Supporting information for

Iron Promoted Conjugate Addition; Implication of the Six-Centered Mechanism Based on the Isolation of the Iron-enolate Intermediate

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Table S2. X-ray Crystallographic Data of (TMEDA)Fe(-O-C(Ph)=CHPh)$_2$ (**7**).

Experimental Procedure

General. All experiments were carried out under an argon atmosphere using standard Schlenk techniques or performed in a N_2-filled glovebox where solvents and reagents were stored. Benzene-d_6, was distilled from benzophenone kethyl. Tetramethylethylenediamine (TMEDA) was distilled from CaH_2. Dehydrated solvents, diethylether, THF, toluene, benzene, and hexane were purchased from Kanto Chemical CO. INC. and used without further purification. The other reagents were used as received. $[Fe(mesityl)_2]_2$[1] and $(TMEDA)_2Fe(mesityl)_2$[2] were prepared according to the literature methods. The ^1H and ^{13}C NMR spectra were recorded on a JEOL Lambda 600 or a Lambda 400 or a JNM−ECS400 spectrometer. Chemical shifts were given in ppm relative to the solvent signal. IR spectra were recorded on a JASCO FT/IR-550 spectrometer. Melting points were measured on a Yanaco micro melting point apparatus. HRMS spectrum was recorded on a JEOL Mstation JMS-70 apparatus. Elemental analyses were performed by a Perkin Elmer 2400/CHN analyzer.

Synthesis of (TMEDA)Fe(-O-C(Ph)=CHCH(Mesityl)(Anisyl))$_2$ (3). In a 50 mL schlenk tube, (TMEDA)Fe(mesityl)$_2$ (**1'**) (410 mg, 1.0 mmol) and 4-methoxychalcone (**2a**) (520 mg, 2.2 mmol) were dissolved in toluene (10 mL). The resulting solution was stirred for 3 h at room temperature. The solvent was removed in vacuo, and the resulting solid was washed with toluene/hexane (1/4). The resulting crude product was dissolved in THF/toluene, and hexane was added to this solution, cooled to –30 ^oC to afford **3** as colorless crystals in 75 % yield (665 mg, 0.75 mmol). M.p.: 196 ^oC. ^1H NMR (600MHz, C_6D_6, r.t.): δ 89.60, 62.13, 59.25, 36.10, 13.2 (br d), 8.68 (d), 8.12, 7.98, 7.30, 7.26, 7.20, 6.64, 6.18, 3.62, 3.56, 3.42, 3.23, 1.55, -12.86. Anal. Calcd. for $C_{56}H_{66}FeN_2O_4$; C, 75.83; H, 7.50; N, 3.16 %. Found C, 75.72; H, 7.77; N,2.99 %.

Reaction of (TMEDA)Fe(-O-C(Ph)=CHCH(Mesityl)(Anisyl))$_2$ (3) with NH_4Cl (aq). In a 20 mL schlenk tube was placed complex **3** (49 mg, 0.055 mmol) in toluene (2.5 mL), and a saturated aqueous solution of NH_4Cl was added to this solution. The mixed solution was stirred at room temperature for 15

min. After a standard aqueous work up, the ^{1}H NMR spectrum of the crude product indicated the quantitative formation of **4a**.

^{1}H NMR (400MHz, $CDCl_3$, r.t.): δ 7.98 (d, *J* = 7.2, 2H, C_6H_5), 7.57 (t, *J* = 7.2, 1H, C_6H_5), 7.47 (t, *J* = 7.2, 2H, C_6H_5), 6.93 (d, *J* = 8.7, 2H, C_6H_4), 6.83 (s, 2H, $C_6H_2Me_3$), 6.76 (d, *J* = 8.7, 2H, C_6H_4), 5.36 (dd, J_1 = 8.2, J_2 = 4.8, 1H, -C*H*CH_2-), 4.06 (dd, J_1 = 17.4, J_2 = 8.2, 1H, -CHC*H*$_2$-), 3.75 (s, 3H, OMe), 3.45 (dd, J_1 = 17.4, J_2 = 4.8, 1H, -CHC*H*$_2$-), 2.39-2.03 (br s, 6H, *ortho*-Me of $C_6H_3Me_3$), 2.25 (s, 3H, *para*-Me of $C_6H_2Me_3$). ^{13}C NMR (100MHz, $CDCl_3$, r.t.): δ 198.7, 157.5, 138.4, 137.0, 136.8, 135.8, 135.3, 133.0, 130.0(br), 128.6, 128.1, 127.7, 113.6, 55.1, 42.5, 37.6, 21.2, 20.7. IR (neat): ν 3058, 3032, 3000, 2953, 2916, 2863, 2835, 1685, 1609 1597, 1580, 1508, 1481, 1463, 1448, 1416, 1377, 1357, 1333, 1298, 1286, 1249, 1203, 1181, 1159, 1114, 1036, 1001, 984, 911, 852, 825, 771, 759, 743, 690, 648 cm^{-1}. HRMS (EI^+): Calcd for $C_{25}H_{26}O_2$ 358.1933 ; Found 358.1930.

