotted to provide the reaction profile as shown in Figure 4.



Time[a] (minutes)	Allene (**9**) (mmol)	PKR product (**25**) (mmol)	Metallacycle (**26**) (mmol)
0	0.183	0	0
10	0.073	0.107	0.003
20	0.028	0.148	0.007
30	0.015	0.160	0.008
40	0.005	0.170	0.008
50	0.0	0.175	0.008
60	0.0	0.175	0.008
90	0.0	0.175	0.008
120	0.0	0.175	0.008

[a]Time measurements were begun immediately following the addition of allene and alkyne.

Initial Rate Kinetics: The order of the reaction was found to be [alkyne]$^{1.6}$:



Each of four small vials were charged with N-methylmorpholine N-oxide (8.10 mg, 0.069 mmol) followed by dry THF (990 µL) under N_2 atmosphere. To each solution was then added $Fe_2(CO)_9$ (12.5 mg, 0.034 mmol) at -50 °C followed by allene **9** (5.0 mg, 0.023 mmol). Quantities of alkyne (1.9-4.9 µL, 0.014-0.034 mmol) were then added to each of the four reactions at -50 °C. An internal standard of 1,3,5-trimethoxybenzene in THF solution (10 µL, 0.595M) was added which established a reaction concentration of 0.023M with respect to allene **9**. After stirring the reaction mixtures at -50 °C for 5 min, each reaction was then allowed to warm to rt by removal of the dry ice bath. Aliquots (~50 µL) were then removed from each reaction periodically and

diluted to 200 µL with THF. These samples were then analyzed by gas chromatography and the amount of PKR product **25** was measured relative to the internal standard.

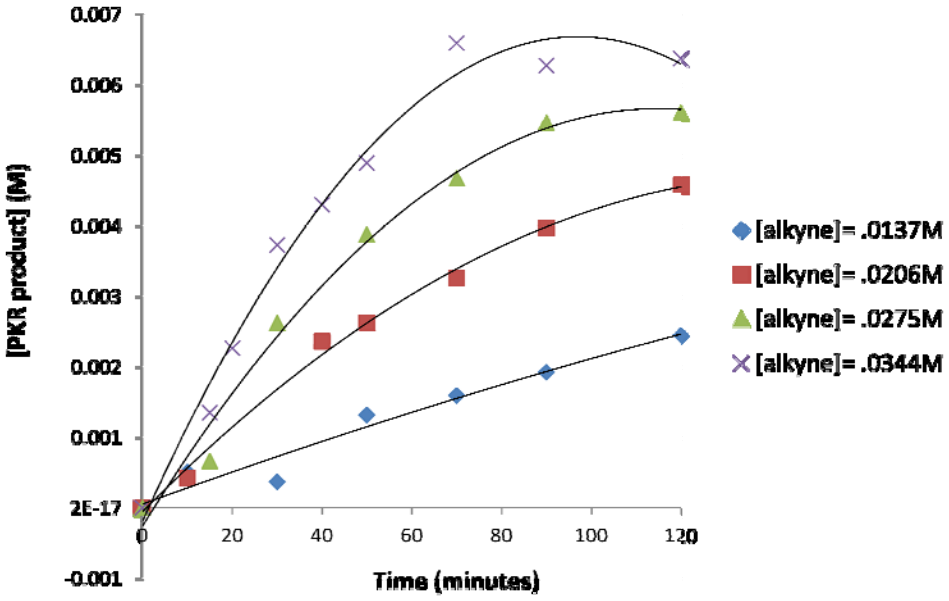


Figure I. Reaction profile dependence on alkyne concentration (an average of three experimental iterations)

For each of the curves shown, data points were selected which fall in the region of linearity of each curve and were plotted as shown in Figure 6.

The rates of the reaction at different alkyne concentrations were determined from the slopes of each plot from Figure 6. These data are tabulated and display the linear behavior as shown in Figure 7. The log/log plot (Figure II) shows the order of the reaction $[alkyne]^{1.6}$. This behavior is indicative of a complex reaction involving a series of steps. In contrast, the cobalt-catalyzed PKR has been shown to demonstrate zero order kinetics with respect to alkyne concentration. These results provide evidence for a different mechanistic pathway compared to the classical PKR.

[Alkyne] (M)	Initial Rate ($mmol.min^{-1}.mL^{-1}$)	Log [Alkyne]	Log (Rate)
0.0137	2.132×10^{-5}	-1.86	-4.67
0.0206	4.517×10^{-5}	-1.69	-4.35
0.0275	6.329×10^{-5}	-1.56	-4.19
0.0344	9.479×10^{-5}	-1.46	-4.02

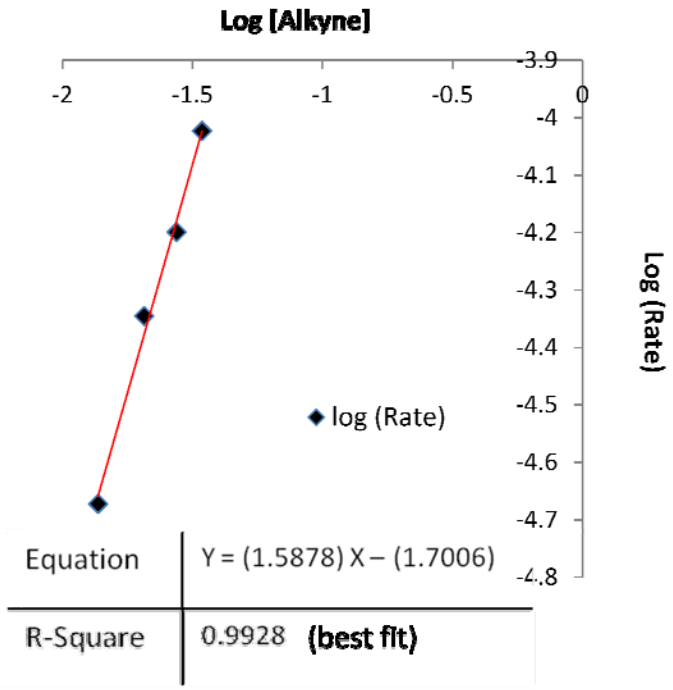
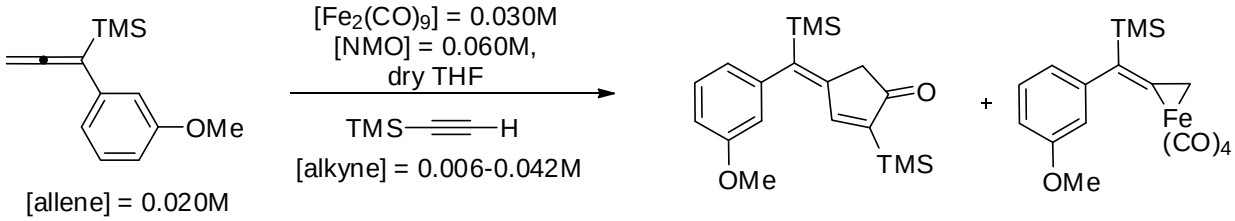


Figure II. Log/log plot of the initial reaction rates vs the alkyne concentration

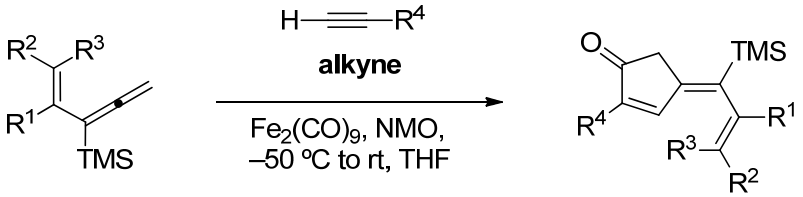
NMR analysis which examines the production of PKR product (25) and metallacycle (26) as a function of alkyne concentration over linear regions of the initial reaction profile:



Seven small vials were charged with N-methylmorpholine N-oxide (13.00 mg, 0.111 mmol) followed by dry THF (1.75 mL) under N_2 atmosphere. To each of the solutions was then added $Fe_2(CO)_9$ (20.0 mg, 0.055 mmol) at -50 °C followed by allene **9** (8.0 mg, 0.037 mmol). Various amounts of alkyne (1.6-11.0 µL, 0.006-0.042 mmol) were then added to each of the seven reactions at -50 °C. An internal standard of 1,3,5-trimethoxybenzene was added in THF solution (10 µL, 2.98M) which established a reaction concentration of 0.020M with respect to allene **9**.

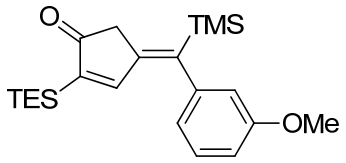
After stirring the reaction mixture at -50 °C for 5 min, it was then allowed to warm to rt by removal of the dry ice bath. Each reaction was then diluted with hexanes (~3.0 mL) after 60 minutes, and the solutions were passed through a pipette plug of Florisil® with diethyl ether elution. These samples were then analyzed by 1H NMR spectroscopy, and the amounts of PKR product **25** and iron metallacycle **26** were measured relative to the internal standard. The readings were plotted to provide the Figure 5.

General Procedure for allenic Pauson-Khand reactions:



1,1-disubstituted allenylsilane **4-alkylidene-2-cyclopenten-1-ones**

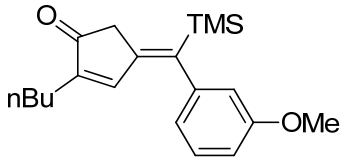
To a solution of N-methylmorpholine N-oxide (3 equiv) in dry THF (~ 0.2M) was added $Fe_2(CO)_9$ (1.5 equiv unless otherwise noted) at -50 °C under N_2. The allene (1.0 equiv) was then added at -50 °C immediately followed by alkyne (freshly distilled before use whenever feasible) (1.5 - 3.0 equiv) addition. After stirring the reaction mixture at -50 °C for 5 min, it was then allowed to warm to rt and was stirred for additional 1-3 hours. All reactions were monitored by TLC for completion. The reaction mixture was then diluted with hexanes and filtered through a plug of Florisil®. After several elutions with diethyl ether/ hexanes or ethyl acetate/ hexanes solvent system, the combined organic layers were concentrated *in vacuo* and crude product was analyzed by GC-MS. The residue was then purified by flash silica gel column chromatography to afford the major product 4-alkylidene-2-cyclopenten-1-one as a pure substance.



12

(E)-4-((3-methoxyphenyl)(trimethylsilyl)methylene)-2-(triethylsilyl)cyclopent-2-enone *(12):*

Following the general procedure, **12** was prepared using triethyl(ethynyl)silane (49.22 µL, 0.276 mmol) and allene **9** (40 mg, 0.184 mmol). The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 10% diethyl ether in hexanes) to afford the desired product (52 mg, 73% yield; >97:3 isomeric ratio) as a clear yellow oil. R_f=0.56 (SiO_2, 20% diethyl ether in hexanes); IR (film) ν_{max} 2954, 2910, 2875, 1697, 1594, 1463, 1285, 1249, 1171, 853, 839 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.56 (1H, s), 7.25 (1H, t, *J* = 7.6Hz), 6.81-6.79 (1H, m), 6.57-6.52 (2H, m), 3.82 (3H, s), 3.09 (2H, s), 0.87 (9H, t, *J* = 8.0Hz), 0.65 (6H, q, *J* = 8.0Hz), 0.13 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 210.7, 165.1, 159.5, 147.4, 146.2, 143.9, 143.7, 129.3, 120.8, 113.8, 111.7, 55.4, 41.5, 7.5, 3.0, -0.1; HRMS *m/e* calcd. for $C_{22}H_{34}O_2Si_2$ $(M)^+$ 386.2092 found 386.2081.

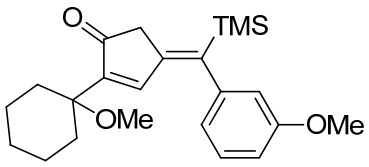


13

(E)-2-butyl-4-((3-methoxyphenyl)(trimethylsilyl)methylene)cyclopent-2-enone *(13):*

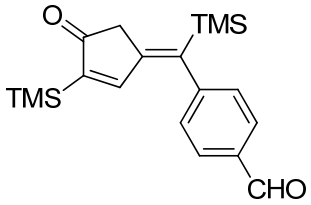
Following the general procedure, **13** was prepared using 1-hexyne (31.50 µL, 0.28 mmol) and allene **9** (20 mg, 0.092 mmol). The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 10% diethyl ether in hexanes) to afford the desired product (13.5 mg, 69% yield; >92:8 isomeric ratio) as a clear yellow oil. R_f =0.48 (SiO_2, 20% diethyl ether in hexanes); IR (film) ν_{max} 2956, 2921, 1703, 1643, 1602, 1482, 1285, 1248, 1045, 838 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.25 (1H, t, *J* = 7.6Hz), 7.17 (1H, s), 6.81-6.79 (1H, m), 6.56-6.51 (2H, m), 3.82 (3H, s), 3.13 (2H, s), 2.19 (2H, t, *J* = 7.6Hz), 1.39-1.23 (4H, m), 0.86 (3H, t, *J* = 7.2Hz), 0.13 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 206.6, 159.5, 152.2, 148.5, 144.9, 144.4,

142.2, 129.3, 120.9, 114.0, 111.4, 55.4, 41.1, 30.2, 24.9, 22.8, 13.9, 0.0; HRMS *m/e* calcd. for $C_{20}H_{28}O_2Si_1$ $(M)^+$ 328.1853 found 328.1842.



14

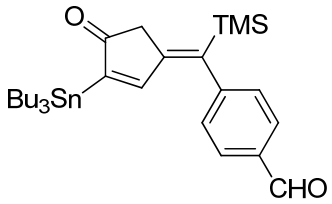
(E)-2-(1-methoxycyclohexyl)-4-((3-methoxyphenyl)(trimethylsilyl)methylene) cyclopent-2-enone *(14):* Following the general procedure, **14** was prepared using 1-ethynyl-1-methoxycyclohexane (57.96 mg, 0.428 mmol) and allene **9** (30 mg, 0.138 mmol). The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 10% diethyl ether in hexanes) to afford the desired product (22 mg, 77% yield brsm; 93:7 isomeric ratio) as a clear yellow oil. R_f =0.26 (SiO_2, 20% diethyl ether in hexanes); IR (film) ν_{max} 2933, 2856, 1698, 1643, 1602, 1482, 1312, 1248, 1152, 1074, 838 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.31 (1H, s), 7.24 (1H, t, *J* = 8.0Hz), 6.79-6.77 (1H, m), 6.55-6.49 (2H, m), 3.81 (3H, s), 3.18 (2H, s), 3.03 (3H, s), 1.79-1.22 (10H, m), 0.13 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 204.8, 159.5, 153.6, 149.7, 144.1, 144.0, 143.7, 129.3, 120.8, 113.9, 111.5, 75.9, 55.4, 50.2, 42.5, 32.7, 25.4, 21.4, -0.1; HRMS *m/e* calcd. for $C_{23}H_{32}O_3Si_1$ $(M)^+$ 384.2115 found 384.2126.



15

(E)-4-((4-oxo-3-(trimethylsilyl)cyclopent-2-en-1-ylidene)(trimethylsilyl)methyl) benzaldehyde *(15):* Following the general procedure, **15** was prepared using (Trimethylsilyl)acetylene (20.46 mg, 0.208 mmol) and allene **10** (30 mg, 0.138 mmol). The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 9% diethyl ether in hexanes) to afford the desired product (39 mg, 81%; 94:6 isomeric ratio) as a clear colorless oil. R_f = 0.40(SiO_2, 20% diethyl ether in hexanes); IR (film) ν_{max} 3045, 2956, 2923, 2850, 1697, 1600,

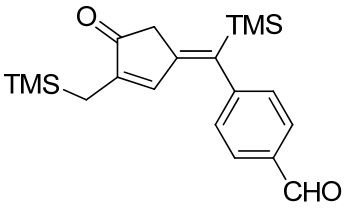
1536, 1249, 1168, 920, 840 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 10.04 (1H, s), 7.88 (2H, d, *J* = 8.0Hz), 7.38 (1H, s), 7.16 (2H, d, *J* = 8.0Hz), 3.13 (2H, s), 0.14 (9H, s), 0.12 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 209.8, 192.1, 162.7, 149.9, 149.8, 147.7, 142.9, 134.7, 129.9, 128.9, 41.5, -0.2, -1.7; HRMS *m/e* calcd. for $C_{19}H_{27}O_2Si_2$ $(M+H)^+$ 343.1544 found 343.1552.



16

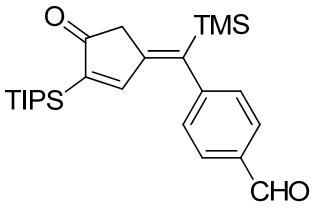
(E)-4-((4-oxo-3-(tributylstannyl)cyclopent-2-en-1-ylidene)(trimethylsilyl)methyl) benzaldehyde *(16):* Following the general procedure, **16** was prepared using tributyl(ethynyl)tin (39.80 µL, 0.138 mmol) and allene **10** (20 mg, 0.092 mmol). The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 15% diethyl ether in hexanes) to afford the desired product (26 mg, 51%; 100:0 isomeric ratio) as a clear colorless oil. R_f = 0.47 (SiO_2, 20% diethyl ether in hexanes); IR (film) ν_{max} 2956, 2925, 2871, 2853, 1695, 1692, 1600, 1250, 1209, 842 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 10.03 (1H, s), 7.88 (2H, d, *J* = 8.0Hz), 7.44 (1H, s), 7.17 (2H, d, *J* = 8.0Hz), 3.09 (2H,s), 1.44-1.38 (6H, m), 1.26-1.21 (6H, m), 0.95 (6H, t, *J* = 8.2Hz), 0.82 (9H, t, *J* = 7.4Hz), 0.15 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 211.1, 192.1, 164.9, 153.6, 150.1, 148.8, 140.6, 134.7, 129.8, 129.1, 40.5, 29.2, 27.4, 13.8, 9.8, -0.1; HRMS *m/e* calcd. for $C_{24}H_{35}O_2SiSn$ $(M-C_4H_9)^+$ 503.1423 found 503.1441.

Note: For **16**, silica gel neutralized with 3% Et_3N was used for flash column chromatography to avoid protodestannylation.



17

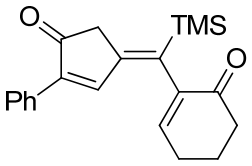
(E)-4-((4-oxo-3-((trimethylsilyl)methyl)cyclopent-2-en-1-ylidene)(trimethylsilyl) methyl)benzaldehyde *(17):* Following the general procedure, **17** was prepared using propargyltrimethylsilane (41.40 µL, 0.286 mmol) and allene **10** (20 mg, 0.092 mmol). $Fe_2(CO)_9$ was used in excess (3 equiv). The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 15% diethyl ether in hexanes) to afford the desired product (12 mg, 52%; 80:20 isomeric ratio) as a white solid. R_f = 0.33 (SiO_2, 20% diethyl ether in hexanes); IR (film) ν_{max} 2955, 2922, 2850, 1702, 1596, 1250, 1210, 929, 841 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 10.03 (1H, s), 7.87 (2H, d, *J* = 8.0Hz), 7.15 (2H, d, *J* = 8.0Hz), 6.87 (1H, s), 3.13 (2H,s), 1.71 (2H, s), 0.14 (9H, s), -0.05 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 205.5, 192.1, 150.6, 148.7, 147.8, 145.6, 138.9, 134.6, 129.9, 129.2, 40.5, 16.0, 0.1, -1.5; HRMS *m/e* calcd. for $C_{20}H_{28}O_2Si_2$ $(M)^+$ 356.1622 found 356.1607.



18

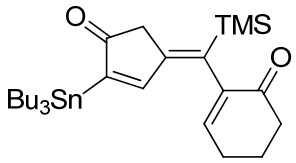
(E)-4-((4-oxo-3-(triisopropylsilyl)cyclopent-2-en-1-ylidene)(trimethylsilyl)methyl) benzaldehyde *(18):* Following the general procedure, **18** was prepared using (Triisopropylsilyl)acetylene (61.32 µL, 0.286 mmol) and allene **10** (20 mg, 0.092 mmol). The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 15% diethyl ether in hexanes) to afford the desired product (24 mg, 61%; >97:3 isomeric ratio) as a white solid. R_f = 0.61 (SiO_2, 20% diethyl ether in hexanes); IR (film) ν_{max} 2943, 2865, 1698, 1600, 1527, 1250, 843 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 10.04 (1H, s), 7.88 (2H, d, *J* = 8.4Hz), 7.47 (1H, s), 7.17 (2H, d, *J* = 8.4Hz), 3.13 (2H, s), 1.26-1.22 (3H, m), 0.96 (18H, d, *J* =

7.6Hz), 0.16 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 210.2, 192.1, 165.3, 149.9, 147.8, 146.1, 142.3, 134.7, 129.6, 128.9, 41.4, 18.8, 11.1, -0.1; HRMS *m/e* calcd. for $C_{22}H_{31}O_2Si_2$ $(M\text{-}C_3H_7)^+$ 383.1857 found 383.1862.



19

(E)-2-((4-oxo-3-phenylcyclopent-2-en-1-ylidene)(trimethylsilyl)methyl)cyclohex-2-enone *(19):* Following the general procedure, **19** was prepared using phenylacetylene (15.98 µL, 0.146 mmol) and allene **11** (20 mg, 0.097 mmol). The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 25% diethyl ether in hexanes) to afford the desired product (24 mg, 74%; 83:17) as a clear yellow oil. R_f = 0.35 (SiO_2, 20% ethyl acetate in hexanes); IR (film) ν_{max} 2953, 2924, 2851, 1698, 1671, 1447, 1341, 1247, 942, 840 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.79 (1H, s), 7.73 (2H, d, *J* = 7.2 Hz), 7.40- 7.26 (3H, m), 6.61 (1H, t, *J* = 4.0Hz), 3.34 (1H, A of AB, *J* = 20.8Hz), 3.25 (1H, B of AB, *J* = 20.8Hz), 2.57-2.50 (4H, m), 2.16-2.09 (2H, m), 0.17 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 204.2, 199.3, 150.5, 145.9, 145.0, 143.0, 141.9, 141.5, 131.6, 129.1, 128.7, 127.8, 42.0, 38.9, 26.4, 23.5, -0.3; HRMS *m/e* calcd. for $C_{21}H_{24}O_2Si_1$ $(M)^+$ 336.1540 found 336.1528.

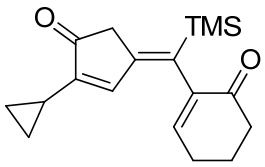


20

(E)-2-((4-oxo-3-(tributylstannyl)cyclopent-2-en-1-ylidene)(trimethylsilyl)methyl) cyclohex-2-enone *(20):* Following the general procedure, **20** was prepared using tributyl(ethynyl)tin (86.74 µL, 0.301 mmol) and allene **11** (20 mg, 0.097 mmol). The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 8% ethyl acetate in hexanes) to afford the desired product (34 mg, 64%; 100:0 isomeric ratio) as a clear colorless oil. R_f = 0.61 (SiO_2, 20% ethyl acetate in hexanes); IR (film) ν_{max} 2956, 2871, 2853, 2056, 1989,

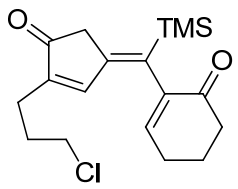
1689, 1678, 1519, 1247, 841 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.76 (1H, s), 6.56 (1H, t, *J* = 4.0Hz), 3.06 (1H, A of AB, *J* = 20.6Hz), 2.97 (1H, B of AB, *J* = 20.6Hz), 2.54-2.47 (4H, m), 2.09-2.07 (2H, br m), 1.52- 1.45 (6H, m), 1.34-1.25 (6H, m), 0.99 (6H, t, *J* = 8.4Hz), 0.88 (9H, t, *J* = 7.6Hz), 0.13 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 211.5, 199.4, 164.7, 152.0, 149.3, 145.8, 141.9, 137.9, 40.3, 38.9, 29.3, 27.5, 26.4, 23.5, 13.9, 9.8, -0.4; HRMS *m/e* calcd. for $C_{27}H_{47}O_2Si_1Sn_1$ $(M+H)^+$ 551.2289 found 551.2341.

Note: For **20**, silica gel neutralized with 3% Et_3N was used for flash column chromatography to avoid protodestannylation.



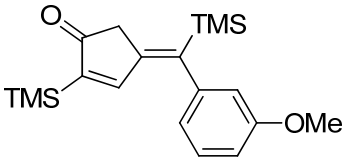
21

(E)-2-((3-cyclopropyl-4-oxocyclopent-2-en-1-ylidene)(trimethylsilyl)methyl) cyclohex-2-enone *(21):* Following the general procedure, **21** was prepared using ethylenecyclopropane (19.88 mg , 0.301 mmol) and allene **11** (20 mg, 0.097 mmol). $Fe_2(CO)_9$ was used in excess (3 equiv).The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 10% ethyl acetate in hexanes) to afford the desired product (13 mg, 72 % yield; >97:3 isomeric ratio) as a clear colorless oil. R_f = 0.29 (SiO_2, 20% ethyl acetate in hexanes); IR (film) ν_{max} 3025, 2923, 1697, 1668, 1650, 1345, 1247, 840 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.03 (1H, s), 6.52 (1H, t, *J* = 4.0Hz), 3.15 (1H, A of AB, *J* = 20.8Hz), 3.05 (1H, B of AB, *J* = 20.8Hz), 2.53-2.46 (4H, m), 2.11-2.04 (2H, m), 1.69- 1.63 (1H, m), 0.93-0.88 (2H, m), 0.75-0.71 (2H, m), 0.12 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 205.5, 199.3, 150.2, 146.7, 145.7, 145.4, 141.9, 137.5, 41.4, 38.9, 26.4, 23.5, 8.9, 8.7, 7.4, -0.3; HRMS *m/e* calcd. for $C_{18}H_{25}O_2Si_1$ $(M+H)^+$ 301.1618 found 301.1608.



22

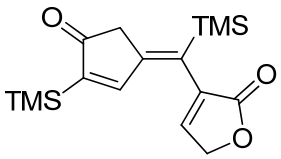
(E)-2-((3-(3-chloropropyl)-4-oxocyclopent-2-en-1-ylidene)(trimethylsilyl)methyl) cyclohex-2-enone *(22):* Following the general procedure, **22** was prepared using 5-Chloro-1-pentyne (30.52 mg, 0.298 mmol) and allene **11** (20 mg, 0.096 mmol). The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 15% ethyl acetate in hexanes) to afford the desired product (13 mg, 61% yield brsm; 97:3 isomeric ratio) as a clear yellow oil. R_f =0.25 (SiO_2, 20% ethyl acetate in hexanes); IR (film) ν_{max} 2954, 1701, 1673, 1590, 1348, 1247, 935, 841 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.39 (1H, s), 6.55 (1H, t, *J* = 4.4Hz), 3.52 (2H, t, *J* = 6.4Hz), 3.14 (1H, A of AB, *J* = 21.0Hz), 3.05 (1H, B of AB, *J* = 21.0Hz), 2.54-2.48 (4H, m), 2.42 (2H, t, *J* = 7.2Hz), 2.13-2.07 (2H, m), 1.99-1.92 (2H, m), 0.13 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 206.0, 199.3, 151.9, 146.2, 145.8, 145.4, 141.8, 139.4, 44.7, 40.7, 38.9, 30.8, 26.4, 23.5, 22.7, -0.4; HRMS *m/e* calcd. for $C_{18}H_{25}ClO_2Si_1$ $(M+H)^+$ 337.1391 found 337.1381.



25

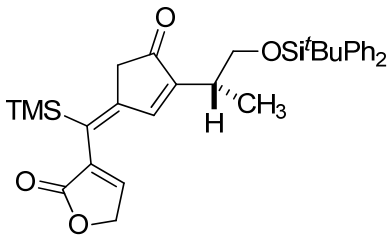
(E)-4-((3-methoxyphenyl)(trimethylsilyl)methylene)-2-(trimethylsilyl)cyclopent-2-enone *(25)*: Following the general procedure, **25** was prepared using trimethylsilyl acetylene (20.23 mg, 0.206 mmol) and allene **9** (30 mg, 0.138 mmol). The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 10% diethylether in hexanes) to afford the desired product (37 mg, 74% yield; 21:1 isomeric ratio) as a clear oil. R_f =0.48 (SiO_2, 20% diethylether in hexanes); IR (film) ν_{max} 2915, 2876, 1694, 1248, 839; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.53 (1H, s), 7.25 (1H, t, *J* = 8.0Hz), 6.82-6.79 (1H, m), 6.57-6.51 (2H, m), 3.82(3H, s), 3.10(2H,s), 0.13 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 210.5, 163.7, 159.5, 148.6, 147.2, 144.0,

143.9, 129.3, 120.8, 113.9, 111.6, 55.4, 41.6, -0.2, -1.6; HRMS *m/e* calcd. for $C_{19}H_{28}O_2Si_2Na$ $(M+Na)^+$ 367.1526 found 367.1528.



7

(E)-3-((4-oxo-3-(trimethylsilyl)cyclopent-2-en-1-ylidene)(trimethylsilyl)methyl)furan-2(5H)-one *(7):* Following the general procedure, **7** was prepared using (Trimethylsilyl)acetylene (67.80 mg, 0.479 mmol) and allene **3a** (30 mg, 0.155 mmol). The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 40% diethyl ether in hexanes) to afford the desired product (31 mg, 62% yield; >97:3 isomeric ratio) as a clear colorless oil. R_f=0.45 (SiO_2, 50% diethyl ether in hexanes); IR (film) ν_{max} 2956, 1756, 1695, 1535, 1249, 1078, 840 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.63 (1H, s), 7.11 (1H, s), 4.96 (2H, d, *J* = 2.0Hz), 3.08 (2H, s), 0.21 (9H, s), 0.19 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 209.3, 173.6, 161.6, 150.9, 150.6, 145.1, 134.9, 131.1, 70.5, 41.5, -0.4, -1.6; HRMS *m/e* calcd. for $C_{16}H_{24}O_3Si_2$ $(M)^+$ 320.1258 found 320.1256.

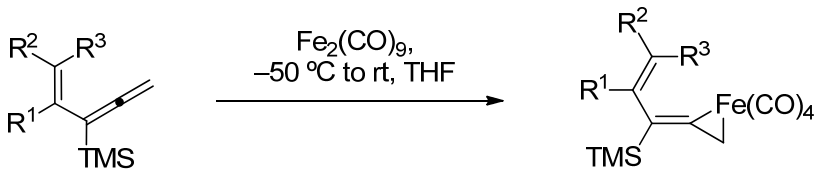


8

(R,E)-3-((3-(1-((tert-butyldiphenylsilyl)oxy)propan-2-yl)-4-oxocyclopent-2-en-1-ylidene)(trimethylsilyl)methyl)furan-2(5H)-one *(8):* Following the general procedure, **8** was prepared using (R)-tert-butyl((2-methylbut-3-yn-1-yl)oxy)diphenylsilane[2] (49.78 mg, 0.077 mmol) and allene **3a** (10 mg, 0.052 mmol). $Fe_2(CO)_9$ was used in excess (3 equiv). The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 40% diethyl ether in hexanes) to afford the desired product (14 mg, 75 % yield

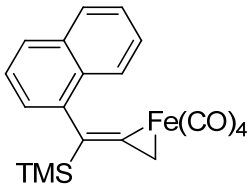
brsm; 95:5) as a clear yellow oil. R_f =0.43 (SiO_2, 50% diethyl ether in hexanes); IR (film) ν_{max} 3024, 2960, 2858, 1759, 1703, 1645, 1428, 1113, 1075, 838 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.59-7.57 (4H, m), 7.46 (1H, s), 7.42-7.35 (6H, m), 6.89 (1H, s), 4.78 (2H, s), 3.73, 3.67 (2H, J_{AB} = 9.6Hz, J_{AX} = 4.8Hz, J_{BX} = 5.2Hz), 3.09 (1H, A of AB, J = 20.8Hz), 3.02 (1H, B of AB, J = 20.8Hz), 2.89-2.85 (1H, m), 1.17 (3H, d, J = 7.2Hz), 1.01 (9H, s), 0.21 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 204.8, 173.0, 151.6, 150.5, 148.6, 145.6, 135.8, 135.7, 135.1, 133.9, 133.6, 130.1, 129.9, 129.8, 127.93, 127.91, 70.4, 66.7, 40.9, 32.9, 27.1, 19.6, 16.1, -0.3; HRMS *m/e* calcd. for $C_{32}H_{41}O_4Si_2$ $(M+H)^+$ 545.2538 found 545.2555.

General procedure for the synthesis of three-membered iron metallacycles:



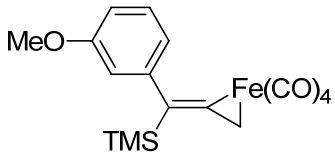
1,1-disubstituted allenylsilane **Three-membered iron metallacycle**

To a solution of $Fe_2(CO)_9$ (1.5 equiv) in dry THF (~ 0.25M) prepared at -50 °C under N_2 was added allene (1.0 equiv) at -50 °C. After stirring the reaction mixture at -50 °C for 5 min, it was then allowed to warm to rt and was stirred for additional 2 hours. The reaction mixture was then diluted with hexanes and filtered through a plug of Florisil®. After several elutions with diethyl ether/ hexanes or ethyl acetate/ hexanes solvent system, the combined organic layers were concentrated *in vacuo*. The crude mixture was purified by flash column chromatography on silica gel to afford the desired iron metallacycle**.**



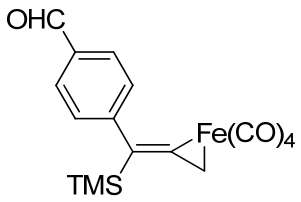
24

Following the general procedure, **24** was prepared from allene **23** (50 mg, 0.21 mmol). The crude mixture was purified by flash column chromatography on silica gel (100% hexanes then gradient to 30% ethyl acetate in hexanes) to afford the desired iron metallacycle (35 mg, 41% yield) as a dark green oil. R_f =0.70 (SiO_2, 10% diethyl ether in hexanes); IR (film) ν_{max} 3060, 2957, 2088 (sh, vs), 2049 (vs), 1987 (br), 1713 (w), 1505, 1390, 1248, 1054, 841 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.88 (1H, d, *J* = 8.0Hz), 7.78 (2H, t, *J* = 7.2Hz), 7.50-7.37 (3H, m), 7.08 (1H, dd, *J* = 7.2, 1.2Hz), 2.39 (1H, A of AB, *J* = 8.0Hz), 2.35 (1H, B of AB, *J* = 8.0Hz), 0.18 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 209.2, 167.7, 143.9, 134.8, 134.2, 132.1, 128.6, 126.4 (2C), 125.8, 125.7, 125.4, 125.3, 7.2, -0.7; HRMS *m/e* calcd. for $C_{20}H_{18}FeO_4Si_1$ $(M)^+$ 406.0318 found $C_{20}H_{18}FeO_4Si_1$ $(M)^+$ 406.0300.



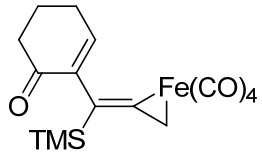
26

Following the general procedure, **26** was prepared from allene **9** (50 mg, 0.23 mmol). The crude mixture was purified by flash column chromatography on silica gel (100% hexanes then gradient to 50% diethyl ether in hexanes) to afford the desired iron metallacycle (33 mg, 67 % yield) as a light yellow/green oil. R_f =0.67 (SiO_2, 10% diethyl ether in hexanes); IR (film) ν_{max} 2957, 2853, 2087 (sh, vs), 2002 (vs), 1712 (w), 1595, 1483, 1284, 1051, 840 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.27 (1H, t, *J* = 8.0Hz), 6.82-6.79 (1H, dd, *J* = 8.4, 1.6Hz), 6.60 (1H, d, *J* =7.6Hz), 6.55 (1H, s), 3.81 (3H, s), 2.25 (2H, s), 0.18 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 209.4, 165.3, 159.7, 148.1, 136.7, 129.5, 120.8, 113.9, 111.3, 55.4, 7.3, -0.8; HRMS *m/e* calcd. for $C_{17}H_{18}FeO_5Si_1$ found for $C_{15}H_{18}FeO_3Si_1$ $(M\text{-}C_2O_2)^+$ 330.0361, $C_{14}H_{18}FeO_2Si_1$ $(M\text{-}C_3O_3)^+$ 302.0418, $C_{13}H_{18}FeO_1Si_1$ $(M\text{-}C_4O_4)^+$ 274.0471.



33

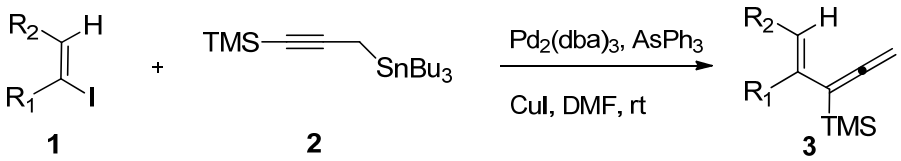
Following the general procedure, **33** was prepared from allene **10** (50 mg, 0.23 mmol). The crude mixture was purified by flash column chromatography on silica gel (100% hexanes then gradient to 30% diethyl ether in hexanes) to afford the desired iron metallacycle as a brown colloidal oil. R_f =0.40 (SiO_2, 10% diethyl ether in hexanes); IR (film) ν_{max} 2957, 2853, 2086 1986, 1700, 1598, 1404 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 10.03 (1H, s), 7.90 (2H, d, *J* = 7.6Hz), 7.18 (2H, d, *J* = 7.6Hz), 2.26 (2H, s), 0.19 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 208.9, 192.2, 166.6, 153.4, 137.1, 134.5, 130.3(2C), 128.9(2C), 7.1, -0.9; HRMS *m/e* calcd. for $C_{17}H_{16}FeO_5Si$ $(M)^+$ 384.0116 found $C_{16}H_{16}FeO_4Si$ $(M\text{-}CO)^+$ 356.0158.



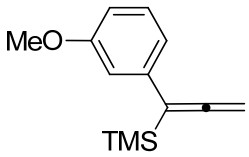
28a

Following the general procedure, **28a** was prepared from allene **11** (45 mg, 0.22 mmol). The crude mixture was purified by flash column chromatography on silica gel (100% hexanes then gradient to 30% ethyl acetate in hexanes) to afford the desired iron metallacycle as a light green oil. R_f =0.50 (SiO_2, 10% ethyl acetate in hexanes); IR (film) ν_{max} 2922, 2048 (sh), 1986, 1645 (br), 1462, 1247, 842 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 6.59 (1H, t, *J* = 4.0Hz), 2.54-2.46 (4H, m), 2.18 (2H, s), 2.13-2.06 (2H, m), 0.13 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 209.5, 198.5, 164.9, 145.6, 144.8, 132.3, 38.9, 26.4, 23.3, 7.1, -1.1; HRMS *m/e* calcd. for $C_{16}H_{18}FeO_5Si_1$ $(M)^+$ 374.0273 found $C_{14}H_{18}FeO_3Si_1$ $(M\text{-}C_2O_2)^+$ 318.0502.

General procedure for the preparation of 1,1-disubstituted allenylsilanes:[3]

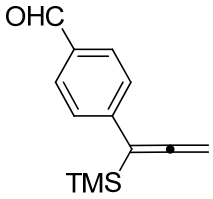


To a solution of propargyl stannane **2 (**1.3 equiv) and iodide **1** (1 equiv.) in DMF (~0.2 M) was added $AsPh_3$ (0.8 equiv) followed by $Pd_2(dba)_3$ (20 mol%) and CuI (0.8 equiv) at rt. The reaction was stirred at 22 °C unless otherwise mentioned for 8-15 hrs. All reactions were monitored by TLC for completion. The reaction mixture then was quenched with saturated aqueous $NaHCO_3$. The aqueous layer was extracted in hexane or diethylether (4 × 15 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated *in vacuo.* The residue was then purified by flash silica gel column chromatography to afford the cross-coupling product **3**.



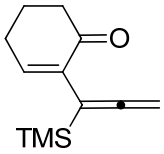
9

1-Methoxy-3-(octa-1,2-dien-3-yl)benzene (9): Following the general procedure, **9** was prepared using 3-iodoanisole **1a** (300 mg, 1.28 mmol). The reaction was stirred at 45°C. The crude product was purified by flash column chromatography on silica gel (100% hexanes then 1% ethyl acetate in hexane) to afford the desired product (115 mg, 82%) as a clear oil. R_f = 0.44 (SiO_2, 8% ethyl acetate in hexane); IR (film) ν_{max} 3068, 3052, 2956, 1915,1595, 1578, 1250, 1049, 841,737, 696 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.21(1H, t, *J* = 8.0 Hz), 6.90(1H, d, *J* = 8.0 Hz), 6.87(1H, t, *J* = 2.0 Hz), 6.74(1H, dd, *J* = 8.8, 2.0 Hz), 4.67(2H, s), 3.80(3H, s), 0.24(9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 211.3, 159.9, 138.8, 129.5, 120.4, 113.5, 111.9, 98.8, 70.8, 55.4, -0.3; HRMS *m/e* calcd. for $C_{13}H_{18}OSi$ $(M)^+$ 218.1121 found 218.1117.



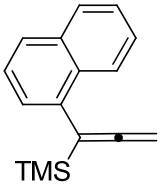
10

4-(1-(Trimethylsilyl)propa-1,2-dienyl)benzaldehyde (10): Following the general procedure, **10** was prepared using **1b** (90 mg, 0.39 mmol). The crude product was purified by flash column chromatography on silica gel (100% pentane then gradient to 5% diethylether in pentane) to afford the desired product (65 mg, 77% yield) as a clear oil. R_f = 0.45 (SiO_2, 10% diethylether in pentane); IR ν_{max} 3051, 2958, 2822, 2732, 1915, 1701, 1600, 1388, 1251, 1213, 841 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 9.97(1H, s), 7.81(2H, d, *J* = 8.1 Hz), 7.46(2H, d, *J* = 8.0 Hz), 4.76(2H, s), 0.26(9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 212.3, 192.0, 144.6, 134.6, 130.2, 128.4, 98.9, 71.4, -0.3; HRMS *m/e* calcd. for $C_{13}H_{16}OSi$ $(M)^+$ 216.0965 found 216.0969.



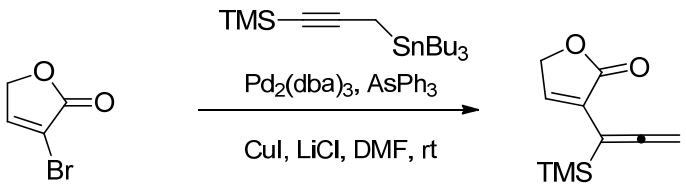
11

2-(1-(Trimethylsilyl)propa-1,2-dienyl)cyclohex-2-enone (11): Following the general procedure, **11** was prepared using **1c** (150 mg, 0.68 mmol). The crude product was purified by flash column chromatography on silica gel (100% pentane then gradient to 5% diethylether in pentane) to afford the desired product (72 mg, 51% yield) as a clear oil. R_f = 0.66 (SiO_2, 20% diethylether in pentane); IR (film) ν_{max} 2953, 1925, 1679, 1358, 1246, 1167, 1129, 842 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 6.79(1H, t, *J* = 4.2 Hz), 4.49(2H, s), 2.48-2.39(4H, m), 2.03-1.97(2H, m), 0.12(9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 210.5, 198.2, 146.2, 137.3, 94.7, 69.0, 38.9, 26.7, 23.2, -0.5; HRMS *m/e* calcd. for $C_{12}H_{19}OSi$ $(M+H)^+$ 207.1200 found 207.1190.



23

Trimethyl(1-(naphthalen-1-yl)propa-1,2-dien-1-yl)silane *(23):* Following the general procedure, **23** was prepared using **1d** (100 mg, 0.39 mmol). The crude product was purified by flash column chromatography on silica gel (100% hexanes then gradient to 10% diethyl ether in hexanes) to afford the desired product (70 mg, 75% yield) as a white solid. R_f = 0.81 (SiO_2, 10% diethyl ether in hexanes); IR (film) ν_{max} 3059, 2957, 2927, 2871, 2160, 1927, 1592, 1389, 1249, 897 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.07-8.04 (1H, m), 7.86-7.83 (1H, m), 7.73 (1H, d, *J* = 8.4Hz), 7.49-7.41 (3H, m), 7.23 (1H, dd, *J* = 7.2, 0.8Hz), 4.54 (2H, s), 0.16 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 209.5, 135.6, 134.2, 131.9, 128.5, 126.7, 126.3, 125.9, 125.7, 125.6, 125.3, 96.8, 68.2, -1.0; HRMS *m/e* calcd. for $C_{16}H_{18}Si_1$ $(M)^+$ 238.1172 found 238.1174.



6 **3a**

3-(1-(Trimethylsilyl)propa-1,2-dien-1-yl)furan-2(5H)-one *(3a):* To a solution of propargyl stannane **(**392 mg, 0.98 mmoles) and iodide (100 mg, 0.61 mmoles) in dry DMF (~0.6 M) was added $AsPh_3$ (0.8 equiv) followed by $Pd_2(dba)_3$ (20 mol%), CuI (0.8 equiv) and LiCl (0.2 equiv) at rt. The reaction was stirred at 22 °C for 9 hrs. The reaction mixture then was quenched with saturated aqueous $NaHCO_3$. The aqueous layer was extracted in diethyl ether (4 × 15 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated *in vacuo.* The crude residue was then purified by flash silica gel column chromatography (100% hexanes then gradient to 40% diethyl ether in hexanes) to afford the desired product (71 mg, 60% yield) as a clear colorless oil. R_f =0.53 (SiO_2, 50% diethyl ether in hexanes); IR (film) ν_{max} 2957, 1919, 1760, 1345, 1250, 1072, 842 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.15 (1H, s), 4.80 (2H, d, *J* = 1.2Hz), 4.73

(2H, d, *J* = 1.2Hz), 0.21 (9H, s); ^{13}C NMR ($CDCl_3$, 101 MHz) δ 212.9, 172.4, 143.2, 129.5, 88.2, 71.3, 69.9, -0.8; HRMS *m/e* calcd. for $C_{10}H_{15}O_2Si_1$ $(M+H)^+$ 195.0836 found 195.0838.

References:

[1]Pangborn, A. B.; Giardellow, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996**, *15*, 1518-1520.

[2]Kim, C. H.; An, H. J.; Shin, W. K.; Yu, W.; Woo, S. K.; Jung, S. K.; Lee, E. *Angew. Chem. Int.Ed.* **2006**, *45*, 8019-8021.

[3]Williams, D. R.; Shah, A. A. *Chem. Commun.* **2010**, *46*, 4297-4299.