Reaction of (TMEDA)Fe(-O-C(Ph)=CHCH(Mesityl)(Anisyl))$_2$ (3) with AcOH-d$_4$. In a 20 mL schlenk tube was placed complex **3** (49 mg, 0.055 mmol) in toluene (2.5 mL), and AcOH-d_4 (21 mg, 0.328 mmol) was added to this solution. The mixed solution was stirred at room temperature for 15 min, then a saturated aqueous solution of NH_4Cl was added to quench the reaction. After a standard aqueous work up, the product was purified by silica-gel column chromatography (hexane : AcOEt = 9 : 1) to give the product ***4a-d$_1$*** (96 %, 38 mg、0.106 mmol).

^{1}H NMR (400MHz, $CDCl_3$, r.t.): δ 7.98 (d, *J* = 7.2, 2H, C_6H_5), 7.57 (t, *J* = 7.2, 1H, C_6H_5), 7.47 (t, *J* = 7.2, 2H, C_6H_5), 6.93 (d, *J* = 8.7, 2H, C_6H_4), 6.83 (s, 2H, $C_6H_2Me_3$), 6.76 (d, *J* = 8.7, 2H, C_6H_4), 5.36 (d, *J* = 8.2, 1H, -C*H*CH_2-), 4.06 (d, *J* = 8.2, 1H, -CHC*H*$_2$-), 3.75 (s, 3H, OMe), 2.39-2.03 (br s, 6H, *ortho*-Me of $C_6H_3Me_3$), 2.25 (s, 3H, *para*-Me of $C_6H_2Me_3$). ^{13}C NMR (100MHz, $CDCl_3$, r.t.): δ 198.7, 157.5, 138.4, 137.0, 136.8, 135.8, 135.3, 133.0, 130.0 (br), 128.6, 128.1, 127.7, 113.6, 55.1, 42.4, 42.2, 42.0, 37.6, 21.2, 20.7.

Reaction of (TMEDA)Fe(-O-C(Ph)=CHCH(Mesityl)(Anisyl))$_2$ (3) with TMSX (X=OTf, Cl). In a 20 mL schlenk tube was placed complex **3** (89 mg, 0.10 mmol) in benzene (3 mL), and trimethylsilyltrifluoromethanesurfonate (TMSOTf) (44 mg, 0.20 mmol) or trimethylsilylchloride (TMSCl) (26 mg, 0.24 mmol) was added to this solution. The mixed solution was stirred at room temperature for 1h, then the solvent was removed under vaccum. The product was extracted with hexane, and the hexane solution was passed through a pad of Celite. The solution was removed in vacuo to give the crude product (50 mg). This crude product was dissolved in hexane, cooled to – 35 ^{o}C to afford **5** in 31 % yield (27 mg, 0.063 mmol).

^{1}H NMR (400MHz, $CDCl_3$, r.t.): δ 7.53 (d, *J* = 6.8, 2H, C_6H_5), 7.31 (t, *J* = 6.8, 2H, C_6H_5), 7.26 (t, *J* = 6.8, 1H, C_6H_5), 7.09 (d, *J* = 8.5, 2H, C_6H_4), 6.83 (s, 2H, $C_6H_2Me_3$), 6.81 (d, *J* = 8.5, 2H, C_6H_4), 5.69 (AB, J_1 = 23.7, J_2 = 9.7, 2H, -C*H*C*H*=C-), 3.79 (s, 3H, OMe), 2.26-2.21 (br s, 6H, *ortho*-Me of $C_6H_3Me_3$), 2.26 (s, 3H, *para*-Me of $C_6H_3Me_3$), 0.01 (s, 9H, $SiMe_3$). ^{13}C NMR (100MHz, $CDCl_3$, r.t.): δ 157.5, 150.6, 139.5, 138.1., 136.9, 136.6, 135.4, 129.9, 128.1, 128.0, 127.7, 126.1, 113.5, 112.0, 55.2, 40.6, 21.5, 20.7, 0.6. IR (KBr): ν 3443, 3065, 3029, 2863, 2838, 1642, 1608, 1578, 1507, 1480, 1445, 1377, 1342, 1322, 1280, 1249, 1213, 1173, 1114, 1102, 1077, 1049, 1036, 1022, 901, 842, 827, 759, 697, 673, 632 cm^{-1}. HRMS (FAB^{+}): Calcd for $C_{28}H_{34}O_2Si$ 430.2328; Found 430.2328.

Reaction of (TMEDA)Fe(mesityl) (1') with 4-methoxychalcone (2a). In a 20 mL schlenk tube was placed (TMEDA)Fe(mesityl)$_2$ (**1'**) (49 mg, 0.12 mmol) in toluene (3 mL), and toluene solution (1 mL) of 4-methoxychalcone (**2a**) (48 mg, 0.20 mmol) was added to this solution. The mixed solution was stirred at room temperature for 3 h, then a saturated aqueous solution of NH_4Cl was added to quench the reaction. After a standard aqueous work up, the product was purified by silica-gel column chromatography (hexane : AcOEt = 9 : 1) to give the product **4a** (97 %, 69.9 mg, 0.195 mmol).

Reaction of (TMEDA)Fe(mesityl) (1') with benzalacetone (2b). In a 20 mL schlenk tube was placed (TMEDA)Fe(mesityl)$_2$ (**1'**) (49 mg, 0.12 mmol) in toluene (3 mL), and toluene solution (1 mL) of

benzalacetone (**2b**) (29 mg, 0.20 mmol) was added to this solution. The mixed solution was stirred at room temperature for 3 h, then a saturated aqueous solution of NH_4Cl was added to quench the reaction. After a standard aqueous work up, the product was purified by silica-gel column chromatography (hexane : AcOEt = 9 : 1) to give the product **4b** (96 %, 50.5 mg, 0.190 mmol).

^{1}H NMR (400MHz, $CDCl_3$, r.t.): δ 7.23 (t, *J* = 7.2, 2H, C_6H_5), 7.15 (t, *J* = 7.2, 1H, C_6H_5), 6.99 (d, *J* = 7.2, 2H, C_6H_5), 6.83 (s, 2H, $C_6H_2Me_3$), 5.20 (dd, J_1 = 8.2, J_2 = 5.8, 1H, -C*H*CH_2-), 3.47 (dd, J_1 = 17.4, J_2 = 8.2, 1H, -CHC*H*$_2$-), 3.01 (dd, J_1 = 17.4, J_2 = 5.8, 1H, -CHC*H*$_2$-), 2.47-1.91 (br s, 6H, *ortho*-Me of $C_6H_3Me_3$), 2.26 (s, 3H, -C(=O)-Me), 2.17 (s, 3H, *para*-Me of $C_6H_3Me_3$). ^{13}C NMR (100MHz, $CDCl_3$, r.t.): δ 207.4, 143.2, 137.9, 136.8, 135.9, 130.0 (br), 128.2, 126.6, 125.6, 47.2, 38.2, 30.3, 21.2, 20.7. IR (neat): ν 3026, 3001, 2964, 2953, 2919, 1718, 1610, 1601, 1495, 1483, 1447, 1415, 1378, 1356, 1234, 1161, 1028, 911, 851, 763, 737, 729, 698, 579 cm^{-1}. HRMS (EI$^+$): Calcd for $C_{19}H_{22}O$ 266.1671 ; Found 266.1671.

Reaction of (TMEDA)Fe(mesityl) (**1'**) **with chalcone** (**2c**)**.** In a 20 mL schlenk tube was placed (TMEDA)Fe(mesityl)$_2$ (**1'**) (49 mg, 0.12 mmol) in toluene (3 mL), and toluene solution (1 mL) of chalcone (**2c**) (42 mg, 0.20 mmol) was added to this solution. The mixed solution was stirred at room temperature for 3 h, then a saturated aqueous solution of NH_4Cl was added to quench the reaction. After a standard aqueous work up, the product was purified by silica-gel column chromatography (hexane : AcOEt = 9 : 1) to give the product **4c** (92 %, 60.7 mg, 0.185 mmol).