AAS-4-232-1H

Data Collected on:
vxr400-inova400
Archive directory:

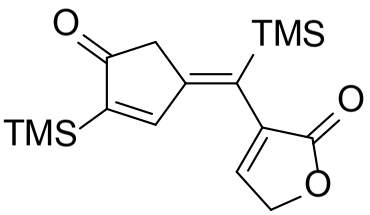
Sample directory:

FidFile: AAS-4-232-1H-again

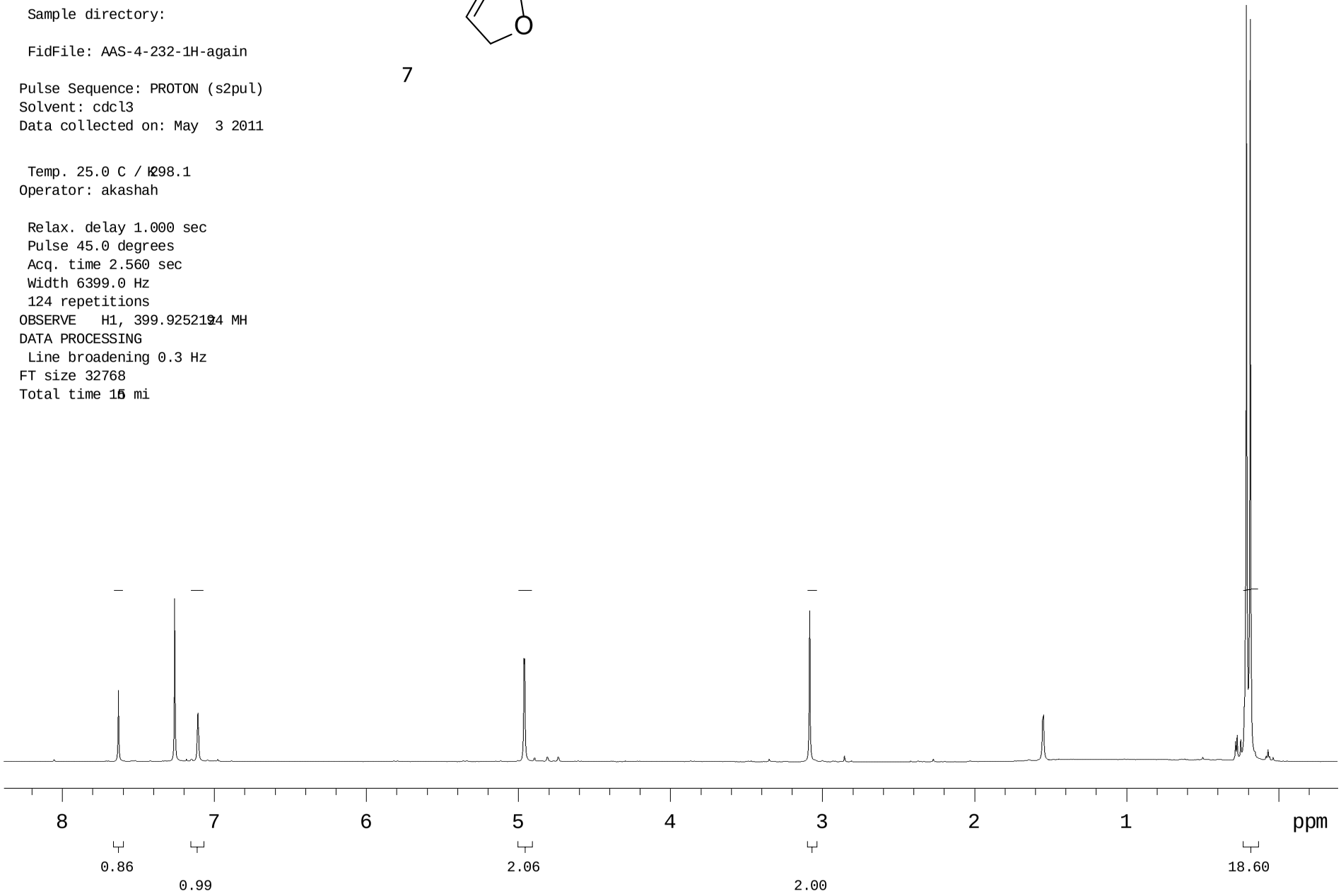
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 3 2011

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
124 repetitions
OBSERVE H1, 399.9252194 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 15 min



7



AAS-4-232-13C

Sample Name:

Data Collected on:
vxr400-inova400
Archive directory:

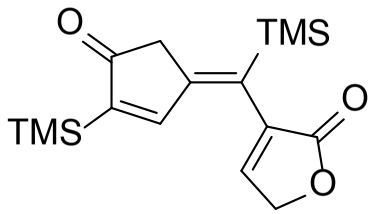
Sample directory:

FidFile: AAS-4-232-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 22 2011

Temp. 25.0 C / 298.1 K
Operator: akashah

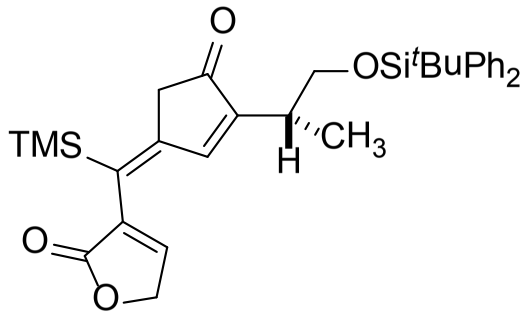
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
12000 repetitions
OBSERVE C13, 100.5612523 MHz
DECOUPLE H1, 399.9272260 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 11 hr, 2 min



7

Data Collected on:
vxr400-inova400
Archive directory:

Sample directory:

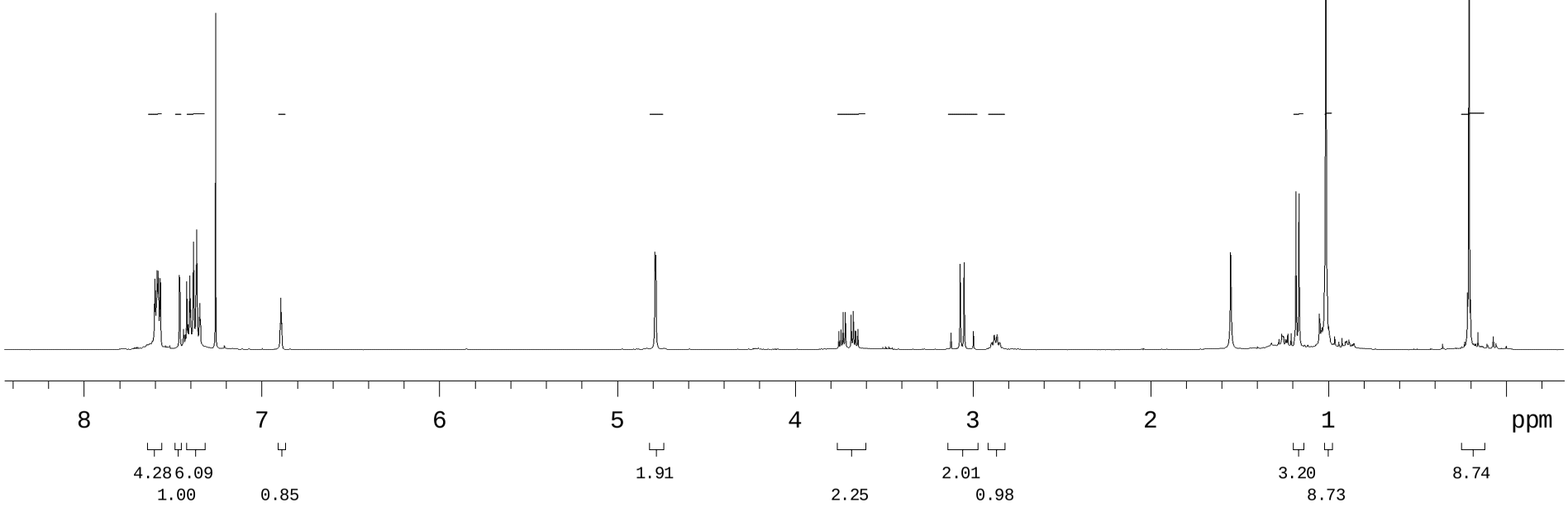


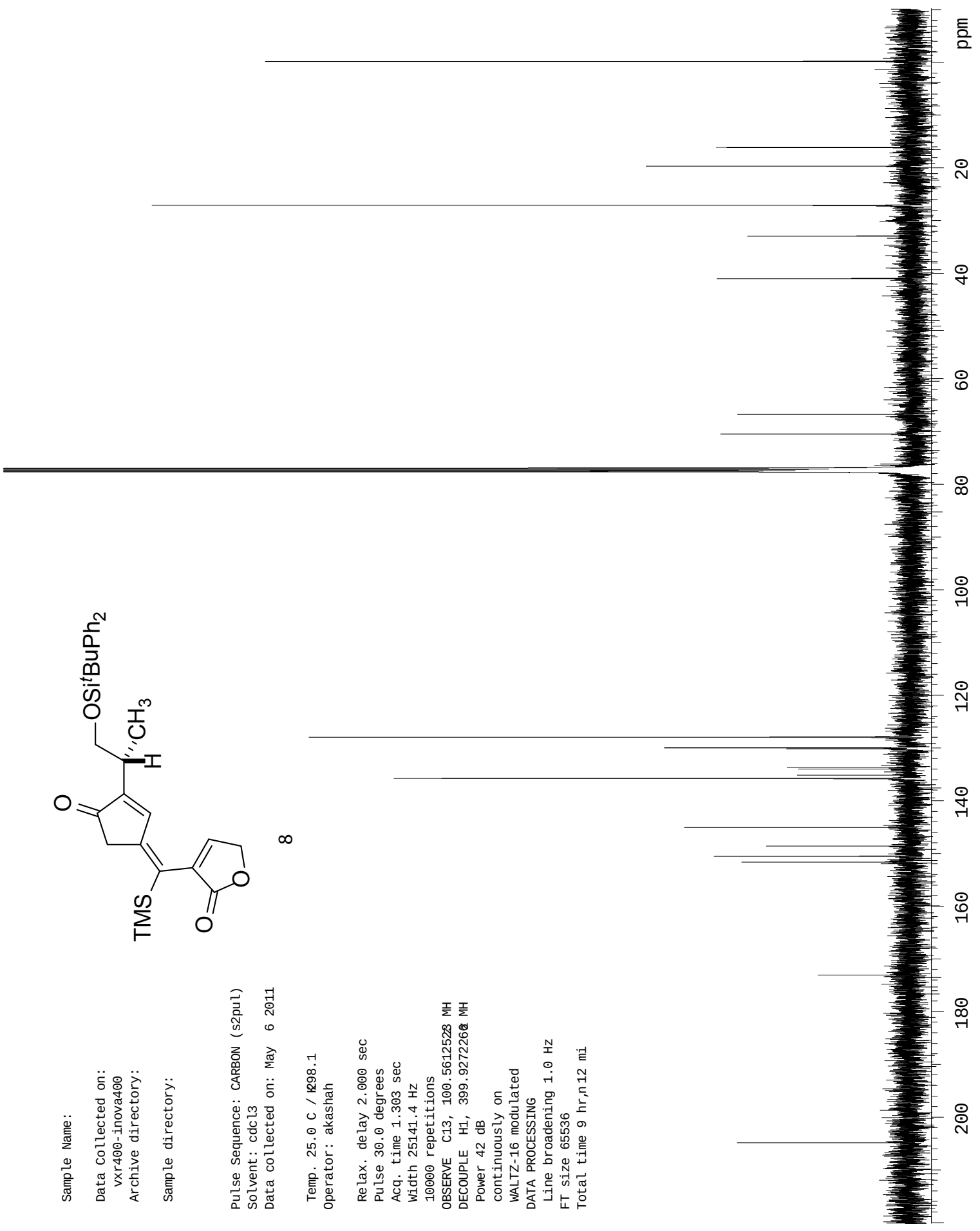
8

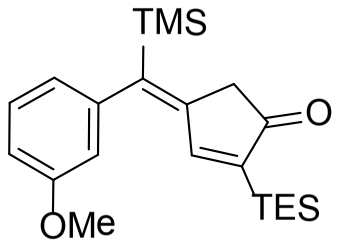
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 6 2011

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
44 repetitions
OBSERVE H1, 399.9252124 MH
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 15 mi




Sample Name:
Data Collected on:
vxr400-inova400
Archive directory:
Sample directory:
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 6 2011
Temp. 25.0 C / 298.1 K
Operator: akashah
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
10000 repetitions
OBSERVE C13, 100.5612523 MH
DECOUPLE H1, 399.9272260 MH
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 hr,n12 mi
OSi^{t}BuPh$_2$
CH$_3$
H
O
TMS
O
O
8
200
180
160
140
120
100
80
60
40
20
ppm



12

Data Collected on:
vxr400-inova400
Archive directory:

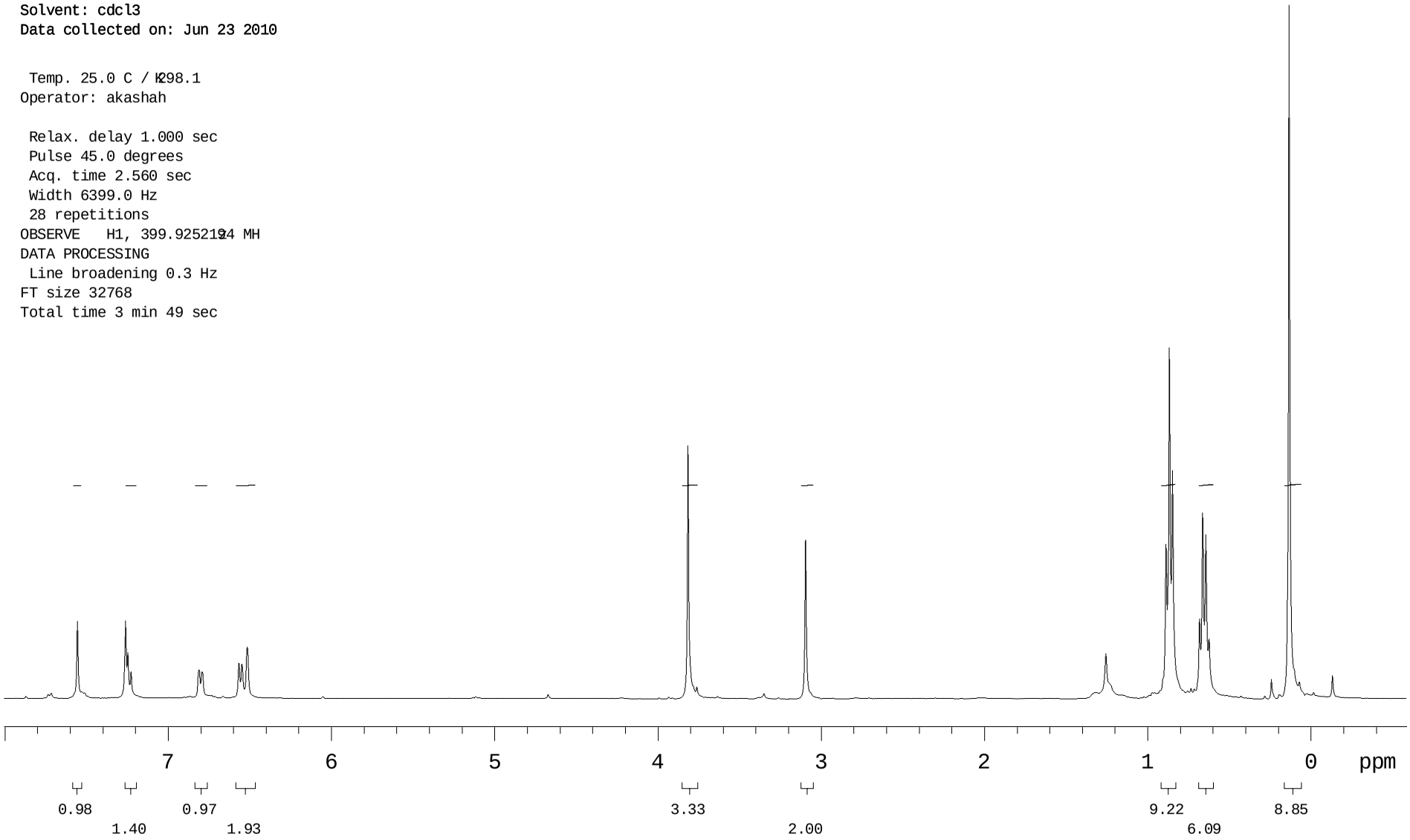
Sample directory:

FidFile: AAS-3-186-1H

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 23 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
28 repetitions
OBSERVE H1, 399.9252194 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 3 min 49 sec



VARIAN

AAS-3-186-13C

Data Collected on:
vxr400-inova400
Archive directory:

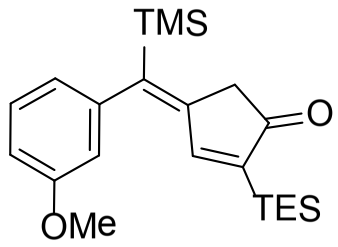
Sample directory:

FidFile: AAS-3-186-a-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 23 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
1232 repetitions
OBSERVE C13, 100.5612531 MH
DECOUPLE H1, 399.9272260 MH
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 3 hr, 40 mi



12

AAS-3-150-1H

Data Collected on:
vxr400-inova400
Archive directory:

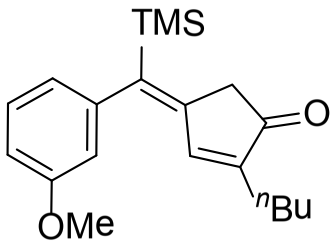
Sample directory:

FidFile: AAS-3-150-1H

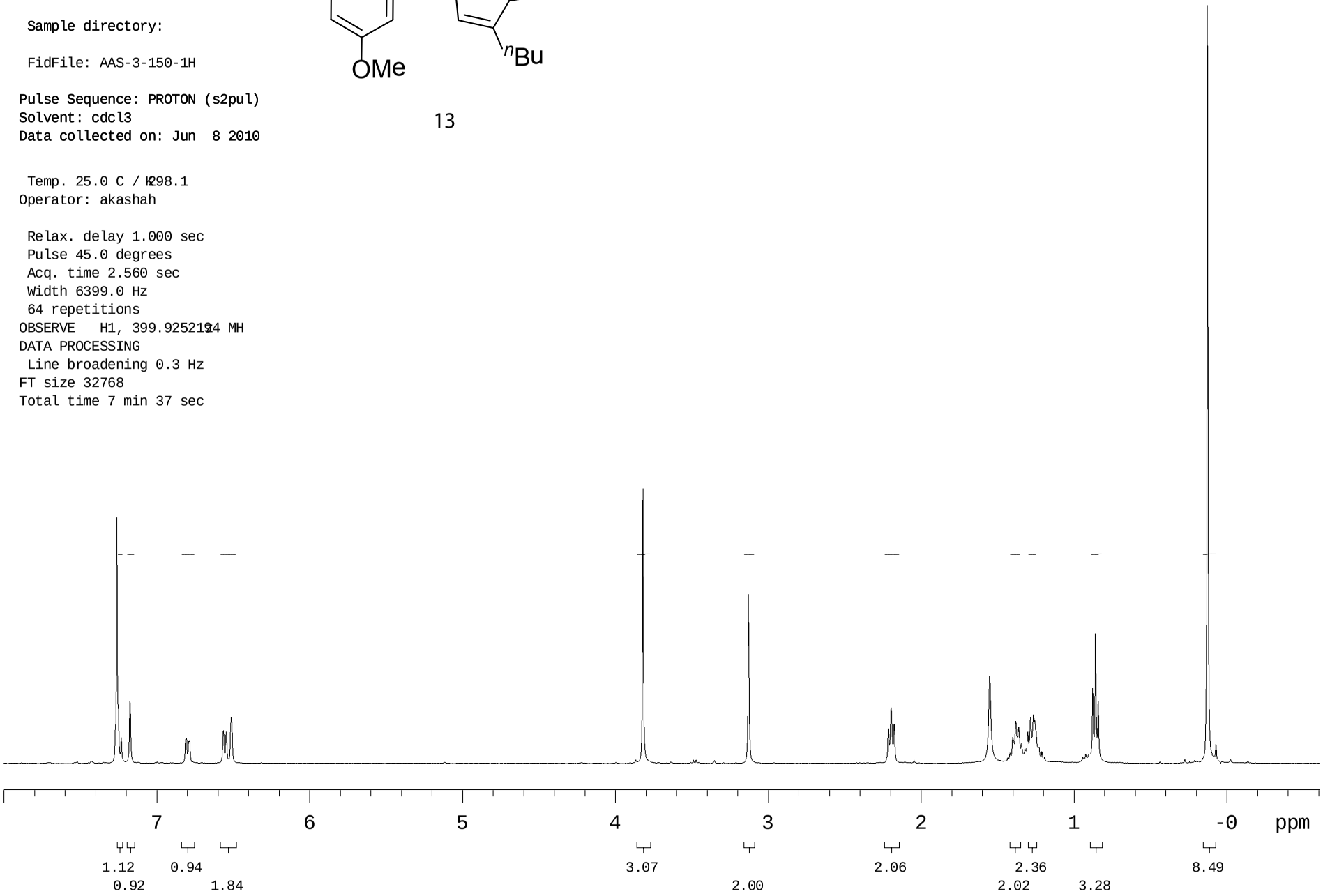
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 8 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
64 repetitions
OBSERVE H1, 399.9252194 MH
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 7 min 37 sec



13



AAS-3-150-13C

Data Collected on:
vxr400-inova400
Archive directory:

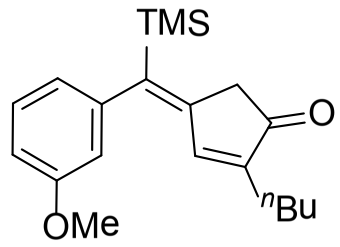
Sample directory:

FidFile: AAS-3-150-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 8 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
10500 repetitions
OBSERVE C13, 100.5612531 MHz
DECOUPLE H1, 399.9272260 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 hr, 39 min



13

AAS-3-188-1H

Data Collected on:
vxr400-inova400
Archive directory:

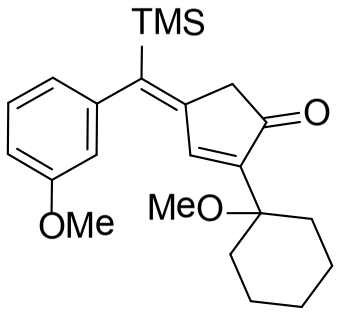
Sample directory:

FidFile: AAS-3-188-1H

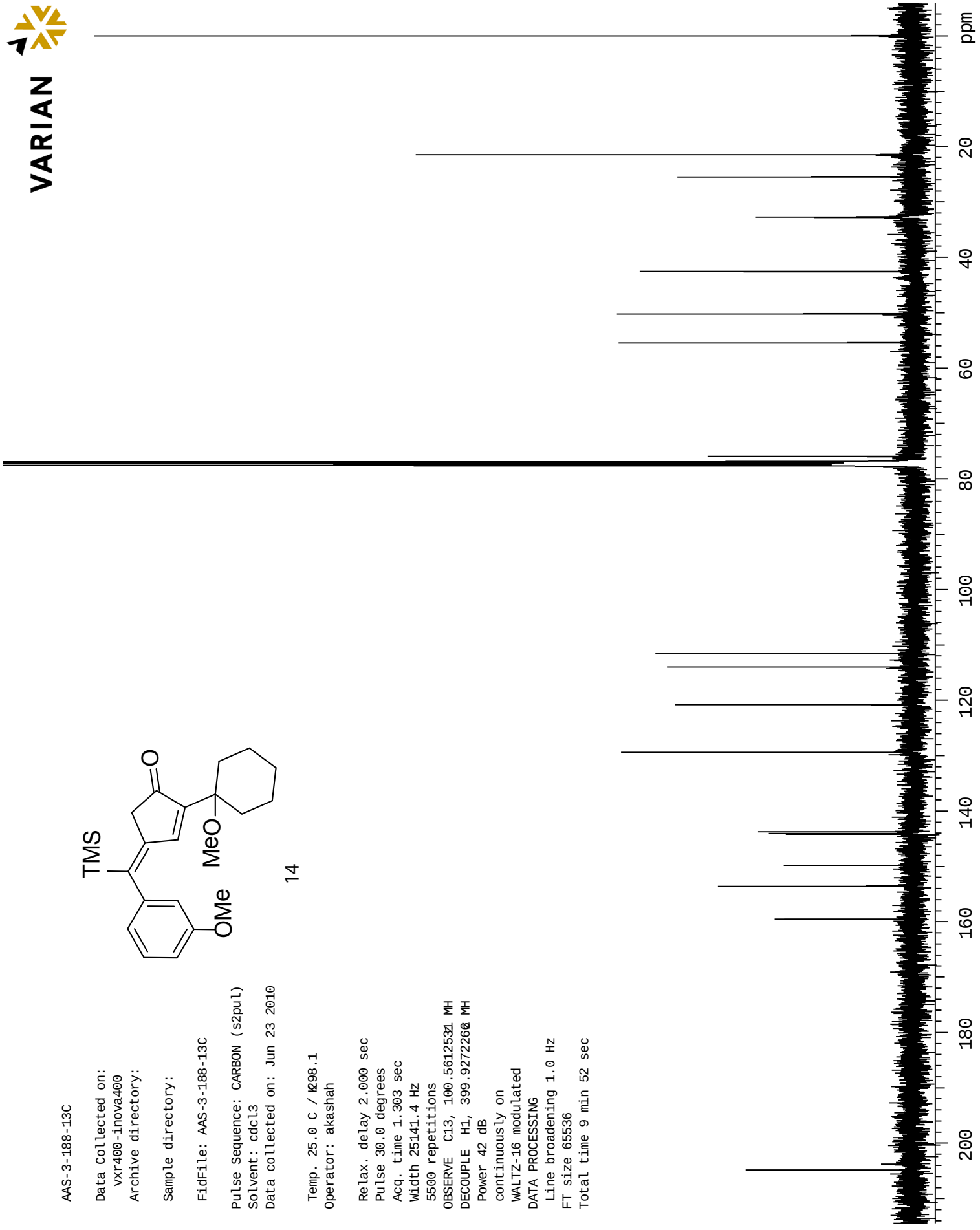
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 23 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
40 repetitions
OBSERVE H1, 399.9252718 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 3 min 49 sec



14


VARIAN
AAS-3-188-13C
Data Collected on:
vxr400-inova400
Archive directory:
Sample directory:
FidFile: AAS-3-188-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 23 2010
Temp. 25.0 C / 298.1
Operator: akashah
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
5500 repetitions
OBSERVE C13, 100.5612532 MH
DECOUPLE H1, 399.9272268 MH
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 min 52 sec
TMS
MeO
OMe
O
14
200
180
160
140
120
100
80
60
40
20
ppm

AAS-3-178-1H
Data Collected on:
vxr400-inova400
Archive directory:

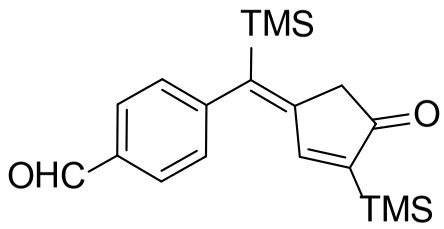
Sample directory:

FidFile: AAS-3-178-1H

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 17 2010

Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
28 repetitions
OBSERVE H1, 399.9252128 MH
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 3 min 49 sec



15

Data Collected on:
vxr400-inova400
Archive directory:

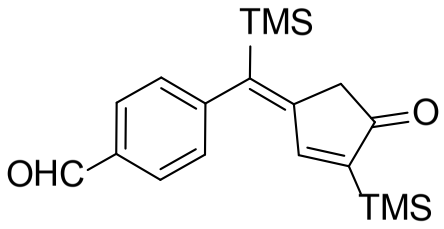
Sample directory:

FidFile: AAS-3-178-13C

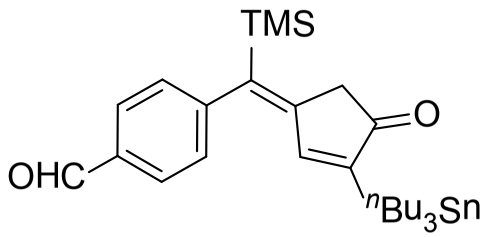
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 6 2011

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
10000 repetitions
OBSERVE C13, 100.5612523 MHz
DECOUPLE H1, 399.9272260 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 hr, 12 min



15



16

AAS-3-308-1H

Data Collected on:
vxr400-inova400
Archive directory:

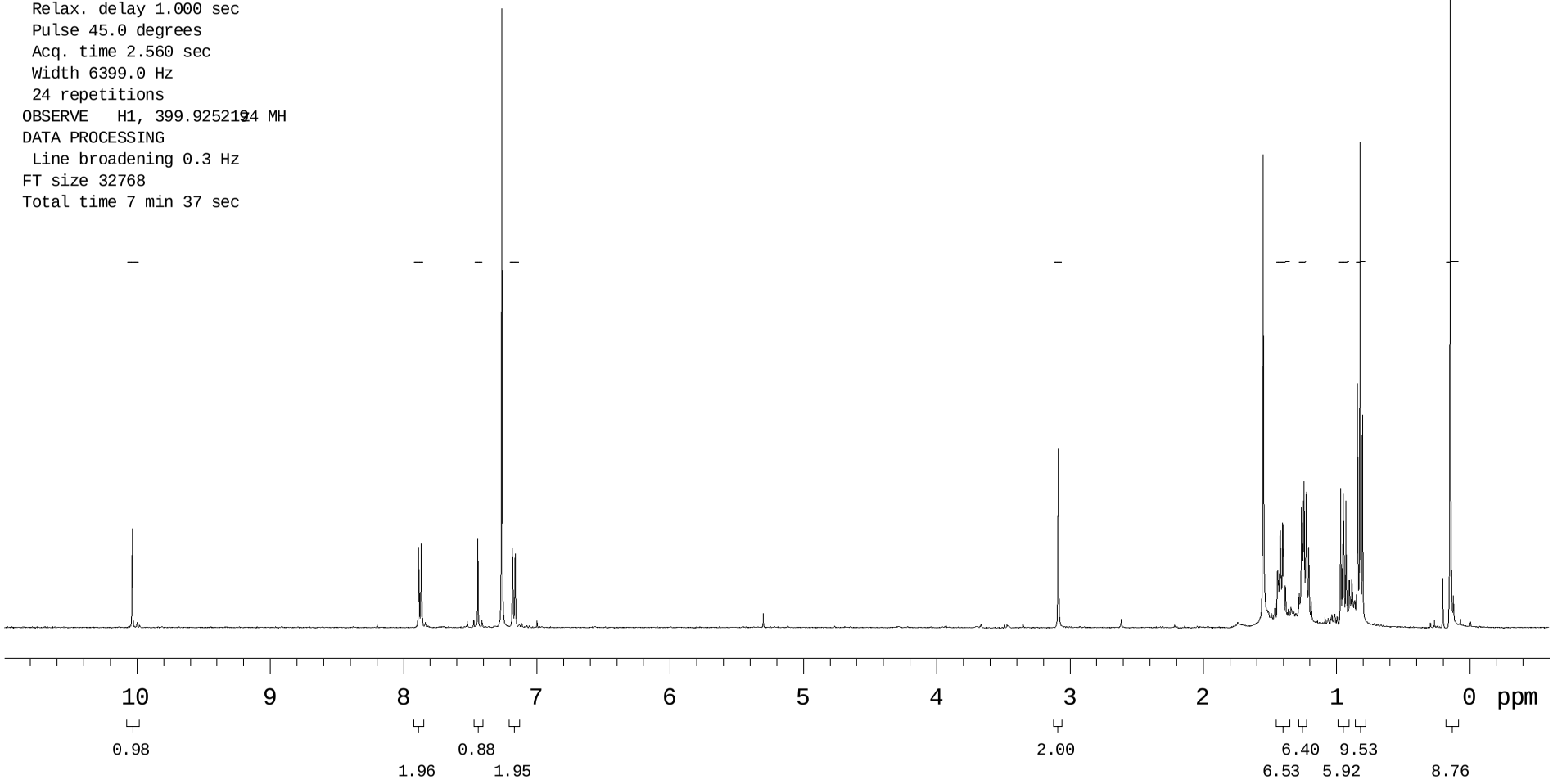
Sample directory:

FidFile: AAS-3-308-1H

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 14 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
24 repetitions
OBSERVE H1, 399.9252124 MH
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 7 min 37 sec



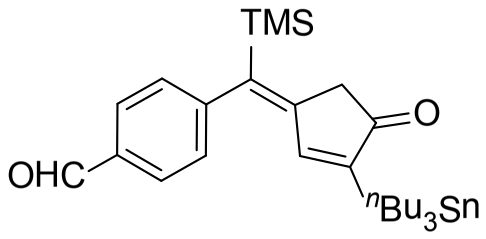
VARIAN

AAS-3-308-13C

Data Collected on:
vxr400-inova400
Archive directory:

Sample directory:

FidFile: AAS-3-308-13C

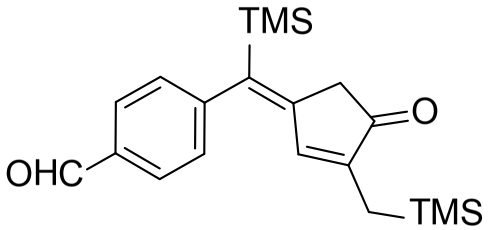


16

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 13 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
11000 repetitions
OBSERVE C13, 100.5612523 MHz
DECOUPLE H1, 399.9272262 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 10 hr, 7 min



17

AAS-3-304-1H

Data Collected on:
vxr400-inova400
Archive directory:

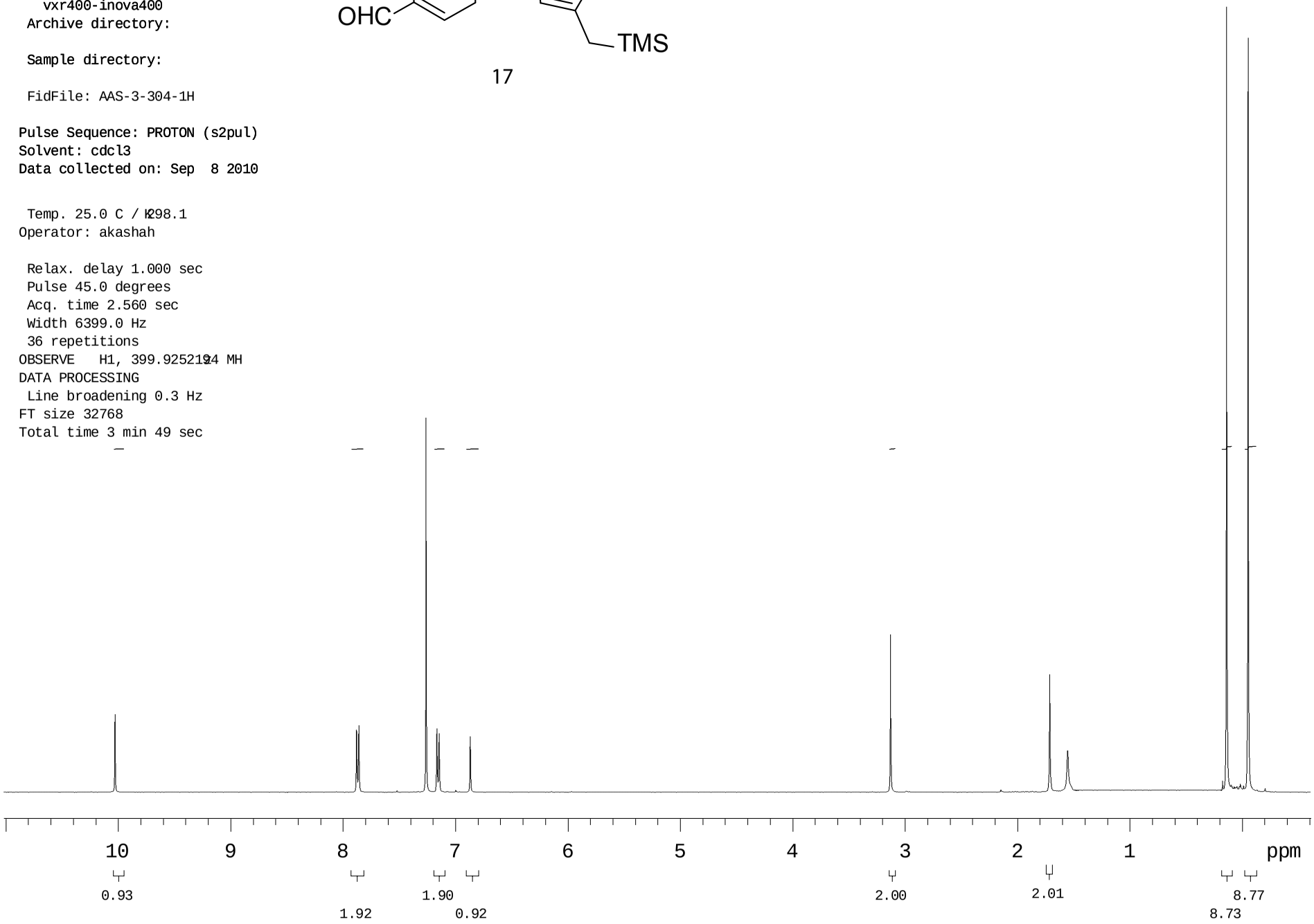
Sample directory:

FidFile: AAS-3-304-1H

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 8 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
36 repetitions
OBSERVE H1, 399.9252194 MH
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 3 min 49 sec



AAS-3-304-13C

Data Collected on:
vxr400-inova400
Archive directory:

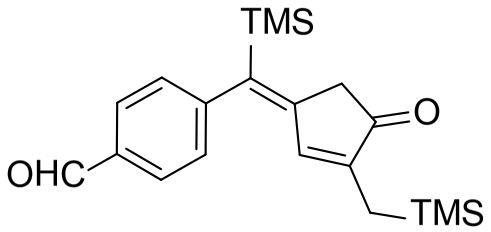
Sample directory:

FidFile: AAS-3-304-a-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 9 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
8000 repetitions
OBSERVE C13, 100.5612531 MH
DECOUPLE H1, 399.9272260 MH
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 min 52 sec



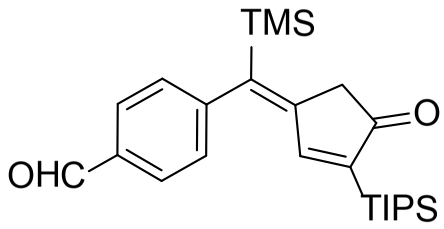
17

AAS-4-46-1H

Data Collected on:
vxr400-inova400
Archive directory:

Sample directory:

FidFile: AAS-4-46-1H



18

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 22 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

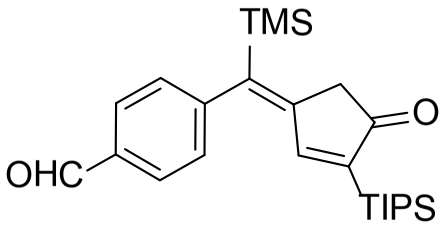
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
128 repetitions
OBSERVE H1, 399.9252128 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 7 min 37 sec

AAS-4-46-13C

Data Collected on:
vxr400-inova400
Archive directory:

Sample directory:

FidFile: AAS-4-46-A-13C



18

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 22 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
5000 repetitions
OBSERVE C13, 100.5612528 MHz
DECOUPLE H1, 399.9272260 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 min 52 sec

AAS-3-130-1H

Data Collected on:
i400-inova400
Archive directory:

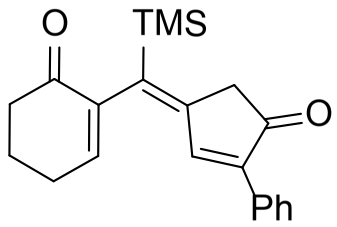
Sample directory:

FidFile: AAS-3-130-1H

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 2 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6401.5 Hz
52 repetitions
OBSERVE H1, 400.1076209 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 7 min 37 sec



19

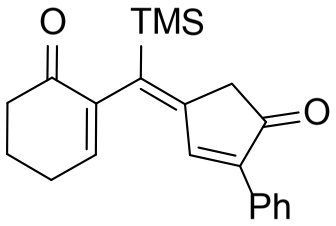
VARIAN

AAS-3-206-13C

Data Collected on:
vxr400-inova400
Archive directory:

Sample directory:

FidFile: AAS-3-206-13C



19

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 10 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
8000 repetitions
OBSERVE C13, 100.5612523 MH
DECOUPLE H1, 399.9272262 MH
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 min 52 sec

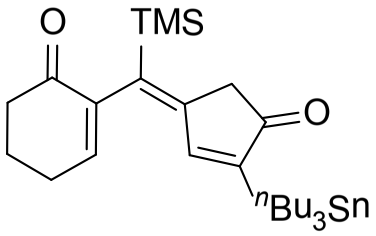
AAS-3-260-1H

Sample Name:

Data Collected on:
vxr400-inova400
Archive directory:

Sample directory:

FidFile: AAS-3-260-1H

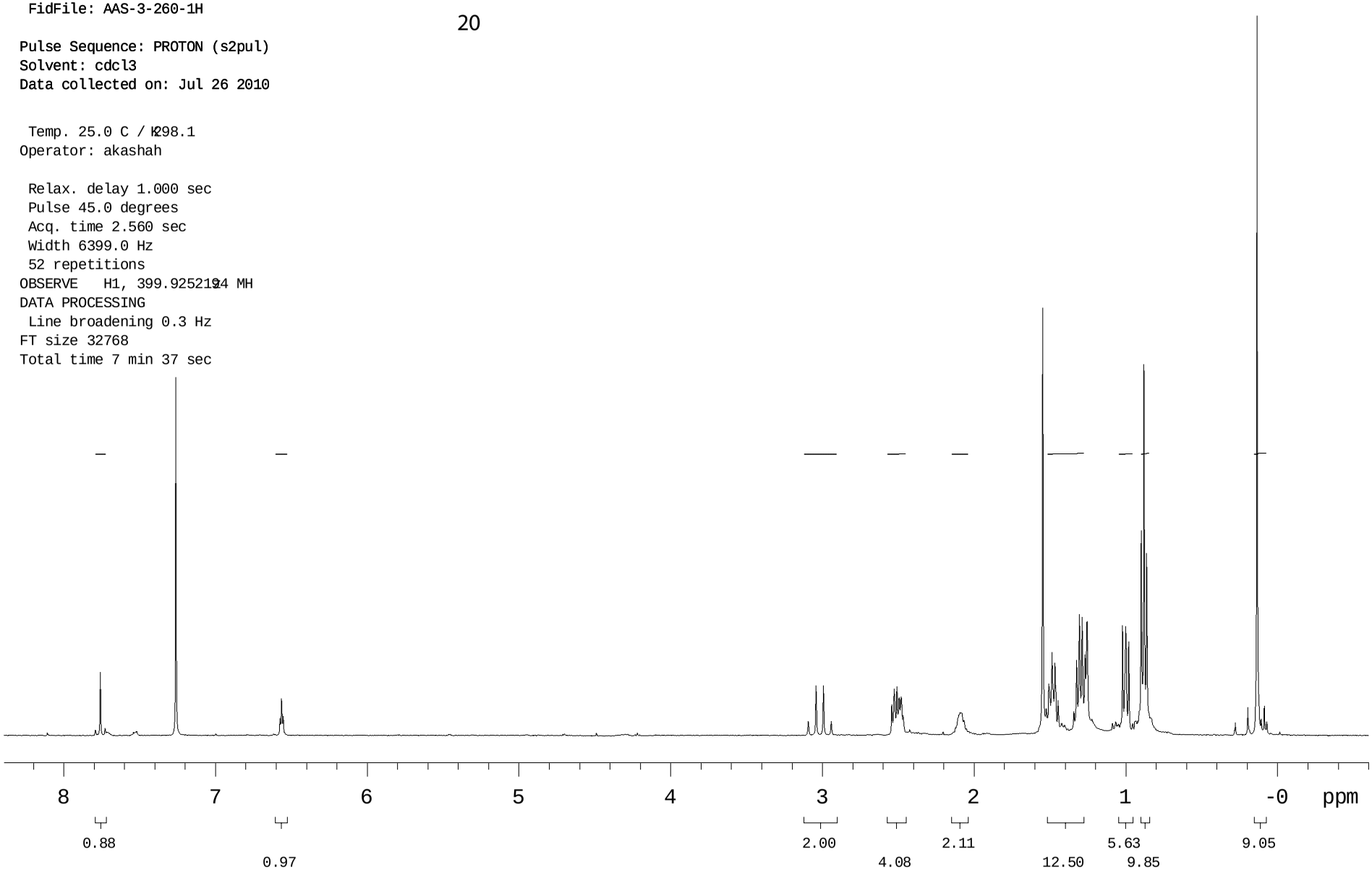


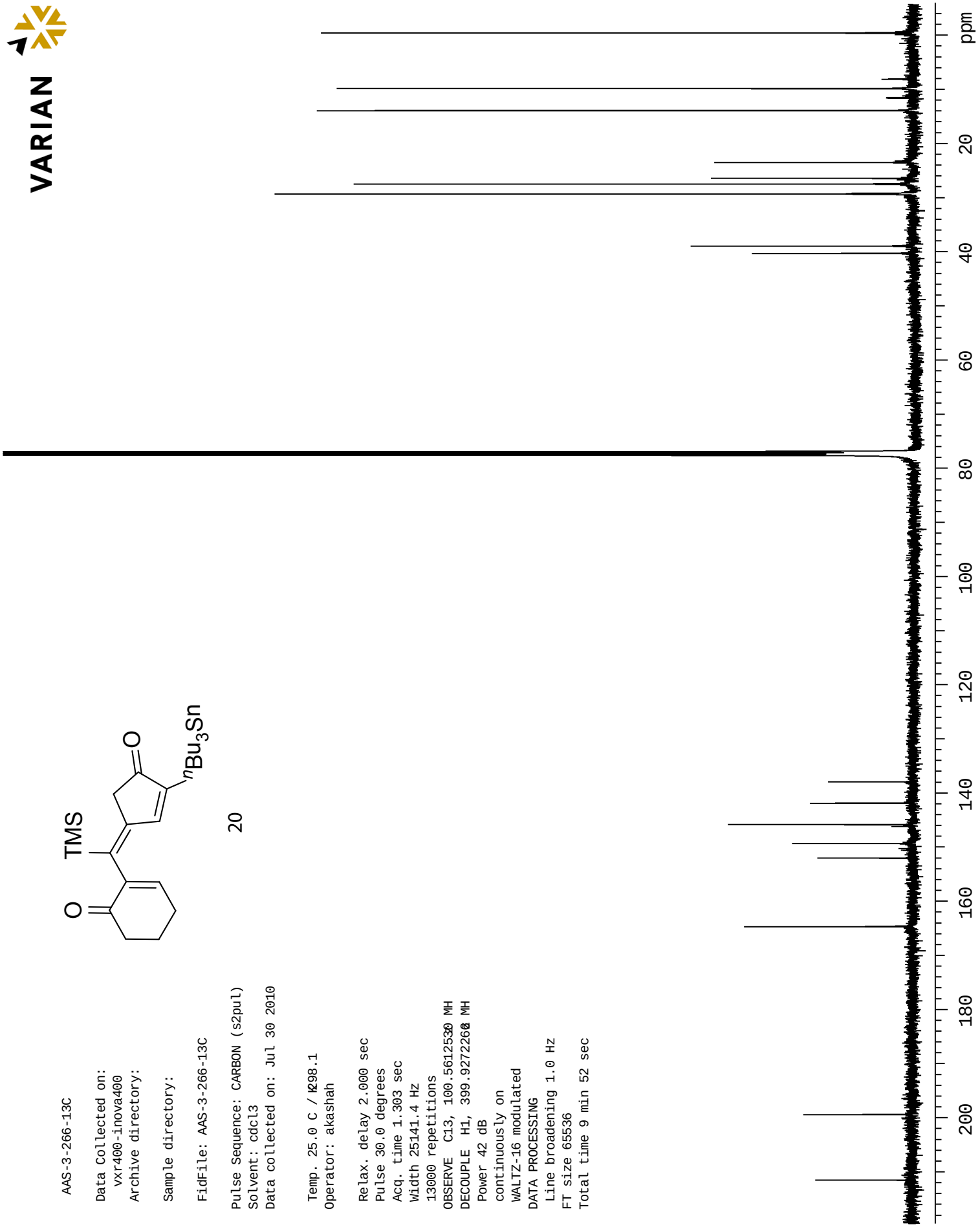
20

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 26 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
52 repetitions
OBSERVE H1, 399.9252194 MH
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 7 min 37 sec




VARIAN
AAS-3-266-13C
Data Collected on:
vxr400-inova400
Archive directory:
Sample directory:
FidFile: AAS-3-266-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 30 2010
Temp. 25.0 C / 298.1
Operator: akashah
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
13000 repetitions
OBSERVE C13, 100.5612530 MH
DECOUPLE H1, 399.9272260 MH
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 min 52 sec
O
TMS
O
nBu3Sn
20
200
180
160
140
120
100
80
60
40
20
ppm

AAS-3-270-1H

Sample Name:

Data Collected on:
vxr400-inova400
Archive directory:

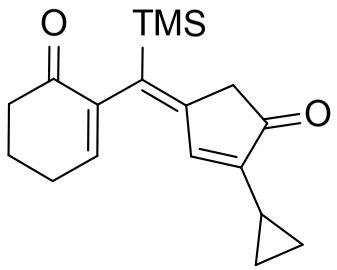
Sample directory:

FidFile: AAS-3-270-1H

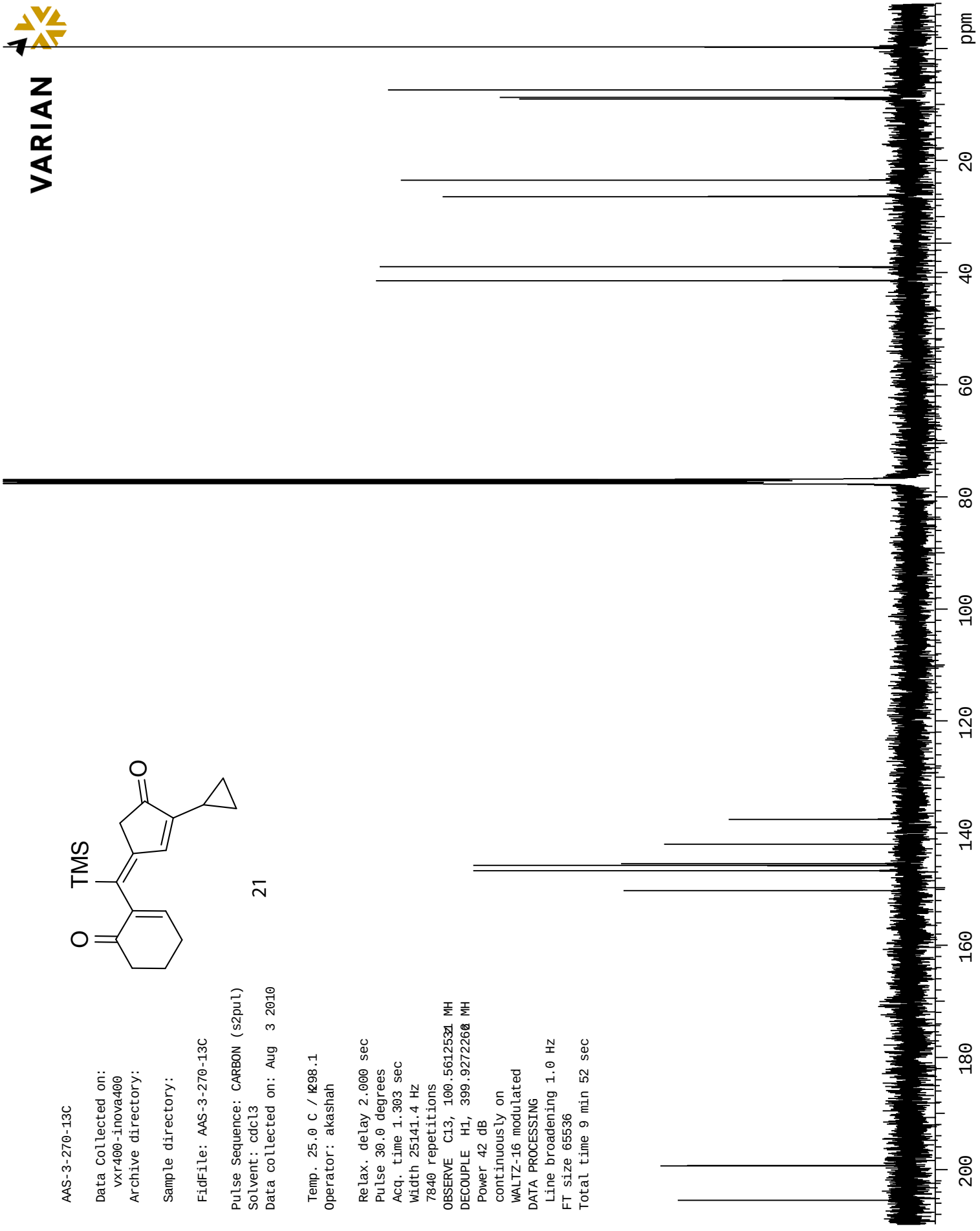
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 6 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
52 repetitions
OBSERVE H1, 399.9252124 MH
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 7 min 37 sec



21


VARIAN
AAS-3-270-13C
Data Collected on:
vxr400-inova400
Archive directory:
Sample directory:
FidFile: AAS-3-270-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 3 2010
Temp. 25.0 C / 298.1
Operator: akashah
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
7840 repetitions
OBSERVE C13, 100.5612531 MH
DECOUPLE H1, 399.9272268 MH
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 min 52 sec
TMS
O
O
21
200
180
160
140
120
100
80
60
40
20
ppm

AAS-3-268-1H

Data Collected on:
vxr400-inova400
Archive directory:

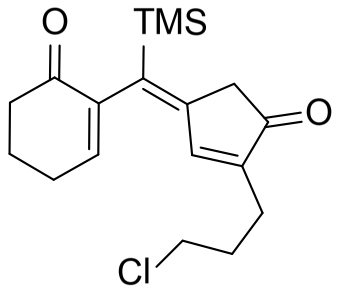
Sample directory:

FidFile: AAS-3-268-1H

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 2 2010

Temp. 25.0 C / K298.1
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
84 repetitions
OBSERVE H1, 399.925219[illegible]4 MH
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 7 min 37 sec



22

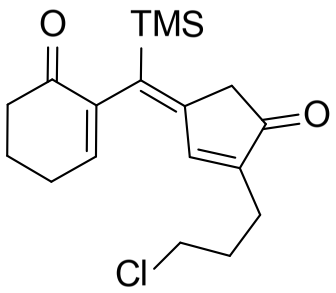
VARIAN

AAS-3-268-13C

Data Collected on:
vxr400-inova400
Archive directory:

Sample directory:

FidFile: AAS-3-268-13C

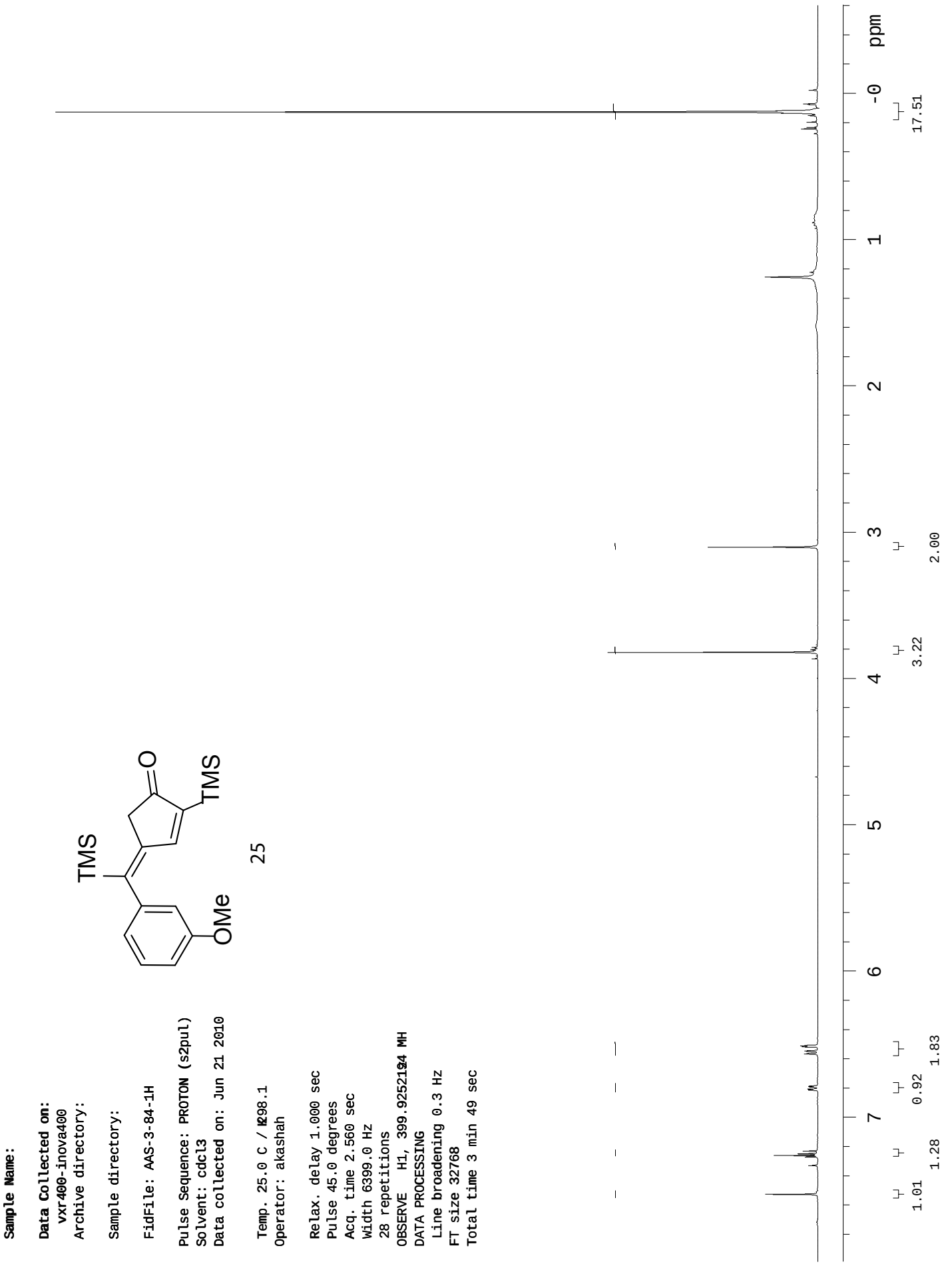


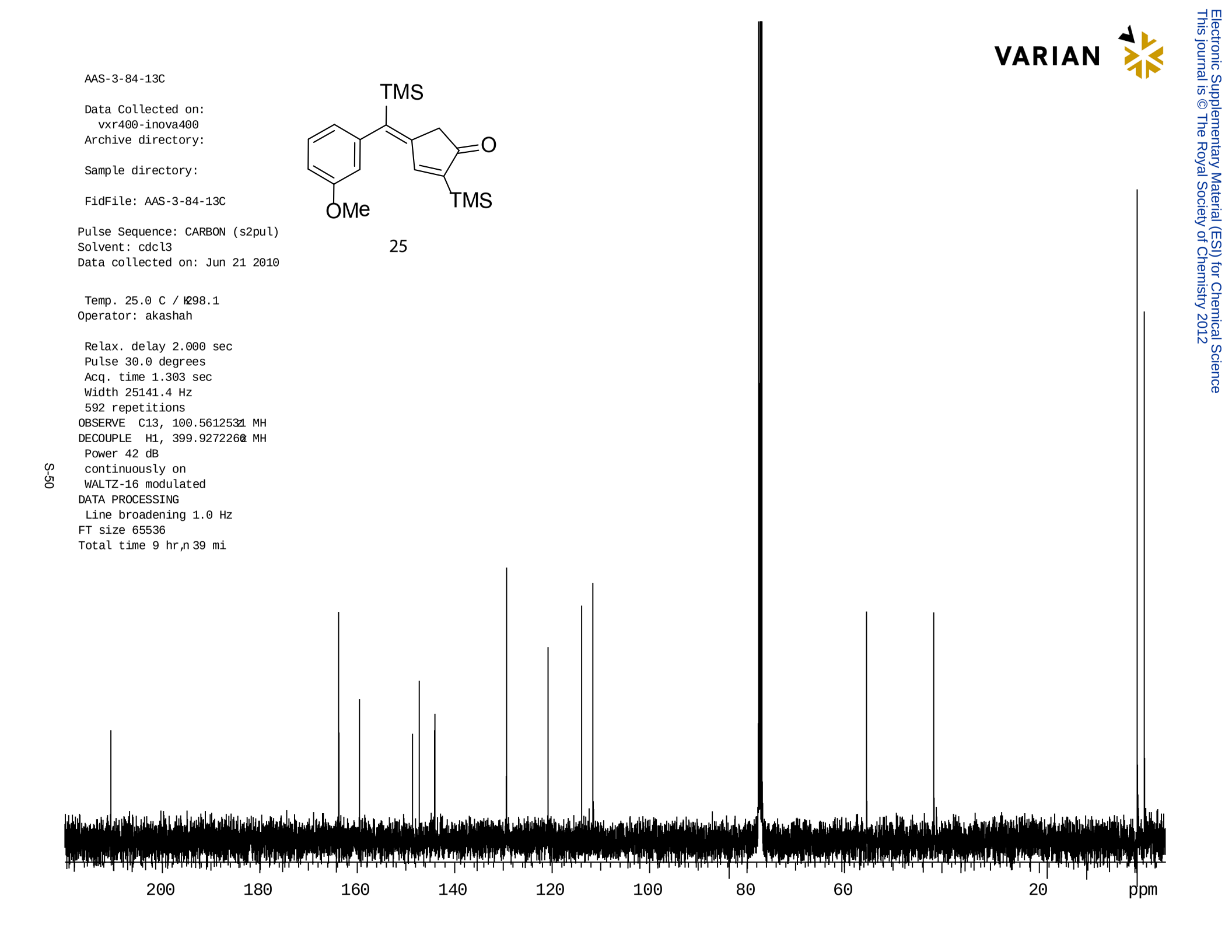
22

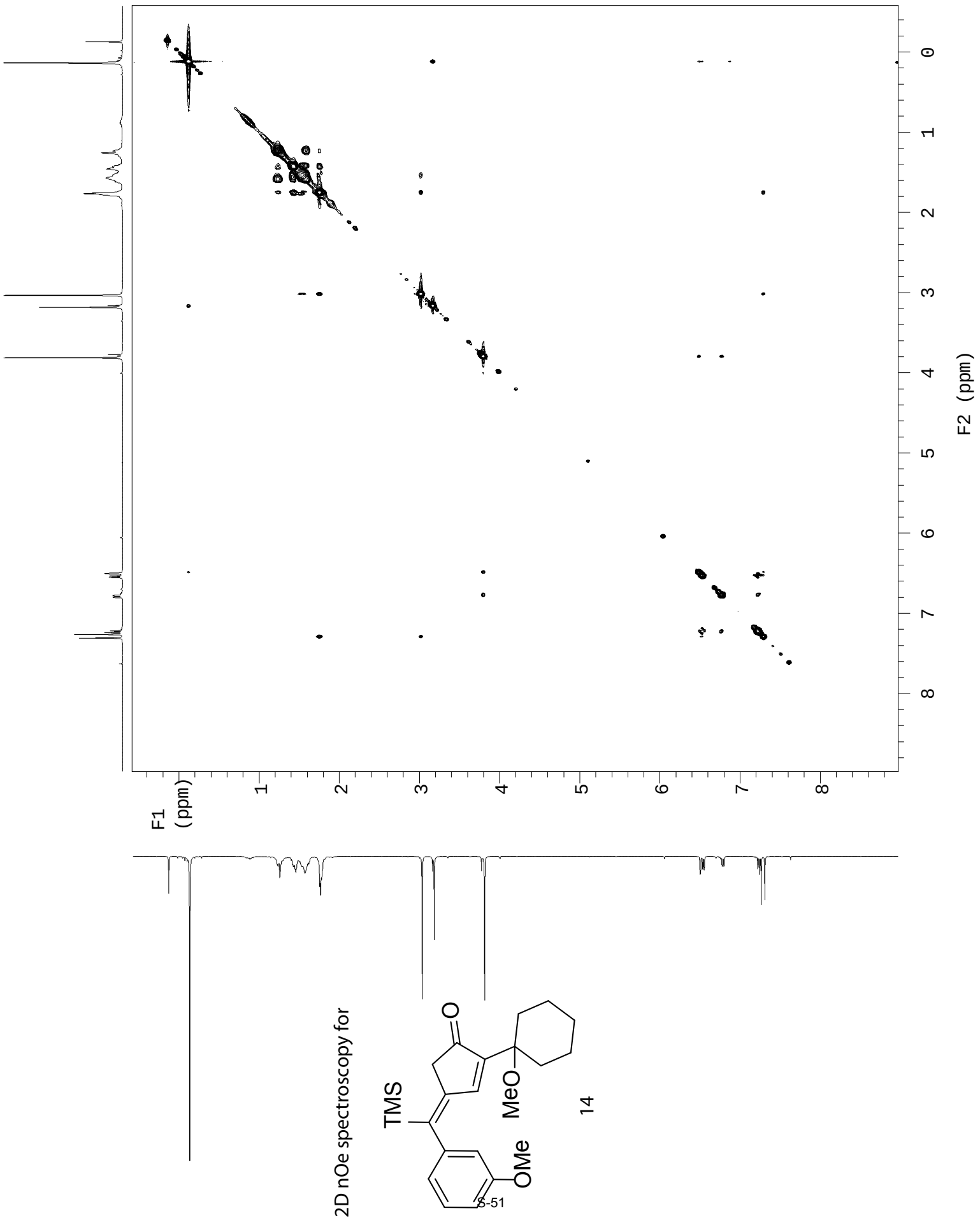
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 26 2010

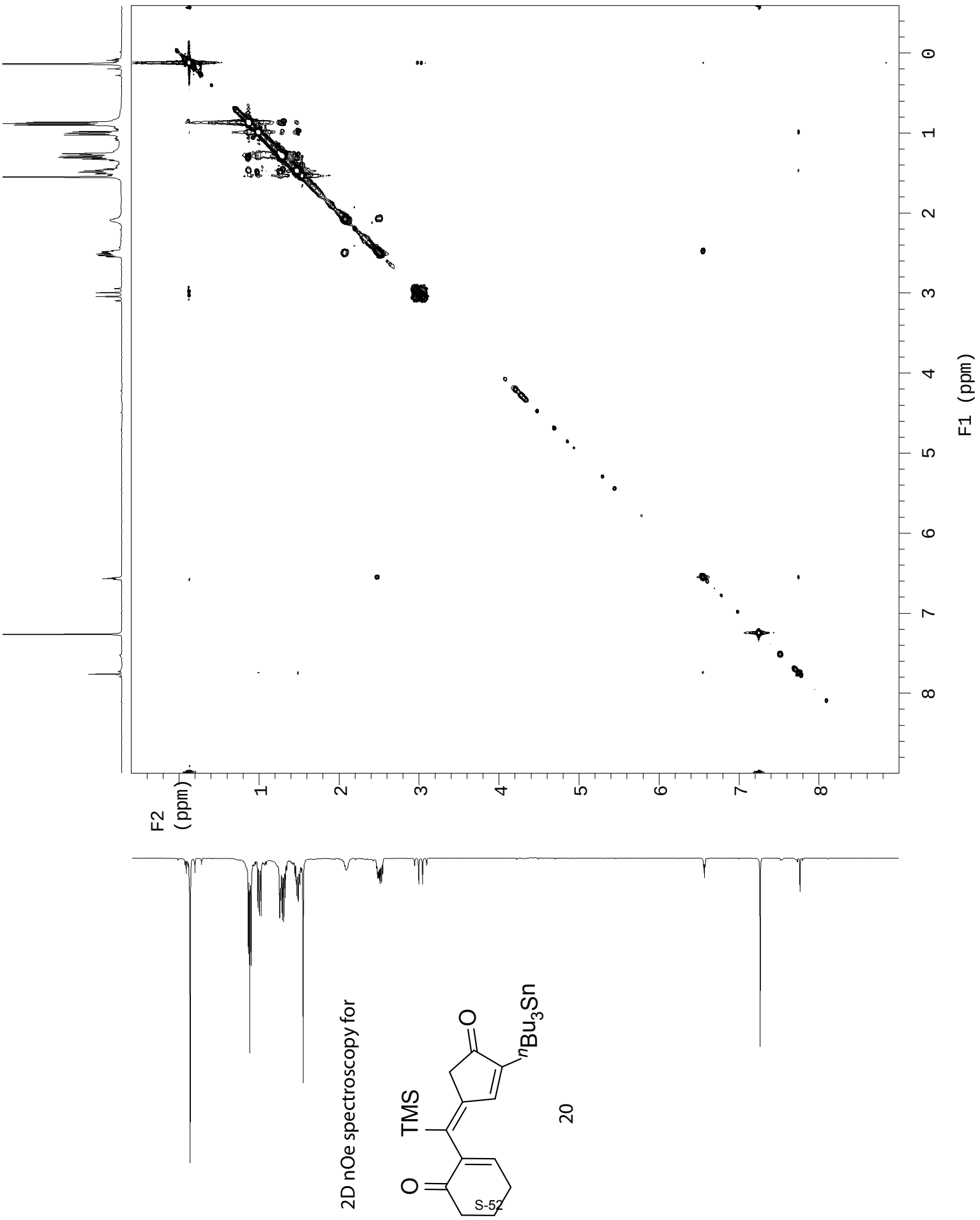
Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
8000 repetitions
OBSERVE C13, 100.5612531 MHz
DECOUPLE H1, 399.9272260 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 min 52 sec


Sample Name:
Data Collected on:
vxr400-inova400
Archive directory:
Sample directory:
FidFile: AAS-3-84-1H
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 21 2010
Temp. 25.0 C / 298.1
Operator: akashah
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
28 repetitions
OBSERVE H1, 399.9252134 MH
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 3 min 49 sec
TMS
O
TMS
OMe
25
ppm
1.01
1.28
0.92
1.83
3.22
2.00
17.51

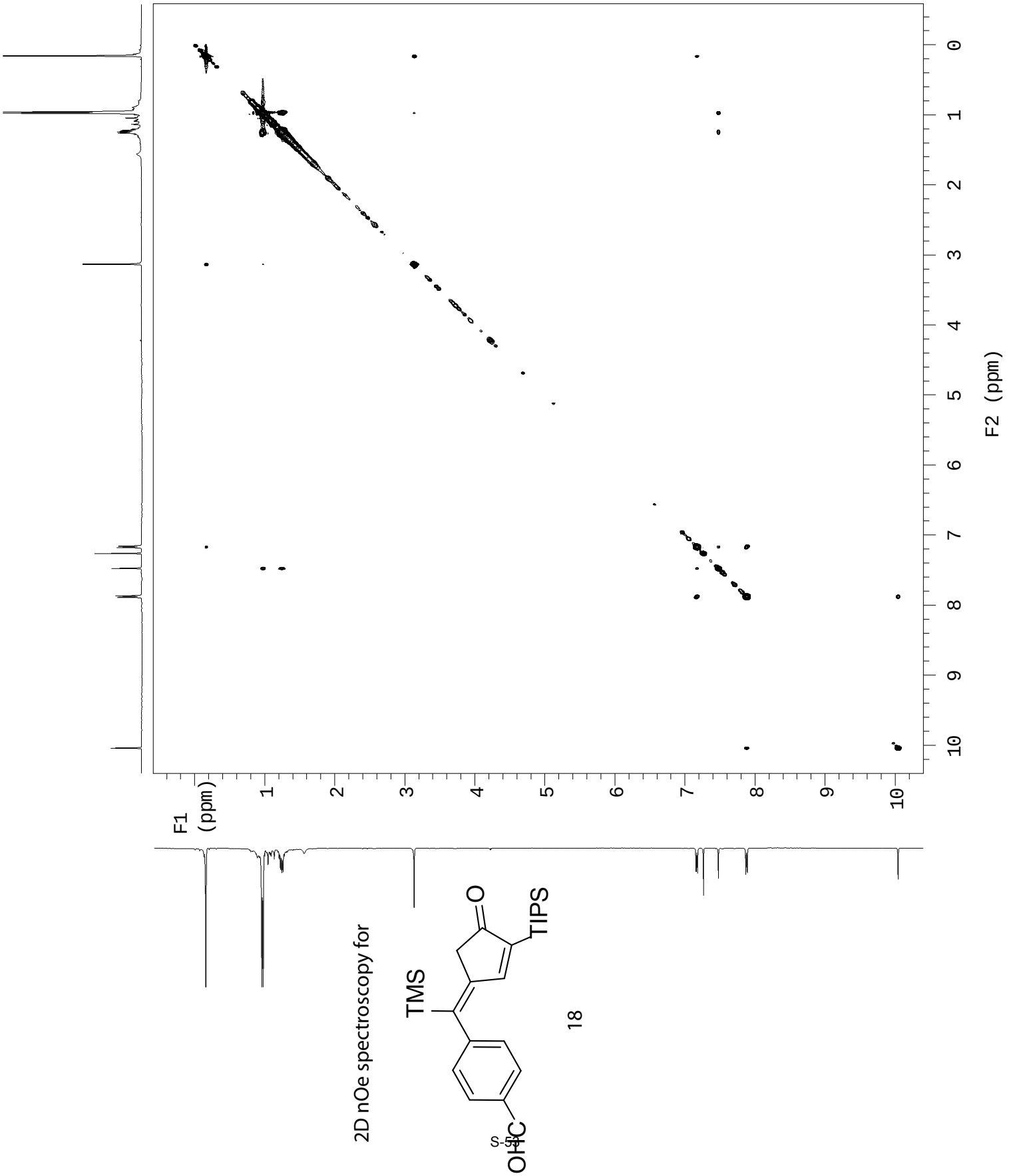


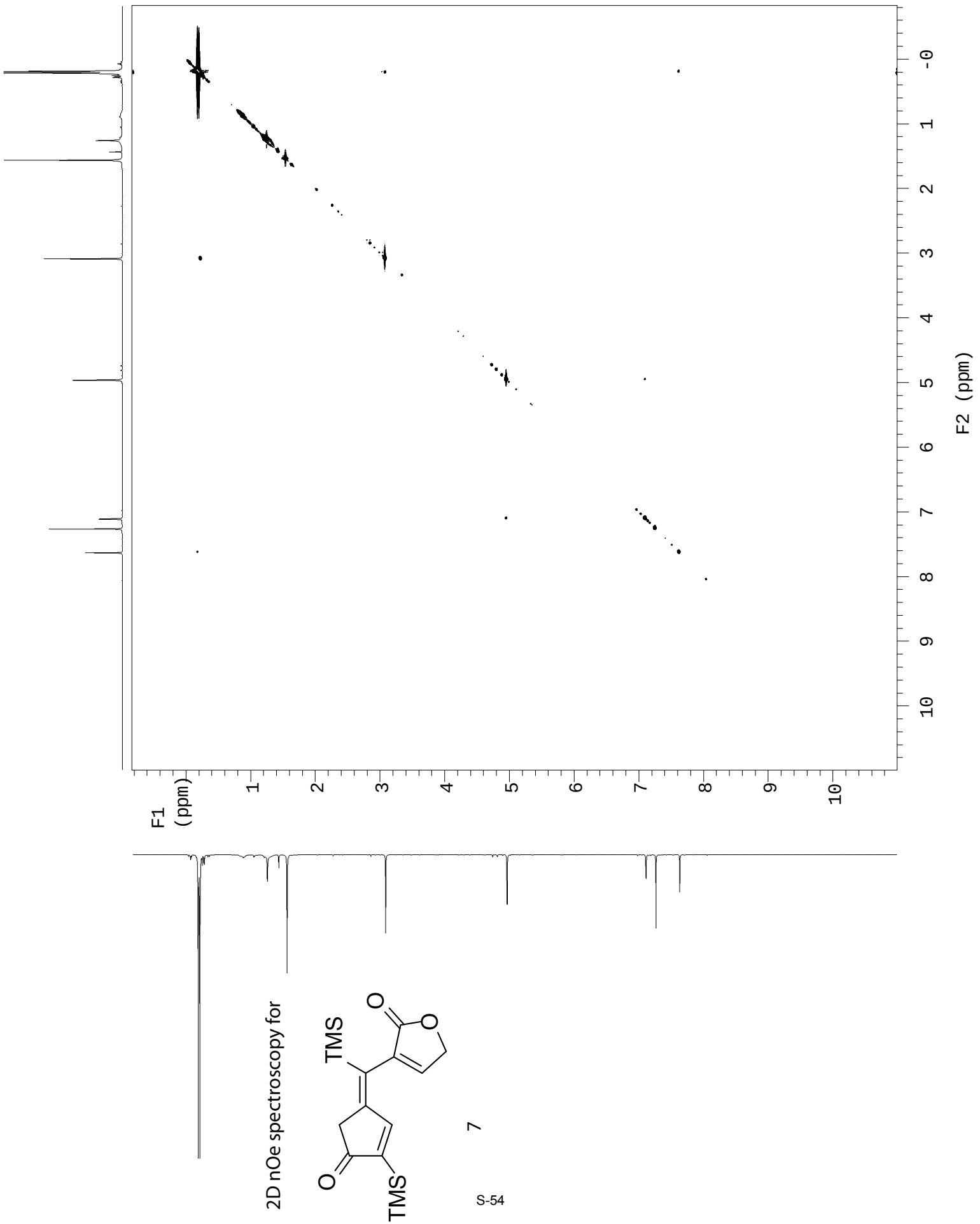




2D nOe spectroscopy for

20





2D nOe spectroscopy for

7

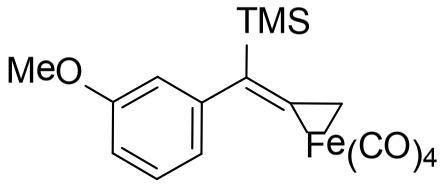
AAS-4-54-1H

Sample Name:

Data Collected on:
vxr400-inova400
Archive directory:

Sample directory:

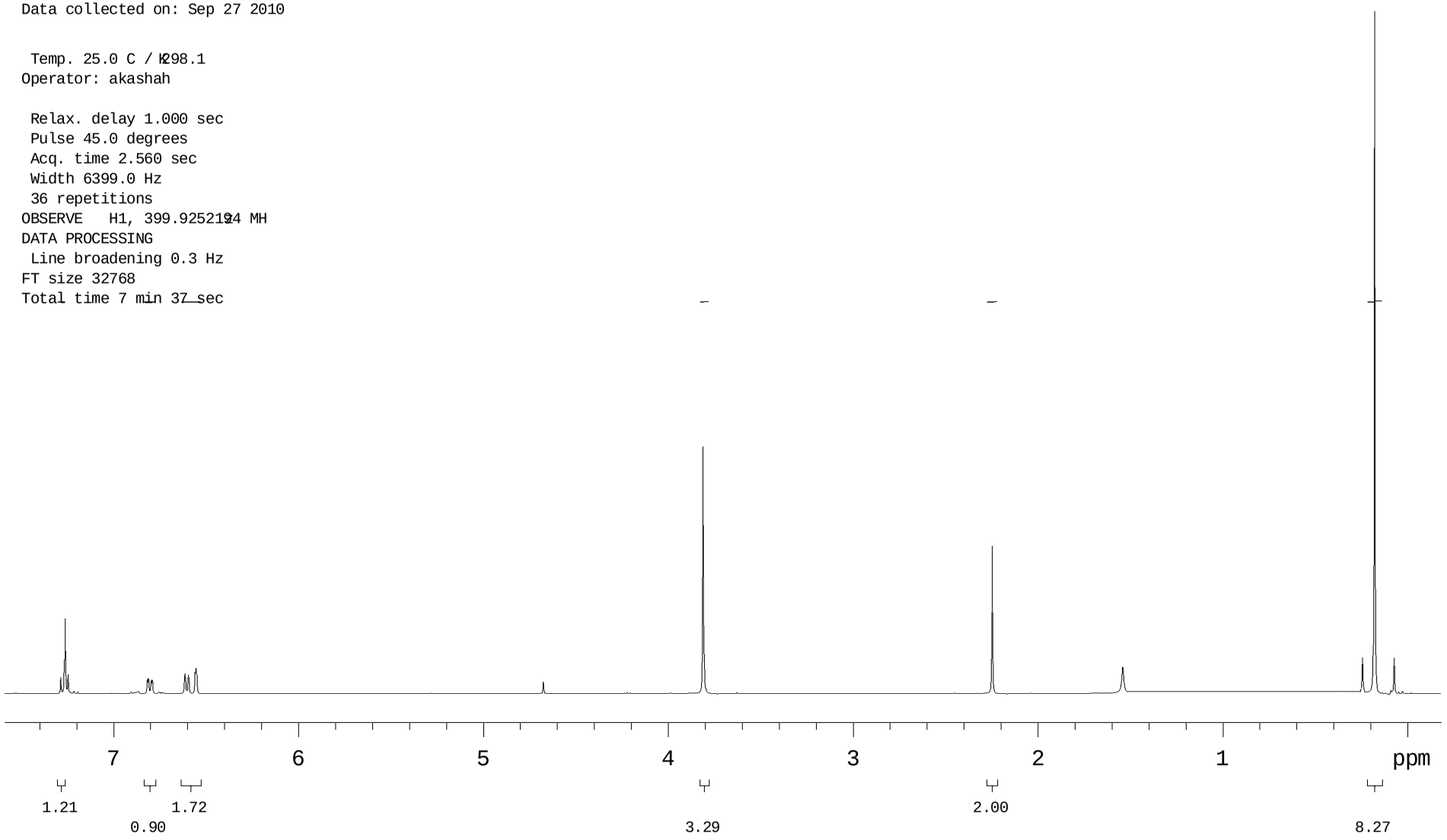
FidFile: AAS-4-54-1H

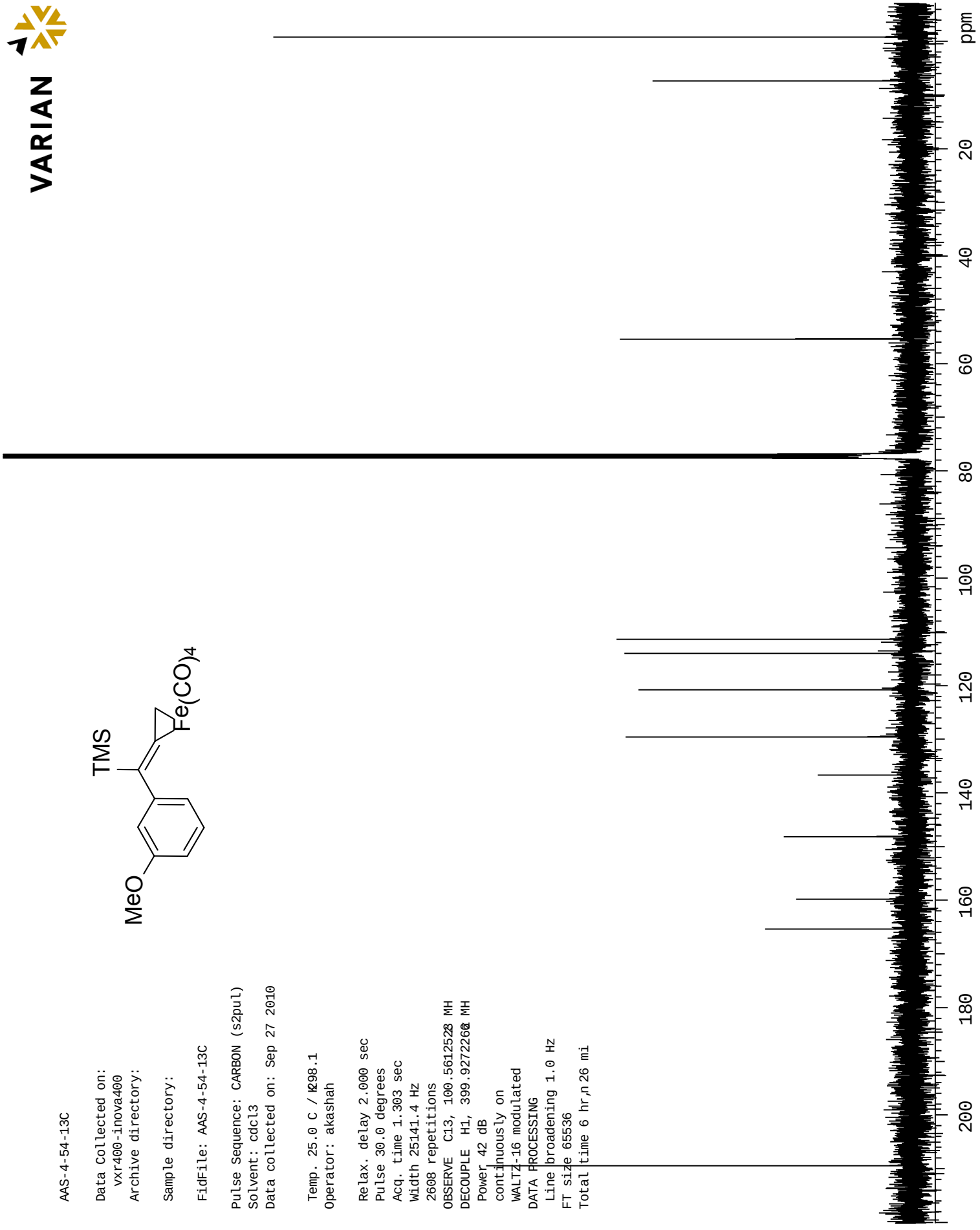


Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 27 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
36 repetitions
OBSERVE H1, 399.9252124 MH
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 7 min 37 sec





AAS-4-54-13C

Data Collected on:
vxr400-inova400
Archive directory:

Sample directory:

FidFile: AAS-4-54-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 27 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
2608 repetitions
OBSERVE C13, 100.5612523 MHz
DECOUPLE H1, 399.9272268 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 6 hr, 26 min

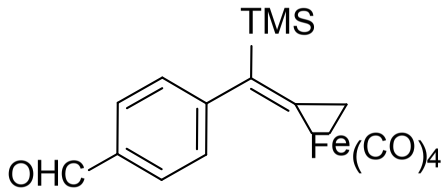
AAS-4-80-1H

Sample Name:

Data Collected on:
vxr400-inova400
Archive directory:

Sample directory:

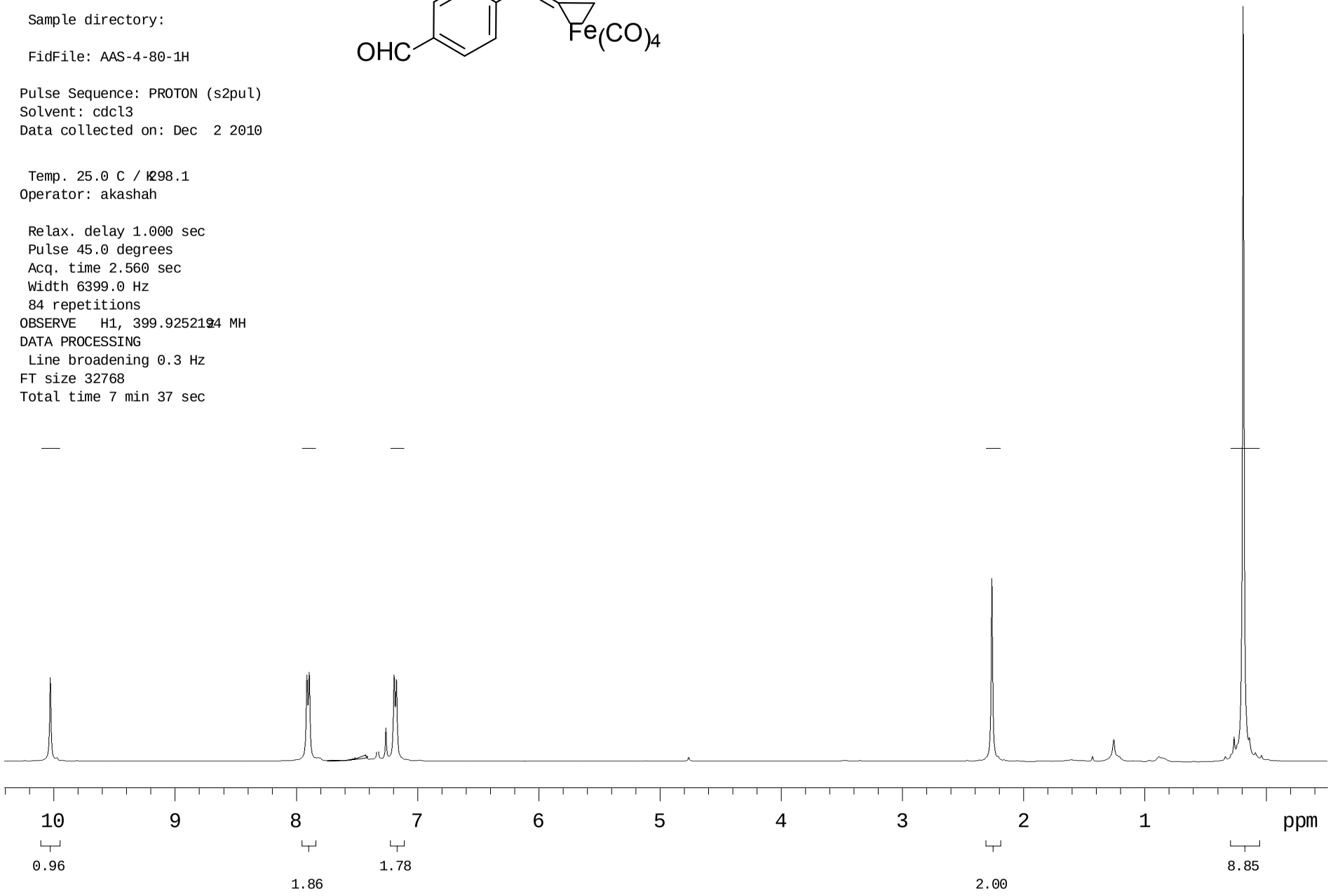
FidFile: AAS-4-80-1H

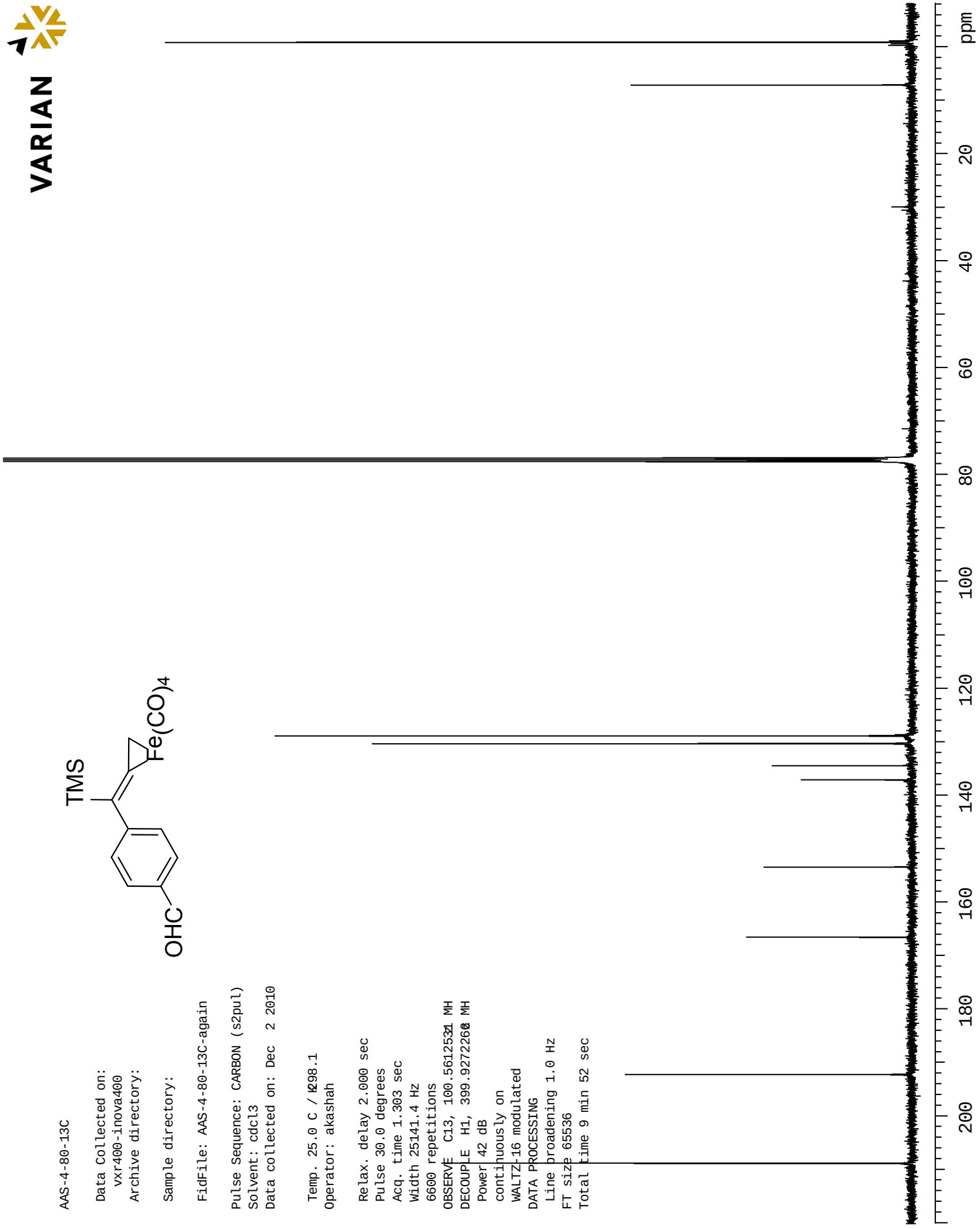


Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 2 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
84 repetitions
OBSERVE H1, 399.9252194 MH
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 7 min 37 sec




VARIAN
AAS-4-80-13C
Data Collected on:
vxr400-inova400
Archive directory:
Sample directory:
FidFile: AAS-4-80-13C-again
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 2 2010
Temp. 25.0 C / 298.1 K
Operator: akashah
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
6600 repetitions
OBSERVE C13, 100.5612531 MH
DECOUPLE H1, 399.9272268 MH
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 min 52 sec
TMS
Fe(CO)4
OHC
200
180
160
140
120
100
80
60
40
20
ppm

AAS-4-106-1H

Sample Name:

Data Collected on:
vxr400-inova400
Archive directory:

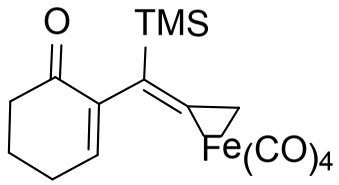
Sample directory:

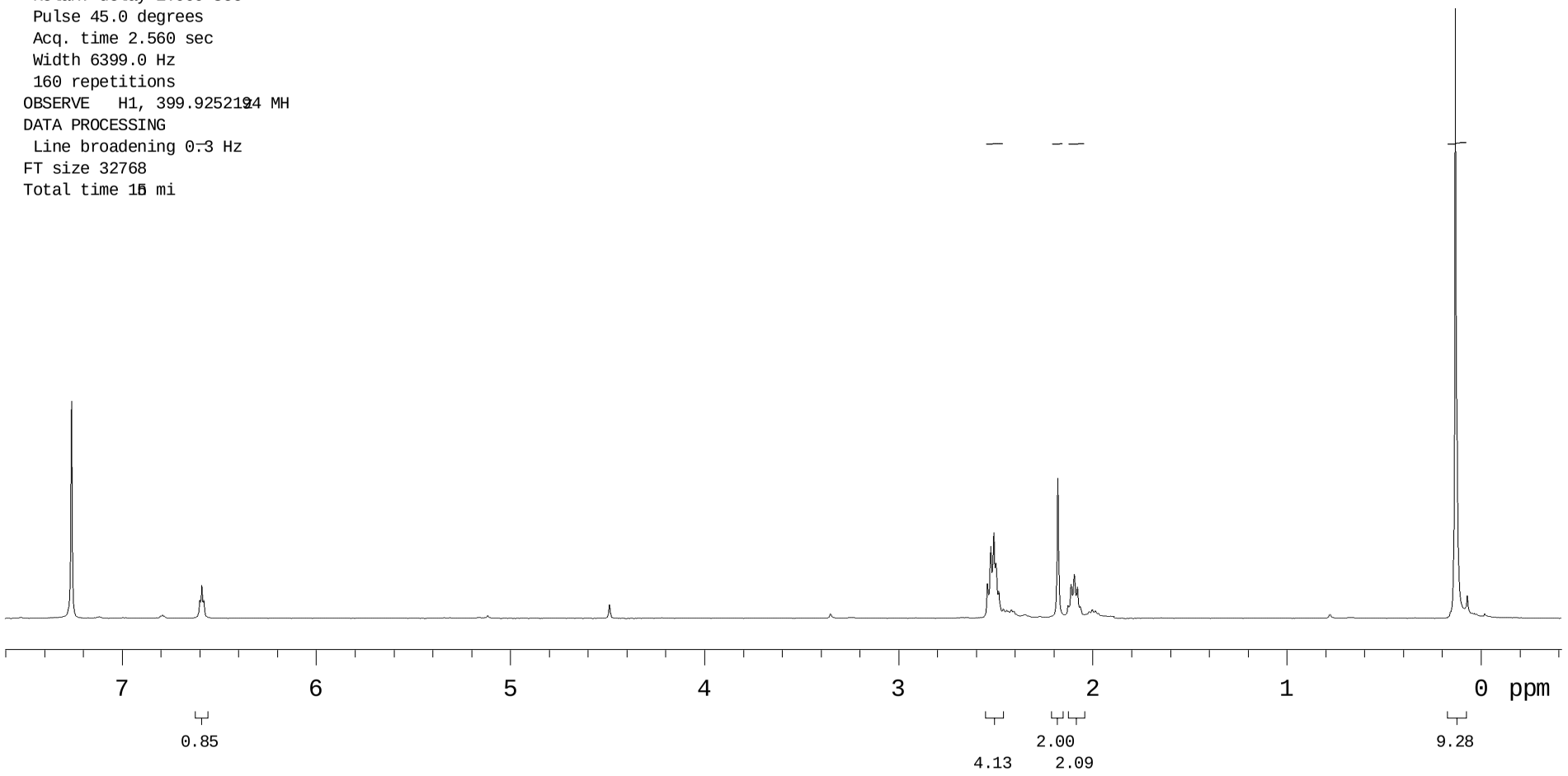
FidFile: AAS-4-106-1H

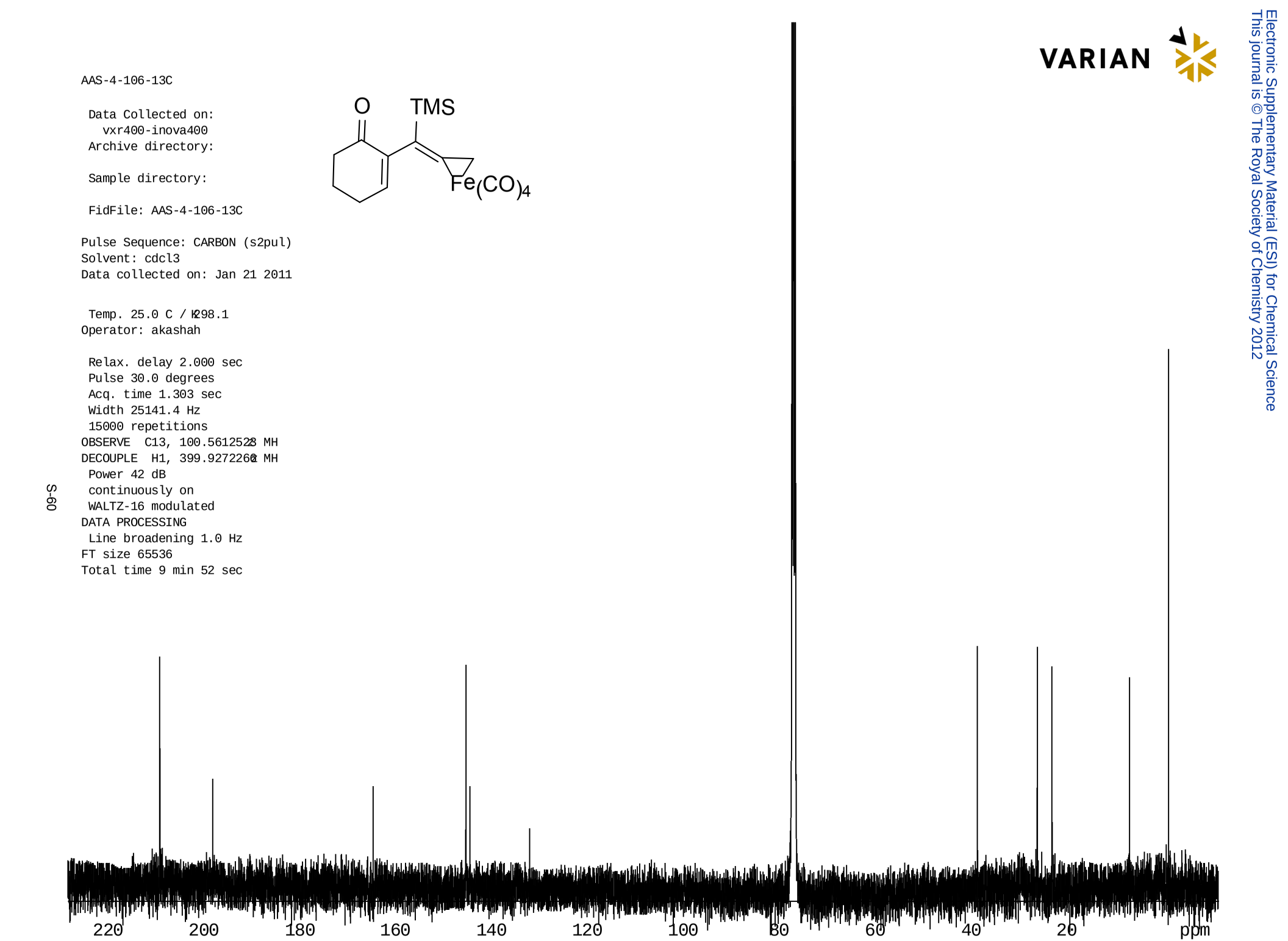
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 21 2011