^{1}H NMR (400MHz, $CDCl_3$, r.t.) δ 7.99 (d, *J* = 7.7, 2H, C_6H_5), 7.58 (t, *J* = 7.2, 1H, C_6H_5), 7.47 (t, *J* = 7.7, 2H, C_6H_5), 7.21 (t, *J* = 7.2, 2H, C_6H_5), 7.14 (t, *J* = 7.2, 1H, C_6H_5), 7.02 (d, *J* = 7.7, 2H, C_6H_5), 6.84 (s, 2H, $C_6H_2Me_3$), 5.44 (dd, J_1 = 8.2, J_2 = 4.8, 1H, -C*H*CH_2-), 4.11 (dd, J_1 = 17.4, J_2 = 8.2, 1H, -CHC*H*$_2$-), 3.46 (dd, J_1 = 17.4, J_2 = 4.8, 1H, -CHC*H*$_2$-), 2.47-1.91 (br s, 6H, *ortho*-Me of $C_6H_3Me_3$), 2.26 (s, 3H, *para*-Me of $C_6H_3Me_3$). ^{13}C NMR (100MHz, $CDCl_3$, r.t.): δ 198.6, 143.4, 138.4, 137.0, 136.9, 133.1, 130.0(br), 128.6, 128.2, 128.1, 126.7, 125.5, 42.4, 38.2, 21.3, 20.7. IR (neat): ν 3085, 3058, 3026, 3002, 2950, 2917, 2864, 1685, 1609, 1597, 1580, 1495, 1482, 1448, 1410, 1377, 1357, 1332, 1315, 1296,

1286, 1259, 1240, 1203, 1180, 1159, 1077, 1049, 1030, 1020, 1002, 983, 967, 920, 911, 852, 784, 768, 750, 739, 722, 697, 690, 650, 628 cm^{-1}. HRMS (EI^+): Calcd for $C_{24}H_{24}O$ 328.1827 ; Found 328.1822.

Reaction of (TMEDA)Fe(mesityl) (1') with 4-phenylpropenylketone (2d). In a 20 mL schlenk tube was placed (TMEDA)Fe(mesityl)$_2$ (**1'**) (49 mg, 0.12 mmol) in toluene (3 mL), and toluene solution (1 mL) of 4-phenylpropenylketone (**2d**) (29 mg, 0.20 mmol) was added to this solution. The mixed solution was stirred at room temperature for 3 h, then a saturated aqueous solution of NH_4Cl was added to quench the reaction. After a standard aqueous work up, the product was purified by silica-gel column chromatography (hexane : AcOEt = 9 : 1) to give the product **4d** (94 %, 50.0 mg, 0.188 mmol).

^{1}H NMR (400MHz, $CDCl_3$, r.t.): δ 7.93 (t, *J* = 7.2, 2H, C_6H_5), 7.55 (t, *J* = 7.2, 1H, C_6H_5), 7.45 (d, *J* = 7.2, 2H, C_6H_5), 6.83 (s, 2H, $C_6H_2Me_3$), 4.02 (ddt, J_1 = 16.4, J_2 = 4.8, J_3 = 7.2, 1H, -C*H*Me), 3.44 (dd, J_1 = 16.4, J_2 = 8.7, 1H, -CHC*H*$_2$-), 3.35 (dd, J_1 = 16.4, J_2 = 4.8, 1H, -CHC*H*$_2$-), 2.61-2.26 (br, 6H, *ortho*-Me of $C_6H_3Me_3$), 2.24 (s, 3H, *para*-Me of $C_6H_3Me_3$), 1.37 (d, *J* = 7.2, 3H, -CH*Me*). ^{13}C NMR (100MHz, $CDCl_3$, r.t.): δ 199.4, 139.3, 137.1, 136.0(br), 135.3, 132.9, 131.1(br), 129.3(br), 128.5, 128.0, 44.4, 30.0, 21.5(br), 20.6, 19.2. IR (neat): ν 2964, 2921, 2873, 1687, 1611, 1597, 1580, 1482, 1459, 1448, 1380, 1369, 1347, 1316, 1286, 1269, 1247, 1221, 1204, 1180, 1028, 1102, 992, 851, 755, 742, 690, 646 cm^{-1}. HRMS (EI^+): Calcd for Calcd for $C_{19}H_{22}O$ 266.1671; Found 266.1669.

Reaction of (TMEDA)Fe(mesityl) (1') with 3-hepten-2-one (2e). In a 20 mL schlenk tube was placed (TMEDA)Fe(mesityl)$_2$ (**1'**) (49 mg, 0.12 mmol) in toluene (3 mL), and toluene solution (1 mL) of 3-hepten-2-one (**2e**) (22 mg, 0.20 mmol) was added to this solution. The mixed solution was stirred at room temperature for 3 h, then a saturated aqueous solution of NH_4Cl was added to quench the reaction. After a standard aqueous work up, the product was purified by silica-gel column chromatography (hexane : AcOEt = 9 : 1) to give the product **4e** (83 %, 38.4 mg, 0.165 mmol).

^{1}H NMR (400MHz, $CDCl_3$, r.t.): δ 6.80 (br s, 1H, C_6H_2Me), 6.78 (br s, 1H, C_6H_2Me), 3.80-3.70 (m, 1H, C*H*(Mes)), 2.88-2.75 (m, 2H,- C(=O)-CH_2-), 2.36 (br s, 3H, *ortho*-Me of $C_6H_3Me_3$), 2.35 (br s, 3H,

ortho-Me of $C_6H_3Me_3$), 2.22 and 2.05 (s, 3H x 2, *para*-Me of $C_6H_3Me_3$ and -C(=O)Me), 2.05 (s, 3H, Me), 1.77-1.57 (m, 2H, -C*H*$_2$-), 1.33-1.06 (m, 2H, -C*H*$_2$-), 0.85 (t, *J* = 7.2, 3H, -CH$_2$*Me*). ^{13}C NMR (100MHz, $CDCl_3$, r.t.): δ: 208.1, 137.8, 137.0 (br), 135.8 (br), 135.2, 131.0 (br), 129.2 (br), 48.8, 36.7, 34.9, 30.3, 21.7(br), 21.4(br), 21.3, 20.6, 14.3. IR (neat): ν 3003, 2956, 2929, 2871, 1717, 1611, 1481, 1465, 1456, 1428, 1423, 1407, 1377, 1355, 1301, 1287, 1258, 1233, 1163, 1107, 1024, 1017, 851, 736 cm^{-1}. HRMS (EI$^+$): Calcd for $C_{16}H_{24}O$ 232.1827; Found 232.1829.

Reaction of (TMEDA)Fe(mesityl) (1') with methylvinylketone (2f). In a 20 mL schlenk tube was placed (TMEDA)Fe(mesityl)$_2$ (**1'**) (49 mg, 0.12 mmol) in toluene (3 mL), and toluene solution (1 mL) of methylvinylketone (**2f**) (14 mg, 0.20 mmol) was added to this solution. The mixed solution was stirred at room temperature for 3 h, then a saturated aqueous solution of NH_4Cl was added to quench the reaction. After a standard aqueous work up, the product was purified by silica-gel column chromatography (hexane : AcOEt = 9 : 1) to give the product **4f** (39 %, 15.1 mg, 0.079 mmol).

^{1}H NMR (400MHz, $CDCl_3$, r.t.): δ 6.84 (s, 2H, C_6H_2Me), 2.91-2.84 (m, 2H, -CH_2CH_2-), 2.61-2.54 (m, 2H, -CH_2CH_2-), 2.27 (s, 6H, *ortho*-Me of $C_6H_3Me_3$), 2.25 and 2.18 (s, 3H x 2, *para*-Me of $C_6H_3Me_3$ and -C(=O)Me). ^{13}C NMR (100MHz, $CDCl_3$, r.t.): δ 208.3, 135.9, 135.4, 134.4, 129.0, 42.8, 29.8, 23.3, 20.7, 19.6. IR (neat): ν 3002, 2962, 2918, 2863, 1715, 1613, 1578, 1485, 1464, 1447, 1412, 1362, 1281, 1257, 1222, 1207, 1160, 1037, 1025, 1014, 945, 853, 723 cm^{-1}. HRMS (EI$^+$): Calcd for $C_{13}H_{18}O$ 190.1358; Found 190.1352.

Reaction of (TMEDA)Fe(mesityl) (1') with *trans*-cinnamaldehyde (2g). In a 20 mL schlenk tube was placed (TMEDA)Fe(mesityl)$_2$ (**1'**) (49 mg, 0.12 mmol) in toluene (3 mL), and toluene solution (1 mL) of *trans*-cinnamaldehyde (**2g**) (26 mg, 0.20 mmol) was added to this solution. The mixed solution was stirred at room temperature for 3 h, then a saturated aqueous solution of NH_4Cl was added to quench the reaction. After a standard aqueous work up, the product was purified by silica-gel column chromatography (hexane : AcOEt = 9 : 1) to give the product **4g** (92 %, 46.2 mg, 0.183 mmol).