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
160 repetitions
OBSERVE H1, 399.9252124 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 15 min

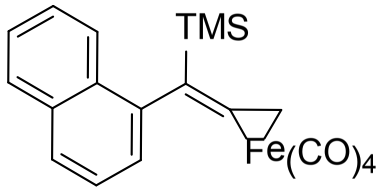






VARIAN

AAs-4-78-1H



Data Collected on:
vxr400-inova400
Archive directory:

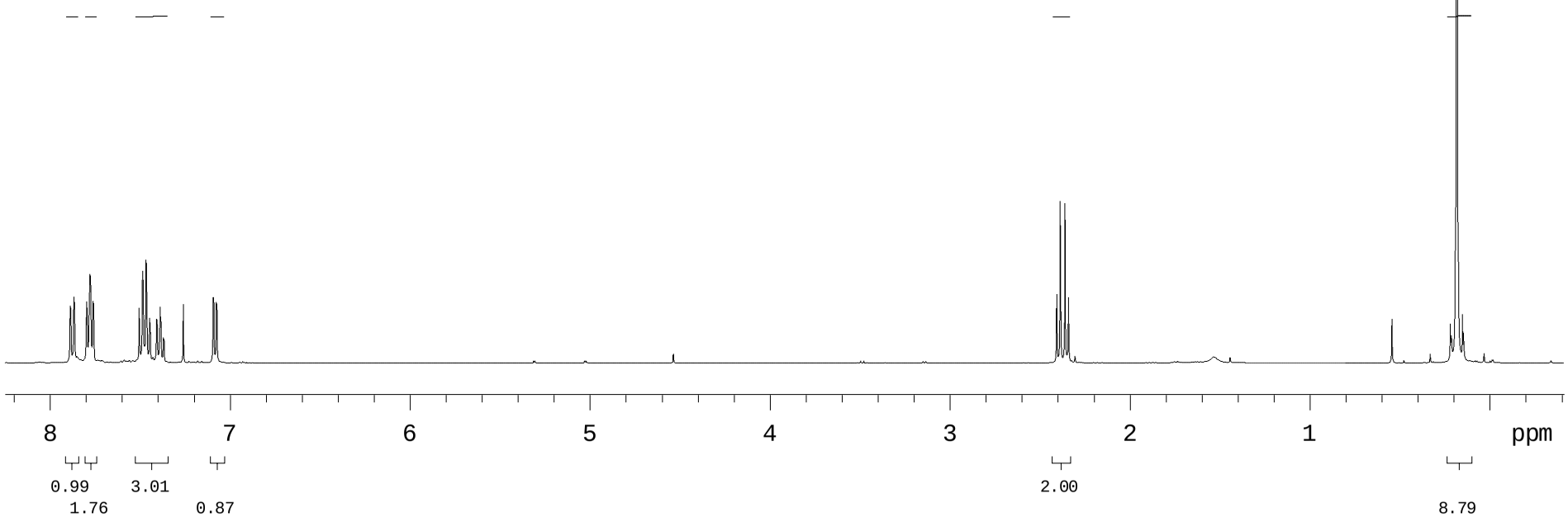
Sample directory:

FidFile: AAS-4-78-1H

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 1 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
104 repetitions
OBSERVE H1, 399.9252124 MH
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 7 min 37 sec



STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
vxr400-inova400
Archive directory:

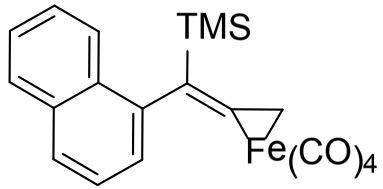
Sample directory:

FidFile: AAS-4-78-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 1 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
7000 repetitions
OBSERVE C13, 100.5612531 MH
DECOUPLE H1, 399.9272266 MH
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 min 52 sec



AAS-4-76-1H

Data Collected on:
vxr400-inova400
Archive directory:

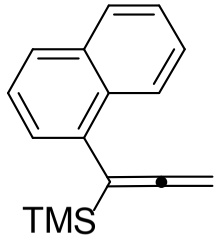
Sample directory:

FidFile: AAS-4-76-1H

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 29 2010

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
20 repetitions
OBSERVE H1, 399.9252194 MH
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 7 min 37 sec



23

AAS-4-76-13C

Data Collected on:
vxr400-inova400
Archive directory:

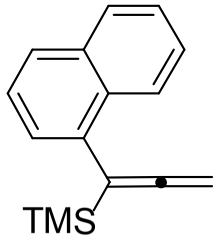
Sample directory:

FidFile: AAS-4-76-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 30 2011

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
928 repetitions
OBSERVE C13, 100.5612538 MH
DECOUPLE H1, 399.9272260 MH
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9 hr, 12 mi



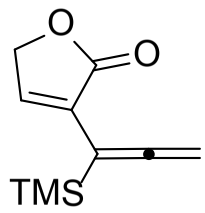
23

AAS-4-268-1H

Data Collected on:
vxr400-inova400
Archive directory:

Sample directory:

FidFile:

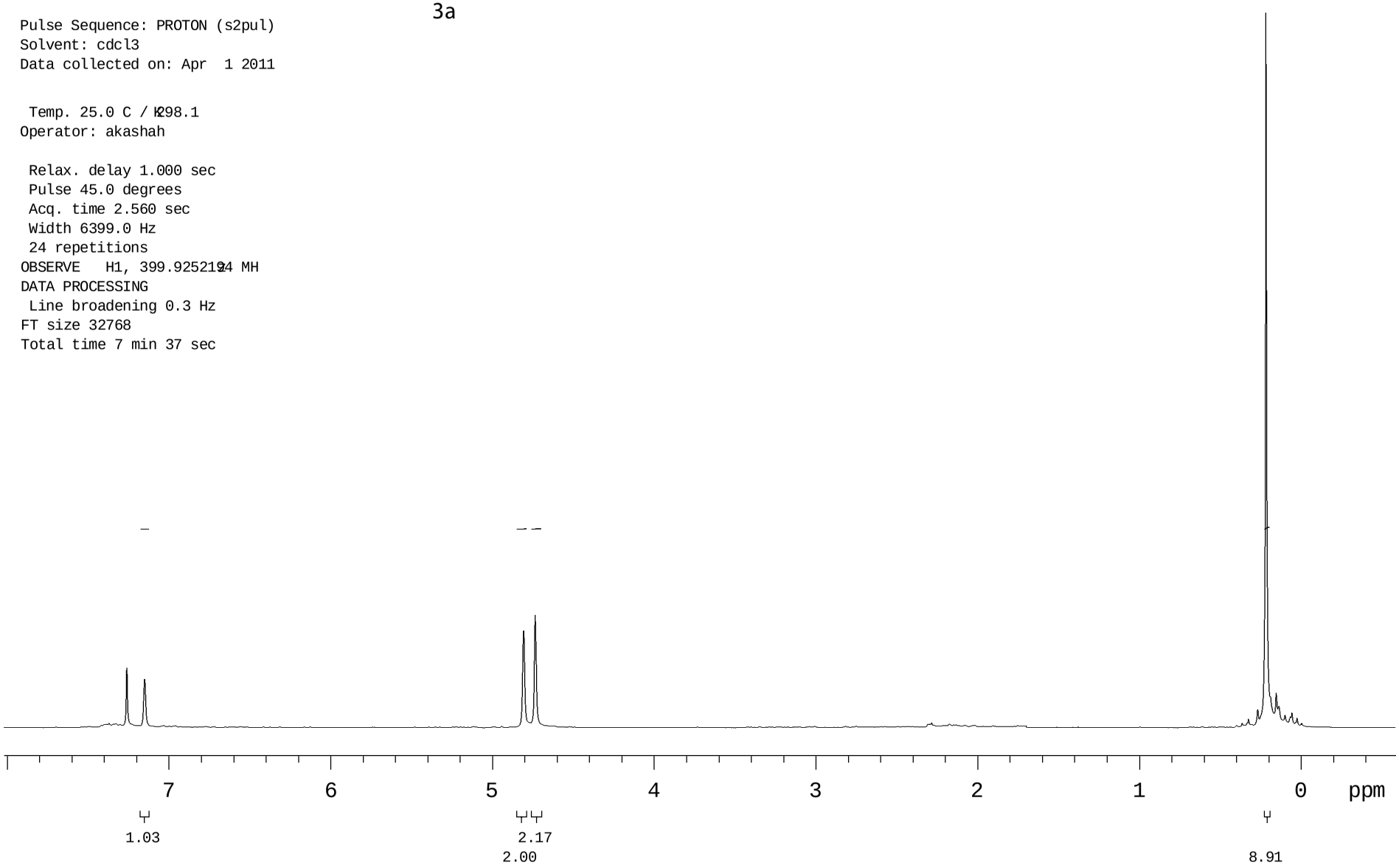


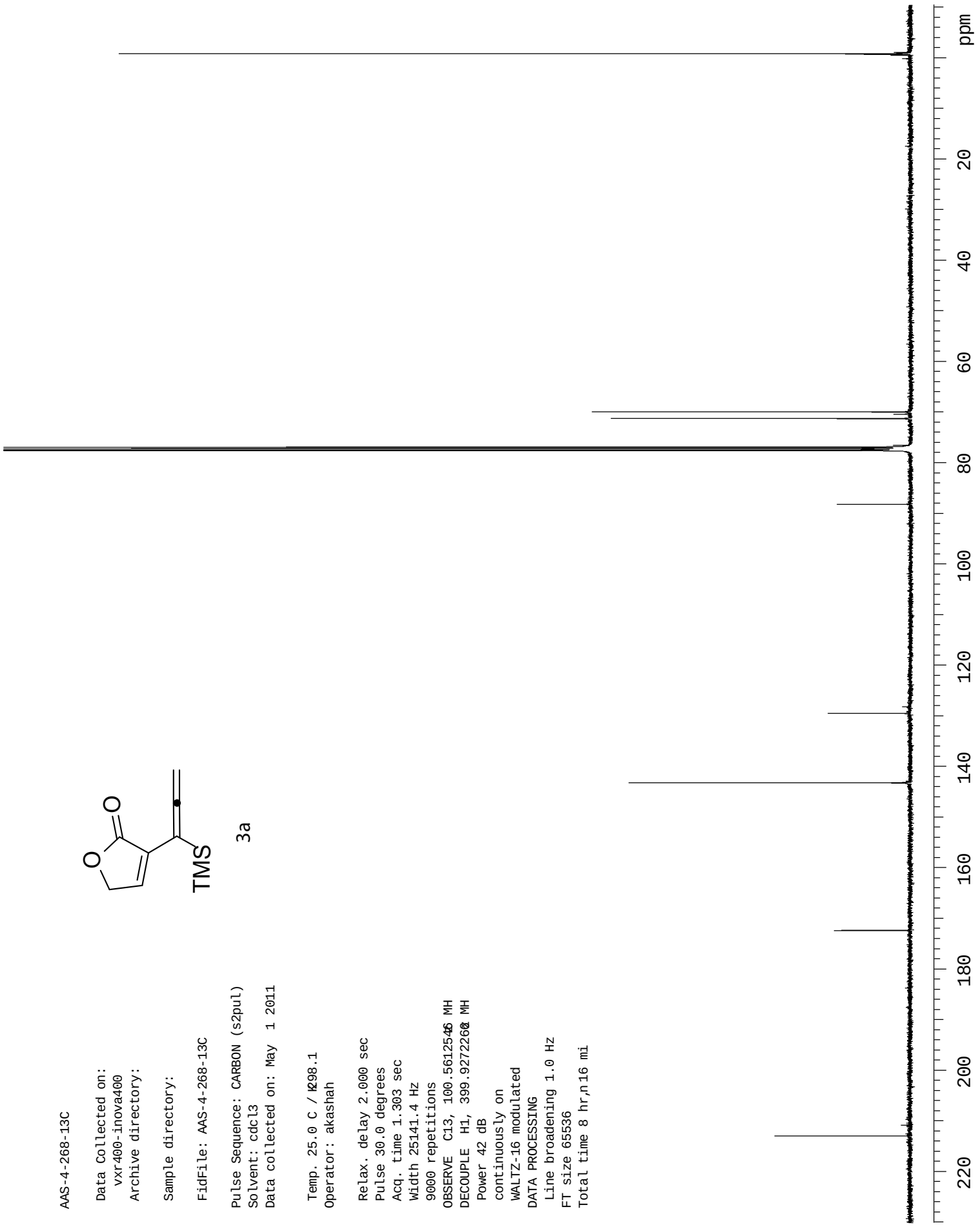
3a

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 1 2011

Temp. 25.0 C / 298.1 K
Operator: akashah

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
24 repetitions
OBSERVE H1, 399.9252194 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 7 min 37 sec




AAS-4-268-13C
Data Collected on:
vxr400-inova400
Archive directory:
Sample directory:
FidFile: AAS-4-268-13C
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 1 2011
Temp. 25.0 C / 298.1 K
Operator: akashah
Relax. delay 2.000 sec
Pulse 30.0 degrees
Acq. time 1.303 sec
Width 25141.4 Hz
9000 repetitions
OBSERVE C13, 100.5612546 MH
DECOUPLE H1, 399.9272260 MH
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 8 hr,n16 mi
O
O
TMS
3a
220
200
180
160
140
120
100
80
60
40
20
ppm

General computational information:

All calculations were carried out using Density Functional Theory as implemented in the Jaguar 7.7[1] suite of ab initio quantum chemistry programs. Geometry optimizations were performed with the B3LYP functional[2] and the 6-31G** basis set. The transition metal was represented using the Los Alamos LACVP[3] basis that includes relativistic effective core potentials. Geometry optimizations have been carried out for singlet spin state. Triplet spin state was tested as well. The energies of the optimized structures were re-evaluated by additional single-point calculations on each optimized geometry using Dunning's correlation-consistent triple-ζ basis set cc-pVTZ(-f)[4] that includes a double set of polarization functions. For transition metal, we used a modified version of LACVP, designated as LACV3P, in which the exponents were decontracted to match the effective core potential with the triple-ζ. Vibrational frequency calculations based on analytical second derivatives at the B3LYP/6-31G** (LACVP) level of theory were carried out to derive the zero-point-energy (ZPE) and entropy corrections at 298K utilizing unscaled frequencies. Note that by entropy here we refer specifically to the vibrational/rotational/translational entropy of the solute(s); the entropy of the solvent is implicitly included in the dielectric continuum model. Solvation energies were evaluated by a self-consistent reaction field (SCRF)[5] approach based on accurate numerical solutions of the Poisson-Boltzmann equation. In the results reported, solvation calculations were carried out at the optimized gas-phase geometry employing the dielectric constant of ϵ = 7.6 (THF). As is the case for all continuum models, the solvation energies are subject to empirical parametrization of the atomic radii that are used to generate the solute surface. We employ the standard set of optimized radii in Jaguar for H (1.150 Å), C (1.900 Å), N (1.600Å), O(1.600Å), Si (2.147 Å) and Fe (1.456 Å).

The energy components have been computed with the following protocol. The free energy in solution phase *G*(Sol) has been calculated as follows:

$G(\text{Sol}) = G(\text{gas}) + G^{\text{solv}}$ (1)

$G(\text{gas}) = H(\text{gas}) - TS(\text{gas})$ (2)

$H(\text{gas}) = E(\text{SCF}) + ZPE$ (3)

$\Delta G(\text{Sol}) = \sum G(\text{Sol})$ for products $- \sum G(\text{Sol})$ for reactants (4)

G(gas) is the free energy in gas phase; G^{solv} is the free energy of solvation as computed using the continuum solvation model; *H*(gas) is the enthalpy in gas phase; *T* is the temperature (298K); *S*(gas) is the entropy in gas phase; *E*(SCF) is the self-consistent field energy, i.e. "raw" electronic energy as computed from the SCF procedure and *ZPE* is the zero point energy.

To locate transition states, the potential energy surface was first explored approximately using the linear synchronous transit (LST)[6] method, followed by a quadratic synchronous transit (QST)[7] search using the LST transition state as an initial guess. In QST, the initial part of the transition state search is restricted to a circular curve connecting the reactant, initial transition state guess and the product, followed by a search along the Hessian eigenvector that is most similar to the tangent of this curve. In some cases, IRC (Intrinsic Reaction Coordinate) scans were performed to verify the convergence of the transition states to appropriate reactants and products.

References

(1) Jaguar 7.7; Schrodinger, LLC, New York, NY, 2010.

(2) (a) Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.* **1980**, *58*, 1200. (b) Lee, C. T.; Yang, W. T.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

(3) (a) Wadt, W. R.; Hay, P. J. *J. Chem. Phys.* **1985**, *82*, 284. (b) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 270. (c) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299.

(4) Dunning, T. H., Jr. *J. Chem. Phys.* **1989**, *90*, 1007.

(5) (a) Marten, B.; Kim, K.; Cortis, C.; Friesner, R. A.; Murphy, R. B.; Ringnalda, M. N.; Sitkoff, D.; Honig, B. *J. Phys. Chem.* **1996**, *100*, 11775. (b) Friedrichs, M.; Zhou, R.; Edinger, S. R.; Friesner, R. A. *J. Phys. Chem. B* **1999**, *103*, 3057. (c) Edinger, S. R.; Cortis, C.; Shenkin, P. S.; Friesner, R. A. *J. Phys. Chem. B* **1997**, *101*, 1190.

(6) Halgren, T. A.; Lipscomb, W. N. *Chem. Phys. Lett.* **1977**, *49*, 225.

(7) Peng, C. Y.; Schlegel, H. B. *Isr. J. Chem.* **1993**, *33*, 449.

Studies of regioselectivity complexation of $FeCO_4$ with 1,1-disubstituted allenes:

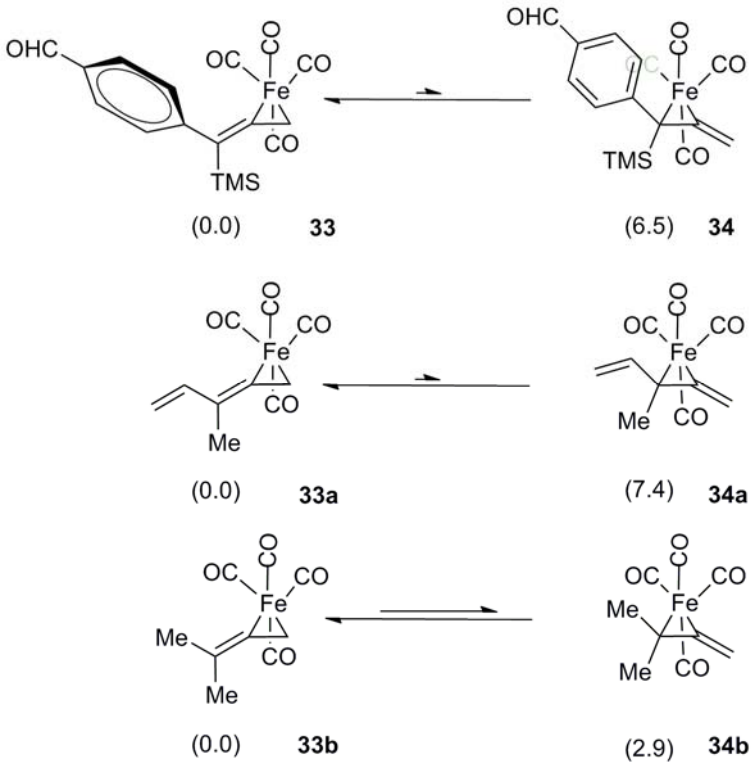


Figure S1. Relative electronic energy in kcal/mol.

Other structural isomers of 41, 42 and their energetic data:

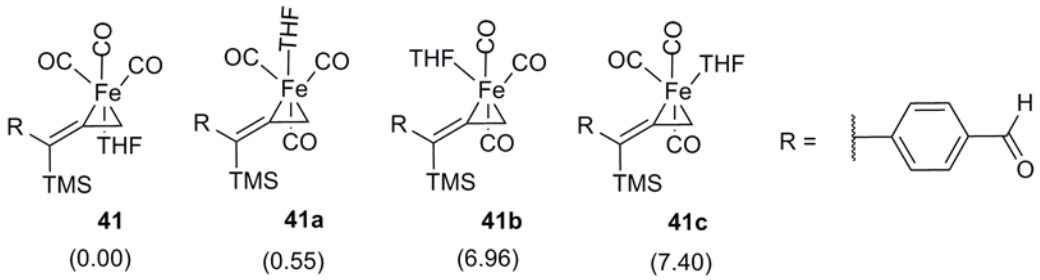


Figure S2. Relative electronic energy in kcal/mol.

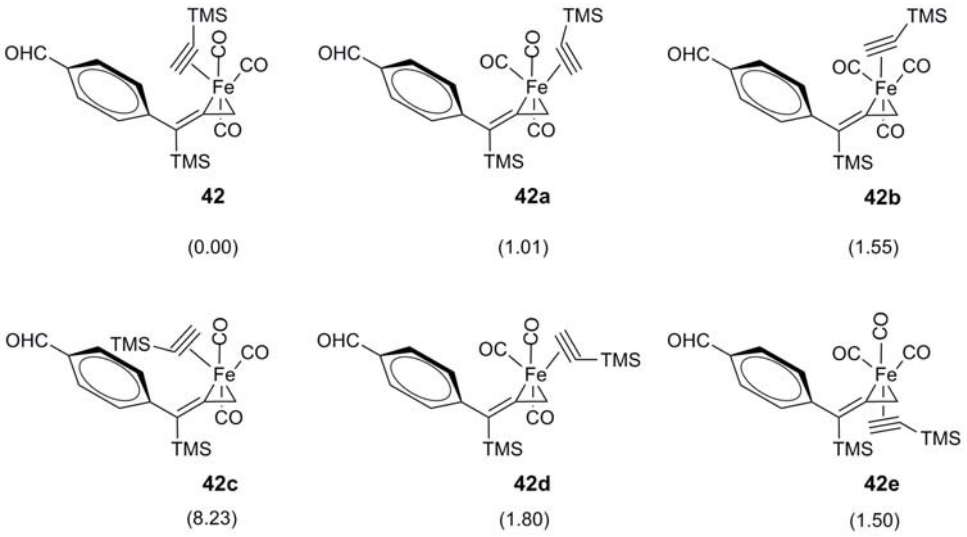


Figure S3. Relative electronic energy in kcal/mol.

Energetics of mechanistic pathway following the insertion of alkyne:

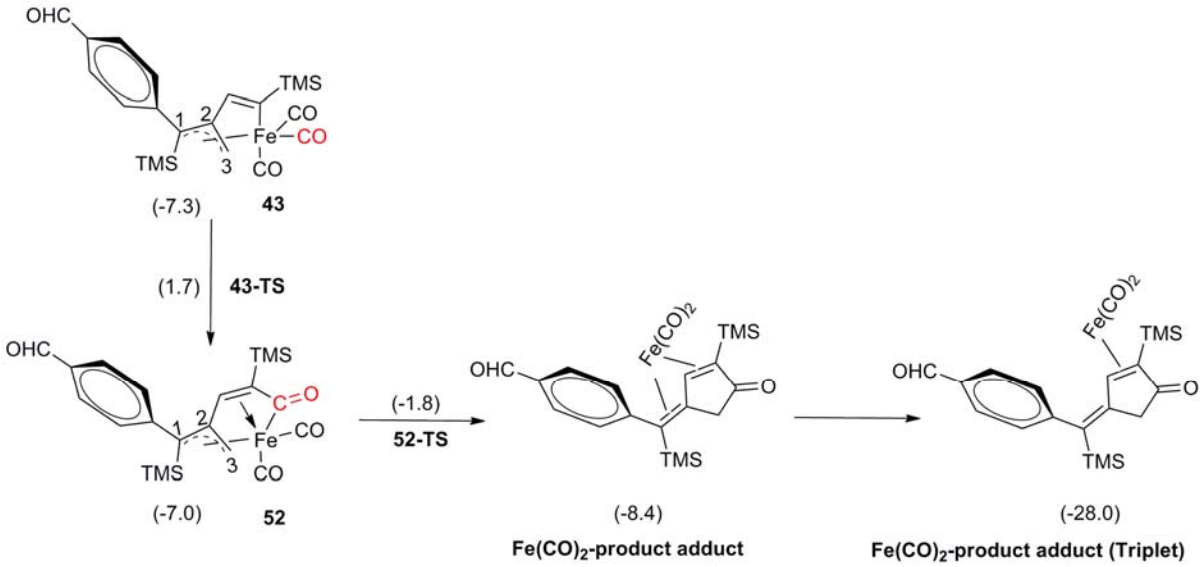


Figure S4. Δ*G*(Sol) in kcal/mol.

As illustrated in Figure S4, ferracyclopentene **43** undergoes insertion of CO traversing the transition state **43-TS** with an activation energy of 9.0 kcal/mol to yield **52**. The energy barrier for the reductive elimination from **52** is 5.2 kcal/mol. The Fe center changes its spin state and becomes high spin triplet while bound to the product α-substituted cyclopentenone. Interestingly the triplet state is downhill by an overall 28.0 kcal/mol. Eventaully the product

cyclopentenone is going to fall off the loosely bound adduct complex upon workup of the reaction mixture.

Exploration of the triplet potential energy surface:

The Fe-complexes contain a number of strong-field CO ligands. Therefore these complexes have been calculated as singlet spin state. However, the ground state for $FeCO_4$ has been modeled as triplet.[8] Any reactivity in the triplet surface was discarded because the triplet surface of $FeCO_4$ was found to be repulsive for allene binding. Complex **33** shows spontaneous dissociation of allene from the Fe center in the triplet surface. In case of other mechanistically important intermediates, both the triplet and singlet states were probed and the later was found to be lower in energy.

(8) Barckholtz, T. A.; Bursten, B. E. *J. Organomet. Chem.* **2000**, *596*, 212-220.

Table S1. Computed energy components of the optimized structures.

	E(SCF)/(ev)	ZPE/(kcal/mol)	S(gas)/(eu)	G(Solv)/(kcal/mol
	cc-pVTZ(-f)/(LACV3P)	6-31G**/LACVP	6-31G**/LACVP	6-31G**/LACVP
THF	-6327.512	73.49	74.267	-2.81
CO	-3084.528	3.16	47.235	0.00
(TMS)CC(H)	-13228.315	81.90	92.977	-3.42
NMO	-10949.708	105.32	82.360	-12.28
CO2	-5133.559	7.28	51.154	-2.25
N-methylmorpholine	-8904.058	102.34	79.630	-4.14
FeCO4	-15700.353	19.88	104.847	-1.81
FeCO5	-18786.149	26.63	109.630	-2.81
10	-23672.358	156.21	135.675	-6.57
Fe2CO9	-34486.533	48.56	160.366	-5.97
33	-39373.403	178.71	191.124	-7.76
34	-39373.101	178.65	186.127	-7.52
35	-39373.258	178.75	188.379	-7.88
36	-29320.892	132.56	158.379	-7.52
37	-29320.966	132.91	157.653	-7.77
38	-39371.799	178.65	189.590	-12.42
39	-45700.238	254.09	218.818	-11.12
40	-36287.424	172.68	172.947	-8.96
41	-42615.680	248.03	208.640	-9.26
42	-49516.396	256.12	229.578	-7.92
47-TS1 (48)	-49516.112	256.65	221.910	-8.01
47-TS2 (49)	-49515.709	256.64	225.232	-9.03
47-TS3	-49515.659	256.68	217.723	-8.27
47-TS4	-49515.539	256.63	224.873	-8.86
43	-49517.226	259.53	212.170	-7.67
44	-49516.892	258.58	215.216	-7.83
45	-49517.135	259.36	212.210	-7.75
46	-49516.913	258.45	217.030	-7.73
43-TS	-49516.798	259.24	210.338	-8.83
52	-49517.113	260.18	213.558	-10.27
52-TS	-49516.847	259.66	211.682	-11.20
Fe(CO)2-product adduct	-49517.114	260.44	213.865	-11.75
Fe(CO)2-product adduct (Triplet)	-49517.700	258.71	230.823	-11.07

Table S2. Cartesian coordinates of the optimized geometries.

==========

THF

==========

O	-0.422113374	-2.904869030	-0.588678555
C	-0.231052984	-3.616368050	0.628791753
C	0.643321609	-4.839864192	0.270127500
C	0.396700033	-5.021347112	-1.253383283
C	-0.617521240	-3.904712998	-1.581820272
H	0.229847953	-2.933732966	1.347498180
H	-1.202865998	-3.943235913	1.035906189
H	1.699114101	-4.637602061	0.469559504
H	0.361932187	-5.723055182	0.850796309
H	1.324802228	-4.877858416	-1.813397552
H	0.009096446	-6.012845193	-1.504387497
H	-1.649116201	-4.293705764	-1.535679613
H	-0.469603552	-3.440084263	-2.560208808

==========

CO

==========

C	-1.140505294	0.249537881	-0.233494810
O	-0.010552800	0.116442996	-0.226535606

==========

(TMS)CC(H)

==========

C	2.986531000	2.052929522	2.905128459
C	2.463461395	1.694860698	1.867888194
H	3.452130113	2.365673128	3.812536814
Si	1.646290835	1.157070860	0.301891830
C	2.985987645	0.726412506	-0.958312004
C	0.577530501	-0.356141325	0.671503493
C	0.576511304	2.577818651	-0.334814703
H	0.075408039	-0.707657207	-0.237153608
H	1.179986356	-1.182183788	1.062603830
H	-0.194158122	-0.125037363	1.412876571
H	2.538793432	0.401976568	-1.904824416
H	3.625960735	1.589433048	-1.168665965
H	3.626264145	-0.083783425	-0.595132304
H	0.072962310	2.296549816	-1.266802074
H	-0.193994156	2.851152091	0.393064901
H	1.178733481	3.469828907	-0.535127144

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NMO

==========

O	0.193015726	1.677315475	0.051827820
C	-0.958424692	0.904268566	-0.268218546
C	-0.949148174	-0.419443744	0.484336404
N	0.299583606	-1.189648889	0.086377398
C	1.505623347	-0.328564206	0.426222109
C	1.381479850	0.990417353	-0.324408555
H	-1.829714550	1.496051590	0.026826381
H	-1.001259578	0.688060206	-1.342680637
H	-0.952017856	-0.258654264	1.568766353
H	-1.788990887	-1.051388339	0.188859823
H	1.388203881	0.775416485	-1.399982662
H	2.219912635	1.645481162	-0.070949106
H	1.547540338	-0.165787500	1.509530371
H	2.374817611	-0.897559682	0.090515928
C	0.365476670	-2.478533069	0.842368733
O	0.277553948	-1.450344654	-1.248380982
H	-0.510104677	-3.057638092	0.549305867
H	0.386749746	-2.315837341	1.925659702
H	1.265042208	-2.992603142	0.504297327

==========

CO2

==========

C	-0.065442570	-0.039494343	-0.291773435
O	0.069357962	-0.983490218	0.386643313

O -0.200274687 0.904397325 -0.970323275

==========

N-methylmorpholine

==========

O 0.193511147 1.668154361 0.008683546
C -0.955513132 0.881917598 -0.279633144
C -0.919070532 -0.444521062 0.476230724
N 0.300467883 -1.176266593 0.130464602
C 1.478677885 -0.356713167 0.416979243
C 1.381505919 0.967393203 -0.337628564
H -1.824552572 1.474982508 0.018643442
H -1.018183635 0.682604731 -1.361271882
H -0.980485659 -0.241399116 1.563150117
H -1.789026109 -1.052326893 0.201130629
H 1.404107440 0.770945459 -1.421228609
H 2.218399044 1.622909611 -0.081351997
H 1.579212211 -0.145847757 1.499703278
H 2.376527251 -0.899740586 0.099214016
C 0.363071748 -2.473247152 0.785829436
H -0.504093347 -3.075801309 0.496746583
H 0.378613111 -2.405960606 1.890354599
H 1.265834865 -3.004467599 0.467642825

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FeCO4

==========

Fe 0.676606696 0.491237709 0.189483590
C 2.470332580 0.743551207 -0.243793233
C 0.014327668 2.184927615 -0.098100284
C 0.063614371 -0.285655245 -1.366776299
C -0.544072003 -0.169957163 1.437506643
O -1.316818827 -0.565596514 2.187595145
O 3.567975188 0.916144101 -0.531335409
O -0.326753353 -0.754083884 -2.341270315
O -0.401267808 3.238857546 -0.294189480

==========

FeCO5

==========

C 2.500520331 -0.050113371 -0.034600279
Fe 0.699943128 0.053627805 0.023653262
C 0.637942079 -0.024376572 -1.790287033
C 0.758201362 0.113169565 1.838077471
C -0.084396889 1.678273931 -0.010481746
C -0.304097893 -1.443248742 0.108560891
O 0.793692223 0.148904957 2.983847479
O 0.599278227 -0.079110337 -2.935238527
O 3.648976017 -0.109668782 -0.072885795
O -0.942836127 -2.399393767 0.153671752
O -0.581405480 2.715854739 -0.030670199

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10

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C -0.587688642 2.054217009 0.201845974
C 0.624851046 1.569990617 0.121300761
C 1.841904865 1.066420109 0.072074660
H -0.770753834 3.125232907 0.256245243
H -1.460132082 1.404334573 0.209591162
Si 2.679239836 0.702464764 1.754320731
C 4.428567805 1.422307465 1.740085650
C 1.669574514 1.531167561 3.117803152
C 2.730428118 -1.161880189 2.088960268
H 3.144058783 -1.350322650 3.086328268
H 1.723304017 -1.591112228 2.062163601
H 3.343524254 -1.714933259 1.370684452
H 2.110448711 1.314778986 4.097394454
H 1.646462628 2.618869108 2.995650727
H 0.634439623 1.177896666 3.129824727
H 4.927681117 1.233597618 2.697267585
H 5.050214878 0.993125002 0.948907423
H 4.401915320 2.506332246 1.587546078
C 2.513055780 0.856027642 -1.243251773

C	2.129403427	1.604482704	-2.377044326
H	1.336844367	2.338864450	-2.275560820
C	2.746351073	1.417813206	-3.602810451
H	2.453514756	1.995590373	-4.473990903
C	3.777897463	0.474412491	-3.740044918
C	4.444311317	0.273927252	-5.042212910
C	4.168256061	-0.273732196	-2.624403778
H	4.962383900	-1.010464683	-2.723359478
C	3.546954025	-0.084136591	-1.393221196
H	3.858677598	-0.684751642	-0.545928423
O	4.173950187	0.883324982	-6.061009020
H	5.243430935	-0.501460840	-5.038283892

==========

Fe2CO9

==========

Fe	-0.069893497	3.669494206	2.770238207
O	-1.380645380	6.052041263	4.033154409
O	1.345214570	1.584363176	1.208071206
C	-0.778001634	5.038953275	4.039100472
C	0.819474847	2.381441629	1.843409004
Fe	0.069988547	3.764155674	5.290947705
C	-0.780374709	2.340879693	3.901602983
C	1.564103076	3.735472227	4.152761763
C	0.745870078	5.053663721	1.888710233
C	-1.592509832	3.704337432	1.811376598
C	0.791876348	2.372787093	6.215446253
C	0.765859958	5.116487286	6.248525777
C	-1.533800219	3.687588135	6.175684734
O	-1.348440759	1.325654801	4.058500413
O	2.733265880	3.737406960	4.004260005
O	1.217723596	5.894484314	1.268533691
O	-2.543961000	3.702073515	1.170089290
O	1.262526226	1.540945783	6.849208130
O	1.208179963	5.959837870	6.888523392
O	-2.496086930	3.647244589	6.797343173

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33

==========

C	-1.990409469	0.522317133	0.048061876
C	-0.610435162	0.327262321	-0.093391382
C	0.606727827	0.863755960	-0.138047366
Si	0.799835458	2.751271259	0.148663118
H	-2.562579647	0.991623883	-0.749392731
H	-2.429414247	0.639121809	1.035951250
Fe	-1.511775295	-1.491850351	-0.385907813
C	-0.346143595	-2.816893139	-0.722764185
C	-3.169242948	-2.190721292	-0.426802183
C	-1.487448931	-1.030711773	-2.142661220
C	-1.271700214	-1.733378513	1.394287983
O	-1.458012610	-0.719069725	-3.246677880
O	-1.099172923	-1.861394658	2.522642930
O	-4.237349534	-2.617068713	-0.448735574
O	0.373108048	-3.687989423	-0.939913551
C	2.520696845	3.089980818	0.856338289
C	0.589933583	3.663792375	-1.498812342
C	-0.508871307	3.344213445	1.377950941
H	-0.379226361	4.413653410	1.580877178
H	-1.525673048	3.199811202	1.000721023
H	-0.426705768	2.813979607	2.333072895
H	2.653149187	4.162107701	1.042439854
H	2.673925974	2.567062174	1.806766206
H	3.312604581	2.769303017	0.172192718
H	0.670614091	4.747652306	-1.354540471
H	1.354438570	3.371543784	-2.226770221
H	-0.389248847	3.459967635	-1.945779939
C	1.831639129	0.051438470	-0.389995113
C	2.584035407	0.234849203	-1.567611665
H	2.241159229	0.948546504	-2.311725984
C	3.741468265	-0.497086334	-1.796518031
H	4.320141254	-0.368488454	-2.706256009

C 4.186917937 -1.427729276 -0.845614859
C 5.421535728 -2.206023790 -1.080171070
C 3.450248210 -1.612426733 0.330307058
H 3.793599265 -2.332015263 1.070862504
C 2.288028688 -0.880082447 0.557219980
H 1.727673075 -1.019877346 1.476609611
H 5.680302203 -2.920499297 -0.266647077
O 6.127075974 -2.104456559 -2.066702307
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26
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C -2.043771129 0.480710479 0.238648931
C -0.675881526 0.329774747 -0.003340279
C 0.543233137 0.850042266 -0.088033244
Si 0.837632568 2.702733880 0.270356565
H -2.680484818 0.966988585 -0.496825063
H -2.418782177 0.540451109 1.257300580
Fe -1.551877332 -1.506573793 -0.320844924
C -0.327354527 -2.734962434 -0.785654196
C -3.173646870 -2.280529339 -0.292779212
C -1.668854397 -0.966553510 -2.047481555
C -1.198946654 -1.818637804 1.430301341
O -1.728485313 -0.600839562 -3.134705232
O -0.965355661 -1.990232646 2.541428414
O -4.219264026 -2.762102467 -0.273337350
O 0.434331624 -3.544264614 -1.083854935
C 2.137420719 2.858220797 1.637663861
C 1.480093782 3.536936331 -1.304583852
C -0.769673162 3.537886465 0.813804897
H -0.586051672 4.597967650 1.025699297
H -1.539848976 3.484894781 0.037377140
H -1.180027023 3.085116240 1.722259930
H 2.396905058 3.909129281 1.811573747
H 1.773420246 2.444325250 2.584418026
H 3.057076665 2.325558911 1.374468318
H 1.711908545 4.591137135 -1.111477104
H 2.391918084 3.054361551 -1.671041356
H 0.737864352 3.503335061 -2.110034505
C 1.731180696 0.033285762 -0.498637949
C 2.102359923 -0.042081083 -1.853760570
H 1.511864453 0.477532312 -2.602161394
C 3.209861576 -0.796023458 -2.230466227
H 3.486470038 -0.859880872 -3.279688577
C 3.976849238 -1.479085697 -1.282980557
H 4.832935532 -2.059894884 -1.602782654
C 3.615977302 -1.399300529 0.066428397
O 4.280953223 -2.024662965 1.082220067
C 2.500434002 -0.640664381 0.452670024
H 2.245265473 -0.599059965 1.506983315
C 5.408636333 -2.818686478 0.752618115
H 5.781221663 -3.220384521 1.696099124
H 5.139802038 -3.649629883 0.088863042
H 6.199202166 -2.224634570 0.277599819
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34
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C -2.064604954 0.425199235 0.116283839
C -0.693559331 0.156545655 0.026225427
C 0.546063776 0.607723252 0.154953880
Si -2.855372717 1.665076027 -1.144066086
Fe -1.520731512 -1.609054621 -0.547596681
C -0.236713836 -2.810767181 -0.881179074
C -3.160811442 -2.327995123 -0.771693742
C -1.360698876 -1.119299956 -2.284194446
C -1.393002738 -2.119283665 1.203706148
O -1.215982598 -0.895306383 -3.401463673
O -1.261147723 -2.498422901 2.276473961
O -4.211744326 -2.776334431 -0.907350059
O 0.574618404 -3.599369874 -1.096420494
H 1.413103485 -0.008968485 -0.059578665

H	0.740287630	1.629309064	0.482442146
C	-3.496010844	3.137286906	-0.138109963
C	-1.537260034	2.332275958	-2.326300413
C	-4.297808382	0.921456370	-2.122152942
H	-4.747838159	1.696466764	-2.754147650
H	-3.983336100	0.105365338	-2.779835314
H	-5.087457329	0.538071052	-1.467962069
H	-1.971298580	3.157803879	-2.903365587
H	-0.680048830	2.730052717	-1.774096024
H	-1.161205093	1.596580091	-3.039885677
H	-3.865886302	3.915717251	-0.815924966
H	-4.313248987	2.861099619	0.533985795
H	-2.701418060	3.580635116	0.471923966
C	-2.729355371	0.431260244	1.466427983
C	-2.018329811	0.842344559	2.611858102
H	-0.966685370	1.093367868	2.517127732
C	-2.641512901	0.928763812	3.849660143
H	-2.095417968	1.250254729	4.731445155
C	-3.999490561	0.606836765	3.983291199
C	-4.672642260	0.708344171	5.294889982
C	-4.715958023	0.189030812	2.853402933
H	-5.768154301	-0.070652285	2.950261149
C	-4.090785127	0.103101941	1.614615071
H	-4.655957684	-0.236088544	0.752428571
H	-5.750865989	0.420834086	5.287530188
O	-4.135314959	1.073671865	6.323002745

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33a

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C	-1.953139638	0.507527264	0.096384732
C	-0.612828761	0.278645143	-0.239786760
C	0.588470397	0.842303373	-0.414854775
C	0.758969165	2.332882657	-0.191894095
H	-2.636567730	0.963739034	-0.617765311
H	-2.251184906	0.641153375	1.134756649
Fe	-1.542104728	-1.519731915	-0.366519713
C	-0.446832297	-2.856096079	-0.847341365
C	-3.189419145	-2.209626355	-0.138173921
C	-1.790613304	-1.079092878	-2.111572277
C	-1.039308234	-1.718099457	1.368361497
O	-1.929441669	-0.775465486	-3.209127382
O	-0.706124289	-1.816819264	2.461640507
O	-4.251605979	-2.623813152	0.013404270
O	0.241031558	-3.726989353	-1.154431015
C	1.759018662	0.059567897	-0.824818439
C	2.993474250	0.541194891	-1.034369389
H	3.241617695	1.590528817	-0.913499049
H	1.521999439	2.530345790	0.569718411
H	1.086901542	2.828564199	-1.112835545
H	-0.176518526	2.791770096	0.131195897
H	1.580443105	-1.003026009	-0.967722965
H	3.802440770	-0.113968238	-1.340176395

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34a

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C	-2.061550406	0.426712711	0.074500709
C	-0.689938172	0.110510910	0.005678077
C	0.527917644	0.602303688	0.170477183
C	-2.703359395	1.272759684	-1.014939341
Fe	-1.498376544	-1.655611670	-0.541967221
C	-0.228050960	-2.862041326	-0.908928402
C	-3.157898532	-2.325278192	-0.760730597
C	-1.345756317	-1.094194448	-2.259845509
C	-1.368121343	-2.172627476	1.195332775
O	-1.203318940	-0.778743100	-3.355061484
O	-1.235595202	-2.545772964	2.272983990
O	-4.226330792	-2.729981194	-0.897377519
O	0.575785406	-3.651011944	-1.152535612
H	1.420789068	0.009582652	-0.004803595
H	0.677697604	1.632301020	0.494685591

C	-2.730516782	0.446119029	1.391340135
H	-3.708644102	0.926870367	-1.274749831
H	-2.795200258	2.302850008	-0.648047236
H	-2.100445910	1.298445561	-1.922759391
H	-2.153115619	0.035116851	2.216464054
C	-3.933473055	0.975747313	1.658258757
H	-4.568946062	1.410276810	0.893426095
H	-4.321551608	0.982406878	2.671630764

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33b

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C	-2.010859084	0.528609385	0.004286007
C	-0.636291172	0.317901890	-0.130724653
C	0.582482264	0.843886796	-0.155848018
C	0.749452076	2.342036154	0.086313855
H	-2.587088528	0.977493739	-0.803188368
H	-2.462517011	0.652951838	0.986883258
Fe	-1.524111785	-1.506386909	-0.392032121
C	-0.341252628	-2.814391878	-0.703699778
C	-3.176986299	-2.214264425	-0.408973425
C	-1.510355164	-1.061946250	-2.150778324
C	-1.273560261	-1.694379064	1.394882537
O	-1.482297020	-0.753850288	-3.256490675
O	-1.096077484	-1.784538625	2.525640995
O	-4.242886354	-2.648017010	-0.416439994
O	0.405715503	-3.668028556	-0.905131991
C	1.827093090	0.012532926	-0.411806664
H	1.793296536	2.650996985	-0.022083414
H	0.151482551	2.929050793	-0.620455016
H	0.422522671	2.621725789	1.094881982
H	2.732281808	0.624460224	-0.362327544
H	1.930067772	-0.793873503	0.323401367
H	1.798029324	-0.457963467	-1.401631882