^{1}H NMR (400MHz, $CDCl_3$, r.t.): δ 7.39-7.18 (m, 5H, C_6H_5), 6.86 (s, 2H, C_6H_2Me), 6.58-6.45 (m, 2H, -C*H*=C*H*-), 5.88 (t, *J* = 3.8, 1H, -C*H*(OH)(Mes)), 2.42 (s, 6H, *ortho*-Me of $C_6H_3Me_3$), 2.27 (s, 3H, *parao*-Me of $C_6H_3Me_3$), 1.89 (d, *J* = 3.8, 1H, -CH(O*H*)(Mes)). ^{13}C NMR (100MHz, $CDCl_3$, r.t.): δ 137.1, 136.9, 136.5, 135.1, 130.3, 130.0, 129.5, 128.5, 127.4, 126.4, 71.1, 20.8, 20.6. IR (neat): ν 3370, 3026, 2918, 2370, 2344, 1609, 1577, 1493, 1448, 1377, 1005, 964, 849, 770, 722, 694 cm^{-1}. HRMS (EI^+): Calcd for $C_{18}H_{20}O$ 252.1514; Found 252.1511.

Reaction of (TMEDA)Fe(mesityl)$_2$ (1') with 2-cyclohexenone. In a 20 mL schlenk tube was placed (TMEDA)Fe(mesityl)$_2$ (**1'**) (49 mg, 0.12 mmol) in toluene (3 mL), and toluene solution (1 mL) of 2-cyclohexenone (19 mg, 0.20 mmol) was added to this solution. The resulting solution was stirred for 3 h at -20 ^{o}C. The solvent was removed in vacuo, and the resulting solid was dissolved in hexane. This hexane solution was passed through a pad of Celite, then the solvent was removed under vacuum to afford colorless oil. The product **6** was characterized by ^{1}H NMR spectrum by comparison with previous literature,[3] and the yield of **6** was determined by ^{1}H-NMR analysis in $CDCl_3$ with ferrocene as an internal standard. Yield: 52 %.

Reaction of (TMEDA)Fe(mesityl) (1') with acetone-d$_6$. In a 20 mL schlenk tube was placed (TMEDA)Fe(mesityl)$_2$ (**1'**) (41 mg, 0.10 mmol) in toluene (3 mL), and acetone-d_6 (13 mg, 0.20 mmol) was added to this solution. The mixed solution was stirred at room temperature for 1 h, then a saturated aqueous solution of NH_4Cl was added to quench the reaction. After a standard aqueous work up, the product was extracted with ethyl acetate, and the solvent was removed in vacuo. The formation of 2-deuterio-1,3,5-trimethylbenzene was determined by GC-MS analysis and ^{1}H NMR spectrum.

Synthesis of (TMEDA)Fe(-O-C(Ph)=CHPh)$_2$ (7). In a 50 mL schlenk tube, (TMEDA)Fe(mesityl)$_2$ (**1'**) (60 mg, 0.15 mmol) and benzylphenylketone (57 mg, 0.29 mmol) were dissolved in toluene (3.5 mL). The resulting solution was stirred for 16 h at 60 ^{o}C. The solvent was removed in vacuo, and the

resulting solid was dissolved in THF. Hexane was added to this solution, cooled to –30 °C to afford **7** as brown crystals in 46 % yield (38 mg, 0.068 mmol). M.p.: 186 °C. ^{1}H NMR (600MHz, C_6D_6, r.t.): δ 95.17, 62.38, 38.69, 26.88, 13.18, 6.07, 3.80, -5.55, -8.85. Anal. Calcd. for $C_{34}H_{38}FeN_2O_2$; C, 72.60; H, 6.81; N, 4.98 %. Found C, 72.21; H, 6.87; N, 4.65 %.

Synthesis of 3-(4-methoxyphenyl)-1,3-diphenylpropan-1-one (9) using a catalytic amount of $FeCl_2$ (no TMEDA condition). To a THF solution (2.0 mL) of 2-(4-methoxyphenyl)-4,4,5,5,-tetramethyl-1,3,2-dioxaborolane (0.176 g, 0.75 mmol) was added n-BuLi (0.44 mL, 1.60 M in hexane, 0.70 mmol) at –42 °C. The reaction mixture was stirred at the same temperature for 30 min and at 0 °C for 30 min. The solvent was removed *in vacuo* at 0 °C. To the residual borate was added THF (2.0 mL) and $FeCl_2$ (3.2 mg, 0.025 mmol, 5.0 mol%) at 0 °C. After 5 min, chalcone (**2c**) (0.104 g, 0.50 mmol) was added at this temperature. The reaction was carried out at 60 °C for 1 h. The resulting mixture was cooled to ambient temperature and was added saturated aqueous NH_4Cl. The aqueous layer was extracted four times with EtOAc. The combined organics were passed through a pad of Florisil® and were concentrated *in vacuo*. ^{1}H NMR analysis using pyrazine as an internal standard revealed that the title compound **9** was obtained in 96% yield; Rf = 0.21 (hexane/EtOAc = 20/1); ^{1}H NMR (392 MHz, $CDCl_3$) δ 3.70 (d, *J* = 7.17 Hz, 2H, $Ar_2HCH_2CC(O)$-), 3.75 (s, 3H, H_3CO-), 4.77 (t, *J* = 7.64 Hz, 1H, $Ar_2HCH_2CC(O)$-), 6.79-6.82 (m, 2H, 3-H_2-4-$MeOC_6H_2$-), 7.14-7.19 (m, 3H, 2-H_2-4-$MeOC_6H_2$- and C_6H_5-), 7.24-7.29 (m, 4H, C_6H_5-), 7.43 (t, *J* = 7.64 Hz, 2H, 3-$H_2C_6H_3C(O)$-), 7.54 (t, *J* = 7.64 Hz, 1H, 4-$HC_6H_4C(O)$-), 7.93 (m, 2H, 2-$H_2C_6H_3C(O)$-); ^{13}C NMR (99 MHz, $CDCl_3$) δ 44.9, 45.1, 55.2, 113.9, 126.3, 127.7, 128.0, 128.5, 128.6, 128.7, 133.0, 136.2, 137.0, 144.5, 158.0, 198.1; IR (neat) ν 3061, 3027, 2930, 2835, 1683, 1610, 1597, 1580, 1509, 1494, 1448, 1361, 1302, 1245, 1204, 1177, 1111, 1076, 1031, 1001, 981, 921, 827, 750, 689; HRMS (FAB) M^+ Calcd for $C_{22}H_{20}O_2$ 316.1463. Found 316.1463.

Synthesis of 3-(4-methoxyphenyl)-1,3-diphenylpropan-1-one (9) using a catalytic amount of $FeCl_2$. To a THF solution (2.0 mL) of 2-(4-methoxyphenyl)-4,4,5,5,-tetramethyl-1,3,2-dioxaborolane (0.176 g, 0.75 mmol) was added n-BuLi (0.44 mL, 1.60 M in hexane, 0.70 mmol) at –42 °C. The reaction mixture was stirred at the same temperature for 30 min and at 0 °C for 30 min. The solvent was removed *in vacuo* at 0 °C. To the residual borate was added THF (2.0 mL), *N*,*N*,*N*',*N*'-tetramethylethylenediamine (2.9 mg, 0.025 mmol, 5.0 mol%) and $FeCl_2$ (3.2 mg, 0.025 mmol, 5.0 mol%) at 0 °C. After 5 min, chalcone (**2c**) (0.104 g, 0.50 mmol) was added at this temperature. The reaction was carried out at 60 °C for 1 h. The resulting mixture was cooled to ambient temperature and was added saturated aqueous NH_4Cl. The aqueous layer was extracted four times with EtOAc. The combined organics were passed through a pad of Florisil® and were concentrated *in vacuo*. ^1H NMR analysis using pyrazine as an internal standard revealed that the title compound **9** was obtained in 97% yield.

X-ray data collection and reduction. X-ray crystallography was performed on a Rigaku Saturn CCD area detector with graphite monochromated Mo-Kα radiation (λ = 0.71070 A). The data were collected at 123(2) K using□ ω scan in the θ range of $3.0 \leq \theta \leq 27.5$ deg (**3**) and $3.2 \leq \theta \leq 27.5$ deg (**7**). The data obtained were processed using Crystal-Clear (Rigaku) on a Pentium computer, and were corrected for Lorentz and polarization effects. The structure was solved by direct methods[4] for **3** and **7**, and expanded using Fourier techniques.[5] The non-hydrogen atoms were refined anisotropically except for the disordered carbon atoms. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement on F^2 was based on 11,203 observed reflections and 634 variable parameters for **3** and 6,279 observed reflections and 390 variable parameters for **7**. Neutral atom scattering factors were taken from Cromer and Waber.[6] All calculations were performed using the CrystalStructure[7,8] crystallographic software package. Details of final refinement as well as the bond distances and angles are summarized in the supporting information, and the numbering scheme employed is also shown in the supporting information, which were drawn with ORTEP at 50%

probability ellipsoid. CCDC 888725 (**3**) and 888724 (**7**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