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34b

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C	-2.013820872	0.413870873	0.071513323
C	-0.646444607	0.146142828	-0.053022156
C	0.582477426	0.630442535	0.029142785
C	-2.740403506	1.230556001	-0.988393570
Fe	-1.484634623	-1.646254875	-0.518904137
C	-0.267265527	-2.905803562	-0.901711284
C	-3.163843304	-2.266867679	-0.657218196
C	-1.362413754	-1.127161333	-2.251892881
C	-1.283294144	-2.108564596	1.222398085
O	-1.237906554	-0.835236963	-3.356002564
O	-1.111537114	-2.443569636	2.307760012
O	-4.251734772	-2.635594686	-0.742723840
O	0.501707435	-3.727396260	-1.150870387
H	1.460787251	0.025119993	-0.173387539
H	0.757018347	1.669756618	0.309104307
C	-2.649640955	0.553127106	1.448069704
H	-3.771773588	0.889870432	-1.127790692
H	-2.787256474	2.276622521	-0.653842249
H	-2.236454143	1.220080661	-1.955391126
H	-2.699573929	1.620670944	1.705247279
H	-3.675449894	0.169825681	1.463100133
H	-2.080034328	0.054675607	2.233082440

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35

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C	-1.760135548	0.689756604	0.123342065
C	-0.418582476	0.330243325	-0.077411947
C	0.833193494	0.780298066	-0.172742739
Si	2.373901436	-0.320693172	-0.466115581
H	-2.349022348	1.098130726	-0.694457197
H	-2.099067689	1.004707332	1.107988007
Fe	-1.518446704	-1.398682897	-0.025594145
C	-0.580817080	-2.913141282	-0.222390677
C	-3.247238403	-1.863469662	0.166090808

C	-1.600247000	-1.199917628	-1.827952210
C	-1.154466605	-1.400147908	1.753748470
O	-1.633486602	-1.054500951	-2.965538297
O	-0.909119448	-1.383391625	2.874221953
O	-4.358623396	-2.130059181	0.289629754
O	-0.005527559	-3.903652944	-0.342769901
C	3.887521368	0.792387978	-0.691806025
C	2.674890309	-1.464590121	1.013265562
C	2.170881882	-1.319407002	-2.062825808
H	3.102319108	-1.852832829	-2.287298713
H	1.374290387	-2.064724791	-2.005960736
H	1.956151562	-0.661716812	-2.912134709
H	4.764356419	0.177638418	-0.926923265
H	3.749114679	1.499552308	-1.516484151
H	4.121849823	1.375522293	0.203504830
H	3.600374701	-2.034607133	0.869417491
H	2.781544111	-0.892188858	1.941376522
H	1.865040371	-2.185186766	1.157268699
C	1.023991881	2.266815661	-0.075086689
C	1.724341354	2.830784402	1.004861942
H	2.119548579	2.183203522	1.782637847
C	1.900572609	4.208490374	1.093946481
H	2.437132704	4.635575059	1.938656717
C	1.389723097	5.054486449	0.101470971
C	1.586999082	6.516106650	0.197819931
C	0.689580761	4.500454349	-0.980608766
H	0.299414245	5.168872163	-1.742193577
C	0.509061332	3.126112534	-1.063988277
H	-0.029773438	2.697246807	-1.904378581
H	2.154003640	6.847372484	1.096946683
O	1.180699251	7.326400931	-0.614537143

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36

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C	-1.960938639	0.518806920	0.019790325
C	-0.593349031	0.254092294	-0.151261569
C	0.614585699	0.811457847	-0.237863855
C	0.765981983	2.319589306	-0.112381810
H	-2.546483269	0.963841492	-0.782266302
H	-2.367430316	0.700228073	1.012850021
Fe	-1.551030616	-1.523142565	-0.338907401
C	-0.429877677	-2.891287584	-0.658097186
C	-3.226652567	-2.181264668	-0.310588697
C	-1.570238821	-1.125731624	-2.113467549
C	-1.284646400	-1.696751266	1.446268624
O	-1.562679132	-0.851469126	-3.226969004
O	-1.087763867	-1.780791337	2.574161158
O	-4.306037060	-2.576645091	-0.286849495
O	0.266672723	-3.783089567	-0.863724944
H	1.459681486	2.577581985	0.697321307
H	1.174733913	2.756766127	-1.031892469
H	-0.197913192	2.792879775	0.087111951
C	1.865564280	0.037094776	-0.473804999
C	2.748119255	0.405030837	-1.510183276
H	2.498559761	1.242396139	-2.155040599
C	3.921230935	-0.301432642	-1.735036671
H	4.596834909	-0.031743878	-2.541192385
C	4.256943647	-1.390463505	-0.916094781
C	5.508567157	-2.143813128	-1.146370643
C	3.397436643	-1.753045733	0.127312617
H	3.660020983	-2.588164111	0.773307090
C	2.218109681	-1.046457050	0.347059088
H	1.568806989	-1.319162325	1.171943966
H	5.677207641	-2.987569292	-0.439821097
O	6.314489350	-1.895415183	-2.023823638

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37

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C	-1.911051268	0.652053166	-0.251359345
C	-0.551429736	0.362482631	-0.097202007

C	0.686739058	0.845086914	0.068619030
C	1.871364809	-0.077084090	0.259419681
H	-2.315078546	0.929644168	-1.223287806
H	-2.498214655	1.017584966	0.589454519
Fe	-1.525446531	-1.424587968	-0.142822504
C	-0.447406502	-2.848789489	0.020934862
C	-3.213631691	-2.033173130	-0.307906605
C	-1.195240022	-1.375922204	-1.929831061
C	-1.592658729	-1.261140891	1.667697928
O	-0.965075995	-1.320847309	-3.052021175
O	-1.614209874	-1.134196506	2.807212822
O	-4.298729439	-2.396552304	-0.416911845
O	0.227409842	-3.775942945	0.123352545
C	0.948972628	2.310643490	0.086869065
C	2.219745137	2.801854895	0.447490439
H	3.011619891	2.114741356	0.719506089
C	2.483414554	4.168015112	0.475761139
H	3.471122504	4.521554860	0.764098240
C	1.491293398	5.092067621	0.134499988
C	1.778358725	6.540520799	0.158008009
C	0.222172045	4.617923368	-0.236766344
H	-0.540064874	5.340287255	-0.512766314
C	-0.040577228	3.258988871	-0.257894562
H	-1.023125215	2.916983349	-0.560813912
H	2.816721843	6.800792526	0.464516901
O	0.976176289	7.411310846	-0.126123518
H	2.663217593	0.134046932	-0.470092034
H	2.313292876	0.036777780	1.258148312
H	1.569866751	-1.117475771	0.146053943

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38

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C	-2.114689944	0.829941514	-0.012976397
C	-0.746144492	0.188390383	-0.183060877
C	0.473039839	0.734717240	-0.089004309
Si	0.722277107	2.609845803	0.258125898
H	-2.317589716	1.657710511	-0.708709047
H	-2.303699098	1.195590821	1.006669228
Fe	-1.469858794	-1.615791280	-0.606835484
C	0.038355999	-2.642776067	-0.857416046
C	-3.012454490	-0.364954215	-0.311325260
C	-1.600427771	-1.067393054	-2.339881224
C	-1.590959173	-1.912447299	1.184000238
O	-1.649308418	-0.713292157	-3.430363247
O	-1.629864061	-2.094549684	2.316804805
O	0.911068895	-3.365706929	-1.035326752
C	2.571643940	2.948778989	0.468393444
C	0.080264015	3.630990108	-1.203280164
C	-0.168244201	3.131869985	1.848540907
H	0.097655309	4.166427864	2.097669197
H	-1.258137799	3.090104744	1.761789722
H	0.125423706	2.503402838	2.696091158
H	2.734066010	4.013861625	0.671424921
H	2.997718938	2.382173214	1.302821497
H	3.142302053	2.689054587	-0.428788697
H	0.256994535	4.698464443	-1.026955162
H	0.596196896	3.359328378	-2.130503529
H	-0.993756309	3.501427579	-1.372061397
C	1.721344363	-0.070897920	-0.263007572
C	2.369084246	-0.148158088	-1.512800985
H	1.928728879	0.357876912	-2.367891906
C	3.550094260	-0.864002964	-1.662662306
H	4.052435215	-0.932038608	-2.623079212
C	4.122778754	-1.517656924	-0.560773083
C	5.385844806	-2.273261895	-0.707901972
C	3.491471032	-1.442357387	0.686582768
H	3.934791298	-1.946436352	1.542999477
C	2.307024035	-0.725390006	0.834339217
H	1.822928211	-0.667189778	1.804877641
H	5.748991911	-2.751431875	0.230166743

O	6.009992596	-2.385527404	-1.746328435
O	-4.213328086	-0.421675431	-0.339637107

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39

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C	-1.321595963	1.194648717	0.186353874
C	-0.202270707	0.207528425	-0.121043829
C	1.119715709	0.431886027	-0.194775706
Si	1.922417316	2.161779458	0.013614463
H	-1.393476800	2.049104312	-0.504512904
H	-1.287730611	1.600797516	1.208016109
Fe	-1.444275119	-1.380683799	-0.399490667
C	-0.337189218	-2.794903406	-0.809894671
O	-3.178600151	-2.626614892	-0.587290804
C	-1.473794233	-0.758673771	-2.100800581
C	-1.246981935	-1.563112021	1.388443829
O	-1.427820787	-0.349959351	-3.175655508
O	-1.054557793	-1.663976078	2.519507119
O	0.283401416	-3.719318405	-1.086171840
C	3.795586461	1.956588705	0.204145924
C	1.570304564	3.210428167	-1.528617688
C	1.277539797	3.067125511	1.551018857
H	1.887909457	3.960083811	1.732000380
H	0.239631208	3.397015648	1.448639963
H	1.343917906	2.437661173	2.445411424
H	4.273994535	2.936489446	0.318081803
H	4.049450716	1.358915257	1.086415247
H	4.244688918	1.464885649	-0.664501387
H	2.027658721	4.203091053	-1.440110485
H	1.975611943	2.739110913	-2.430771523
H	0.495679541	3.354060028	-1.686496210
C	2.066946686	-0.684862843	-0.496078568
C	2.552430739	-0.895180199	-1.802959270
H	2.203002721	-0.251519278	-2.606049335
C	3.453592590	-1.916452299	-2.076108941
H	3.823740759	-2.089466153	-3.082374609
C	3.904116166	-2.754498958	-1.044328550
C	4.862813834	-3.843004326	-1.325080930
C	3.434811369	-2.549943607	0.259266830
H	3.782091367	-3.198341092	1.061438184
C	2.530531184	-1.526566768	0.530315726
H	2.170171552	-1.371120633	1.543438181
H	5.148261384	-4.446782308	-0.433540958
O	5.328104212	-4.095535911	-2.421454725
C	-3.975505826	-2.892554358	0.592207175
C	-5.133419991	-3.755924406	0.080211821
C	-5.300532058	-3.314629193	-1.401398999
C	-4.136182283	-2.336308600	-1.638298276
H	-3.329836930	-3.396499877	1.313120685
H	-4.321152006	-1.936413844	1.002211908
H	-4.874248374	-4.816292656	0.137806185
H	-6.039171183	-3.599129564	0.671036236
H	-5.236345736	-4.175100974	-2.071658250
H	-6.259890611	-2.823315601	-1.581518693
H	-4.450730512	-1.292239878	-1.537440340
H	-3.621513721	-2.481491503	-2.589474666
C	-2.508281642	0.254599129	0.034812957
O	-3.689289456	0.487664357	0.149056951

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40

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C	-1.503875195	1.070129381	-1.806745056
C	-0.403591432	0.593276332	-1.059378795
C	0.549268161	0.893104086	-0.162421286
Si	0.676678329	2.668938296	0.549898150
H	-1.335340770	1.642022297	-2.717715928
H	-2.456087091	1.298894376	-1.323255804
Fe	-1.242374555	-0.931521189	-1.896869144
C	-0.482089368	-2.417860949	-1.176149565
C	-2.758114035	-1.467746279	-2.760936783

C	-0.223092120	-0.961164165	-3.305516798
O	0.466141597	-0.928376922	-4.229148591
O	-3.717701422	-1.771262459	-3.317859693
O	-0.029810059	-3.363213883	-0.703867677
C	-0.366415445	3.865811411	-0.474805966
C	0.068119751	2.721345888	2.347762022
C	2.493377450	3.193820019	0.481438655
H	2.619695946	4.202104156	0.892556850
H	3.132211586	2.515623842	1.055650792
H	2.865083734	3.206622370	-0.549066996
H	-0.219889093	4.888707752	-0.108273847
H	-0.088873960	3.849441290	-1.533564216
H	-1.434643927	3.638727357	-0.406758517
H	0.041038574	3.759994332	2.699290455
H	-0.944736699	2.314879237	2.444109707
H	0.721307462	2.164918719	3.027458706
C	1.573615151	-0.106285157	0.258119160
C	2.432815361	-0.700470489	-0.689213141
H	2.333401812	-0.424533403	-1.734085275
C	3.400241095	-1.618218508	-0.302002378
H	4.063813673	-2.078195457	-1.028170833
C	3.539504317	-1.970209036	1.048712919
C	4.565399862	-2.949106776	1.468285910
C	2.694796503	-1.384267604	1.999314382
H	2.793516907	-1.660130316	3.047307537
C	1.730445599	-0.458711226	1.611136827
H	1.072683808	-0.023261458	2.356528054
H	4.583741539	-3.158955833	2.561863041
O	5.344851623	-3.502480683	0.715010965

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41

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C	-1.924434679	0.420253799	-0.064191052
C	-0.543802980	0.162581317	-0.184818026
C	0.666806913	0.731490479	-0.261217517
Si	0.727434634	2.641960365	-0.198244873
H	-2.499404464	0.725172729	-0.936140286
H	-2.335041328	0.763582138	0.883829466
Fe	-1.482919634	-1.579126587	-0.225116411
C	-0.300849702	-2.904150704	-0.570804256
O	-1.652454422	-1.275458974	-2.356579139
C	-3.142674507	-2.304365496	-0.138384646
C	-1.214898999	-1.702376769	1.506277503
O	-4.211300609	-2.727288741	-0.040136499
O	-1.024560336	-1.751445981	2.642965516
O	0.428242575	-3.764533676	-0.808887838
C	2.497706758	3.285729731	-0.397265568
C	-0.350868164	3.378155024	-1.572056766
C	0.072280843	3.198477875	1.490873408
H	0.058171684	4.292084800	1.568549955
H	-0.947345139	2.839046455	1.664113805
H	0.701565086	2.815673852	2.302117302
H	2.515050409	4.371715842	-0.247277924
H	3.177377169	2.839341237	0.336039790
H	2.909840982	3.085281011	-1.391510954
H	-0.372029579	4.472112088	-1.503602953
H	0.031939443	3.116310745	-2.565080212
H	-1.383388434	3.021180696	-1.505473028
C	1.917588128	-0.075448050	-0.315264016
C	2.803041759	0.036001689	-1.408629193
H	2.561436834	0.720561224	-2.217478343
C	3.963169684	-0.722792858	-1.476488474
H	4.638650947	-0.649130838	-2.323710179
C	4.286428270	-1.610082182	-0.438136365
C	5.517413621	-2.423529373	-0.502577836
C	3.426774170	-1.716619198	0.661880649
H	3.676610732	-2.397872966	1.472916966
C	2.260006298	-0.959769360	0.723295934
H	1.604645441	-1.042230626	1.583660125
H	5.676316849	-3.090482405	0.375067645

O	6.318926762	-2.400959839	-1.419335159
C	-2.873829404	-1.463126432	-3.121821000
C	-2.468324971	-1.357415241	-4.601968052
C	-1.086459349	-0.680458099	-4.546521201
C	-0.513945404	-1.244492918	-3.252046426
H	-3.307286777	-2.436356540	-2.872176485
H	-3.570510245	-0.678526928	-2.811019293
H	0.248590790	-0.629128873	-2.776513448
H	-0.126158162	-2.263340789	-3.387324427
H	-2.382236625	-2.354974487	-5.045029480
H	-3.199614585	-0.794793457	-5.187854296
H	-0.464405618	-0.910276262	-5.415548648
H	-1.186081051	0.407519165	-4.470238863

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C	-1.907838621	0.638297717	-0.476655065
C	-0.547006407	0.283734281	-0.382131602
C	0.676719930	0.729006910	-0.067193453
Si	0.881935090	2.530671423	0.534588040
H	-2.252105363	1.259038536	-1.301805870
H	-2.509426259	0.722041476	0.426594203
Fe	-1.562755972	-1.345083137	-0.863671915
C	-0.451703407	-2.772843727	-0.908816296
O	-1.778700441	-1.608190792	1.280824616
C	-3.236429370	-1.972919262	-1.169193952
C	-1.272022862	-0.978615923	-2.556199690
O	-4.304254132	-2.342509478	-1.400406844
O	-1.068877716	-0.698854597	-3.656432127
O	0.224250960	-3.705522039	-0.948900364
C	2.573392249	3.187455391	-0.008174936
C	-0.457155531	3.637566907	-0.215241976
C	0.749870671	2.607759685	2.428124695
H	0.814671104	3.642777058	2.783462300
H	-0.206625746	2.198725203	2.772431658
H	1.549317640	2.042655694	2.920238896
H	2.712618421	4.220477717	0.331677272
H	3.398063942	2.589396239	0.391703749
H	2.664174957	3.183128089	-1.100196300
H	-0.275820623	4.682186884	0.064438024
H	-0.452775979	3.581527764	-1.309251495
H	-1.460826222	3.368725532	0.127291230
C	1.888195125	-0.134535139	-0.166094065
C	2.252941342	-0.760786590	-1.375653026
H	1.635229897	-0.604451116	-2.253792988
C	3.390248894	-1.552932458	-1.460940502
H	3.672687504	-2.033594249	-2.392923359
C	4.206638932	-1.745056866	-0.335707395
C	5.420037120	-2.582909264	-0.416951242
C	3.862152434	-1.123060791	0.870634759
H	4.491847129	-1.266194532	1.746783960
C	2.725525301	-0.324356122	0.951109946
H	2.470252320	0.151178728	1.893820496
H	5.985681783	-2.667667025	0.539407893
O	5.808973161	-3.151740735	-1.420606700
C	-3.001593912	-2.008145246	1.934326895
C	-2.733562362	-1.748343100	3.419700374
C	-1.199680483	-1.957873690	3.560729341
C	-0.698785796	-2.103684221	2.110088758
H	-3.810879209	-1.414132504	1.508318367
H	-3.190609086	-3.072577751	1.732597409
H	-3.006093192	-0.721022920	3.677113604
H	-3.313490935	-2.418162810	4.060336042
H	-0.732889086	-1.105540891	4.060351912
H	-0.960928466	-2.852744337	4.142301472
H	-0.511457603	-3.155341220	1.856872612
H	0.183754336	-1.514559995	1.865527138

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C	-1.928176681	0.671423771	-0.777599982
C	-0.588923518	0.345748437	-0.438756625
C	0.567185182	0.838324838	0.020280176
Si	0.789232851	2.706673595	0.347440727
H	-2.133747892	1.187265163	-1.715070758
H	-2.640301170	0.921032135	0.007338163
Fe	-1.567372884	-1.328553954	-0.997959020
C	-1.889442308	-1.550842283	0.776251660
O	-0.407658627	-3.158588236	-1.018765643
C	-3.190371714	-1.821010252	-1.552257568
C	-0.850674693	-1.002022807	-2.639216098
O	-4.283418854	-1.983254791	-1.892028795
O	-0.362445572	-0.807567654	-3.662729829
O	-2.069283771	-1.686073021	1.905071913
C	1.903434186	3.423416070	-1.009816888
C	-0.871863432	3.608913205	0.345023304
C	1.629929364	3.001926175	2.022933085
H	1.772353655	4.077313003	2.183580288
H	1.029266743	2.622760857	2.857437538
H	2.615161977	2.527953088	2.074992398
H	2.107826651	4.485431452	-0.828580852
H	2.867163628	2.904311901	-1.055191800
H	1.434877866	3.338191292	-1.996497661
H	-0.712484535	4.673252421	0.555334028
H	-1.383348148	3.532248809	-0.618653111
H	-1.546692515	3.217404079	1.113430826
C	1.771951669	-0.030380822	0.184592059
C	2.432137421	-0.566518808	-0.941391412
H	2.040071646	-0.349182900	-1.929741611
C	3.565723496	-1.357486262	-0.801439948
H	4.075422877	-1.770520761	-1.667129331
C	4.079673229	-1.636348564	0.474983661
C	5.275519579	-2.488094708	0.635845076
C	3.437546469	-1.104509671	1.601039023
H	3.829440587	-1.320338839	2.593195367
C	2.303428115	-0.309233706	1.457491092
H	1.808745558	0.089178863	2.337263372
H	5.605487069	-2.625586576	1.690851566
O	5.879204629	-3.020208111	-0.278187734
C	0.463645415	-3.594850597	0.048208852
C	1.182513554	-4.798676058	-0.552321030
C	0.079689772	-5.469342984	-1.408633003
C	-0.954220488	-4.343959781	-1.645308854
H	1.107670731	-2.754590708	0.302200291
H	-0.140057875	-3.873486062	0.924927041
H	2.011264499	-4.457162311	-1.179273232
H	1.587575607	-5.465775387	0.213305395
H	0.478928640	-5.860464383	-2.347682316
H	-0.382792745	-6.304344065	-0.874350922
H	-1.924571079	-4.572923797	-1.187642725
H	-1.113514393	-4.100466060	-2.697844943

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C	-1.894673181	0.658804548	-0.247012902
C	-0.506041180	0.348328491	-0.257432711
C	0.718338623	0.883354926	-0.255639282
Si	0.892568269	2.784179364	-0.196425356
H	-2.346253881	1.117061697	-1.126751944
H	-2.363577481	0.973282561	0.684673218
Fe	-1.457856274	-1.366722519	-0.404104191
C	-0.283411435	-2.703171028	-0.492052434
O	-3.399047242	-2.309508204	-0.625604556
C	-1.415584330	-1.124364569	-2.210248600
C	-1.519513323	-1.430897741	1.405840429
O	-1.392088384	-0.952429793	-3.345444430
O	-1.551026222	-1.448389987	2.556339052
O	0.515245753	-3.536258991	-0.549777673
C	2.707241308	3.250019486	0.078392007
C	0.284795691	3.538818420	-1.827241509

C	-0.134309153	3.481322096	1.234174770
H	-0.039304031	4.572807573	1.277232251
H	-1.196972151	3.243467155	1.126262774
H	0.202761927	3.080395924	2.196501369
H	2.815887881	4.339096440	0.142417965
H	3.092596629	2.822577866	1.010678550
H	3.351286784	2.897187641	-0.733327579
H	0.348830825	4.633294579	-1.803938928
H	0.879510071	3.190155819	-2.678825174
H	-0.759626019	3.271183771	-2.021818140
C	1.942784847	0.034732135	-0.317600471
C	2.764533287	0.037641317	-1.463123080
H	2.479765742	0.647727371	-2.316519252
C	3.912768669	-0.739970002	-1.523079107
H	4.542798671	-0.750253700	-2.407541959
C	4.281231733	-1.538484763	-0.428909248
C	5.501650334	-2.367055825	-0.481552081
C	3.477127320	-1.542604556	0.717457859
H	3.759806492	-2.160127300	1.567834423
C	2.324245670	-0.764773021	0.772714508
H	1.705268674	-0.768241419	1.664663138
H	5.692698015	-2.963860570	0.439641976
O	6.264904172	-2.425931266	-1.428921348
C	-3.596843942	-3.725039577	-0.461850787
C	-5.047970940	-3.947212595	-0.896154282
C	-5.755509830	-2.627677617	-0.484955553
C	-4.597825502	-1.658991559	-0.155040823
H	-2.857006524	-4.232435077	-1.082183731
H	-3.434846411	-4.001666926	0.589937881
H	-5.095115531	-4.087089072	-1.979302971
H	-5.487294722	-4.828736365	-0.423224039
H	-6.377261957	-2.245211577	-1.297289476
H	-6.400614244	-2.766620179	0.386264298
H	-4.510278294	-1.483969069	0.925018346
H	-4.655453818	-0.694610976	-0.660159528

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42

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C	-1.872778108	0.337344044	0.186407239
C	-0.502286948	0.322867658	-0.108350981
C	0.567843794	1.049720188	-0.429051256
Si	0.435653654	2.943304839	-0.669920724
H	-2.603301215	0.461418764	-0.610513991
H	-2.216054169	0.683803481	1.158823545
Fe	-1.114017709	-1.596803137	0.254414012
C	-2.677297669	-2.290784022	0.764489701
C	-1.381023541	-1.766801971	-1.540492615
C	-0.447475884	-1.306966243	1.924063304
O	-1.510227158	-1.875590210	-2.676754038
O	0.021456157	-1.130210802	2.958648979
O	-3.716844929	-2.666801663	1.098033422
C	1.946061718	3.761435989	0.129227846
C	0.429214706	3.339102778	-2.523699205
C	-1.137932292	3.615876081	0.132068404
H	-1.173118685	4.706382073	0.024586876
H	-2.043358397	3.207198205	-0.326295350
H	-1.172196837	3.387370318	1.202636945
H	1.913518687	4.848014972	-0.012725968
H	1.988170356	3.569545950	1.207211936
H	2.881734715	3.398027858	-0.308092460
H	0.369976001	4.421609557	-2.687953823
H	1.340308118	2.982389038	-3.015963401
H	-0.426434328	2.878292037	-3.029164358
C	1.929729717	0.464495598	-0.619753198
C	2.435948341	0.211415600	-1.910774801
H	1.803528114	0.401690433	-2.773293604
C	3.719819249	-0.290835740	-2.090091468
H	4.111938843	-0.496727571	-3.081722005
C	4.539972721	-0.544266592	-0.979750397
C	5.907642706	-1.076640057	-1.161725027

C	4.049011996	-0.288824793	0.307315768
H	4.682039842	-0.483467805	1.170777097
C	2.761647995	0.211596462	0.485474907
H	2.387332096	0.407811821	1.485656180
H	6.470102678	-1.238292757	-0.214321291
O	6.415276626	-1.331275683	-2.238098750
C	0.708948047	-2.649833729	-0.146118856
C	-0.028477660	-3.574013433	0.258746468
H	1.608565325	-2.192622338	-0.507069483
Si	-0.597653110	-5.274510233	0.757513508
C	-1.119505004	-5.226930206	2.570495501
C	-2.027205425	-5.797874004	-0.356404077
C	0.879633561	-6.432870897	0.529776486
H	-1.395652403	-6.229989197	2.915668095
H	-0.302307379	-4.869748332	3.206634684
H	-1.981542937	-4.571141258	2.727047533
H	0.616377207	-7.457265514	0.818941612
H	1.212641622	-6.454631626	-0.513203228
H	1.729095147	-6.119840222	1.146076947
H	-2.335411782	-6.823346953	-0.121307371
H	-2.899313940	-5.149718523	-0.227414706
H	-1.737281299	-5.771618643	-1.412365427

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42a

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C	-1.950338356	0.873473954	0.371543704
C	-0.622565188	0.577247863	0.032137904
C	0.654204850	0.933077085	0.169343826
Si	1.082310228	2.445821797	1.257134449
H	-2.478071967	1.686757880	-0.122202505
H	-2.321911925	0.647751441	1.369667776
Fe	-1.756763125	-0.836504590	-0.846841802
C	-0.561782028	-1.830759830	-1.720814811
C	-2.006878724	0.259251634	-2.281802333
C	-1.595486047	-1.829456230	0.673099013
O	-2.186536765	0.963896361	-3.170030161
O	-1.510246106	-2.437975885	1.643127953
O	0.201929381	-2.479429506	-2.293459678
C	2.831500498	3.040133402	0.847455402
C	-0.146546410	3.853547782	0.959073014
C	1.016770591	1.918137706	3.076750591
H	1.258490768	2.757198556	3.739694055
H	0.020882745	1.553150436	3.351298581
H	1.733055480	1.115359296	3.283974443
H	3.101962563	3.893015381	1.480779929
H	3.575570510	2.254092051	1.011504849
H	2.918824011	3.361893174	-0.195814565
H	0.104130202	4.717321680	1.586368989
H	-0.128307137	4.184432747	-0.084983978
H	-1.172665474	3.557146335	1.198586013
C	1.772768313	0.132207185	-0.409014755
C	2.361267657	0.482017914	-1.639424656
H	1.972751111	1.336660342	-2.186548824
C	3.413894622	-0.258589802	-2.161308801
H	3.865606483	-0.003763200	-3.115502612
C	3.917270021	-1.363434250	-1.456851335
C	5.037252261	-2.157528129	-2.002962712
C	3.346743366	-1.711941383	-0.227247120
H	3.733253112	-2.569393350	0.320221965
C	2.288632244	-0.971104454	0.291399716
H	1.846386411	-1.245861796	1.244773431
H	5.347209741	-3.015845322	-1.363955847
O	5.603640319	-1.930358984	-3.056299537
C	-3.883804671	-1.072854363	-0.730683965
C	-3.572234828	-2.060821529	-1.426292309
H	-4.552811815	-0.416819928	-0.209123114
Si	-3.692737949	-3.625544852	-2.426418323
C	-2.593452886	-4.940157640	-1.636712999
C	-5.504344452	-4.164168534	-2.375246972
C	-3.155210202	-3.254524348	-4.196098915

H	-2.693979260	-5.890891156	-2.171681126
H	-1.538394535	-4.654246244	-1.666868259
H	-2.870078034	-5.115194577	-0.591973339
H	-3.271266811	-4.144156054	-4.824811395
H	-3.759685530	-2.454968069	-4.636855198
H	-2.105518035	-2.950569315	-4.240505585
H	-5.650074909	-5.085225002	-2.950786154
H	-5.830544601	-4.357244415	-1.348306212
H	-6.161841767	-3.397932385	-2.797806680

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42b

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C	-1.896632281	-0.089554349	0.008613763
C	-0.511930079	0.005175547	-0.160391802
C	0.586025499	0.753380224	-0.018819643
Si	0.415889753	2.550358227	0.613406425
H	-2.570593472	0.406642947	-0.685996291
H	-2.303335264	-0.253492288	1.003731974
Fe	-1.073903523	-1.864003443	-0.722950252
C	-2.675209224	-2.641331447	-0.880532184
C	-1.018192824	-1.171040130	-2.347006679
C	0.123433618	-3.112940022	-1.240604712
O	-0.981002089	-0.718829776	-3.407340620
O	0.869854768	-3.934519326	-1.547212021
O	-3.735057704	-3.075230525	-1.028881966
C	1.739073007	3.608908472	-0.231069885
C	-1.292584502	3.229125686	0.173290738
C	0.646807346	2.621513699	2.495496784
H	0.489636845	3.642890681	2.862256036
H	-0.069716535	1.970727795	3.008534099
H	1.653287785	2.316779030	2.801838590
H	1.672636845	4.651142054	0.102086597
H	2.749922206	3.251549341	-0.010216187
H	1.617291738	3.600768646	-1.319981750
H	-1.365581098	4.281714645	0.470962152
H	-1.475786973	3.175745901	-0.905431004
H	-2.096765530	2.684067748	0.676160378
C	1.948997103	0.232172080	-0.330518526
C	2.311985447	-0.187115524	-1.626577637
H	1.582114202	-0.121752443	-2.426622017
C	3.590292081	-0.660761153	-1.893627824
H	3.874528028	-0.980316943	-2.891916062
C	4.549243112	-0.731388788	-0.871366274
C	5.912137386	-1.233196182	-1.147926893
C	4.204251761	-0.313346920	0.419020401
H	4.942908799	-0.365604717	1.216489697
C	2.924755624	0.168384822	0.683556104
H	2.669581487	0.491064244	1.688811400
H	6.586613127	-1.247419861	-0.261425732
O	6.307074159	-1.608050657	-2.236190977
C	0.001537722	-2.160668529	1.177719219
C	-1.051619980	-2.779752078	1.410537727
H	0.995405567	-1.775951665	1.280147975
Si	-2.187211686	-3.927928095	2.348219387
C	-2.371389975	-5.523394087	1.359467782
C	-1.320837285	-4.274588703	3.992007287
C	-3.850410659	-3.087924886	2.633025978
H	-2.957402561	-6.255036958	1.927702855
H	-2.879668596	-5.356526452	0.405552980
H	-1.393660725	-5.970135300	1.149996383
H	-4.503572985	-3.736672843	3.228180010
H	-3.732851812	-2.145517169	3.178491295
H	-4.362092094	-2.874914841	1.689710256
H	-1.919946907	-4.957887755	4.605269637
H	-0.342692510	-4.740345076	3.832350485
H	-1.166197796	-3.356210332	4.567643886

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42c

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C	-1.732469327	0.604796892	0.169096804

C	-0.401362431	0.358342769	-0.205034040
C	0.759986073	0.981072275	-0.409617859
Si	0.729339853	2.905635985	-0.371471513
H	-2.456436391	0.968833831	-0.556678577
H	-1.952813237	0.892577369	1.195283634
Fe	-1.428133251	-1.434709797	-0.052093948
C	-3.053082192	-1.683562035	0.624605318
C	-1.879017866	-1.282092132	-1.810015286
C	-0.458008260	-1.561082157	1.480041290
O	-2.141657431	-1.193724402	-2.925854356
O	0.170798227	-1.669781148	2.437640647
O	-4.108115609	-1.792957473	1.077570105
C	2.495205882	3.584173175	-0.438232201
C	-0.246960991	3.541802547	-1.866299423
C	-0.070525131	3.512679961	1.233084748
H	-0.030390216	4.607450095	1.280337925
H	-1.120492961	3.217144770	1.315115435
H	0.458428553	3.125292512	2.110924049
H	2.475925835	4.679400168	-0.389472110
H	3.096705776	3.225405525	0.403981731
H	3.017392496	3.301360697	-1.357089579
H	-0.301868533	4.636726709	-1.862484618
H	0.223069335	3.236936545	-2.807769849
H	-1.272968015	3.157917450	-1.869364201
C	2.086720602	0.339714292	-0.628080629
C	2.747873517	0.435828057	-1.870709805
H	2.230549577	0.892434543	-2.710921459
C	4.044226678	-0.036436346	-2.032573706
H	4.554331134	0.029724470	-2.989087068
C	4.728904479	-0.603534929	-0.946819597
C	6.112063674	-1.098568281	-1.106684857
C	4.083988240	-0.702370127	0.292253766
H	4.611020878	-1.141448370	1.137106517
C	2.778447430	-0.241990775	0.449456668
H	2.292793682	-0.312282606	1.416805862
H	6.561258248	-1.521587243	-0.179538098
O	6.744478987	-1.068102787	-2.146492728
C	-1.325924199	-3.562229792	-0.199650331
C	-0.328549496	-3.255186472	-0.894378300
H	-1.999242695	-4.259596540	0.261429616
Si	1.024427077	-3.752986077	-2.094334603
C	0.513286575	-5.457675088	-2.742217685
C	1.112605758	-2.535662813	-3.528527526
C	2.657659795	-3.891832321	-1.166369429
H	1.257841728	-5.829420691	-3.456454897
H	0.436135544	-6.190190518	-1.931946312
H	-0.452642895	-5.420353191	-3.256542381
H	3.459057536	-4.188933603	-1.852775358
H	2.943904835	-2.943050182	-0.706478514
H	2.595598306	-4.648637780	-0.376983235
H	1.863563599	-2.867832907	-4.254712093
H	0.152582476	-2.461729948	-4.049393585
H	1.393984764	-1.536323183	-3.188495504

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42d

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C	-2.038566145	0.808192322	0.109129118
C	-0.684702639	0.511405381	-0.085018927
C	0.572528765	0.860942986	0.184280615
Si	0.955723412	2.409063327	1.237319920
H	-2.507665850	1.617885395	-0.443711228
H	-2.503731653	0.605746248	1.070672647
Fe	-1.727663306	-0.927290420	-1.055882322
C	-0.405887816	-1.863525885	-1.799233175
C	-1.921760592	0.163322475	-2.503077868
C	-1.712310998	-1.894105585	0.487602148
O	-2.079526555	0.860590433	-3.401581621
O	-1.725538981	-2.488048722	1.470646067
O	0.422786395	-2.487017596	-2.301864931
C	2.005150680	3.615272713	0.219678070

C	-0.632942457	3.280772534	1.779047892
C	1.934200813	1.875349243	2.769965212
H	2.219012521	2.747247338	3.370640246
H	1.345483398	1.209640552	3.411106193
H	2.852839889	1.346337380	2.495888282
H	2.282735970	4.487221067	0.823706511
H	2.930860935	3.149441002	-0.133627711
H	1.458836238	3.980655130	-0.657088693
H	-0.381614261	4.165809102	2.376032451
H	-1.226925601	3.617089152	0.923162873
H	-1.267748208	2.635673042	2.394729476
C	1.747536782	0.055621656	-0.266686912
C	2.473360555	0.409103142	-1.420996885
H	2.150008838	1.264808935	-2.007040731
C	3.579750110	-0.329497597	-1.821464339
H	4.138257632	-0.070316242	-2.715964917
C	3.996642799	-1.438576551	-1.070020753
C	5.171902250	-2.231223737	-1.488463490
C	3.288403114	-1.791300897	0.085130319
H	3.609666007	-2.651089180	0.669641845
C	2.179498805	-1.050682010	0.484749870
H	1.632752441	-1.327842691	1.381466404
H	5.407131084	-3.092484007	-0.822477105
O	5.854345634	-1.999114928	-2.469291460
C	-3.173163276	-2.276022226	-1.917393647
C	-3.890742933	-1.493161862	-1.258209019
H	-2.955994241	-3.108274070	-2.558289631
Si	-5.437993405	-0.759117931	-0.527965874
C	-5.635151261	1.025257132	-1.110010650
C	-6.892052469	-1.800044720	-1.143577081
C	-5.341168060	-0.852779031	1.355899882
H	-6.592052170	1.429570249	-0.761041707
H	-4.840904016	1.670960019	-0.725862458
H	-5.625479493	1.091250659	-2.202685822
H	-6.283570899	-0.510955767	1.798470656
H	-5.168216227	-1.879322710	1.694364020
H	-4.539286320	-0.227356016	1.758316568
H	-7.835789288	-1.420937204	-0.734768955
H	-6.966758634	-1.775334904	-2.235360033
H	-6.791682271	-2.846128118	-0.837226871

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42e

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C	-1.818818530	0.815436197	0.572491945
C	-0.493969900	0.470894246	0.281122438
C	0.782140546	0.867820393	0.254335271
Si	1.173573219	2.633367631	0.880407648
H	-2.374777022	1.443914556	-0.119102335
H	-2.160905507	0.855862778	1.604172841
Fe	-1.657607363	-1.114477270	-0.202742475
C	-3.399955405	-1.456954967	0.002247161
C	-1.154414282	-1.721628579	1.375425804
C	-0.957190967	-2.588796157	-0.975898112
O	-0.823640322	-2.121463963	2.405691395
O	-0.540655291	-3.527571155	-1.497286432
O	-4.513276725	-1.665684865	0.227233208
C	3.038466156	2.813850863	1.148459093
C	0.572270529	3.909361340	-0.385797289
C	0.295435995	2.912685039	2.532922178
H	0.526294350	3.909481373	2.926367051
H	-0.791760267	2.836724596	2.436819292
H	0.617672787	2.178252039	3.279370171
H	3.270343461	3.807398438	1.549656667
H	3.408500413	2.073136716	1.866073314
H	3.608631504	2.686700864	0.223085370
H	0.732505046	4.930459593	-0.020206309
H	1.099653865	3.814378923	-1.341650139
H	-0.498529247	3.791692281	-0.585047281
C	1.871454342	0.004573154	-0.283683550
C	2.613275496	0.429036821	-1.407927814

H	2.380689353	1.388014587	-1.864959846
C	3.621216942	-0.360461907	-1.945798486
H	4.184577709	-0.041998887	-2.817819996
C	3.932136735	-1.598067778	-1.363256947
C	5.006403701	-2.442119744	-1.928872606
C	3.215395595	-2.023179988	-0.237554415
H	3.458738707	-2.978775355	0.222760743
C	2.198726545	-1.234021370	0.295184411
H	1.658664353	-1.568512046	1.173816500
H	5.170814783	-3.403193117	-1.391203835
O	5.679254596	-2.149018612	-2.900536687
C	-1.029576444	-0.255199926	-2.157243798
C	-2.257066753	-0.332536381	-2.324197631
H	0.016264442	-0.105405232	-2.331978549
Si	-3.867254758	-0.315887491	-3.272272422
C	-5.132116582	0.751661006	-2.370438621
C	-3.457175205	0.426462383	-4.961318076
C	-4.457371424	-2.097063863	-3.467055367
H	-6.058910834	0.806293745	-2.953936538
H	-5.381210606	0.343766989	-1.386333319
H	-4.765262890	1.774936108	-2.234126114
H	-5.348163726	-2.134959735	-4.105406339
H	-3.684806461	-2.715931723	-3.936479376
H	-4.716488343	-2.549239654	-2.504960460
H	-4.354691741	0.460027523	-5.591049725
H	-3.073437296	1.448314204	-4.871260442
H	-2.703872203	-0.171633022	-5.485373667

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47-TS1 (48)

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C	-0.329249336	-0.430851263	0.023851629
C	0.403057172	-2.193598974	0.769100655
C	-1.729412114	-0.616734819	0.063501070
C	0.601981711	0.541800701	0.111048643
Si	0.111123002	2.259252140	0.805407406
H	-2.359195100	0.052655369	-0.514864334
H	-2.188398865	-1.025201289	0.958882206
Fe	-0.810088723	-2.156856041	-0.986600723
C	-2.370233623	-2.987454892	-1.140107680
C	-0.846519648	-1.201733084	-2.493614812
C	0.326769977	-3.347892603	-1.739123742
O	-0.891462432	-0.579465930	-3.461936669
O	1.041211838	-4.125711622	-2.193104906
O	-3.405796789	-3.489144524	-1.216406679
C	1.394431595	3.532290836	0.241936612
C	-1.576219475	2.797632643	0.139000476
C	0.045173674	2.204525260	2.700201641
H	-0.280545020	3.170876456	3.103299965
H	-0.659973974	1.442713860	3.050003304
H	1.022603396	1.978644310	3.140487403
H	1.118121193	4.530752109	0.600543998
H	2.398510711	3.310038230	0.614901156
H	1.452875609	3.578671723	-0.851222200
H	-1.761553811	3.841974585	0.417336365
H	-1.614708651	2.737111706	-0.954182495
H	-2.398474739	2.198734034	0.540330573
C	2.032466185	0.293411999	-0.211288529
C	2.458806084	-0.106429356	-1.494613249
H	1.723198866	-0.223650002	-2.282290252
C	3.804944278	-0.317357146	-1.768904354
H	4.137724616	-0.612873516	-2.759556768
C	4.768902051	-0.142446398	-0.765051733
C	6.204181000	-0.356296973	-1.051532692
C	4.360129070	0.248973692	0.515877452
H	5.103018582	0.383033030	1.299626018
C	3.013645250	0.470838896	0.786185342
H	2.709322220	0.773949926	1.783995783
H	6.877928831	-0.193122549	-0.179742565
O	6.654535496	-0.681200981	-2.134203445
C	-0.471808710	-3.107708753	0.913500169

H	1.398842599	-1.870243272	1.027818368
Si	-1.062373165	-4.631646493	1.800202231
C	-1.048777037	-6.073026940	0.578482673
C	0.125232376	-4.969630573	3.234326022
C	-2.808247410	-4.331474196	2.455124069
H	-1.328708228	-7.005058814	1.083070293
H	-1.757855724	-5.913040071	-0.240233709
H	-0.055176404	-6.216254627	0.140474697
H	-3.173807187	-5.213164189	2.994083168
H	-2.833376406	-3.484081115	3.148838886
H	-3.509504935	-4.123156336	1.640858642
H	-0.190980928	-5.850925958	3.804764876
H	1.142235141	-5.153991900	2.871760752
H	0.165279208	-4.121857218	3.926822445

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47-TS2 (49)

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C	0.016198432	0.004644026	0.019166022
C	0.030208662	0.019630692	2.004860921
C	1.222871487	-0.003411523	-0.796231133
C	1.514193030	-0.053894949	-2.102701962
Si	0.207007066	-0.096754085	-3.493902806
H	-0.586962840	-0.901592588	-0.022935889
H	-0.589637761	0.907070122	-0.044072049
Fe	2.014018589	0.018933796	0.970224919
C	3.769255130	0.026708166	1.015253576
C	2.089806238	-1.805731558	0.965265309
C	2.079170298	1.840304802	0.948147139
O	2.157325659	-2.950604673	0.957409768
O	2.147340180	2.985846651	0.924418231
O	4.923630606	0.034994778	1.048251937
C	0.058708312	-1.841652242	-4.224972522
C	-1.499983915	0.432847773	-2.861319531
C	0.740707314	1.097304857	-4.864125952
H	0.025034356	1.077611545	-5.694465655
H	0.797957160	2.128974720	-4.499612752
H	1.724217377	0.834236112	-5.266948494
H	-0.710134308	-1.862138530	-5.006861374
H	0.996835206	-2.174297334	-4.681114300
H	-0.222909473	-2.578114158	-3.464181987
H	-2.199641778	0.475834659	-3.704754154
H	-1.917215034	-0.266830156	-2.130058006
H	-1.478408554	1.428466415	-2.405005810
C	2.946268905	-0.052893185	-2.540008703
C	3.532905474	-1.202526503	-3.106320045
H	2.939078721	-2.106949531	-3.203797140
C	4.860778101	-1.201257993	-3.514480162
H	5.321898160	-2.088061220	-3.939032209
C	5.639826506	-0.042622362	-3.377254708
C	7.053147536	-0.032826776	-3.807147189
C	5.064543503	1.108293604	-2.824639832
H	5.665276431	2.009387390	-2.717938828
C	3.734450770	1.103860456	-2.414479378
H	3.291325015	2.000380537	-1.991051918
H	7.577508901	0.936430197	-3.645310593
O	7.636693136	-0.980301364	-4.301239935
C	1.068578880	0.019533640	2.767241768
H	-1.046240140	0.027096468	2.089309673
Si	1.507202761	-0.004565705	4.576386488
C	2.668850731	1.444699211	4.923948843
C	-0.064877523	0.149892985	5.623057456
C	2.366727965	-1.647580476	4.943778930
H	2.962208244	1.468571619	5.979714133
H	3.582103587	1.369501380	4.324114186
H	2.192504690	2.403155821	4.689807337
H	2.658261054	-1.707189271	5.998617633
H	1.707476515	-2.496765551	4.732792237
H	3.271989262	-1.767895747	4.339496945
H	0.168553168	0.130399681	6.694021053
H	-0.591307129	1.088137969	5.416009060

H	-0.758886299	-0.673671160	5.421318154

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47-TS3

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C	-0.225168129	-0.329428345	0.176173976
C	-0.667633641	-2.883142230	1.290678010
C	-1.632534671	-0.452745918	0.281909384
C	0.674931886	0.660992879	-0.020054114
Si	-0.027854165	2.441253501	0.206111820
H	-2.249706680	0.176163983	-0.356021418
H	-2.086261858	-0.717324239	1.231085222
Fe	-0.846853920	-2.164303655	-0.592756588
C	-2.444015198	-2.921676168	-0.643085797
C	-0.900542314	-1.403213872	-2.216579202
C	0.212497670	-3.507736070	-1.186807047
O	-0.993383796	-0.919784003	-3.257026097
O	0.869700424	-4.385710573	-1.531885327
O	-3.496713760	-3.389981713	-0.635712968
C	1.306655273	3.779182865	0.377510046
C	-1.013677633	2.861847694	-1.360372188
C	-1.130596604	2.551789961	1.740634288
H	-1.515641843	3.573010944	1.845747040
H	-1.987944086	1.875313671	1.697219700
H	-0.565458253	2.316257108	2.649287809
H	0.812738607	4.758011726	0.340437723
H	1.845666221	3.727484884	1.329482513
H	2.043307087	3.751645222	-0.430726939
H	-1.440001439	3.869660745	-1.288762080
H	-0.364998736	2.839923653	-2.243422026
H	-1.838980395	2.166218839	-1.542340151
C	2.060946429	0.471387221	-0.525470926
C	2.349882497	-0.334946419	-1.649229702
H	1.540117329	-0.841051019	-2.156569080
C	3.645134107	-0.468808243	-2.133216405
H	3.857924419	-1.084858055	-3.001931418
C	4.708227450	0.201737375	-1.511407996
C	6.090083150	0.067952465	-2.018703408
C	4.441928258	1.007994653	-0.397581091
H	5.259558510	1.529681598	0.095856511
C	3.143696122	1.144427056	0.080135751
H	2.964811773	1.769619264	0.946600957
H	6.850181316	0.643647133	-1.442937826
O	6.415356122	-0.603995019	-2.979895263
C	0.322308355	-2.078332929	1.359675408
H	-1.150677255	-3.681705468	1.829517063
Si	1.866565514	-1.961058315	2.436555664
C	1.986537435	-0.282005371	3.288614688
C	1.574114890	-3.282145116	3.762842293
C	3.411751295	-2.408183313	1.454539936
H	2.908604355	-0.219509417	3.878247269
H	1.983382000	0.545224570	2.577071673
H	1.143143284	-0.140889825	3.973155011
H	3.648527518	-1.674687096	0.681892328
H	4.272763578	-2.478484201	2.129940098
H	3.291641724	-3.383112789	0.969979440
H	2.400226177	-3.283535674	4.483723281
H	0.649281906	-3.097523389	4.319546331
H	1.511673195	-4.283856791	3.325373400