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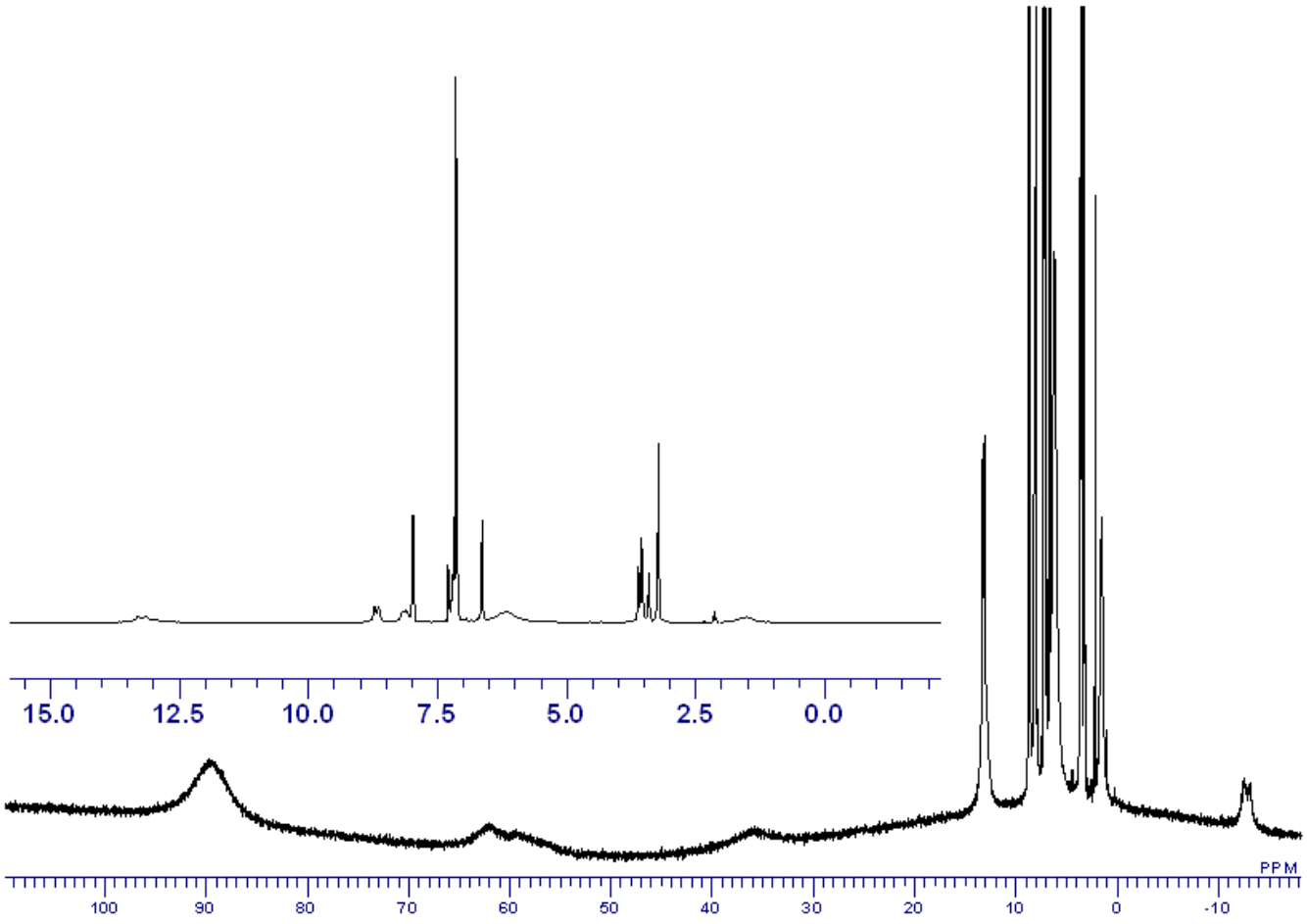