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47-TS4

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C	0.049048777	-0.011967773	-0.235314615
C	0.954240174	-0.057310932	2.528429768
C	1.313271851	0.001406642	-0.958744384
C	1.679836390	-0.028593940	-2.248191616
Si	0.431510422	-0.076252727	-3.694002596
H	-0.540368257	-0.919804475	-0.343482268
H	-0.546425207	0.892528562	-0.327147751
Fe	1.982594083	-0.017187707	0.861872884
C	3.718301356	-0.015488253	1.126952459

C	2.065871346	-1.837879516	0.773483929
C	2.047581058	1.802093282	0.848004163
O	2.138997716	-2.981051965	0.712897700
O	2.113449994	2.948328410	0.830743236
O	4.858448947	-0.013334696	1.308780739
C	0.144349978	-1.858731401	-4.279616376
C	-1.243019506	0.655789884	-3.184331455
C	1.115119472	0.947499868	-5.132006785
H	0.423134099	0.929236836	-5.982122149
H	1.259637527	1.994681105	-4.843921877
H	2.080051274	0.564220305	-5.478820614
H	-0.604647590	-1.882406067	-5.080401454
H	1.059165452	-2.313195357	-4.674291016
H	-0.219235426	-2.496474931	-3.466241300
H	-1.891014369	0.725935955	-4.066364321
H	-1.768010776	0.041632288	-2.445756850
H	-1.138871978	1.666564020	-2.774569689
C	3.130782977	-0.008831597	-2.611113471
C	3.731325339	-1.103684129	-3.265761558
H	3.135350450	-1.986834834	-3.478007082
C	5.074413677	-1.079588338	-3.618513042
H	5.543839283	-1.925278242	-4.112368515
C	5.858300924	0.049212536	-3.335390026
C	7.285811174	0.086341154	-3.712741860
C	5.271353981	1.145367144	-2.691087782
H	5.874340218	2.024550948	-2.472459614
C	3.926002955	1.116847530	-2.336110709
H	3.474403765	1.973958320	-1.846866506
H	7.810783707	1.029533848	-3.437584252
O	7.880065873	-0.813520492	-4.278660024
C	-0.121720638	-0.039170374	1.808393824
H	1.131408200	-0.076919554	3.595434762
Si	-1.975289559	-0.006535300	2.111514447
C	-2.804378861	-1.521614002	1.339490059
C	-2.190048879	-0.037499236	3.988421373
C	-2.735127200	1.573291800	1.400111333
H	-3.864381779	-1.551351423	1.617881326
H	-2.758204934	-1.515993412	0.245383227
H	-2.343196572	-2.450635402	1.691096871
H	-3.792920595	1.639124583	1.680920441
H	-2.233111397	2.465985172	1.788102828
H	-2.688748610	1.609247725	0.306569968
H	-3.253972679	-0.018044018	4.251907016
H	-1.754705434	-0.941407619	4.426923132
H	-1.714361039	0.828733022	4.459872570

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43

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C	0.260112205	-0.539935817	0.164223310
C	0.313619651	-0.725889330	1.656126939
C	1.530215420	-0.636676283	-0.471194612
C	-0.796718485	0.230125275	-0.393500938
Si	-1.270429031	0.298968321	-2.271921997
H	1.615437203	-0.625181675	-1.550098303
H	2.311831200	-1.178810210	0.049565200
Fe	1.181852077	1.322454541	0.299541833
C	2.850738315	1.501641223	0.841305573
C	1.475906502	2.075468406	-1.315055831
C	0.427191366	2.768592459	1.026067116
O	1.755939257	2.625586890	-2.286883763
O	-0.052184591	3.706987785	1.487339393
O	3.941622426	1.601761537	1.197049881
C	-1.829413632	2.036763600	-2.775694765
C	0.059180467	-0.289944990	-3.489456918
C	-2.736671196	-0.886077868	-2.489051893
H	-3.039029417	-0.904645330	-3.542804900
H	-2.475685033	-1.911629169	-2.204032221
H	-3.606295145	-0.586864819	-1.897027934
H	-2.130302748	2.022584262	-3.830362803
H	-2.693583671	2.373242844	-2.196005281

H	-1.036563869	2.783111496	-2.671732992
H	-0.390954472	-0.272193075	-4.490032085
H	0.950303186	0.341562245	-3.528699319
H	0.370095858	-1.322005293	-3.297292306
C	-2.039282667	0.398191097	0.439590660
C	-2.676502459	1.644104591	0.605455440
H	-2.223629423	2.534018909	0.183767924
C	-3.863691811	1.756446801	1.318259727
H	-4.346950299	2.719161122	1.455122030
C	-4.463863584	0.619617966	1.879207600
C	-5.733748441	0.726703320	2.628638131
C	-3.849665184	-0.626642750	1.711983077
H	-4.312250630	-1.515720755	2.135959137
C	-2.659521871	-0.734787596	1.000642374
H	-2.209452873	-1.711942130	0.856858413
H	-6.116559718	-0.240179129	3.027492883
O	-6.343941701	1.762862949	2.815396839
C	0.916413781	0.356031033	2.154059931
H	-0.088897784	-1.591485523	2.180948316
Si	1.264706471	0.676247538	3.975739301
C	0.769720937	2.432275314	4.477396987
C	0.249078476	-0.570353297	4.983366153
C	3.104404322	0.418246542	4.351053211
H	0.926781842	2.571500903	5.553504018
H	1.362531843	3.193180366	3.958998765
H	-0.285586471	2.634924698	4.266751501
H	3.296831172	0.556997576	5.421585113
H	3.426242533	-0.594536239	4.084296582
H	3.739239687	1.122448066	3.804692625
H	0.416108189	-0.426634932	6.057201726
H	-0.824062791	-0.457819403	4.795028994
H	0.523645244	-1.604369770	4.745954898

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44

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C	-2.477692987	0.916199405	0.432570559
C	-1.070760170	0.561467912	0.006864662
C	0.096783774	1.059169756	0.498153247
Si	0.241676164	2.526153628	1.718511865
H	-2.772418128	1.890087665	0.006613786
H	-2.560992734	1.040324118	1.522918827
Fe	-1.041264783	-0.899318095	-1.383163962
C	-0.866791028	-2.219733320	-2.618366641
C	-1.733639815	0.330011533	-2.515031121
C	-0.797406752	-1.957330511	0.066946573
O	-2.240587629	1.108657266	-3.191099407
O	-0.720282840	-2.611369714	1.007059848
O	-0.693721014	-3.042199502	-3.403074985
C	1.847863332	3.478335130	1.379608152
C	-1.164529860	3.775098740	1.472969726
C	0.218975189	1.925739245	3.519048138
H	0.286131337	2.773538482	4.211116723
H	-0.706846991	1.385843958	3.746804911
H	1.052419803	1.250679885	3.741933617
H	1.905285650	4.349077504	2.043567203
H	2.754345971	2.886709584	1.532890769
H	1.870049460	3.851392051	0.349450043
H	-0.930542351	4.689007895	2.031887767
H	-1.274824709	4.056625872	0.419907579
H	-2.133572926	3.415721023	1.828718714
C	1.308633324	0.353187339	0.024671032
C	1.333966760	-0.224670118	-1.274199924
H	0.598495389	0.112616982	-2.019315864
C	2.389271488	-1.022217993	-1.709446222
H	2.397541579	-1.454835577	-2.705263720
C	3.481059477	-1.254949937	-0.864639574
C	4.614236849	-2.090437571	-1.311488351
C	3.485122428	-0.673315578	0.413065475
H	4.330836942	-0.853072197	1.073948958
C	2.425907200	0.112608822	0.849948917

H	2.443055557	0.512491323	1.858157204
H	5.429966564	-2.202774802	-0.562369618
O	4.688646393	-2.628817211	-2.400585334
C	-3.419336063	-0.154602004	-0.056626125
C	-3.016250587	-1.113797077	-0.908798955
H	-4.451300338	-0.106371955	0.300031117
Si	-4.175960052	-2.438953203	-1.571654852
C	-3.513707366	-4.165946404	-1.155271215
C	-5.888108639	-2.239676959	-0.774299728
C	-4.369056920	-2.270053221	-3.451164690
H	-4.227527155	-4.934961148	-1.472765051
H	-2.562133723	-4.381201581	-1.651303221
H	-3.361560423	-4.281567220	-0.076471325
H	-5.091715217	-3.004650157	-3.825714098
H	-4.739785511	-1.275082426	-3.721639592
H	-3.430036800	-2.434867757	-3.988600387
H	-6.576050221	-3.007171711	-1.147189861
H	-5.841959680	-2.340624189	0.315579106
H	-6.331513201	-1.263872895	-1.001041092

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45

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C	0.182083039	-0.563293409	0.204520866
C	0.198736816	-0.794823307	1.711637620
C	1.456692993	-0.695767607	-0.410271955
C	-0.816684192	0.268954754	-0.383850744
Si	-1.205039649	0.374554385	-2.283984725
H	1.565086107	-0.664512964	-1.486209605
H	2.220643089	-1.253041588	0.120224686
Fe	1.134034858	1.290948794	0.359318215
C	2.789459423	1.384645017	0.968985983
C	1.505389763	2.077000997	-1.233704618
C	0.443229087	2.731818099	1.145695784
O	1.829220000	2.653797230	-2.175425946
O	0.028694691	3.648183884	1.704293946
O	3.858663320	1.412336615	1.394503768
C	-1.722599453	2.130402572	-2.768219230
C	0.163029752	-0.196488575	-3.469754487
C	-2.672221512	-0.786122892	-2.603277355
H	-2.920968751	-0.773191963	-3.671215549
H	-2.436228812	-1.822024578	-2.334216945
H	-3.567661795	-0.492626144	-2.048697724
H	-1.986554132	2.143330099	-3.832618465
H	-2.601328676	2.466482379	-2.210451610
H	-0.924236584	2.863757632	-2.620608382
H	-0.244994677	-0.119122749	-4.485527805
H	1.071553440	0.410278443	-3.444754505
H	0.437915004	-1.244991811	-3.316792223
C	-2.098592856	0.503849818	0.368577674
C	-2.648518621	1.790271410	0.538059953
H	-2.094154602	2.655124886	0.191667988
C	-3.882751800	1.972830267	1.148913431
H	-4.298458627	2.966367038	1.286920048
C	-4.621336072	0.869131382	1.599242360
C	-5.941826785	1.052579955	2.237752241
C	-4.096899000	-0.416280632	1.423119883
H	-4.667545520	-1.280676659	1.757032057
C	-2.858649298	-0.593936635	0.813725981
H	-2.478487603	-1.596444137	0.654827029
H	-6.435372578	0.106255403	2.556078567
O	-6.482880974	2.127737153	2.417325921
C	0.771757869	0.343658952	2.115203328
Si	-0.170978595	-2.347231588	2.730028568
H	1.029686007	0.637947005	3.130908063
C	1.442132099	-2.865824500	3.580826771
C	-1.464196863	-1.993455776	4.066731614
C	-0.747108535	-3.753566533	1.593239248
H	-1.670504908	-2.897296189	4.651914482
H	-1.107897880	-1.225967099	4.762979438
H	-2.408006788	-1.638954862	3.642067268

H	-0.770226779	-4.702626181	2.141053457
H	-1.753008936	-3.590865285	1.192749280
H	-0.067976017	-3.884702230	0.743460797
H	1.286967805	-3.732815779	4.233471444
H	2.215108466	-3.131415614	2.851188785
H	1.838800076	-2.052763787	4.198997352

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46

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C	-2.446912901	0.927918974	0.409946052
C	-1.034677258	0.577981224	-0.016749659
C	0.130427493	1.085204634	0.469497798
Si	0.263862183	2.561209351	1.676528133
H	-2.740957270	1.893161477	-0.034586128
H	-2.511143651	1.079196937	1.497705198
Fe	-0.994828928	-0.893419711	-1.392840596
C	-0.950171516	-2.254832004	-2.595399051
C	-1.676951125	0.335392724	-2.532956614
C	-0.732501930	-1.938927571	0.065829772
O	-2.183187453	1.113554687	-3.209738801
O	-0.646374951	-2.585547950	1.009832829
O	-0.935492528	-3.124260015	-3.346254156
C	1.891165295	3.487784447	1.366400889
C	-1.120933198	3.822071949	1.379036365
C	0.184030753	1.980914540	3.482192139
H	0.242963363	2.835506281	4.166853545
H	-0.754868770	1.455372749	3.689455992
H	1.001960211	1.297730316	3.735969275
H	1.945202946	4.367412928	2.018900274
H	2.784913995	2.885239290	1.550417546
H	1.944242567	3.844817061	0.331508444
H	-0.892582944	4.739268090	1.934890764
H	-1.199255190	4.093452819	0.320443103
H	-2.103441714	3.475213006	1.710508955
C	1.345383846	0.377521150	0.006625427
C	1.375050635	-0.223039537	-1.282032009
H	0.642200648	0.098458732	-2.037528776
C	2.431470858	-1.028528364	-1.698598229
H	2.442909533	-1.477493201	-2.687347762
C	3.518349829	-1.251550123	-0.844912087
C	4.649993084	-2.099416176	-1.271837304
C	3.517999617	-0.648662478	0.422960087
H	4.358800569	-0.821154556	1.092133150
C	2.458888669	0.147726478	0.840788218
H	2.471573484	0.562391206	1.842988754
H	5.460572883	-2.203981457	-0.515761486
O	4.728611997	-2.655738180	-2.351662030
C	-3.409718939	-0.157694502	-0.050108121
C	-2.910334947	-1.077256358	-0.893406365
Si	-5.212335768	-0.166380900	0.525930509
H	-3.516905861	-1.885705196	-1.300469388
C	-6.147460386	-1.599338162	-0.281815057
C	-5.272682746	-0.359305014	2.412593630
C	-6.033631861	1.475246070	0.045659572
H	-6.308190003	-0.361735983	2.773292348
H	-4.807988106	-1.299326402	2.730782126
H	-4.750711637	0.457792689	2.923654889
H	-7.192262895	-1.608103929	0.050026272
H	-6.150194942	-1.518358681	-1.374380504
H	-5.711053030	-2.569204613	-0.018746976
H	-7.076736302	1.506300160	0.382091201
H	-5.519566690	2.333829437	0.492949087
H	-6.030734207	1.617409936	-1.040978031

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43-TS

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C	-0.016867616	0.007450732	0.035342568
C	-0.060703367	0.054072803	1.894655707
C	2.331021161	-0.045973125	2.025792845
C	1.015282348	0.287961058	2.673793988

C	2.546289678	0.658446037	0.801810129
C	2.922192188	-1.299288521	2.309404792
Si	4.645009038	-1.939465268	1.722559935
H	3.491508236	0.566345423	0.284447742
H	2.042292606	1.609917756	0.669197536
Fe	1.309133187	-1.027812678	0.537409815
C	2.178835424	-1.381241464	-0.951861502
C	0.494839592	-2.620345954	0.594404805
O	2.690037288	-1.578401544	-1.967705721
O	-0.020089670	-3.650553751	0.595663325
O	-0.827046300	0.613922261	-0.563497747
C	4.487485183	-3.718926348	1.097476549
C	5.505016329	-0.908504149	0.383911204
C	5.789329459	-1.925475842	3.236039057
H	6.780842856	-2.299916881	2.954954100
H	5.921156256	-0.913017846	3.634462351
H	5.413158092	-2.555696878	4.047228075
H	5.477102875	-4.098238268	0.816034343
H	4.085399629	-4.391540320	1.861165927
H	3.843804831	-3.784904770	0.214305550
H	6.496349549	-1.349728800	0.220867596
H	4.989541678	-0.915517889	-0.580186155
H	5.664388777	0.131000524	0.688658880
C	2.504849870	-1.988928337	3.580403661
C	2.011462232	-3.308608856	3.611877090
H	1.855926893	-3.840523581	2.680024913
C	1.702049535	-3.932702264	4.814506196
H	1.313421152	-4.946463500	4.836197498
C	1.884299309	-3.260124688	6.031850231
C	1.564925356	-3.920665549	7.315529706
C	2.382309639	-1.951545762	6.017584116
H	2.534824257	-1.423490039	6.956845806
C	2.692497589	-1.329985734	4.812058685
H	3.102382373	-0.323580033	4.816192985
H	1.750874444	-3.292844805	8.216418385
O	1.135088875	-5.053825946	7.423488878
H	0.948883631	0.539008997	3.731522634
Si	-1.855342481	0.070919156	2.526790581
C	-2.770735186	-1.410592439	1.796493587
C	-1.794575158	-0.051347241	4.415791576
C	-2.687846188	1.687281071	2.015082278
H	-3.806530991	-1.431964887	2.154508587
H	-2.800808748	-1.360660268	0.702952001
H	-2.303046486	-2.359543909	2.078597473
H	-3.728991672	1.710457822	2.357694212
H	-2.175800848	2.553390963	2.448580456
H	-2.682230014	1.802468715	0.927556636
H	-2.810161931	-0.072645876	4.827798740
H	-1.280688808	-0.959303485	4.748572468
H	-1.282772523	0.807631009	4.864702738

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52

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C	0.002782551	0.083815432	-0.008743760
C	-0.001113600	0.017115615	1.477243827
C	2.515076781	-0.014200878	1.474115420
C	1.202635103	-0.122200974	2.155307243
C	2.443914250	0.736304508	0.260698492
C	3.417488127	-1.090419210	1.680470148
Si	5.128275692	-1.358192462	0.842914151
H	3.298388523	0.781567601	-0.397592154
H	1.817435894	1.622290634	0.249307227
Fe	1.445420717	-1.125945797	0.190427790
C	1.886459966	-1.307288373	-1.495122841
C	0.779147935	-2.779958609	0.317452037
O	2.174874251	-1.387834597	-2.609714153
O	0.333720188	-3.842164514	0.371235961
O	-0.716635929	0.614300279	-0.810528428
C	5.278745302	-3.168444353	0.310500431
C	5.502917455	-0.276766257	-0.667805138

C	6.455691387	-0.983400918	2.146579503
H	7.453282683	-1.163808117	1.729022511
H	6.418781621	0.062815893	2.470912906
H	6.348763161	-1.611507439	3.035997643
H	6.258926436	-3.335979699	-0.151607112
H	5.191518859	-3.859784052	1.153754830
H	4.513790859	-3.434585769	-0.426912566
H	6.507897135	-0.542168402	-1.018788635
H	4.816139202	-0.443157368	-1.503016144
H	5.517680441	0.792894804	-0.434435098
C	3.315629157	-1.869478990	2.960817536
C	3.072860234	-3.257501029	2.999983602
H	2.884843710	-3.786877416	2.072049576
C	3.043583672	-3.947358935	4.205724872
H	2.844002055	-5.014309526	4.236953903
C	3.262672865	-3.272180699	5.415759815
C	3.228085901	-4.000778824	6.702171088
C	3.513324083	-1.894945771	5.392455754
H	3.688055362	-1.364066796	6.326196271
C	3.546396187	-1.206130060	4.184007975
H	3.756739662	-0.140273212	4.174661336
H	3.418862120	-3.366540843	7.597464368
O	3.012432579	-5.192768233	6.817496303
H	1.187479777	-0.504302016	3.170356677
Si	-1.705694935	-0.266375307	2.309506658
C	-2.656710185	-1.584654815	1.355177284
C	-1.429711118	-0.785874900	4.105652870
C	-2.579055758	1.404147744	2.204476051
H	-3.665767768	-1.702257716	1.766125584
H	-2.754746132	-1.305919198	0.301069071
H	-2.161892069	-2.560274519	1.402480537
H	-3.606383494	1.336315072	2.580271742
H	-2.057610487	2.169109530	2.789758404
H	-2.619109245	1.744856104	1.164672301
H	-2.394409463	-0.921536899	4.608029385
H	-0.887077539	-1.734644745	4.179825771
H	-0.872621050	-0.031925037	4.672861539

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52-TS

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C	-0.011014080	-0.096893314	0.065421774
C	-0.013193585	0.022454110	1.931451516
C	1.417667921	-0.002878161	-0.162717149
C	1.310666637	0.612373617	2.203538068
C	2.117507974	0.411344022	0.999193371
C	1.497956806	1.764479892	3.002189608
Si	0.432723020	2.295896682	4.514342552
H	-0.885205996	0.351903317	2.480499721
H	0.015521634	-1.066143187	1.859014050
Fe	0.559377125	1.798711310	0.804551238
C	-0.972753325	2.671694149	0.636830064
C	1.435272166	3.068286838	-0.046378308
O	-1.982291942	3.222827841	0.539757275
O	2.024043553	3.861528707	-0.643520507
O	-0.960341423	-0.559478253	-0.520696722
C	0.178026165	4.170300884	4.493768699
C	-1.275998656	1.486169386	4.642375839
C	1.412675894	1.815604846	6.066163518
H	0.885530977	2.149962690	6.967429375
H	1.541449416	0.729809138	6.141923749
H	2.408423523	2.269998372	6.076029106
H	-0.444658638	4.460704298	5.348425861
H	1.118929334	4.722537595	4.572077688
H	-0.335128219	4.498188988	3.583225795
H	-1.744581574	1.851668528	5.564696729
H	-1.943938971	1.754628655	3.817272825
H	-1.231411232	0.395140624	4.716825745
C	2.877366171	2.353391851	3.054279317
C	3.125083533	3.716615458	2.793459040
H	2.302615417	4.353053780	2.484801743

C	4.404685949	4.245783972	2.895813839
H	4.597835305	5.292724820	2.681900991
C	5.482296677	3.428603447	3.269698367
C	6.847543819	3.986871981	3.376783400
C	5.250531683	2.074510279	3.537705182
H	6.080515087	1.434622527	3.830724150
C	3.966763222	1.545971066	3.438083589
H	3.794445894	0.497581052	3.663925172
H	7.626703871	3.249198665	3.674704578
O	7.138195437	5.149238983	3.164885203
H	3.157422312	0.708565641	0.959832881
Si	2.144170140	-0.299161223	-1.893255814
C	1.008463931	0.477044467	-3.180687911
C	3.875707007	0.457728332	-1.951931626
C	2.228676699	-2.175301263	-2.121402332
H	1.338819280	0.231126258	-4.196417870
H	-0.014504348	0.109182247	-3.054345809
H	0.987700546	1.568273038	-3.088800464
H	2.626418018	-2.434309611	-3.109094767
H	2.873262159	-2.644603441	-1.369851157
H	1.232126986	-2.620970519	-2.034089875
H	4.335825996	0.278677267	-2.930368683
H	3.848998298	1.541649840	-1.795091477
H	4.540856157	0.022936421	-1.197041635

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Fe(CO)2-product adduct

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C	0.025774654	0.078312957	0.071143585
C	-0.070549569	-0.241709903	1.580180125
C	1.463901694	0.039425522	-0.315376093
C	1.377362447	-0.155772686	2.017045718
C	2.207891653	-0.346454473	0.821212703
C	1.898833052	0.482545722	3.145189410
Si	0.965204963	0.960552956	4.758663824
H	-0.751889123	0.440746942	2.084646704
H	-0.463160507	-1.262395477	1.697780632
Fe	2.062767096	1.656165112	1.177926034
C	1.021656072	2.986542867	1.638186657
C	2.923651646	2.644007074	0.000695010
O	0.248779492	3.799634321	1.934821456
O	3.530956675	3.296567566	-0.735433723
O	-0.930218110	0.260064164	-0.665146159
C	1.699364981	2.559560536	5.448090076
C	-0.897848613	1.198498974	4.547492735
C	1.284709892	-0.462279570	5.969856180
H	0.831324188	-0.245518313	6.943993976
H	0.856901168	-1.403924489	5.608735507
H	2.355733760	-0.621684230	6.131426454
H	1.210294629	2.805053546	6.398016415
H	2.773180782	2.479829602	5.641965596
H	1.535493620	3.401807528	4.767346475
H	-1.310621326	1.524824264	5.510079923
H	-1.138254607	1.974189824	3.813768185
H	-1.419712150	0.278838875	4.267059245
C	3.398347582	0.456181468	3.280652185
C	4.160665927	1.643996038	3.261773245
H	3.651635634	2.599935818	3.181568445
C	5.550811222	1.601073481	3.341033482
H	6.143243415	2.510439279	3.309501009
C	6.211464799	0.373819178	3.473773062
C	7.689708199	0.320806423	3.568418859
C	5.461778261	-0.809988804	3.520222355
H	5.972626947	-1.764258879	3.631535591
C	4.075913533	-0.770987049	3.420777264
H	3.502248065	-1.692980273	3.444952166
H	8.111437430	-0.704506639	3.666489392
O	8.415378181	1.295649517	3.544545028
H	3.241246041	-0.667247589	0.822796639
Si	1.990796913	-0.056163097	-2.139254074
C	1.311608855	1.420957243	-3.092681082

C	3.880909594	-0.138451153	-2.225648396
C	1.258160831	-1.664395205	-2.821206373
H	1.466852461	1.291177846	-4.169865842
H	0.237005639	1.512362411	-2.908748830
H	1.791819604	2.358165106	-2.795467438
H	1.493558450	-1.779371150	-3.885625225
H	1.650534328	-2.543499994	-2.297932106
H	0.168831888	-1.665224294	-2.715060726
H	4.204178113	-0.289609922	-3.262309192
H	4.352845901	0.781948295	-1.867581140
H	4.278394356	-0.974942165	-1.639248867

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Fe(CO)2-product adduct (Triplet)

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C	-0.033950158	0.031496233	0.281956145
C	-0.026976599	0.155098488	1.818587003
C	1.375319101	0.087430522	-0.204015726
C	1.442276851	0.282197548	2.189680464
C	2.208276309	0.185387670	0.930714692
C	1.994333951	0.438007837	3.426724861
Si	1.033746800	0.554248833	5.078856003
H	-0.642953630	1.004063181	2.125233700
H	-0.485035547	-0.744092861	2.247967366
Fe	1.892163191	2.127697330	0.174783099
C	0.544561506	3.412493424	0.106781337
C	3.460979182	3.097828643	0.152565307
O	-0.279959758	4.209296949	-0.006152708
O	4.441830936	3.705341071	0.186834079
O	-1.035259955	-0.133948957	-0.396865333
C	1.951599109	1.735069670	6.239052745
C	-0.737096520	1.196295222	4.883139552
C	1.001586887	-1.179744385	5.845612949
H	0.510086837	-1.160629242	6.825535654
H	0.455801432	-1.889717952	5.214321749
H	2.014004238	-1.571560987	5.990853699
H	1.451191693	1.750932756	7.214552559
H	2.991462785	1.437467525	6.402840415
H	1.955160150	2.762330054	5.857576128
H	-1.153171747	1.382605466	5.880777142
H	-0.774490065	2.144396119	4.335558430
H	-1.401256927	0.486867807	4.381494024
C	3.486482530	0.428150768	3.551842322
C	4.221377933	1.622692470	3.689004056
H	3.693367537	2.572076656	3.690418051
C	5.605142769	1.599727002	3.810670586
H	6.177793330	2.517394470	3.905049011
C	6.293242671	0.376805412	3.811697564
C	7.766185760	0.345948843	3.947678922
C	5.572121793	-0.816472783	3.684978675
H	6.102722445	-1.766503167	3.685233326
C	4.184750338	-0.793341050	3.556892323
H	3.630612362	-1.721942608	3.455771144
H	8.211532251	-0.674366105	3.928862319
O	8.469185258	1.330851140	4.072493570
H	3.277718553	0.008530067	0.931584903
Si	1.823112048	-0.376889124	-1.992460000
C	1.085152411	0.920029503	-3.154387277
C	3.709709119	-0.418863511	-2.149147727
C	1.091338673	-2.077977233	-2.368594027
H	1.268019440	0.657579145	-4.202958609
H	0.002681306	0.986353015	-3.004525194
H	1.511577993	1.916977276	-2.988103901
H	1.276067133	-2.360889173	-3.411464830
H	1.528042312	-2.853867465	-1.730031891
H	0.010049485	-2.068580899	-2.202373835
H	4.003095447	-0.714636300	-3.163251336
H	4.161607442	0.558968320	-1.949321066
H	4.157007987	-1.141765897	-1.457200230

Table S3. Computed vibrational frequencies (cm $^{-1}$) of the optimized structures.

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THF

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16.44 277.75 642.94 651.95 803.84 871.29
906.44 936.34 948.05 969.31 1051.87 1116.46
1154.53 1221.95 1232.31 1266.10 1275.34
1317.03 1321.22 1367.84 1409.18 1500.74
1519.28 1522.03 1540.60 2971.39 2979.70
3070.22 3079.81 3103.56 3111.35 3115.70
3131.25

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CO

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2210.32

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(TMS)CC(H)

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126.96 127.15 147.84 164.28 164.89 201.85
202.07 225.35 358.28 358.40 548.30 653.76
685.73 686.17 697.11 697.34 700.52 787.21
787.59 881.38 881.54 900.15 1309.88 1310.03
1320.04 1466.62 1471.49 1471.62 1479.56
1479.59 1489.69 2152.51 3042.95 3043.14
3044.53 3118.84 3119.11 3121.41 3128.54
3129.56 3129.84 3477.34

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NMO

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179.90 244.48 263.52 312.45 338.32 382.23
446.18 465.69 507.69 523.01 622.96 703.13
792.03 880.55 914.77 938.49 988.39 992.76
1017.15 1064.18 1094.93 1132.71 1175.27
1190.11 1192.97 1261.12 1300.59 1318.92
1341.87 1357.08 1392.08 1395.47 1422.93
1441.14 1464.98 1484.09 1485.86 1488.72
1503.67 1514.70 3046.87 3051.10 3053.36
3054.11 3063.29 3118.52 3119.45 3142.62
3144.09 3157.49 3187.27

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CO2

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645.21 645.23 1367.99 2430.49

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N-methylmorpholine

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163.18 230.83 270.42 325.38 358.47 418.76
433.42 498.07 618.26 791.31 868.89 882.85
915.63 1022.52 1053.59 1079.49 1102.48 1115.35
1147.81 1175.72 1184.74 1230.80 1248.69
1319.76 1320.14 1341.75 1367.90 1403.90
1414.84 1433.12 1468.54 1492.75 1496.89
1496.92 1509.55 1518.20 1519.33 2925.60
2930.45 2944.57 2995.63 3001.75 3069.93
3070.48 3073.68 3108.11 3110.40 3116.45

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FeCO4

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55.00 72.47 77.50 80.34 87.69 306.11 308.58
310.72 352.96 408.98 425.85 429.04 485.08
496.07 496.66 523.74 528.00 2091.17 2096.49
2100.99 2170.00

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FeCO5

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50.43 53.43 97.92 98.41 107.00 107.25
109.47 368.54 368.72 370.24 410.57 435.46
445.40 450.35 463.39 488.43 490.34 570.94
571.30 616.40 665.41 666.10 2096.12 2096.92
2120.94 2121.72 2189.51

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10

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22.01 45.58 60.88 90.43 113.96 125.40
130.21 139.72 156.43 166.28 183.68 189.41
209.69 223.67 244.39 264.35 330.00 342.46
373.86 425.95 468.55 480.05 526.21 554.08
618.97 622.45 643.49 686.53 690.55 695.46
701.63 744.64 778.52 782.80 836.49 846.29
847.50 865.87 875.68 880.00 882.01 930.67
968.09 998.10 1010.30 1032.30 1033.85 1133.50
1167.41 1195.97 1245.06 1278.73 1311.55
1312.17 1321.94 1334.95 1353.62 1430.56
1455.86 1466.39 1468.91 1471.08 1471.46
1478.99 1480.43 1488.62 1544.95 1613.71
1658.46 1794.98 2014.37 2894.60 3043.12
3045.49 3047.59 3117.14 3119.09 3122.10
3126.69 3132.54 3134.47 3136.51 3176.00
3199.87 3209.93 3214.74 3216.94

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Fe2CO9

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28.10 52.76 56.74 61.69 65.43 82.85 84.24
89.84 94.46 95.58 96.13 107.93 126.06
129.77 151.12 158.23 232.47 251.62 329.02
338.39 383.86 386.52 392.51 413.99 428.75
432.39 440.99 442.73 456.29 457.72 461.71
474.20 475.61 488.56 505.72 549.79 554.99
556.64 596.28 612.30 628.59 639.23 642.15
652.12 701.44 1892.45 1905.52 1944.16 2120.69
2121.50 2125.04 2125.49 2140.57 2185.26

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33

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14.13 23.09 23.29 38.85 42.59 43.30 68.31
76.08 87.50 88.70 94.42 106.51 113.85
118.27 151.79 157.34 166.00 167.30 174.98
175.96 187.06 194.50 213.20 233.82 248.94
268.01 312.15 341.40 365.88 407.02 410.26
411.30 418.30 423.05 443.97 468.57 479.63
495.30 501.00 502.97 514.90 561.38 573.86
577.98 608.87 619.83 643.56 650.64 653.60
689.08 691.57 692.06 698.63 737.83 768.08
777.68 784.62 827.17 848.58 863.92 878.77
879.64 883.13 905.05 926.07 971.37 992.02
1018.38 1033.97 1035.05 1079.42 1133.18
1193.50 1238.62 1260.47 1308.10 1310.42
1320.25 1324.56 1343.43 1426.36 1451.89
1466.66 1469.60 1471.48 1478.33 1479.88
1480.30 1488.99 1542.99 1610.33 1656.32
1781.65 1797.58 2098.94 2106.63 2115.36
2162.64 2898.41 3037.96 3041.32 3043.10
3112.83 3114.20 3116.88 3119.59 3127.30

3127.59 3130.31 3172.43 3187.69 3202.36
3202.40 3211.56

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34

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24.76 30.12 33.64 44.80 60.59 67.61 82.83
91.92 94.59 108.05 110.51 114.32 117.32
118.09 131.02 138.65 147.22 164.00 167.54
183.06 191.12 204.30 209.82 236.45 246.80
260.90 283.22 339.93 376.90 384.22 398.35
407.91 417.69 423.61 425.25 454.74 459.29
478.64 488.71 504.76 517.49 549.11 570.75
588.00 606.48 615.95 642.14 648.88 650.83
659.01 685.17 689.53 701.12 704.70 742.01
780.24 782.58 838.12 848.86 870.10 875.74
880.67 882.95 889.80 916.98 974.49 996.99
1031.85 1039.10 1040.76 1091.21 1140.40
1193.87 1239.74 1241.31 1310.67 1313.80
1323.94 1327.98 1344.83 1430.46 1455.20
1466.67 1466.99 1468.61 1471.62 1480.60
1481.01 1489.45 1539.69 1609.01 1652.44
1791.54 1802.20 2089.20 2102.48 2116.91
2162.27 2873.87 3042.32 3043.84 3049.33
3113.95 3115.42 3120.06 3123.51 3130.38
3135.18 3156.93 3173.94 3199.94 3206.78
3213.95 3219.27

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35

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22.47 28.90 34.27 41.13 49.15 55.51 67.65
83.04 89.41 94.35 98.85 106.96 110.51
119.47 127.39 136.34 161.91 167.80 171.63
178.55 192.20 198.83 215.03 231.62 246.88
265.47 328.28 337.73 382.51 403.10 408.02
415.10 420.81 422.66 443.26 452.33 473.20
482.58 501.42 506.28 509.32 567.51 575.09
594.80 608.92 614.33 648.50 649.27 652.90
686.38 690.62 693.68 697.49 742.61 774.17
778.05 781.24 832.77 848.58 864.71 873.12
876.17 878.45 916.14 931.57 968.91 990.30
1017.04 1033.84 1034.93 1089.27 1132.46
1192.46 1233.14 1238.61 1307.88 1310.69
1321.99 1323.78 1343.61 1426.72 1452.25
1467.27 1468.20 1468.52 1477.81 1479.16
1481.19 1486.52 1540.05 1610.28 1653.96
1758.31 1797.37 2091.81 2114.67 2117.73
2165.89 2896.09 3042.82 3043.99 3046.29
3112.55 3113.15 3117.56 3128.39 3131.96
3135.82 3148.24 3171.85 3188.45 3192.86
3201.87 3211.32

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36

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23.84 25.15 48.85 52.41 63.51 72.35 88.93
94.82 104.87 107.11 119.27 143.18 163.07
176.67 194.60 225.03 256.39 263.58 324.23
340.04 387.66 407.54 410.12 416.05 423.91
440.95 442.04 472.83 480.27 499.00 504.21
508.16 536.68 575.59 578.73 607.56 639.08
649.45 653.12 661.81 735.94 745.41 771.74
849.80 852.28 864.83 917.61 946.97 974.29
991.51 1014.54 1032.15 1035.15 1058.09 1085.20
1132.68 1171.20 1194.32 1239.89 1296.21
1329.57 1348.46 1415.47 1427.09 1453.24
1485.59 1495.91 1500.56 1546.93 1613.03
1659.13 1797.49 1798.65 2101.35 2111.37
2119.52 2166.91 2897.42 3033.06 3086.46

3121.35 3138.78 3175.10 3192.89 3192.98 3211.99 3215.04

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37

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22.09 31.20 40.04 51.60 66.95 77.56 91.58 91.64 94.91 105.73 120.41 160.26 183.09 191.78 201.12 240.48 269.21 281.90 330.54 382.36 400.82 401.50 409.37 418.29 423.31 439.47 465.37 469.91 474.38 481.34 498.91 507.91 574.62 581.73 589.65 604.01 607.40 649.95 650.41 655.01 723.51 740.24 779.21 847.27 853.79 862.21 921.27 933.34 968.88 993.02 1015.08 1030.01 1034.47 1069.87 1089.11 1141.05 1194.09 1202.65 1250.91 1282.56 1335.52 1354.04 1417.85 1432.25 1458.06 1482.01 1501.94 1508.55 1547.75 1610.71 1658.15 1779.21 1794.98 2096.38 2118.00 2119.31 2168.12 2895.24 3030.60 3080.34 3117.09 3169.39 3174.89 3188.50 3205.49 3225.69 3228.43

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38

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11.51 17.83 32.25 37.58 45.70 60.07 82.73 83.83 86.70 89.48 95.10 103.72 114.17 132.65 145.54 153.88 166.94 169.14 178.44 183.91 194.39 203.01 217.03 239.23 249.92 254.27 289.92 330.57 355.43 367.47 375.41 400.43 414.79 421.80 449.55 467.48 479.44 494.12 524.45 527.47 554.69 557.56 583.06 585.34 599.52 616.01 640.11 652.71 687.03 688.75 691.89 697.35 743.83 778.60 781.01 826.72 841.35 847.61 864.95 876.82 878.42 879.20 897.37 943.64 970.79 993.15 1032.96 1035.87 1060.96 1110.27 1129.58 1190.63 1208.63 1235.29 1249.20 1309.24 1311.39 1320.20 1321.87 1339.75 1412.32 1425.80 1451.00 1467.55 1469.08 1471.18 1479.82 1481.68 1488.85 1538.59 1607.58 1653.63 1659.04 1799.03 1829.68 2097.89 2112.52 2158.64 2893.30 3009.90 3040.09 3040.94 3043.54 3065.13 3112.02 3114.40 3118.19 3122.69 3128.91 3129.43 3171.97 3184.91 3196.61 3209.93

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39

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18.13 21.37 23.73 28.51 35.00 44.21 45.20 54.61 73.46 77.28 84.10 88.87 91.56 93.31 97.72 102.85 110.54 137.71 138.53 152.74 154.68 161.86 170.90 174.96 179.23 184.25 196.88 203.36 216.05 224.01 239.67 253.75 281.60 300.33 324.93 346.65 369.73 381.85 394.33 415.76 422.76 449.44 455.72 473.23 484.68 504.36 524.68 539.45 563.04 568.83 583.97 600.14 618.89 621.42 643.62 644.12 653.76 681.79 684.87 687.48 695.36 697.55 746.05 779.35 781.04 815.15 829.80 845.57 850.43 865.16 867.96 876.44 877.96 881.03 901.15 909.75 920.14 959.84 966.67 975.38 978.37 993.15 1033.43 1035.73 1065.48 1066.69 1069.69 1107.70 1129.87 1152.85 1190.98 1215.99 1228.27 1237.19 1237.64 1257.87 1265.24 1278.82 1306.91 1309.65 1320.12 1320.78 1324.48 1334.07 1340.97 1378.90 1408.92 1411.92 1426.36 1451.00 1468.17

1470.24 1472.90 1480.12 1482.25 1489.68
1501.69 1518.89 1521.15 1539.18 1539.31
1606.21 1652.86 1654.56 1796.19 1813.09
2077.32 2105.56 2143.30 2890.37 3001.75
3036.01 3039.63 3041.65 3055.10 3061.25
3071.07 3080.03 3089.18 3110.11 3111.01
3115.13 3116.63 3119.51 3126.85 3129.95
3134.71 3145.42 3150.87 3169.08 3183.78
3194.15 3208.87

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6.15 25.55 31.93 37.39 39.48 61.64 79.48
82.99 90.46 95.33 111.34 118.86 138.14
153.46 163.30 167.70 173.91 180.34 186.21
200.53 211.25 237.41 241.86 277.72 313.80
323.22 361.75 404.01 414.40 423.35 435.31
446.50 451.57 462.31 489.90 503.91 530.43
550.89 569.60 587.54 595.41 613.15 631.41
652.63 680.21 686.36 692.88 699.00 710.07
738.65 778.29 780.90 831.72 846.74 865.11
875.57 877.83 881.55 900.56 925.01 970.47
992.50 999.75 1033.65 1035.17 1070.06 1134.37
1193.75 1238.12 1251.35 1306.96 1309.11
1318.60 1324.75 1343.07 1426.69 1451.66
1455.90 1467.13 1469.66 1471.20 1479.13
1481.56 1488.72 1540.16 1608.07 1654.09
1722.99 1797.30 2085.62 2094.49 2139.22
2893.76 3037.74 3041.13 3044.02 3090.10
3110.02 3114.69 3118.06 3124.57 3127.96
3131.33 3169.46 3172.70 3199.74 3207.49
3214.10

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41

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22.77 23.80 27.86 30.90 41.55 51.20 55.30
58.29 68.41 73.27 82.74 88.86 96.27 99.43
102.85 116.33 135.50 152.95 155.29 163.02
166.54 169.20 173.65 179.70 192.33 194.84
213.57 231.91 239.40 251.95 271.76 276.69
313.45 362.90 375.22 418.14 427.01 438.37
446.95 468.72 479.17 481.11 498.47 512.91
523.58 558.39 582.36 587.76 588.78 622.27
626.59 631.75 647.42 686.67 687.81 691.72
696.89 702.07 740.39 744.62 775.68 782.84
831.86 841.16 850.19 864.97 874.98 876.46
881.49 882.93 894.43 900.70 924.32 931.78
933.80 975.71 980.28 991.24 1004.36 1033.29
1035.55 1052.40 1073.28 1076.29 1133.18
1166.90 1192.80 1196.25 1216.85 1240.16
1253.91 1258.53 1276.07 1303.67 1308.27
1319.01 1324.45 1330.92 1343.96 1353.12
1382.10 1409.04 1427.45 1450.26 1453.62
1468.10 1470.43 1472.26 1480.00 1482.11
1489.73 1500.84 1512.41 1528.60 1542.05
1543.95 1607.43 1654.23 1737.17 1794.33
2070.57 2075.67 2123.79 2893.65 3035.10
3037.73 3038.58 3042.32 3063.69 3069.95
3072.23 3107.22 3109.84 3111.77 3115.70
3116.49 3122.77 3124.58 3125.39 3126.29
3133.66 3169.68 3171.85 3180.82 3190.42
3207.77 3215.11

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42

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16.68 20.58 24.25 25.31 38.54 41.08 44.31
49.50 69.60 76.60 82.36 87.12 94.60 98.28

109.27 117.04 119.84 148.15 152.54 154.86
156.66 162.39 168.24 171.86 172.31 175.67
179.53 185.50 194.49 201.82 208.62 211.06
217.45 236.00 245.23 249.02 270.68 301.58
318.98 351.15 364.36 374.67 377.63 403.66
423.38 426.79 431.81 474.57 489.80 490.95
502.55 508.04 522.41 563.79 566.96 575.77
592.09 609.19 621.42 637.77 649.82 657.59
685.83 688.18 691.76 695.92 699.05 699.98
707.33 720.42 737.98 748.08 772.87 776.59
782.37 785.34 789.10 825.44 849.70 868.16
878.10 879.63 882.15 883.28 883.95 893.07
910.43 935.42 974.65 995.78 1017.23 1034.54
1035.36 1083.81 1130.74 1193.05 1236.73
1255.36 1306.79 1309.04 1310.11 1311.72
1318.68 1320.94 1321.40 1340.00 1425.47
1450.76 1466.53 1467.10 1469.97 1470.84
1471.26 1471.28 1475.67 1479.28 1479.80
1480.07 1480.42 1489.22 1489.23 1540.74
1607.13 1652.40 1776.63 1797.84 1940.15
2078.36 2093.78 2135.50 2894.96 3037.81
3039.63 3039.84 3042.91 3043.05 3043.97
3111.97 3112.77 3115.26 3116.16 3116.80
3118.50 3121.15 3121.90 3124.18 3125.77
3130.52 3130.97 3133.19 3172.39 3191.66
3195.45 3202.57 3210.58 3391.66

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47-TS1 (48)

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-287.19 21.93 22.49 29.18 33.35 38.93 43.19
45.45 57.80 69.54 84.26 88.14 94.97 104.34
107.19 109.99 130.85 139.82 153.24 155.38
159.82 163.98 165.05 169.89 172.02 173.64
177.21 185.44 190.43 204.61 210.48 216.58
224.08 238.49 252.76 256.68 288.74 314.17
336.74 362.22 375.45 394.52 416.29 422.87
425.60 436.13 467.93 470.49 484.58 489.13
516.41 529.24 538.56 576.37 581.46 593.01
598.50 623.15 625.46 634.11 653.38 681.55
688.33 689.29 690.44 696.53 699.24 701.86
705.09 739.89 767.13 777.23 780.51 781.72
786.52 797.08 834.22 847.46 864.45 875.71
879.03 880.90 881.44 882.25 891.40 913.94
938.67 970.39 985.41 995.00 1028.34 1033.92
1035.42 1093.87 1135.70 1194.31 1238.04
1254.15 1307.31 1308.79 1310.09 1310.25
1319.52 1320.35 1324.50 1343.68 1426.27
1451.34 1460.95 1467.32 1468.24 1470.33
1471.38 1472.14 1473.15 1479.78 1479.90
1480.52 1481.25 1489.80 1490.20 1540.42
1605.62 1651.45 1682.53 1798.25 1813.78
2082.96 2092.35 2131.42 2892.51 3036.87
3038.61 3041.57 3041.61 3042.77 3043.44
3110.93 3112.39 3114.26 3115.55 3116.30
3118.22 3119.32 3122.36 3127.33 3129.01
3131.12 3133.55 3144.92 3171.58 3195.13
3204.66 3225.76 3227.29 3281.45

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47-TS2 (49)

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-174.53 19.23 21.10 24.97 27.89 30.37
35.48 40.22 50.20 51.87 74.32 87.39 90.76
99.48 101.50 113.36 123.88 149.14 151.17
153.16 161.09 163.58 166.79 170.61 174.60
181.27 193.56 194.65 196.66 201.27 206.44
212.61 227.58 234.70 245.25 252.48 281.96
313.60 351.27 367.66 390.44 401.93 403.06
411.40 423.28 429.29 431.36 452.57 465.51

491.85 511.51 520.37 530.88 581.37 597.87
607.14 631.75 640.15 643.75 645.29 666.71
670.56 680.57 684.15 687.63 690.55 696.36
697.87 699.80 731.11 755.12 775.55 781.63
783.71 784.44 829.54 846.82 860.19 864.45
875.74 876.56 877.70 878.46 881.95 891.48
913.15 959.39 974.97 993.66 1034.27 1035.55
1088.76 1116.14 1131.86 1162.94 1191.99
1237.25 1240.25 1306.55 1306.82 1307.37
1308.37 1317.14 1318.41 1323.35 1343.56
1426.27 1451.42 1453.66 1467.30 1468.44
1470.60 1471.45 1472.26 1473.19 1479.42
1480.35 1480.59 1483.53 1488.84 1490.75
1541.08 1609.14 1654.47 1692.61 1751.69
1796.29 2078.60 2106.02 2149.77 2891.62
3037.00 3037.14 3038.76 3039.79 3040.42
3041.06 3101.58 3109.41 3110.92 3112.71
3114.02 3115.53 3117.41 3118.00 3121.55
3122.50 3123.26 3124.02 3124.52 3170.65
3179.55 3190.69 3199.00 3210.54 3259.16

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47-TS3

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-295.65 28.42 30.82 37.29 41.42 45.15
55.24 64.36 70.09 77.92 82.95 91.26 96.11
105.00 108.81 114.97 120.06 131.24 133.40
143.48 151.98 154.78 160.84 165.13 171.20
176.14 181.00 192.16 209.65 217.71 224.90
229.05 234.30 245.39 254.53 261.88 279.52
303.47 323.95 347.69 366.84 400.44 420.99
429.23 436.60 454.58 465.57 474.81 490.43
503.44 508.16 535.32 540.80 563.83 583.34
590.26 597.18 620.36 623.91 633.15 649.00
678.06 679.59 685.54 690.35 701.05 701.29
703.48 707.36 738.98 745.66 775.47 779.38
781.89 786.61 806.37 834.15 849.72 854.93
857.25 874.75 877.40 878.32 881.04 882.60
888.68 912.45 941.15 979.55 989.77 1025.59
1032.87 1034.84 1082.57 1138.90 1194.96
1241.27 1248.84 1304.83 1308.18 1308.66
1309.65 1317.39 1320.13 1325.96 1344.92
1427.26 1451.43 1462.08 1464.27 1467.48
1469.47 1469.85 1471.16 1472.81 1475.85
1478.51 1480.03 1484.81 1488.15 1490.51
1540.76 1603.60 1639.83 1660.06 1772.80
1796.82 2091.38 2095.49 2135.35 2891.64
3038.38 3039.86 3040.37 3043.49 3046.86
3048.59 3108.56 3111.17 3113.39 3114.51
3115.39 3117.63 3123.26 3126.52 3132.29
3136.19 3140.89 3161.99 3163.82 3172.62
3205.51 3221.44 3226.15 3255.84 3307.33

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47-TS4

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-226.69 15.13 19.88 24.02 28.01 30.85
38.87 45.57 47.14 57.43 80.64 86.64 90.74
101.65 108.13 114.49 127.09 150.50 153.43
157.02 157.62 167.47 168.60 171.71 172.10
180.69 182.45 192.02 195.66 197.36 205.47
216.60 226.61 239.52 246.07 257.27 278.44
294.16 323.64 364.42 391.45 397.70 404.11
417.72 424.69 433.89 437.43 454.78 495.56
504.33 510.25 529.16 549.04 581.07 596.40
604.84 631.25 641.22 644.69 661.75 666.04
683.01 688.44 690.53 691.41 697.46 700.01
702.30 737.52 743.80 769.94 774.99 781.33
782.88 793.06 830.00 846.54 856.43 862.77
875.64 875.75 878.33 879.99 880.30 890.30

897.17 919.74 969.22 990.51 1010.56 1033.85
1035.54 1084.10 1117.96 1132.82 1191.92
1238.05 1240.69 1305.65 1308.33 1309.76
1311.89 1318.26 1321.20 1323.82 1343.85
1426.57 1451.59 1454.77 1467.41 1468.18
1470.04 1471.80 1472.05 1472.65 1480.13
1480.23 1481.74 1484.15 1489.47 1490.43
1541.33 1608.53 1653.97 1681.58 1718.91
1794.52 2081.85 2104.28 2149.77 2890.30
3036.45 3038.32 3040.28 3040.78 3041.08
3043.00 3108.84 3110.43 3113.38 3114.37
3114.75 3118.47 3119.87 3120.60 3123.59
3123.66 3125.73 3126.36 3127.68 3170.65
3189.68 3204.32 3205.34 3209.68 3253.49

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43

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18.80 26.31 32.93 51.12 58.87 67.50 71.47
80.90 93.24 97.18 107.35 109.90 116.33
118.38 125.05 133.07 140.55 153.53 156.23
161.05 171.97 176.70 180.87 188.87 190.47
196.11 199.44 210.49 215.19 220.76 238.36
241.57 249.34 259.78 262.62 304.58 326.51
350.90 368.91 375.37 391.10 428.24 439.08
457.95 459.56 464.02 476.13 487.89 511.96
515.28 534.77 546.23 576.58 590.68 602.15
616.08 623.33 638.10 645.43 679.90 686.14
688.35 688.70 690.06 699.62 706.86 709.77
739.30 773.59 779.45 781.70 785.67 823.82
824.97 829.05 839.53 844.14 866.57 875.46
877.58 877.76 881.03 883.98 899.61 911.89
943.00 962.18 973.31 999.18 1032.22 1035.78
1055.22 1136.52 1195.88 1223.72 1240.45
1241.17 1305.42 1309.48 1309.61 1310.02
1312.10 1319.20 1322.12 1333.91 1345.98
1417.39 1429.16 1453.81 1468.80 1469.25
1469.69 1472.44 1473.09 1475.38 1481.04
1481.51 1482.53 1487.13 1489.87 1493.09
1519.94 1540.11 1608.58 1639.57 1654.78
1797.74 2086.32 2093.48 2131.21 2893.04
3037.66 3040.18 3040.38 3041.88 3043.03
3047.25 3109.73 3110.93 3112.61 3112.96
3115.30 3119.29 3119.43 3125.19 3130.72
3133.86 3142.09 3143.71 3144.06 3171.82
3181.95 3201.84 3206.10 3224.11 3274.65

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29.38 32.46 38.55 43.13 52.03 55.86 70.24
77.22 83.97 93.93 98.39 102.94 108.70
112.49 124.31 129.82 136.45 138.49 150.57
151.67 154.41 162.56 170.86 172.76 175.56
178.47 188.81 200.01 202.17 208.02 228.62
235.37 243.82 263.09 271.93 274.10 292.30
333.79 366.26 381.75 392.29 414.42 422.65
432.94 436.64 460.88 466.76 484.44 501.66
513.75 522.20 530.93 578.95 598.71 604.55
612.52 616.15 622.43 642.51 667.11 682.20
682.74 687.21 688.06 698.46 700.23 707.02
752.62 768.82 771.34 780.49 783.45 809.33
830.71 850.86 858.02 870.17 874.60 875.21
876.36 878.77 887.63 902.70 923.67 949.98
977.25 991.23 1000.53 1024.36 1034.95 1075.85
1133.11 1179.25 1190.31 1236.23 1249.39
1278.93 1305.69 1308.40 1308.86 1310.15
1311.97 1317.47 1322.34 1326.92 1344.42
1424.46 1447.27 1448.43 1469.44 1469.98
1471.07 1472.06 1473.82 1474.01 1480.10

1482.52 1482.90 1484.98 1490.97 1491.23
1527.69 1568.58 1597.79 1641.92 1646.81
1795.47 2095.83 2102.21 2148.26 2899.31
2983.80 3019.68 3021.49 3036.85 3038.83
3040.71 3041.98 3042.56 3043.82 3110.34
3111.30 3111.42 3112.51 3113.80 3114.05
3115.92 3116.39 3119.01 3126.36 3127.55
3135.04 3137.54 3173.25 3210.03 3211.99

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25.74 32.61 37.29 38.83 60.95 64.76 74.52
78.78 83.80 91.54 102.36 109.99 116.80
120.68 121.53 129.97 140.88 144.26 155.58
159.15 164.76 170.28 176.08 176.68 192.34
199.21 204.83 211.88 217.05 226.66 239.50
240.85 252.49 255.77 273.60 298.08 299.29
328.95 350.12 378.35 398.70 431.36 452.95
457.59 464.66 473.66 487.82 515.60 520.61
534.83 544.24 549.69 582.52 592.73 602.94
619.01 631.71 633.48 647.87 668.69 679.02
685.49 688.05 690.45 696.56 698.77 710.85
739.44 750.65 779.06 781.25 785.34 790.00
820.83 831.47 844.36 848.68 867.37 876.06
878.01 878.93 881.57 882.90 886.90 915.31
953.49 971.99 986.28 1001.06 1033.86 1034.94
1054.34 1134.31 1144.44 1195.74 1229.19
1241.89 1297.74 1308.00 1309.68 1310.16
1312.76 1319.63 1322.92 1330.09 1344.33
1405.35 1427.70 1452.96 1468.29 1469.47
1470.14 1471.89 1473.36 1476.05 1479.81
1481.79 1482.72 1487.83 1488.70 1493.82
1519.78 1541.00 1597.52 1608.71 1653.97
1798.08 2090.24 2098.09 2136.13 2892.90
3036.89 3040.11 3041.01 3042.25 3043.33
3047.35 3109.10 3111.82 3112.09 3113.08
3115.28 3117.06 3119.40 3121.06 3132.15
3136.32 3140.92 3145.90 3162.90 3171.71
3185.06 3205.92 3221.31 3223.24 3280.52

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28.11 29.37 32.80 39.14 46.15 52.63 58.61
67.68 78.42 87.54 96.18 99.66 107.24
113.46 117.63 129.45 142.78 146.44 156.44
157.55 166.29 168.70 171.23 174.89 176.26
178.36 189.31 195.07 199.89 203.60 225.79
229.78 244.97 263.90 267.53 286.59 308.42
321.99 342.57 379.20 411.83 419.57 429.23
433.33 446.27 458.99 464.29 478.40 494.41
519.17 528.06 570.70 579.28 598.45 606.89
611.20 613.71 633.05 636.24 657.89 679.66
683.59 686.40 688.52 691.00 697.82 699.53
751.53 768.70 777.54 780.49 782.26 820.34
835.65 847.48 857.16 871.03 875.33 876.52
877.32 879.22 887.85 899.33 911.67 942.41
978.73 993.01 1020.14 1022.73 1035.27 1074.45
1134.27 1186.52 1192.76 1202.97 1237.14
1254.46 1307.67 1308.87 1309.22 1310.21
1312.16 1318.03 1321.93 1325.21 1344.14
1424.62 1448.42 1451.01 1469.57 1469.92
1471.16 1472.29 1473.26 1474.15 1480.21
1482.15 1482.18 1485.01 1490.92 1491.21
1527.70 1565.91 1597.18 1602.39 1645.60
1795.29 2101.20 2111.08 2153.33 2897.57
2987.19 3015.65 3023.12 3034.29 3035.23
3035.94 3038.95 3041.11 3043.03 3108.13
3109.73 3110.06 3110.39 3112.92 3113.34

3114.24 3115.28 3115.69 3118.81 3133.47
3135.11 3149.18 3172.49 3207.90 3212.28

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43-TS

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-281.31 26.53 29.08 33.90 42.37 57.03
58.74 62.55 76.13 85.35 95.49 101.60
113.87 115.40 125.12 132.35 136.39 153.91
160.47 162.12 171.61 173.35 175.03 180.74
185.35 186.03 195.05 197.25 210.39 217.59
232.92 238.56 243.17 248.35 260.21 263.64
319.46 330.42 355.45 376.42 386.77 418.26
428.66 436.54 467.28 475.39 483.86 499.60
516.70 529.75 547.82 569.09 589.25 608.04
619.65 626.93 633.13 649.68 665.75 681.16
688.84 689.62 692.18 697.60 704.90 705.72
707.74 740.84 777.07 779.64 783.42 786.05
827.66 834.41 846.49 850.28 867.09 872.30
879.44 879.95 882.82 883.78 886.18 898.40
928.53 943.28 966.69 975.02 1000.65 1033.24
1035.62 1056.95 1135.01 1195.68 1226.69
1241.01 1273.79 1304.10 1308.30 1308.94
1310.13 1311.24 1319.83 1320.74 1329.69
1341.97 1425.73 1438.29 1454.09 1466.20
1468.59 1472.42 1472.90 1472.96 1475.02
1478.42 1480.34 1482.48 1487.29 1491.27
1493.02 1518.86 1539.51 1594.98 1606.49
1652.85 1798.66 1964.70 2076.97 2110.82
2893.96 3038.82 3039.56 3041.87 3042.12
3043.85 3044.06 3108.71 3110.62 3111.53
3114.47 3116.47 3118.26 3123.02 3128.40
3131.35 3132.96 3139.66 3141.50 3150.27
3170.04 3181.25 3190.63 3205.57 3223.98
3279.94

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52

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25.69 26.77 29.27 34.74 42.52 58.86 59.36
61.47 68.08 92.40 94.83 114.00 114.73
123.30 128.62 139.02 153.00 160.65 162.83
166.92 174.22 174.74 180.05 183.16 190.81
198.15 201.69 211.79 215.53 229.47 241.86
250.25 258.61 259.96 268.30 314.60 320.82
340.48 358.29 376.87 402.24 416.85 427.18
464.67 469.55 479.41 492.02 516.48 528.80
545.23 564.57 582.57 596.94 613.04 623.22
636.38 648.64 671.19 680.47 683.98 688.69
698.11 701.15 705.23 707.52 711.73 741.12
764.19 779.51 780.80 785.15 791.99 829.28
839.47 848.81 868.17 878.28 879.22 881.77
883.06 886.70 888.22 912.71 927.74 960.30
968.68 972.53 999.38 1005.80 1033.25 1035.42
1054.01 1133.17 1194.39 1227.79 1239.73
1297.72 1307.84 1308.90 1309.36 1311.33
1319.29 1320.72 1325.82 1328.07 1340.47
1426.11 1438.76 1452.96 1465.44 1468.21
1471.46 1473.03 1473.17 1475.37 1477.63
1479.65 1481.12 1486.16 1489.10 1490.94
1495.08 1534.57 1537.48 1604.54 1651.96
1797.98 1841.37 2074.49 2104.30 2894.52
3039.39 3039.83 3040.53 3041.79 3042.70
3045.45 3108.81 3111.76 3114.38 3114.89
3118.28 3119.75 3121.52 3128.67 3129.98
3131.95 3132.92 3133.68 3171.28 3179.93
3194.30 3203.84 3209.98 3218.28 3295.82

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52-TS

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-229.41 23.21 25.72 30.99 31.48 43.72
49.08 53.69 65.89 76.51 95.77 99.11 115.83
118.28 120.63 134.95 156.52 158.95 161.50
163.46 172.37 175.62 176.52 181.76 189.14
197.58 203.01 209.44 214.37 224.76 233.75
238.71 245.68 260.71 262.98 283.26 310.08
337.10 347.93 374.89 421.64 428.06 430.91
437.43 466.38 478.58 484.81 509.07 520.52
536.25 555.75 585.29 594.51 614.77 623.99
630.65 650.00 650.40 682.30 688.65 689.68
695.35 701.33 704.71 705.76 729.78 740.36
773.21 778.27 782.82 785.25 806.70 823.36
832.14 853.06 869.76 879.57 880.38 880.72
882.67 886.36 892.30 913.19 929.84 969.39
979.36 1001.99 1033.53 1035.11 1054.08 1074.19
1116.71 1134.50 1194.86 1226.19 1239.49
1245.70 1276.33 1308.61 1308.92 1308.94
1311.96 1319.58 1320.55 1325.42 1340.56
1408.66 1427.27 1441.26 1453.70 1465.93
1468.80 1472.65 1473.57 1473.78 1475.71
1477.63 1479.91 1482.39 1485.83 1490.75
1493.47 1495.77 1538.73 1605.85 1653.37
1797.92 1814.92 2067.42 2096.71 2895.31
3038.13 3038.84 3039.50 3040.23 3042.45
3043.40 3107.39 3111.91 3112.68 3114.41
3115.27 3116.16 3117.92 3120.22 3124.08
3126.45 3128.86 3133.86 3134.30 3171.75
3196.60 3203.41 3217.37 3244.41 3263.16

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Fe(CO)2-product adduct

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21.73 26.28 32.34 43.38 52.10 58.46 61.34
66.21 73.63 81.30 95.48 102.98 107.28
111.27 123.84 133.63 153.96 156.32 158.60
161.43 169.29 171.34 173.73 178.14 182.46
190.14 194.63 205.51 212.61 220.18 233.46
241.59 244.79 254.43 261.96 286.78 310.94
350.31 354.16 420.69 424.67 426.30 439.01
463.01 471.31 491.20 502.09 517.14 522.61
546.78 564.94 583.22 615.13 618.34 637.85
651.55 658.35 666.05 689.76 690.99 692.66
697.22 700.69 707.26 707.87 737.34 767.09
774.16 781.73 786.07 790.66 804.53 831.80
846.74 865.70 874.23 879.24 880.97 882.03
885.64 887.91 898.56 929.49 953.34 972.22
980.18 996.52 1032.43 1035.56 1130.85 1141.62
1165.91 1192.36 1207.43 1232.78 1238.76
1242.67 1274.26 1304.87 1308.66 1309.21
1312.44 1318.07 1322.14 1324.32 1341.88
1422.45 1427.70 1449.79 1456.84 1467.42
1469.98 1473.10 1474.05 1474.71 1476.44
1478.77 1481.01 1484.70 1486.27 1492.64
1493.43 1510.60 1535.37 1605.18 1650.58
1776.53 1802.54 2034.99 2074.45 2902.82
3029.61 3039.22 3040.43 3040.80 3042.61
3044.79 3047.10 3108.84 3113.07 3113.37
3115.53 3117.70 3123.23 3124.59 3126.74
3130.00 3132.96 3136.90 3141.38 3174.20
3177.25 3195.39 3199.07 3213.82 3244.50

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Fe(CO)2-product adduct (Triplet)

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15.19 18.68 24.95 26.28 28.32 31.05 32.32
36.24 46.62 65.29 74.96 82.34 95.60 103.08
111.84 119.22 144.18 155.26 158.08 162.10
166.86 170.12 175.68 179.14 180.46 181.78
190.25 197.79 207.63 214.59 220.71 228.36
239.61 242.70 253.82 270.14 299.13 313.33

316.87 334.93 347.95 382.37 393.99 395.49

421.72 439.04 446.17 463.80 476.26 498.71

527.03 557.29 587.11 613.18 615.30 642.97

647.56 669.16 687.94 690.27 694.17 695.83

696.19 701.90 702.10 740.36 763.95 779.08

783.17 784.37 788.72 828.61 845.79 865.09

869.45 877.07 878.53 879.05 881.92 884.10

884.98 902.40 931.16 948.27 951.24 972.58

995.00 1033.95 1035.43 1130.80 1155.83 1165.73

1192.87 1209.49 1236.02 1238.19 1246.38

1276.75 1304.23 1308.00 1308.40 1312.29

1317.61 1320.58 1322.30 1339.21 1424.73

1442.70 1446.05 1450.47 1464.87 1468.88

1471.60 1471.68 1473.22 1473.88 1476.94

1480.31 1481.56 1484.56 1490.66 1491.33

1538.20 1606.39 1617.56 1653.28 1774.74

1799.48 2046.73 2097.59 2896.82 3032.97

3036.91 3037.71 3040.64 3040.89 3042.36

3062.68 3102.80 3109.75 3110.79 3112.03

3113.83 3114.26 3115.78 3120.70 3123.83

3127.43 3132.45 3134.17 3136.27 3172.62

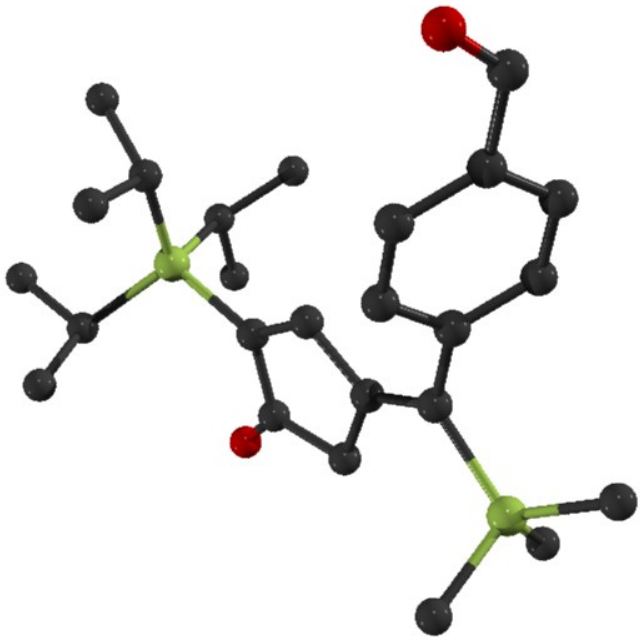
3190.50 3198.57 3212.99 3222.59

INDIANA UNIVERSITY DEPARTMENT OF CHEMISTRY

Molecular Structure Center

X-Ray Crystal Structure Data for PKR Product (18)

Report No. 10101



$C_{25}H_{38}O_2Si_2$

David R. Williams* and Akshay A. Shah

Department of Chemistry, Indiana University,

800 E. Kirkwood ave., Bloomington, IN 47405-7102

IUMSC
Indiana University Molecular Structure Center

The sample was submitted by Akshay Shah (research group of Williams, Department of Chemistry, Indiana University). A yellow crystal (approximate dimensions 0.259 x 0.193 x 0.076 mm^3) was placed onto the tip of a glass capillary and mounted on an Apex Kappa Duo diffractometer and measured at 150 K.

Data collection

The X-ray crystal structure and data collection was performed by **C. Chen**. A preliminary set of cell constants was calculated from reflections harvested from three sets of 12 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 295 reflections. The data collection was carried out using Mo Kα radiation (graphite monochromator) with a frame time of 30 seconds and a detector distance of 5.0 cm. A randomly oriented region of reciprocal space was surveyed to achieve complete data with a redundancy of 4. Sections of frames were collected with 0.50º steps in ω and ϕ scans. Data to a resolution of 0.84 Å were considered in the reduction. Final cell constants were calculated from the xyz centroids of 1810 strong reflections from the actual data collection after integration (SAINT).[1] The intensity data were corrected for absorption (SADABS).[2] Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The space group $P2_1/n$ was determined based on intensity statistics and systematic absences. The structure was solved using SIR-92[3] and refined (full-matrix-least squares) using the Oxford University *Crystals for Windows* system.[4] A direct-methods solution was calculated, which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed, which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were placed in ideal positions and refined with individual relative isotropic displacement parameters. The final full matrix least squares refinement converged to R1 =

0.0491 ($I > 2\sigma(I)$, 2830 data) and wR2 = 0.1221 (F^2, 4475 data, 376 parameters).

Structure description

The structure was found as proposed.

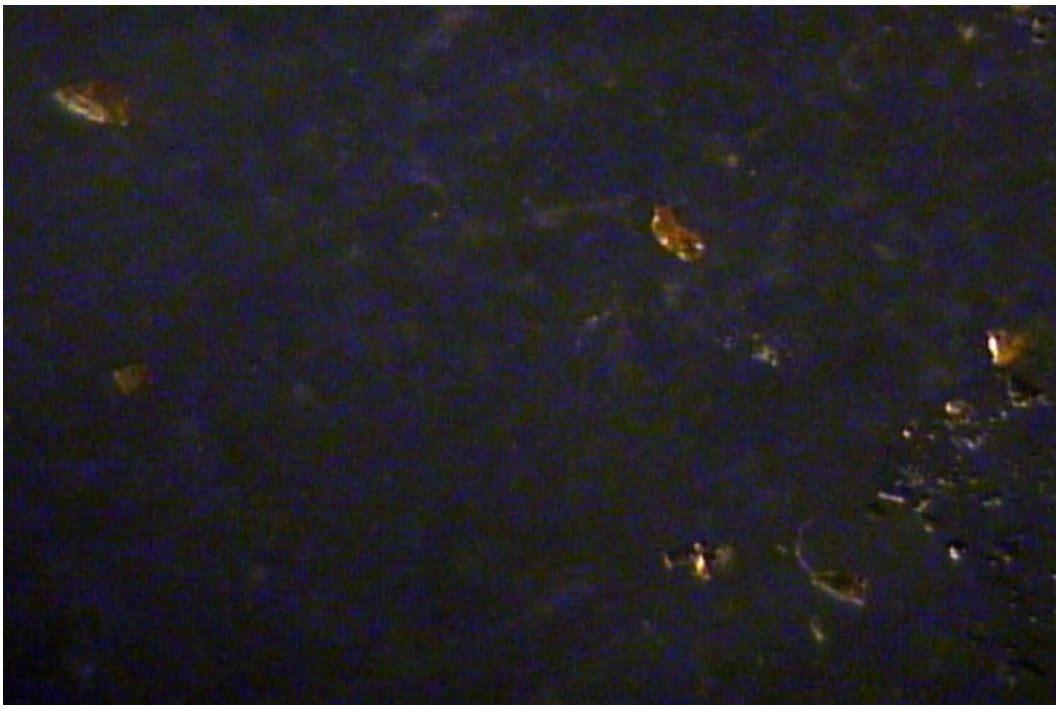
1 SAINT, Bruker Analytical X-Ray Systems,Madison, WI, current version.

2 An empirical correction for absorption anisotropy,R. Blessing, Acta Cryst. A51, 33 - 38 (1995).

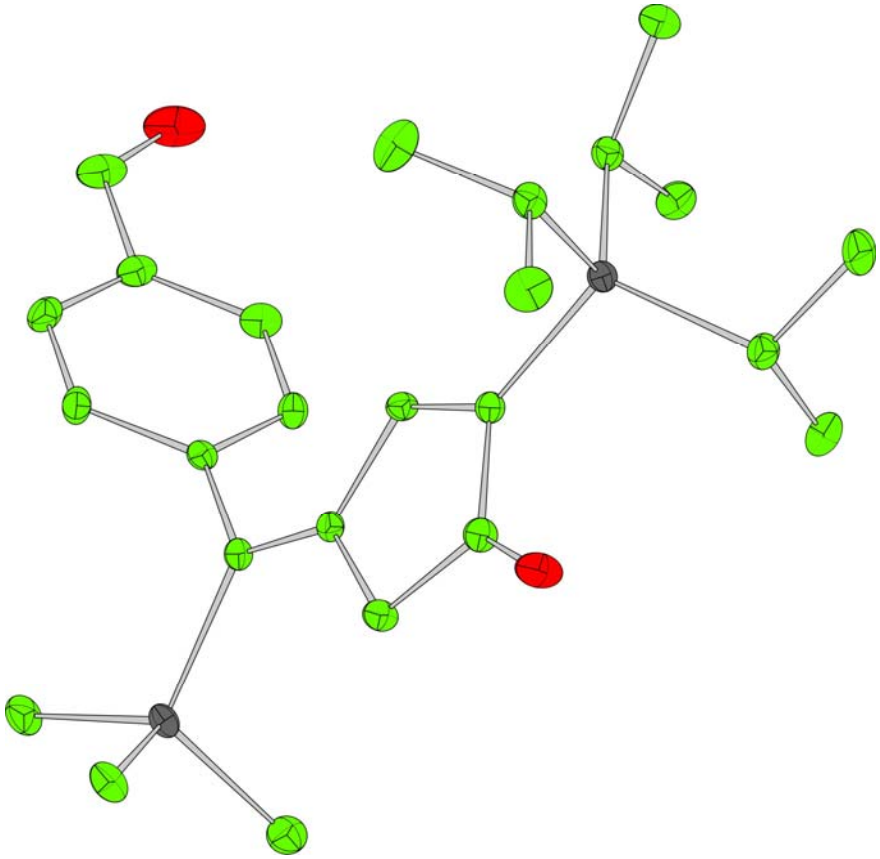
3 Altomare, A; Cascarano, G; Giacovazzo, G.; Guagliardi, A.; Burla, M. C.; Polidori, G.; Camalli, M. *J. Appl. Cryst*. **1994**, *27*, 435.

4 Betteridge, P. W.; Carruthers, J. R.; Cooper, R. I.; Prout, K.; Watkin, D. J. *J. Appl. Cryst.* **2003**, *36*, 1487.

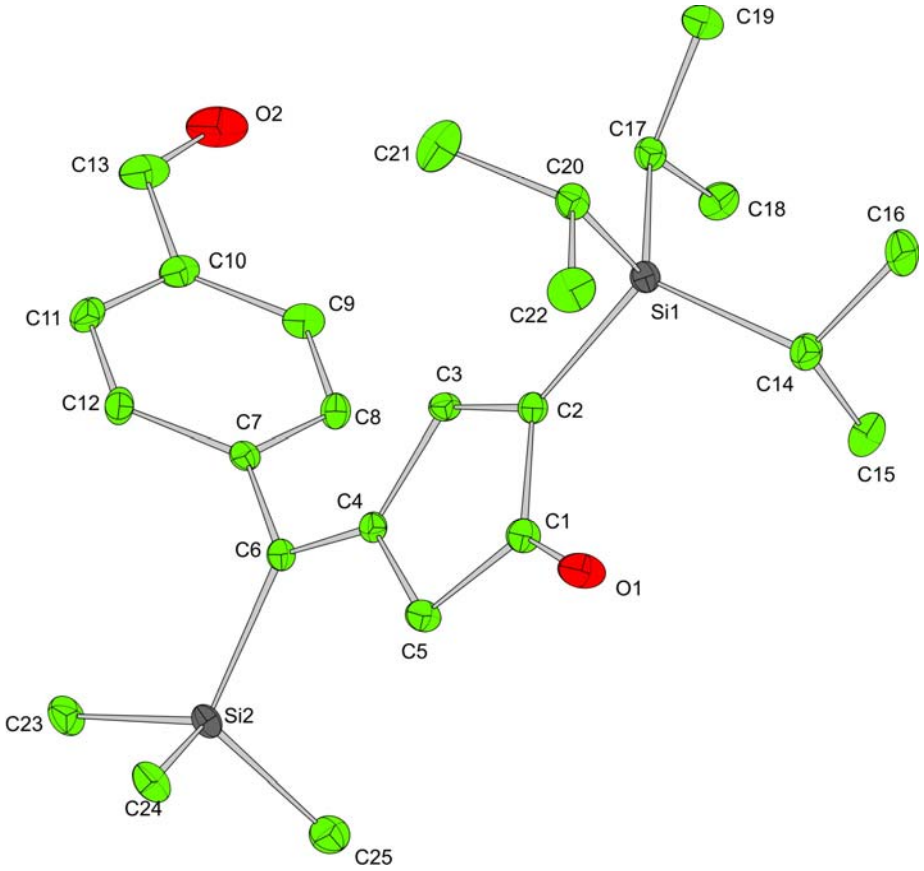
5 PLATON, A. L. Spek, Acta Cryst. A46, C34 (1990).



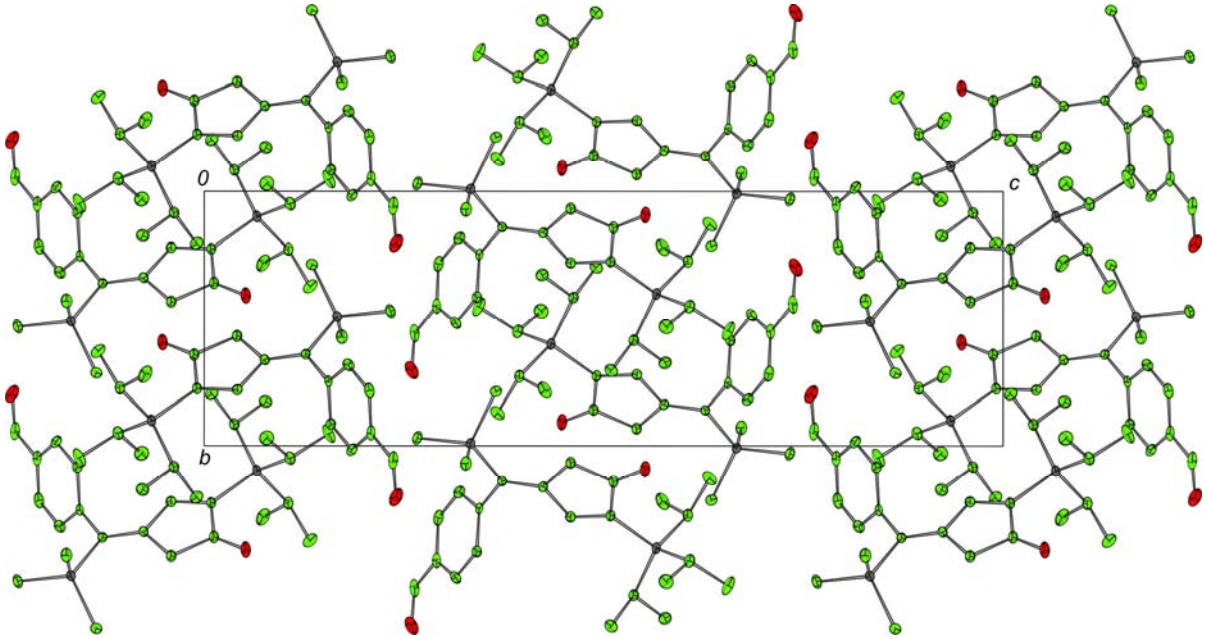
Bulk material



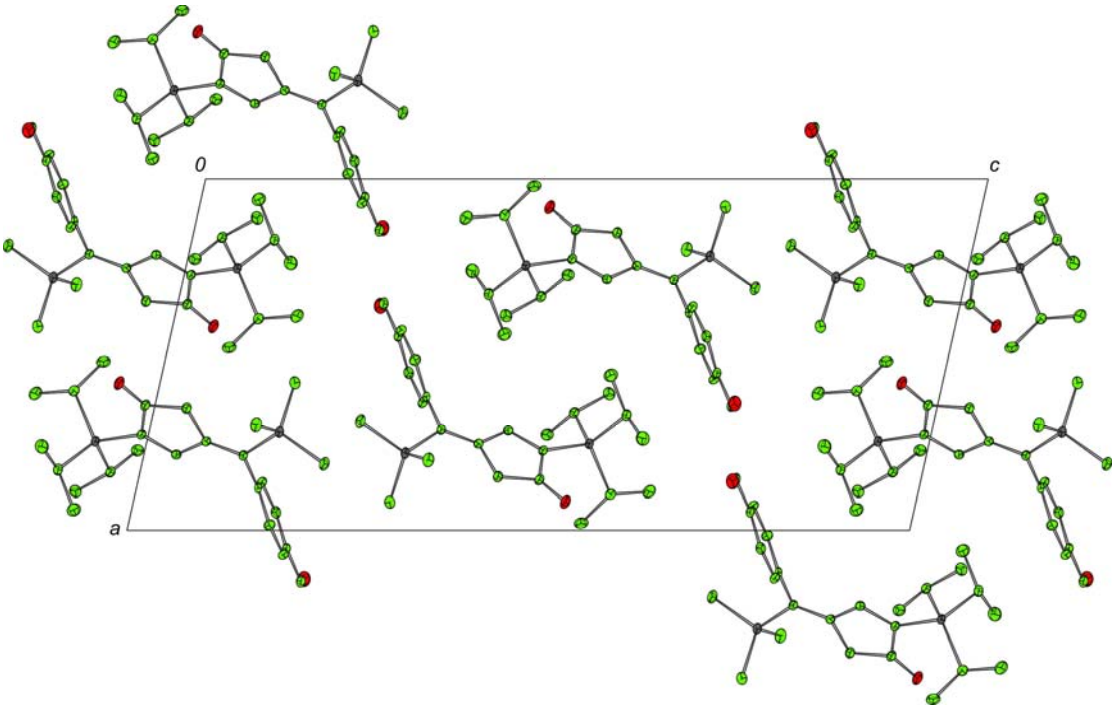
Formula units



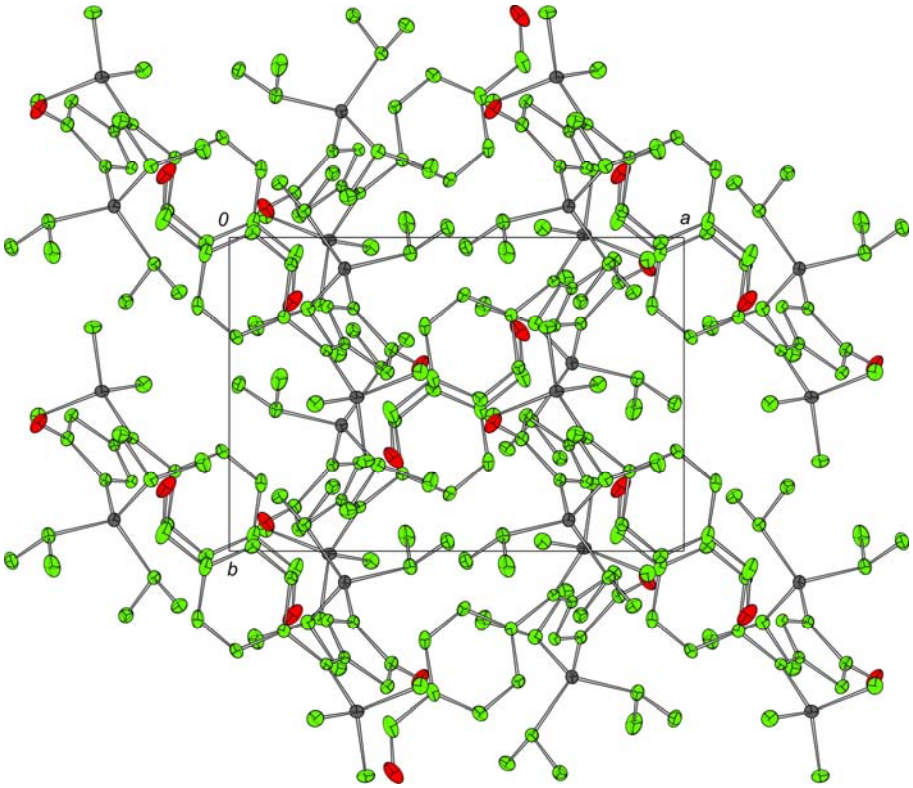
Formula units with labeling



Cell plot, viewed along *a*- axis



Cell plot, viewed along *b*- axis



Cell plot, viewed along *c*- axis

Table 1. Crystal data and structure refinement for 10101.

Empirical formula	C25 H38 O2 Si2	
Formula weight	426.75	
Crystal color, shape, size	yellow plate fragment, 0.259 x 0.193 x 0.076 mm^3	
Temperature	150 K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, P 1 21/n 1	
Unit cell dimensions	a = 12.129(3) Å	α= 90°.
	b = 8.192(2) Å	β= 102.587(5)°.
	c = 26.318(6) Å	γ = 90°.
Volume	2552.2(11) $Å^3$	
Z	4	
Density (calculated)	1.111 Mg/m^3	
Absorption coefficient	0.156 mm^{-1}	
F(000)	928	
Data collection		
Diffractometer	ApexII Kappa Duo, Bruker, Bruker	
Theta range for data collection	1.730 to 25.036°.	
Index ranges	-14<=h<=14, -9<=k<=5, -31<=l<=31	
Reflections collected	17208	
Independent reflections	4475 [R(int) = 0.075]	
Observed Reflections	2830	
Completeness to theta = 25.036°	99.1 %	
Solution and Refinement		
Absorption correction	Numerical	
Max. and min. transmission	0.99 and 0.97	
Solution	Direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting scheme	$w = [\sigma^2 Fo^2 + AP^2 + BP]^{-1}$, with	
	$P = (Fo^2 + 2\,Fc^2)/3$, A = 0.057, B = 5.750	
Data / restraints / parameters	4475 / 0 / 376	
Goodness-of-fit on F^2	0.9997	
Final R indices [I>2sigma(I)]	R1 = 0.0491, wR2 = 0.1064	
R indices (all data)	R1 = 0.0934, wR2 = 0.1221	
Largest diff. peak and hole	0.62 and -0.60 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 10101. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C1	8564(2)	1418(4)	5124(1)	30
C2	7729(2)	2746(4)	5088(1)	25
C3	7154(2)	2798(4)	4585(1)	25
C4	7533(2)	1620(4)	4243(1)	24
C5	8476(3)	677(4)	4588(1)	30
C6	7132(2)	1398(4)	3728(1)	23
C7	6199(2)	2467(4)	3445(1)	24
C8	6360(3)	4149(4)	3414(1)	29
C9	5514(3)	5155(5)	3149(1)	34
C10	4477(2)	4498(4)	2911(1)	34
C11	4302(3)	2834(5)	2933(1)	37
C12	5152(3)	1825(4)	3194(1)	33
C13	3550(3)	5569(6)	2634(1)	47
C14	8978(3)	4506(4)	6076(1)	34
C15	9797(3)	5308(5)	5783(2)	45
C16	8900(4)	5474(6)	6561(2)	58
C17	6655(3)	5840(4)	5378(1)	29
C18	7274(3)	7038(5)	5094(1)	38
C19	6107(3)	6736(5)	5770(1)	39
C20	6727(3)	2733(4)	6054(1)	32
C21	5583(3)	2192(6)	5738(2)	54
C22	7386(3)	1281(5)	6327(2)	49
C23	6890(3)	-310(5)	2669(1)	40
C24	8001(3)	-2138(4)	3651(1)	38
C25	9202(3)	709(5)	3277(2)	40
Si1	7536(1)	4010(1)	5659(1)	25
O1	9195(2)	926(3)	5521(1)	47
Si2	7803(1)	-93(1)	3334(1)	26
O2	3609(2)	7030(4)	2598(1)	62

Table 3. Bond lengths [Å] and angles [°] for 10101.

C1-C2	1.476(4)	C1-C5	1.519(4)
C1-O1	1.222(3)	C2-C3	1.355(4)
C2-Si1	1.881(3)	C3-C4	1.462(4)
C3-H31	0.94(3)	C4-C5	1.509(4)
C4-C6	1.348(4)	C5-H51	0.88(3)
C5-H52	1.01(3)	C6-C7	1.495(4)
C6-Si2	1.896(3)	C7-C8	1.396(4)
C7-C12	1.399(4)	C8-C9	1.381(4)
C8-H81	0.95(3)	C9-C10	1.386(5)
C9-H91	0.93(3)	C10-C11	1.383(5)
C10-C13	1.486(5)	C11-C12	1.383(5)
C11-H111	0.97(3)	C12-H121	0.95(3)
C13-O2	1.204(5)	C13-H131	1.01(4)
C14-C15	1.532(5)	C14-C16	1.524(5)
C14-Si1	1.895(3)	C14-H141	1.00(3)
C15-H151	1.01(4)	C15-H152	0.95(4)
C15-H153	1.01(4)	C16-H161	1.03(4)
C16-H162	1.00(4)	C16-H163	1.04(4)
C17-C18	1.525(5)	C17-C19	1.531(4)
C17-Si1	1.896(3)	C17-H171	0.95(3)
C18-H181	0.99(3)	C18-H182	1.00(3)
C18-H183	0.98(3)	C19-H191	1.02(4)
C19-H192	0.99(3)	C19-H193	1.00(4)
C20-C21	1.520(5)	C20-C22	1.523(5)
C20-Si1	1.893(3)	C20-H201	0.93(3)
C21-H211	0.91(4)	C21-H212	1.05(4)
C21-H213	0.90(4)	C22-H221	1.06(4)
C22-H222	0.99(4)	C22-H223	0.97(4)
C23-Si2	1.866(3)	C23-H231	0.97(4)
C23-H232	0.98(4)	C23-H233	0.99(4)
C24-Si2	1.864(4)	C24-H241	0.95(4)
C24-H242	0.98(3)	C24-H243	0.99(3)
C25-Si2	1.856(4)	C25-H251	0.99(4)
C25-H252	0.94(3)	C25-H253	0.87(4)

C2-C1-C5	109.1(2)	C2-C1-O1	126.2(3)
C5-C1-O1	124.6(3)	C1-C2-C3	106.6(3)
C1-C2-Si1	123.9(2)	C3-C2-Si1	129.5(2)
C2-C3-C4	114.6(3)	C2-C3-H31	123.9(18)

C4-C3-H31	121.5(17)	C3-C4-C5	105.5(2)
C3-C4-C6	128.0(3)	C5-C4-C6	126.5(3)
C1-C5-C4	104.2(2)	C1-C5-H51	108(2)
C4-C5-H51	114(2)	C1-C5-H52	111.5(17)
C4-C5-H52	111.9(18)	H51-C5-H52	107(3)
C4-C6-C7	119.4(3)	C4-C6-Si2	122.2(2)
C7-C6-Si2	118.21(19)	C6-C7-C8	120.4(3)
C6-C7-C12	121.7(3)	C8-C7-C12	117.9(3)
C7-C8-C9	121.3(3)	C7-C8-H81	120.0(19)
C9-C8-H81	118.7(19)	C8-C9-C10	119.9(3)
C8-C9-H91	122(2)	C10-C9-H91	118(2)
C9-C10-C11	119.8(3)	C9-C10-C13	120.5(4)
C11-C10-C13	119.7(3)	C10-C11-C12	120.3(3)
C10-C11-H111	120(2)	C12-C11-H111	120(2)
C7-C12-C11	120.8(3)	C7-C12-H121	121.9(20)
C11-C12-H121	117.3(20)	C10-C13-O2	125.0(4)
C10-C13-H131	114(2)	O2-C13-H131	121(2)
C15-C14-C16	111.4(3)	C15-C14-Si1	114.8(2)
C16-C14-Si1	112.2(2)	C15-C14-H141	108.4(18)
C16-C14-H141	110.9(19)	Si1-C14-H141	98.4(19)
C14-C15-H151	112(2)	C14-C15-H152	109(2)
H151-C15-H152	108(3)	C14-C15-H153	110(2)
H151-C15-H153	113(3)	H152-C15-H153	105(3)
C14-C16-H161	112(2)	C14-C16-H162	109(2)
H161-C16-H162	112(3)	C14-C16-H163	114(2)
H161-C16-H163	103(3)	H162-C16-H163	107(3)
C18-C17-C19	110.7(3)	C18-C17-Si1	113.9(2)
C19-C17-Si1	114.0(2)	C18-C17-H171	107.2(18)
C19-C17-H171	106.6(18)	Si1-C17-H171	103.8(19)
C17-C18-H181	107.4(20)	C17-C18-H182	112.9(19)
H181-C18-H182	106(3)	C17-C18-H183	110.2(19)
H181-C18-H183	111(3)	H182-C18-H183	109(3)
C17-C19-H191	111.5(19)	C17-C19-H192	110.5(19)
H191-C19-H192	108(3)	C17-C19-H193	111.8(19)
H191-C19-H193	110(3)	H192-C19-H193	104(3)
C21-C20-C22	110.7(3)	C21-C20-Si1	112.4(2)
C22-C20-Si1	114.1(2)	C21-C20-H201	110.5(19)
C22-C20-H201	106.9(19)	Si1-C20-H201	101.8(19)
C20-C21-H211	113(3)	C20-C21-H212	111(2)
H211-C21-H212	108(3)	C20-C21-H213	112(3)
H211-C21-H213	106(4)	H212-C21-H213	107(3)
C20-C22-H221	110(2)	C20-C22-H222	114(2)
H221-C22-H222	113(3)	C20-C22-H223	111(2)

H221-C22-H223	109(3)	H222-C22-H223	100(3)
Si2-C23-H231	109.8(20)	Si2-C23-H232	111(2)
H231-C23-H232	108(3)	Si2-C23-H233	112.2(19)
H231-C23-H233	107(3)	H232-C23-H233	108(3)
Si2-C24-H241	106(2)	Si2-C24-H242	112(2)
H241-C24-H242	101(3)	Si2-C24-H243	110(2)
H241-C24-H243	115(3)	H242-C24-H243	113(3)
Si2-C25-H251	109.0(19)	Si2-C25-H252	109(2)
H251-C25-H252	109(3)	Si2-C25-H253	112(2)
H251-C25-H253	109(3)	H252-C25-H253	109(3)
C17-Si1-C14	115.25(16)	C17-Si1-C20	109.65(14)
C14-Si1-C20	108.95(14)	C17-Si1-C2	106.29(13)
C14-Si1-C2	108.69(13)	C20-Si1-C2	107.74(15)
C6-Si2-C23	109.71(15)	C6-Si2-C24	111.29(15)
C23-Si2-C24	109.06(18)	C6-Si2-C25	109.01(16)
C23-Si2-C25	108.86(18)	C24-Si2-C25	108.87(18)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 10101. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	31(2)	36(2)	22(2)	1(2)	0(1)	4(2)
C2	25(2)	29(2)	21(2)	-1(1)	2(1)	1(1)
C3	23(2)	27(2)	25(2)	0(1)	5(1)	4(1)
C4	22(1)	26(2)	22(2)	-2(1)	3(1)	-2(1)
C5	32(2)	33(2)	23(2)	0(2)	4(1)	7(2)
C6	25(2)	24(2)	20(2)	1(1)	3(1)	-2(1)
C7	27(2)	31(2)	14(1)	-2(1)	6(1)	1(1)
C8	30(2)	30(2)	23(2)	0(1)	0(1)	-2(2)
C9	39(2)	36(2)	28(2)	10(2)	11(1)	7(2)
C10	29(2)	56(2)	18(2)	1(2)	4(1)	10(2)
C11	24(2)	59(3)	26(2)	-6(2)	1(1)	0(2)
C12	30(2)	36(2)	32(2)	-6(2)	4(1)	-8(2)
C13	41(2)	80(3)	22(2)	5(2)	6(2)	21(2)
C14	31(2)	42(2)	28(2)	-4(2)	3(1)	-4(2)
C15	32(2)	50(3)	50(2)	3(2)	3(2)	-8(2)
C16	47(2)	83(3)	40(2)	-31(2)	0(2)	-12(2)
C17	30(2)	31(2)	24(2)	-2(2)	2(1)	1(2)
C18	36(2)	39(2)	40(2)	7(2)	7(2)	3(2)
C19	43(2)	37(2)	39(2)	-2(2)	13(2)	8(2)
C20	35(2)	38(2)	22(2)	0(2)	5(1)	-1(2)
C21	43(2)	69(3)	47(2)	20(2)	4(2)	-12(2)
C22	53(2)	46(3)	49(2)	18(2)	14(2)	2(2)
C23	47(2)	45(2)	24(2)	-8(2)	3(2)	2(2)
C24	54(2)	29(2)	32(2)	-2(2)	7(2)	4(2)
C25	42(2)	50(2)	31(2)	-1(2)	11(2)	1(2)
Si1	26(1)	31(1)	17(1)	-2(1)	3(1)	1(1)
O1	48(1)	64(2)	25(1)	-2(1)	-2(1)	26(1)
Si2	34(1)	25(1)	20(1)	-2(1)	5(1)	0(1)
O2	65(2)	77(2)	45(2)	22(2)	13(1)	36(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 10101.

	x	y	z	U(eq)
H31	6560(20)	3540(40)	4458(11)	30
H51	9140(30)	780(40)	4504(12)	37
H52	8310(20)	-530(40)	4587(12)	37
H81	7060(30)	4630(40)	3588(11)	35
H91	5600(30)	6280(40)	3139(13)	42
H111	3570(30)	2380(40)	2776(12)	46
H121	4980(30)	700(40)	3209(12)	42
H131	2840(30)	4950(50)	2470(14)	60
H141	9240(30)	3370(40)	6168(12)	43
H151	9890(30)	4640(50)	5472(14)	56
H152	10520(30)	5410(40)	6012(14)	56
H153	9560(30)	6470(50)	5689(13)	56
H161	8340(30)	4960(50)	6760(15)	73
H162	9670(30)	5580(50)	6786(15)	73
H163	8590(30)	6650(50)	6484(15)	73
H171	6060(30)	5380(40)	5126(12)	35
H181	7650(30)	6390(40)	4860(13)	49
H182	7890(30)	7640(40)	5334(13)	49
H183	6740(30)	7830(40)	4899(13)	49
H191	5640(30)	5960(40)	5945(13)	50
H192	6690(30)	7250(40)	6046(13)	50
H193	5630(30)	7670(40)	5605(13)	50
H201	6640(30)	3470(40)	6314(12)	39
H211	5140(30)	3050(50)	5599(15)	69
H212	5150(30)	1510(50)	5968(15)	69
H213	5650(30)	1560(50)	5466(16)	69
H221	8150(30)	1690(50)	6570(14)	61
H222	6940(30)	580(50)	6513(14)	61
H223	7550(30)	500(50)	6079(14)	61
H231	7280(30)	-930(40)	2451(14)	50
H232	6690(30)	760(50)	2505(13)	50
H233	6180(30)	-900(40)	2672(13)	50
H241	8160(30)	-2870(40)	3397(13)	49
H242	8700(30)	-2210(40)	3915(13)	49
H243	7330(30)	-2420(40)	3787(13)	49
H251	9530(30)	-30(40)	3052(13)	49
H252	9680(30)	730(40)	3609(14)	49

H253	9160(30)	1690(50)	3145(14)	49

Table 6. Torsion angles [°] for 10101.

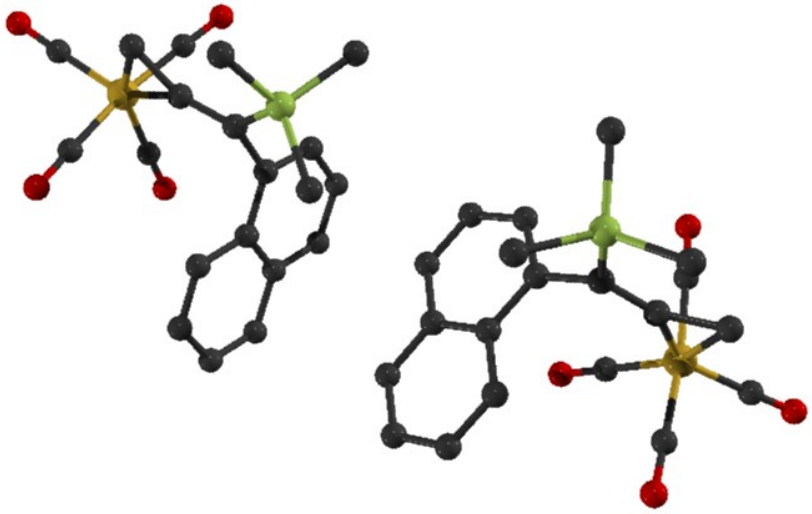
C20-Si1-C14-C15	171.0(2)	C2-Si1-C14-C16	-177.7(3)
C17-Si1-C14-C16	63.2(3)	C20-Si1-C14-C16	-60.6(3)
C2-Si1-C17-C18	-69.3(3)	C14-Si1-C17-C18	51.2(3)
C14-Si1-C2-C1	41.2(3)	C17-Si1-C2-C1	165.8(2)
C20-Si1-C2-C1	-76.7(3)	C14-Si1-C2-C3	-141.0(3)
C17-Si1-C2-C3	-16.3(3)	C20-Si1-C2-C3	101.1(3)
C17-Si1-C20-C21	56.5(3)	C2-Si1-C14-C15	53.8(3)
C17-Si1-C14-C15	-65.3(3)	C17-Si1-C20-C22	-176.4(2)
C14-Si1-C17-C19	-77.1(3)	C20-Si1-C17-C19	46.2(3)
C2-Si1-C20-C21	-58.8(3)	C14-Si1-C20-C21	-176.5(3)
C14-Si1-C20-C22	-49.4(3)	C20-Si1-C17-C18	174.5(2)
C2-Si1-C17-C19	162.4(2)	C2-Si1-C20-C22	68.3(3)
C24-Si2-C6-C7	-135.7(2)	C23-Si2-C6-C4	171.0(3)
C25-Si2-C6-C4	-69.9(3)	C23-Si2-C6-C7	-14.9(3)
C24-Si2-C6-C4	50.2(3)	C25-Si2-C6-C7	104.2(2)
O1-C1-C2-C3	-175.2(3)	C5-C1-C2-Si1	180.0(2)
C5-C1-C2-C3	1.7(3)	O1-C1-C2-Si1	3.1(4)
C2-C1-C5-C4	-1.1(3)	O1-C1-C5-C4	175.8(3)
Si1-C2-C3-C4	-179.8(2)	C1-C2-C3-C4	-1.7(3)
C2-C3-C4-C6	-179.4(3)	C2-C3-C4-C5	0.9(4)
C6-C4-C5-C1	-179.5(3)	C3-C4-C6-Si2	175.3(2)
C3-C4-C5-C1	0.2(3)	C5-C4-C6-Si2	-5.1(4)
C5-C4-C6-C7	-179.1(3)	C3-C4-C6-C7	1.3(5)
C4-C6-C7-C12	-118.9(3)	C4-C6-C7-C8	62.4(4)
Si2-C6-C7-C8	-111.9(3)	Si2-C6-C7-C12	66.9(3)
C12-C7-C8-C9	0.4(4)	C6-C7-C8-C9	179.2(3)
C6-C7-C12-C11	-179.8(3)	C8-C7-C12-C11	-1.0(4)
C7-C8-C9-C10	0.6(5)	C8-C9-C10-C11	-1.1(5)
C8-C9-C10-C13	178.6(3)	C13-C10-C11-C12	-179.3(3)
C9-C10-C11-C12	0.4(5)	C9-C10-C13-O2	-0.8(5)
C11-C10-C13-O2	178.9(3)	C10-C11-C12-C7	0.6(5)

Symmetry transformations used to generate equivalent atoms:

INDIANA UNIVERSITY DEPARTMENT OF CHEMISTRY

Molecular Structure Center

X-Ray Crystal Structure Data for a Three-Membered Iron Metallacycle (24)



$C_{20}H_{18}O_4SiFe$

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IUMSC
Indiana University Molecular Structure Center

Data collection

The X-ray crystal structure and data collection was performed by **C. Chen**. A colorless crystal (approximate dimensions 0.491 x 0.124 x 0.114 mm^3) was placed onto the tip of a glass capillary and mounted on an Apex Kappa Duo diffractometer and measured at 150 K.

A preliminary set of cell constants was calculated from reflections harvested from three sets of 12 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 217 reflections. The data collection was carried out using Mo Kα radiation (graphite monochromator) with a frame time of 60 seconds and a detector distance of 5.0 cm. A randomly oriented region of reciprocal space was surveyed to achieve complete data with a redundancy of 4. Sections of frames were collected with 0.50º steps in ω and ϕ scans. Data to a resolution of 0.71 Å were considered in the reduction. Final cell constants were calculated from the xyz centroids of 9909 strong reflections from the actual data collection after integration (SAINT).[1] The intensity data were corrected for absorption (SADABS).[2] Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The space group $P2_1$ was determined based on intensity statistics and systematic absences. The structure was solved using SIR-92[3] and refined (full-matrix-least squares) using the Oxford University *Crystals for Windows* system.[4] A direct-methods solution was calculated, which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed, which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were placed in ideal positions and refined as riding atoms. The final full matrix least squares refinement converged to R1 = 0.0358 ($I > 2\sigma(I)$, 9275 data) and wR2 = 0.0910 (F^2, 11113 data, 469 parameters).

Structure description

The structure was found as proposed, with two molecules in the asymmetric unit.

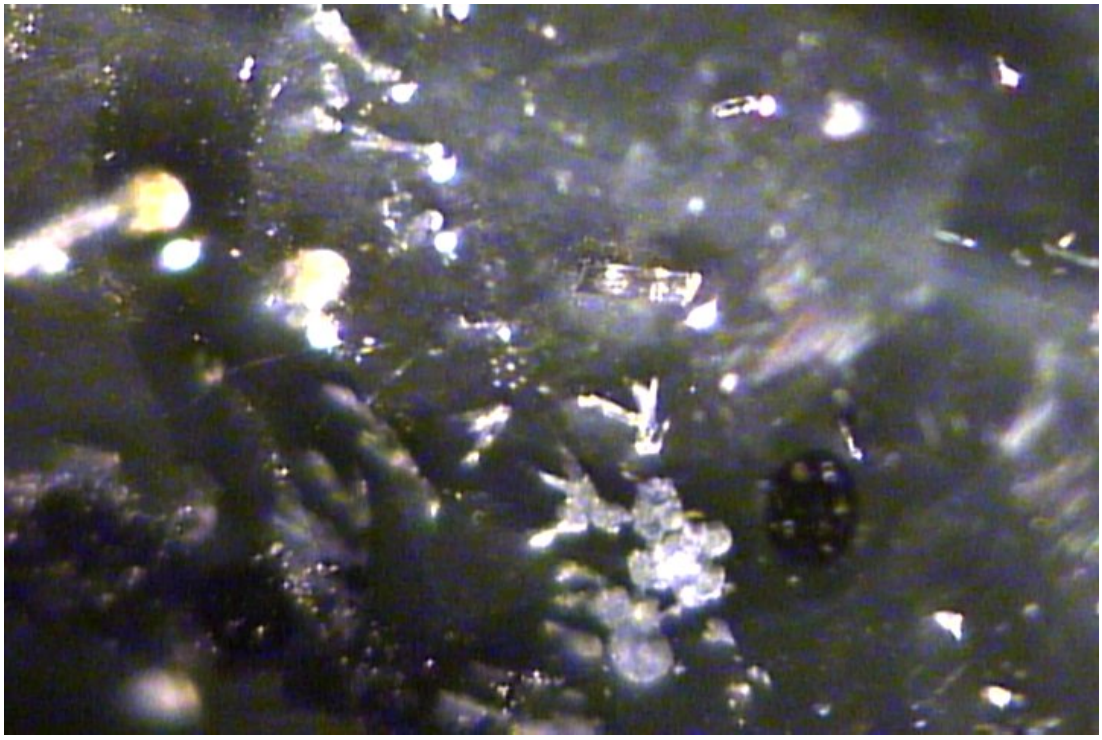
[1] SAINT, Bruker Analytical X-Ray Systems,Madison, WI, current version.

[2] An empirical correction for absorption anisotropy,R. Blessing, Acta Cryst. A51, 33 - 38 (1995).

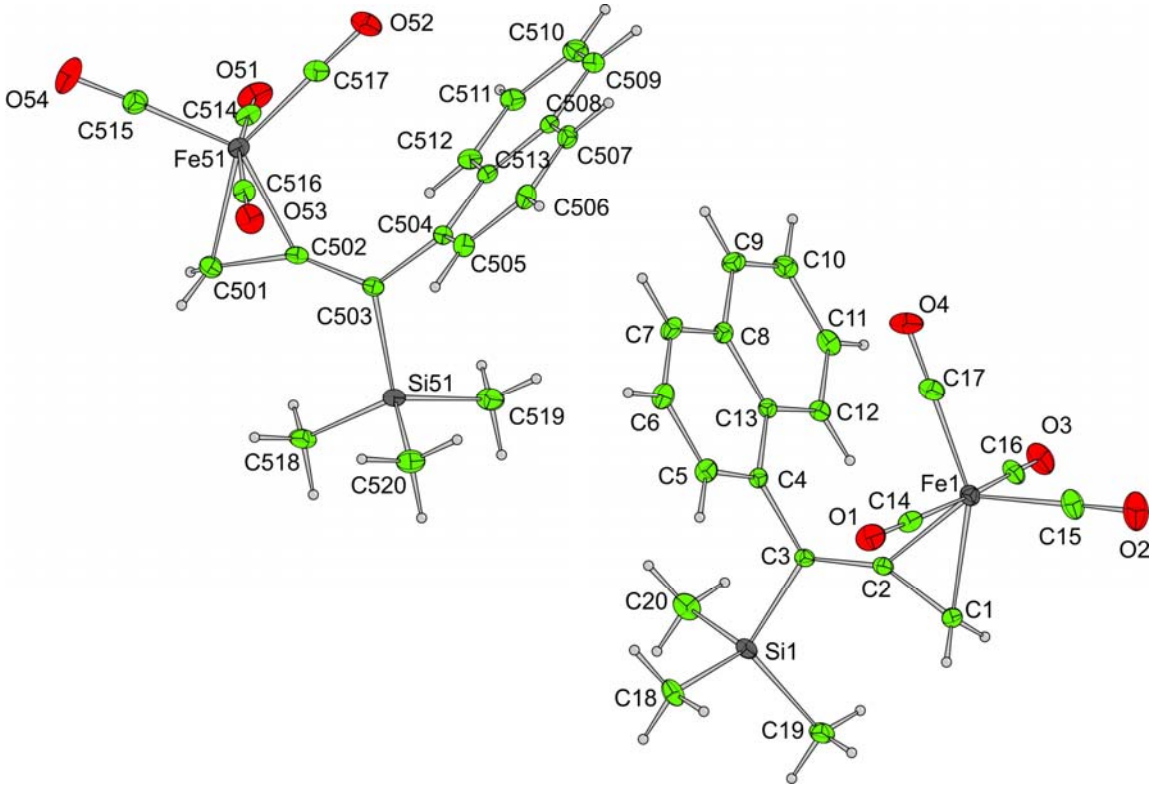
[3] Altomare, A; Cascarano, G; Giacovazzo, G.; Guagliardi, A.; Burla, M. C.; Polidori, G.; Camalli, M. *J. Appl. Cryst*. **1994**, *27*, 435.

[4] Betteridge, P. W.; Carruthers, J. R.; Cooper, R. I.; Prout, K.; Watkin, D. J. *J. Appl. Cryst.* **2003**, *36*, 1487.

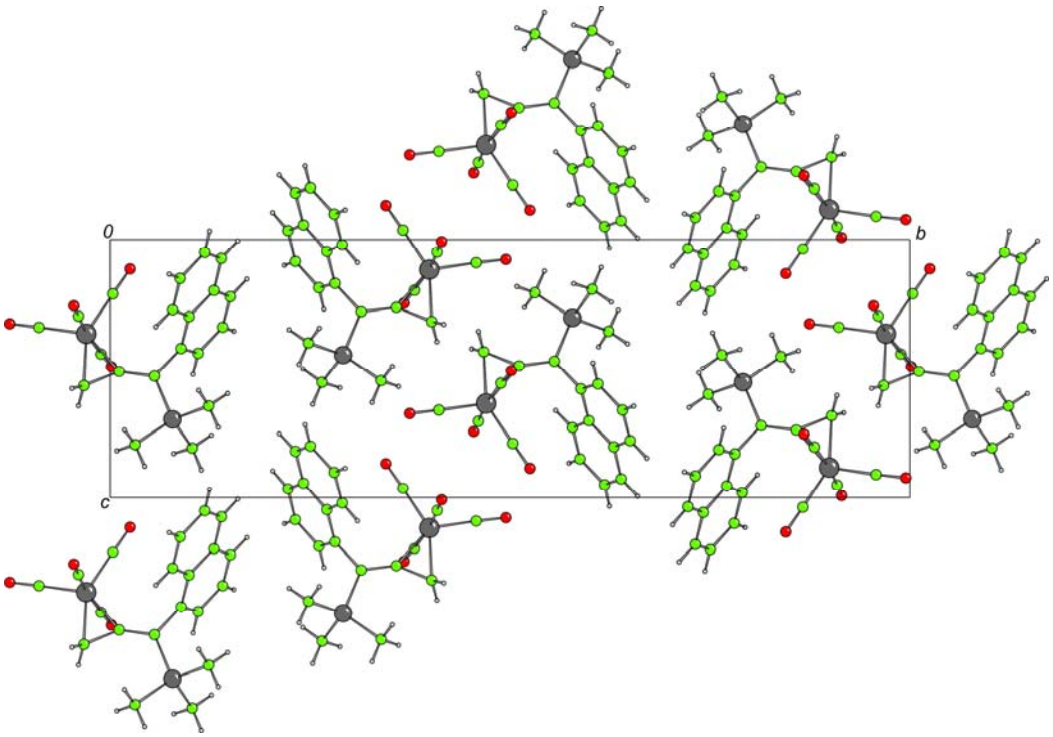
[5] PLATON, A. L. Spek, Acta Cryst. A46, C34 (1990).



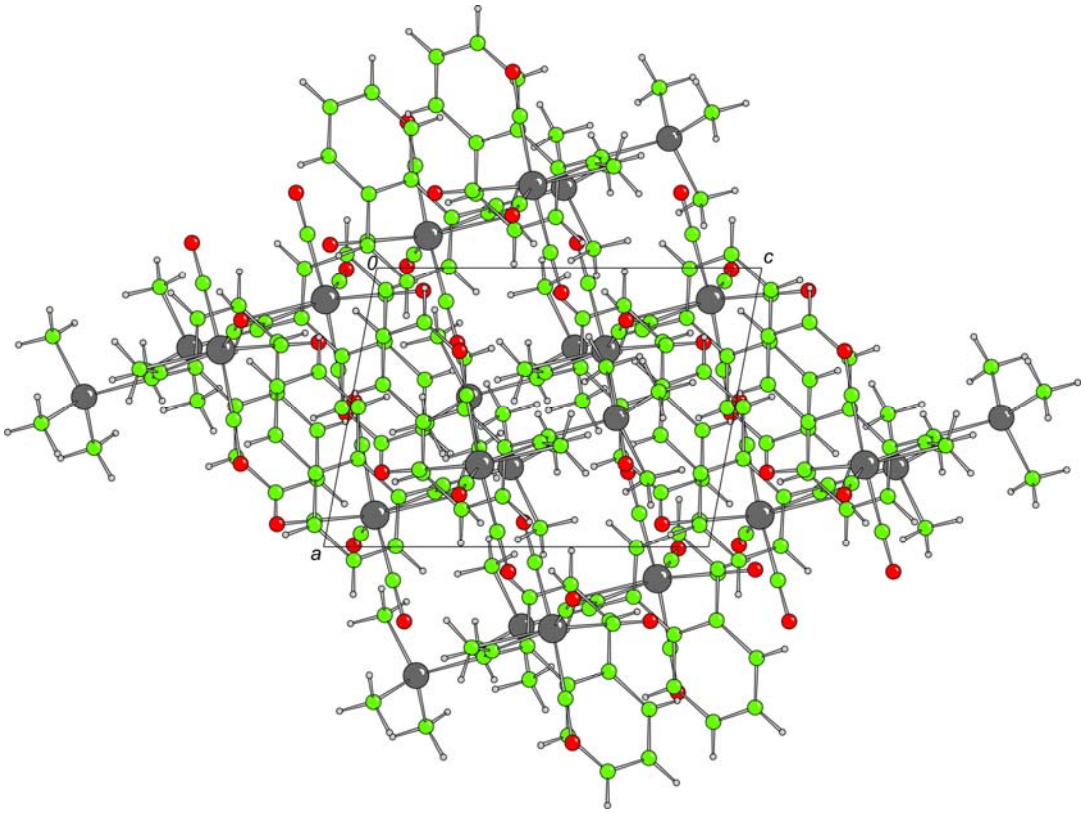
Bulk material



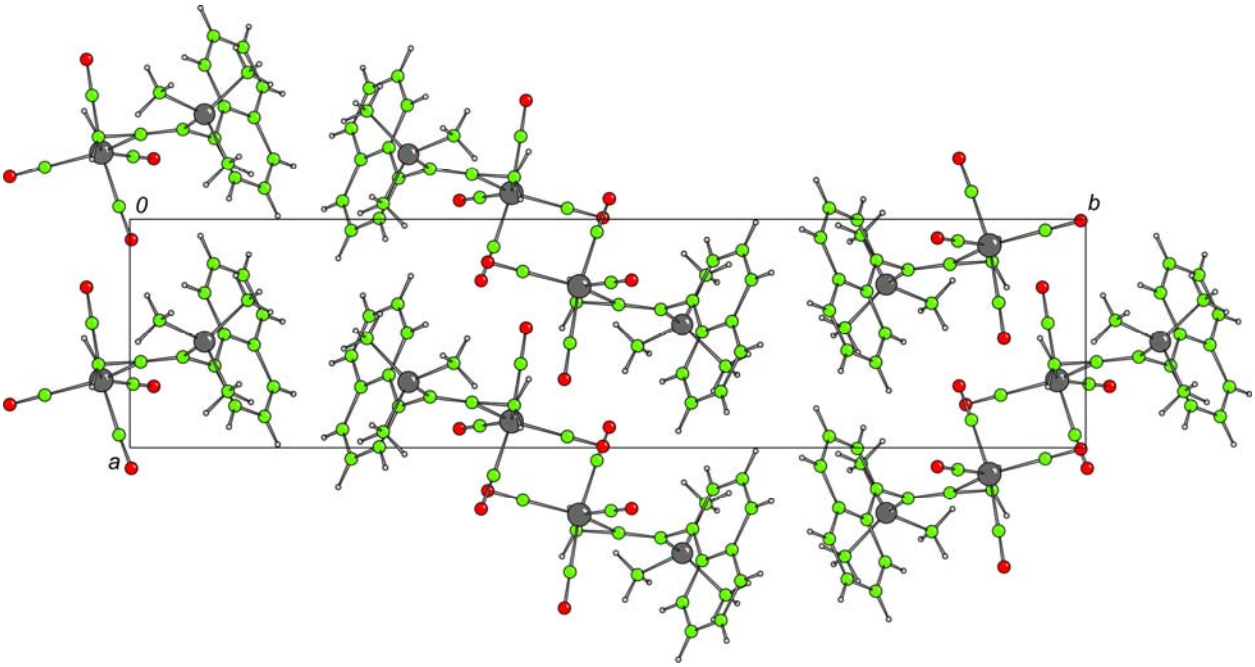
Formula unit (Ellipsoid view) with labeling



Cell plot, viewed along *a*- axis



Cell plot, viewed along *b*- axis



Cell plot, viewed along *c*- axis

Table 1. Crystal data and structure refinement for 10118.

Empirical formula	C20 H18 Fe1 O4 Si1	
Formula weight	406.29	
Crystal color, shape, size	colorless acicular, 0.491 x 0.124 x 0.114 mm^3	
Temperature	150 K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, P 21	
Unit cell dimensions	a = 7.1510(8) Å	α = 90°.
	b = 29.386(3) Å	β = 100.773(2)°.
	c = 9.6851(10) Å	γ = 90°.
Volume	1999.4(4) $Å^3$	
Z	4	
Density (calculated)	1.350 Mg/m^3	
Absorption coefficient	0.835 mm^{-1}	
F(000)	840	
Data collection		
Diffractometer	ApexII Kappa Duo, Bruker	
Theta range for data collection	2.141 to 30.036°.	
Index ranges	-10<=h<=10, -41<=k<=41, -13<=l<=7	
Reflections collected	21632	
Independent reflections	11113 [R(int) = 0.026]	
Observed Reflections	9275	
Completeness to theta = 29.135°	99.5 %	
Solution and Refinement		
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.91 and 0.90	
Solution	Direct methods	
Refinement method	Full-matrix least-squares on F^2	
Weighting scheme	$w = [\sigma^2 Fo^2 + AP^2 + BP]^{-1}$, with	
	$P = (Fo^2 + 2\,Fc^2)/3$, A = 0.043, B = 0.660	
Data / restraints / parameters	11113 / 1 / 469	
Goodness-of-fit on F^2	0.9951	
Final R indices [I>2sigma(I)]	R1 = 0.0358, wR2 = 0.0852	
R indices (all data)	R1 = 0.0443, wR2 = 0.0910	
Largest diff. peak and hole	0.61 and -0.30 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 10118. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe1	2941(1)	4701(1)	6353(1)	27
Fe51	1148(1)	8992(1)	8827(1)	27
Si1	4621(1)	5779(1)	3039(1)	27
Si51	2862(1)	7913(1)	5534(1)	26
O1	-897(3)	5016(1)	5078(2)	46
O2	1876(4)	3744(1)	6737(3)	64
O3	7023(3)	4546(1)	7435(3)	50
O4	2672(3)	5249(1)	8854(2)	52
O51	5226(3)	9145(1)	9920(3)	53
O52	826(3)	8448(1)	11324(2)	52
O53	-2687(3)	8675(1)	7537(2)	47
O54	62(4)	9948(1)	9221(3)	65
C1	3628(4)	4671(1)	4341(3)	32
C2	3739(3)	5112(1)	4892(2)	24
C3	3953(3)	5554(1)	4710(2)	23
C4	3566(3)	5887(1)	5784(3)	23
C5	1821(3)	6100(1)	5601(3)	31
C6	1362(4)	6407(1)	6604(3)	35
C7	2652(4)	6503(1)	7789(3)	31
C8	4477(3)	6298(1)	8028(3)	26
C9	5826(4)	6391(1)	9263(3)	33
C10	7560(4)	6182(1)	9492(3)	35
C11	8046(4)	5875(1)	8489(3)	33
C12	6777(3)	5781(1)	7282(3)	26
C13	4948(3)	5986(1)	7015(2)	22
C14	558(4)	4886(1)	5568(3)	33
C15	2290(4)	4110(1)	6603(3)	41
C16	5444(4)	4604(1)	7034(3)	35
C17	2768(4)	5034(1)	7896(3)	36
C18	2453(4)	6026(1)	1929(3)	38
C19	5567(5)	5311(1)	2062(3)	43
C20	6451(4)	6232(1)	3553(3)	42
C501	1847(4)	9020(1)	6823(3)	35
C502	1973(3)	8578(1)	7377(2)	26
C503	2215(3)	8139(1)	7203(2)	25
C504	1799(3)	7811(1)	8299(2)	24
C505	34(3)	7610(1)	8133(3)	29

C506	-487(4)	7316(1)	9148(3)	30
C507	798(4)	7224(1)	10349(3)	30
C508	2642(3)	7416(1)	10572(2)	24
C509	4002(4)	7317(1)	11801(3)	33
C510	5761(4)	7504(1)	12002(3)	38
C511	6283(4)	7803(1)	10990(3)	33
C512	5011(3)	7902(1)	9793(3)	29
C513	3157(3)	7709(1)	9539(2)	24
C514	3650(4)	9089(1)	9506(3)	36
C515	481(4)	9576(1)	9097(3)	38
C516	-1207(4)	8805(1)	8034(3)	33
C517	953(4)	8661(1)	10370(3)	36
C518	3680(4)	8388(1)	4530(3)	38
C519	4765(4)	7479(1)	6000(3)	40
C520	690(4)	7650(1)	4466(3)	40

Table 3. Bond lengths [Å] and angles [°] for 10118.

Fe1-C1	2.098(2)	Fe1-C2	2.022(2)
Fe1-C14	1.815(3)	Fe1-C15	1.825(3)
Fe1-C16	1.811(3)	Fe1-C17	1.809(3)
Fe51-C501	2.095(3)	Fe51-C502	2.026(2)
Fe51-C514	1.810(3)	Fe51-C515	1.815(3)
Fe51-C516	1.801(3)	Fe51-C517	1.809(3)
Si1-C3	1.890(2)	Si1-C18	1.860(3)
Si1-C19	1.868(3)	Si1-C20	1.868(3)
Si51-C503	1.884(3)	Si51-C518	1.857(3)
Si51-C519	1.859(3)	Si51-C520	1.866(3)
O1-C14	1.126(3)	O2-C15	1.129(4)
O3-C16	1.136(3)	O4-C17	1.136(4)
O51-C514	1.135(3)	O52-C517	1.133(3)
O53-C516	1.144(3)	O54-C515	1.146(4)
C1-C2	1.399(4)	C1-H11	0.950
C1-H12	0.950	C2-C3	1.322(4)
C3-C4	1.492(3)	C4-C5	1.377(3)
C4-C13	1.429(3)	C5-C6	1.408(4)
C5-H51	0.950	C6-C7	1.361(4)
C6-H61	0.950	C7-C8	1.416(3)
C7-H71	0.950	C8-C9	1.416(3)
C8-C13	1.429(3)	C9-C10	1.363(4)
C9-H91	0.950	C10-C11	1.418(4)
C10-H101	0.950	C11-C12	1.367(3)
C11-H111	0.950	C12-C13	1.419(3)
C12-H121	0.950	C18-H181	0.950
C18-H182	0.950	C18-H183	0.950
C19-H191	0.950	C19-H192	0.950
C19-H193	0.950	C20-H201	0.950
C20-H202	0.950	C20-H203	0.950
C501-C502	1.401(4)	C501-H5011	0.950
C501-H5012	0.950	C502-C503	1.317(4)
C503-C504	1.504(3)	C504-C505	1.376(3)
C504-C513	1.428(3)	C505-C506	1.411(4)
C505-H5051	0.950	C506-C507	1.368(4)
C506-H5061	0.950	C507-C508	1.414(3)
C507-H5071	0.950	C508-C509	1.420(3)
C508-C513	1.420(3)	C509-C510	1.353(4)
C509-H5091	0.950	C510-C511	1.416(4)
C510-H5101	0.950	C511-C512	1.365(4)
C511-H5111	0.950	C512-C513	1.419(3)

C512-H5121	0.950	C518-H5181	0.950
C518-H5182	0.950	C518-H5183	0.950
C519-H5191	0.950	C519-H5192	0.950
C519-H5193	0.950	C520-H5201	0.950
C520-H5202	0.950	C520-H5203	0.950

C1-Fe1-C2	39.65(10)	C1-Fe1-C14	89.34(12)
C2-Fe1-C14	83.89(11)	C1-Fe1-C15	101.13(13)
C2-Fe1-C15	140.69(13)	C14-Fe1-C15	95.60(13)
C1-Fe1-C16	86.83(11)	C2-Fe1-C16	87.74(11)
C14-Fe1-C16	170.67(13)	C15-Fe1-C16	93.48(13)
C1-Fe1-C17	148.61(13)	C2-Fe1-C17	109.06(13)
C14-Fe1-C17	88.84(12)	C15-Fe1-C17	110.23(14)
C16-Fe1-C17	90.01(13)	C501-Fe51-C502	39.71(11)
C501-Fe51-C514	86.51(12)	C502-Fe51-C514	87.18(11)
C501-Fe51-C515	102.13(13)	C502-Fe51-C515	141.76(13)
C514-Fe51-C515	93.78(13)	C501-Fe51-C516	89.04(12)
C502-Fe51-C516	83.79(11)	C514-Fe51-C516	170.14(13)
C515-Fe51-C516	95.76(14)	C501-Fe51-C517	148.82(13)
C502-Fe51-C517	109.17(12)	C514-Fe51-C517	90.49(13)
C515-Fe51-C517	109.04(14)	C516-Fe51-C517	88.76(13)
C3-Si1-C18	108.34(12)	C3-Si1-C19	110.40(13)
C18-Si1-C19	109.61(14)	C3-Si1-C20	107.36(13)
C18-Si1-C20	110.08(14)	C19-Si1-C20	110.99(16)
C503-Si51-C518	109.66(12)	C503-Si51-C519	108.61(12)
C518-Si51-C519	110.82(15)	C503-Si51-C520	108.03(12)
C518-Si51-C520	109.44(14)	C519-Si51-C520	110.23(15)
Fe1-C1-C2	67.24(14)	Fe1-C1-H11	118.8
C2-C1-H11	119.0	Fe1-C1-H12	118.7
C2-C1-H12	118.5	H11-C1-H12	109.5
C1-C2-Fe1	73.12(15)	C1-C2-C3	149.1(2)
Fe1-C2-C3	137.31(19)	Si1-C3-C2	120.84(18)
Si1-C3-C4	118.46(18)	C2-C3-C4	120.6(2)
C3-C4-C5	119.3(2)	C3-C4-C13	121.7(2)
C5-C4-C13	119.0(2)	C4-C5-C6	121.6(2)
C4-C5-H51	119.0	C6-C5-H51	119.4
C5-C6-C7	120.4(2)	C5-C6-H61	119.9
C7-C6-H61	119.7	C6-C7-C8	120.5(2)
C6-C7-H71	120.1	C8-C7-H71	119.3
C7-C8-C9	121.2(2)	C7-C8-C13	119.3(2)
C9-C8-C13	119.5(2)	C8-C9-C10	120.5(3)

C8-C9-H91	119.9	C10-C9-H91	119.6
C9-C10-C11	120.5(2)	C9-C10-H101	120.0
C11-C10-H101	119.5	C10-C11-C12	120.4(2)
C10-C11-H111	119.5	C12-C11-H111	120.1
C11-C12-C13	120.8(2)	C11-C12-H121	119.5
C13-C12-H121	119.7	C4-C13-C8	119.2(2)
C4-C13-C12	122.4(2)	C8-C13-C12	118.4(2)
Fe1-C14-O1	177.6(3)	Fe1-C15-O2	179.0(3)
Fe1-C16-O3	178.5(2)	Fe1-C17-O4	178.8(3)
Si1-C18-H181	109.5	Si1-C18-H182	109.5
H181-C18-H182	109.5	Si1-C18-H183	109.4
H181-C18-H183	109.5	H182-C18-H183	109.5
Si1-C19-H191	109.2	Si1-C19-H192	110.1
H191-C19-H192	109.5	Si1-C19-H193	109.1
H191-C19-H193	109.5	H192-C19-H193	109.5
Si1-C20-H201	109.4	Si1-C20-H202	109.3
H201-C20-H202	109.5	Si1-C20-H203	109.6
H201-C20-H203	109.5	H202-C20-H203	109.5
Fe51-C501-C502	67.49(14)	Fe51-C501-H5011	118.7
C502-C501-H5011	118.9	Fe51-C501-H5012	118.5
C502-C501-H5012	118.7	H5011-C501-H5012	109.5
C501-C502-Fe51	72.80(16)	C501-C502-C503	149.3(2)
Fe51-C502-C503	137.54(19)	Si51-C503-C502	120.93(19)
Si51-C503-C504	119.49(17)	C502-C503-C504	119.4(2)
C503-C504-C505	119.4(2)	C503-C504-C513	122.3(2)
C505-C504-C513	118.2(2)	C504-C505-C506	122.6(2)
C504-C505-H5051	118.6	C506-C505-H5051	118.8
C505-C506-C507	119.4(2)	C505-C506-H5061	120.3
C507-C506-H5061	120.2	C506-C507-C508	120.6(2)
C506-C507-H5071	119.8	C508-C507-H5071	119.6
C507-C508-C509	121.2(2)	C507-C508-C513	119.5(2)
C509-C508-C513	119.2(2)	C508-C509-C510	120.6(3)
C508-C509-H5091	119.6	C510-C509-H5091	119.8
C509-C510-C511	120.7(2)	C509-C510-H5101	119.8
C511-C510-H5101	119.5	C510-C511-C512	120.0(3)
C510-C511-H5111	120.0	C512-C511-H5111	119.9
C511-C512-C513	121.0(3)	C511-C512-H5121	119.4
C513-C512-H5121	119.6	C504-C513-C508	119.6(2)
C504-C513-C512	121.9(2)	C508-C513-C512	118.5(2)
Fe51-C514-O51	178.9(3)	Fe51-C515-O54	177.7(3)
O53-C516-Fe51	178.2(3)	Fe51-C517-O52	179.0(3)
Si51-C518-H5181	109.8	Si51-C518-H5182	109.3
H5181-C518-H5182	109.5	Si51-C518-H5183	109.2

H5181-C518-H5183	109.5	H5182-C518-H5183	109.5
Si51-C519-H5191	109.5	Si51-C519-H5192	109.4
H5191-C519-H5192	109.5	Si51-C519-H5193	109.5
H5191-C519-H5193	109.5	H5192-C519-H5193	109.5
Si51-C520-H5201	109.8	Si51-C520-H5202	109.5
H5201-C520-H5202	109.5	Si51-C520-H5203	109.1
H5201-C520-H5203	109.5	H5202-C520-H5203	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 10118. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe1	28(1)	28(1)	26(1)	3(1)	8(1)	3(1)
Fe51	27(1)	27(1)	27(1)	-3(1)	7(1)	-2(1)
Si1	25(1)	32(1)	22(1)	5(1)	2(1)	3(1)
Si51	25(1)	31(1)	21(1)	-2(1)	4(1)	-1(1)
O1	32(1)	56(1)	47(1)	-8(1)	1(1)	8(1)
O2	62(2)	42(1)	94(2)	18(1)	27(2)	-6(1)
O3	33(1)	63(2)	55(1)	19(1)	6(1)	12(1)
O4	51(1)	74(2)	32(1)	-9(1)	12(1)	2(1)
O51	33(1)	67(2)	58(1)	-23(1)	4(1)	-8(1)
O52	60(2)	66(2)	33(1)	7(1)	15(1)	0(1)
O53	34(1)	51(1)	53(1)	4(1)	0(1)	-8(1)
O54	65(2)	36(1)	95(2)	-15(1)	21(2)	10(1)
C1	43(1)	28(1)	26(1)	0(1)	12(1)	7(1)
C2	24(1)	30(1)	20(1)	1(1)	4(1)	6(1)
C3	21(1)	27(1)	20(1)	0(1)	4(1)	3(1)
C4	21(1)	23(1)	25(1)	1(1)	6(1)	2(1)
C5	22(1)	33(1)	36(1)	-2(1)	2(1)	5(1)
C6	27(1)	34(1)	46(2)	-1(1)	9(1)	9(1)
C7	31(1)	28(1)	38(1)	-5(1)	14(1)	4(1)
C8	26(1)	23(1)	28(1)	1(1)	8(1)	-2(1)
C9	38(1)	31(1)	29(1)	-6(1)	6(1)	-7(1)
C10	35(1)	38(2)	29(1)	1(1)	1(1)	-7(1)
C11	20(1)	41(2)	36(1)	8(1)	-1(1)	0(1)
C12	20(1)	32(1)	26(1)	2(1)	5(1)	4(1)
C13	22(1)	22(1)	23(1)	2(1)	6(1)	0(1)
C14	32(1)	34(1)	33(1)	-8(1)	8(1)	0(1)
C15	33(1)	40(2)	52(2)	14(1)	12(1)	2(1)
C16	36(1)	38(2)	31(1)	12(1)	10(1)	6(1)
C17	35(1)	47(2)	28(1)	3(1)	9(1)	2(1)
C18	33(1)	41(2)	35(2)	13(1)	-2(1)	4(1)
C19	56(2)	48(2)	26(1)	4(1)	14(1)	18(2)
C20	34(1)	50(2)	40(2)	6(1)	1(1)	-8(1)
C501	44(1)	33(1)	30(1)	3(1)	15(1)	-1(1)
C502	24(1)	34(1)	20(1)	-2(1)	6(1)	-5(1)
C503	22(1)	29(1)	22(1)	0(1)	3(1)	-2(1)
C504	25(1)	24(1)	22(1)	0(1)	4(1)	1(1)
C505	25(1)	29(1)	34(1)	0(1)	5(1)	0(1)

C506	25(1)	24(1)	40(1)	-1(1)	8(1)	-3(1)
C507	34(1)	24(1)	36(1)	0(1)	13(1)	-2(1)
C508	29(1)	22(1)	23(1)	-3(1)	8(1)	4(1)
C509	40(2)	32(1)	26(1)	-1(1)	7(1)	3(1)
C510	36(1)	42(2)	31(1)	-4(1)	-2(1)	4(1)
C511	27(1)	40(2)	30(1)	-4(1)	1(1)	-1(1)
C512	25(1)	36(1)	28(1)	-4(1)	6(1)	-2(1)
C513	24(1)	25(1)	24(1)	-4(1)	7(1)	2(1)
C514	38(1)	36(2)	35(1)	-11(1)	10(1)	-2(1)
C515	42(2)	37(2)	38(2)	-2(1)	16(1)	-2(1)
C516	33(1)	33(1)	33(1)	2(1)	6(1)	1(1)
C517	34(1)	43(2)	29(1)	-3(1)	5(1)	0(1)
C518	45(2)	46(2)	24(1)	-2(1)	11(1)	-5(1)
C519	34(1)	54(2)	32(1)	-2(1)	6(1)	10(1)
C520	34(1)	50(2)	34(1)	-7(1)	2(1)	-5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 10118.

	x	y	z	U(eq)
H51	906	6037	4778	39
H61	142	6546	6456	45
H71	2337	6710	8463	37
H91	5518	6596	9945	40
H101	8452	6243	10329	42
H111	9272	5738	8652	38
H121	7115	5571	6624	31
H181	2762	6141	1082	46
H182	1981	6266	2424	46
H183	1508	5796	1713	46
H191	5896	5430	1228	53
H192	6662	5180	2630	53
H193	4613	5084	1824	53
H201	6820	6352	2734	51
H202	5928	6468	4033	51
H203	7531	6107	4153	51
H5051	-868	7672	7303	33
H5061	-1714	7180	8995	36
H5071	444	7032	11047	36
H5091	3678	7114	12483	38
H5101	6654	7437	12833	45
H5111	7511	7938	11151	41
H5121	5390	8093	9104	37
H5181	4010	8275	3688	45
H5182	4760	8528	5087	45
H5183	2685	8605	4304	45
H5191	5105	7362	5167	50
H5192	5848	7615	6568	50
H5193	4316	7238	6506	50
H5201	978	7532	3617	48
H5202	-283	7873	4255	48
H5203	267	7410	4989	48
H11	4767	4521	4228	38
H12	2648	4604	3562	38
H5011	2984	9172	6712	43
H5012	868	9087	6042	43

Table 6. Torsion angles [°] for 10118.

C14-Fe1-C1-C2	81.21(17)	C15-Fe1-C1-C2	176.81(16)
C16-Fe1-C1-C2	-90.28(17)	C17-Fe1-C1-C2	-5.5(3)
C1-Fe1-C2-C3	173.6(3)	C14-Fe1-C2-C1	-96.36(17)
C14-Fe1-C2-C3	77.3(3)	C15-Fe1-C2-C1	-5.0(2)
C15-Fe1-C2-C3	168.7(2)	C16-Fe1-C2-C1	87.76(17)
C16-Fe1-C2-C3	-98.6(3)	C17-Fe1-C2-C1	176.98(17)
C17-Fe1-C2-C3	-9.4(3)	C516-Fe51-C502-C503	-78.1(3)
C517-Fe51-C502-C501	-177.49(17)	C517-Fe51-C502-C503	8.5(3)
C514-Fe51-C502-C501	-87.96(17)	C514-Fe51-C502-C503	98.0(3)
C514-Fe51-C501-C502	89.76(17)	C515-Fe51-C501-C502	-177.12(16)
C516-Fe51-C501-C502	-81.44(17)	C517-Fe51-C501-C502	4.6(3)
C501-Fe51-C502-C503	-174.0(3)	C515-Fe51-C502-C503	-169.5(2)
C516-Fe51-C502-C501	96.00(17)	C515-Fe51-C502-C501	4.6(2)
C19-Si1-C3-C4	167.06(19)	C20-Si1-C3-C2	-137.4(2)
C18-Si1-C3-C2	103.7(2)	C18-Si1-C3-C4	-72.9(2)
C19-Si1-C3-C2	-16.3(2)	C20-Si1-C3-C4	46.0(2)
C518-Si51-C503-C504	-170.66(17)	C519-Si51-C503-C502	136.0(2)
C518-Si51-C503-C502	14.8(2)	C520-Si51-C503-C502	-104.4(2)
C520-Si51-C503-C504	70.1(2)	C519-Si51-C503-C504	-49.4(2)
Fe1-C1-C2-C3	-171.5(4)	C1-C2-C3-Si1	-8.1(5)
Fe1-C2-C3-C4	0.4(4)	Fe1-C2-C3-Si1	-176.17(14)
C1-C2-C3-C4	168.4(4)	Si1-C3-C4-C5	79.9(3)
Si1-C3-C4-C13	-101.3(2)	C2-C3-C4-C5	-96.8(3)
C2-C3-C4-C13	82.1(3)	C13-C4-C5-C6	-0.8(4)
C5-C4-C13-C8	0.7(3)	C3-C4-C13-C8	-178.2(2)
C3-C4-C13-C12	1.1(4)	C3-C4-C5-C6	178.1(2)
C5-C4-C13-C12	180.0(2)	C4-C5-C6-C7	0.3(4)
C5-C6-C7-C8	0.4(4)	C6-C7-C8-C9	-179.2(3)
C6-C7-C8-C13	-0.5(4)	C13-C8-C9-C10	-0.3(4)
C7-C8-C13-C4	0.0(4)	C7-C8-C13-C12	-179.4(2)
C7-C8-C9-C10	178.4(3)	C9-C8-C13-C4	178.7(2)
C9-C8-C13-C12	-0.6(4)	C8-C9-C10-C11	0.7(4)
C9-C10-C11-C12	-0.3(4)	C10-C11-C12-C13	-0.6(4)
C11-C12-C13-C4	-178.3(2)	C11-C12-C13-C8	1.1(4)
Fe51-C501-C502-C503	172.1(4)	Fe51-C502-C503-Si51	175.28(14)
Fe51-C502-C503-C504	0.7(4)	C501-C502-C503-Si51	6.5(5)
C501-C502-C503-C504	-168.1(4)	Si51-C503-C504-C505	-80.4(3)
Si51-C503-C504-C513	101.5(2)	C502-C503-C504-C505	94.2(3)
C502-C503-C504-C513	-83.8(3)	C503-C504-C505-C506	-177.0(2)
C513-C504-C505-C506	1.1(4)	C503-C504-C513-C508	176.5(2)
C503-C504-C513-C512	-2.0(4)	C505-C504-C513-C508	-1.6(3)

C505-C504-C513-C512	179.9(2)	C504-C505-C506-C507	0.0(4)
C505-C506-C507-C508	-0.7(4)	C506-C507-C508-C509	-178.8(3)
C506-C507-C508-C513	0.3(4)	C507-C508-C509-C510	-179.9(3)
C513-C508-C509-C510	1.0(4)	C507-C508-C513-C504	0.9(3)
C507-C508-C513-C512	179.5(2)	C509-C508-C513-C504	180.0(2)
C509-C508-C513-C512	-1.5(4)	C508-C509-C510-C511	-0.1(5)
C509-C510-C511-C512	-0.5(5)	C510-C511-C512-C513	0.0(4)
C511-C512-C513-C504	179.5(3)	C511-C512-C513-C508	1.0(4)

Symmetry transformations used to generate equivalent atoms: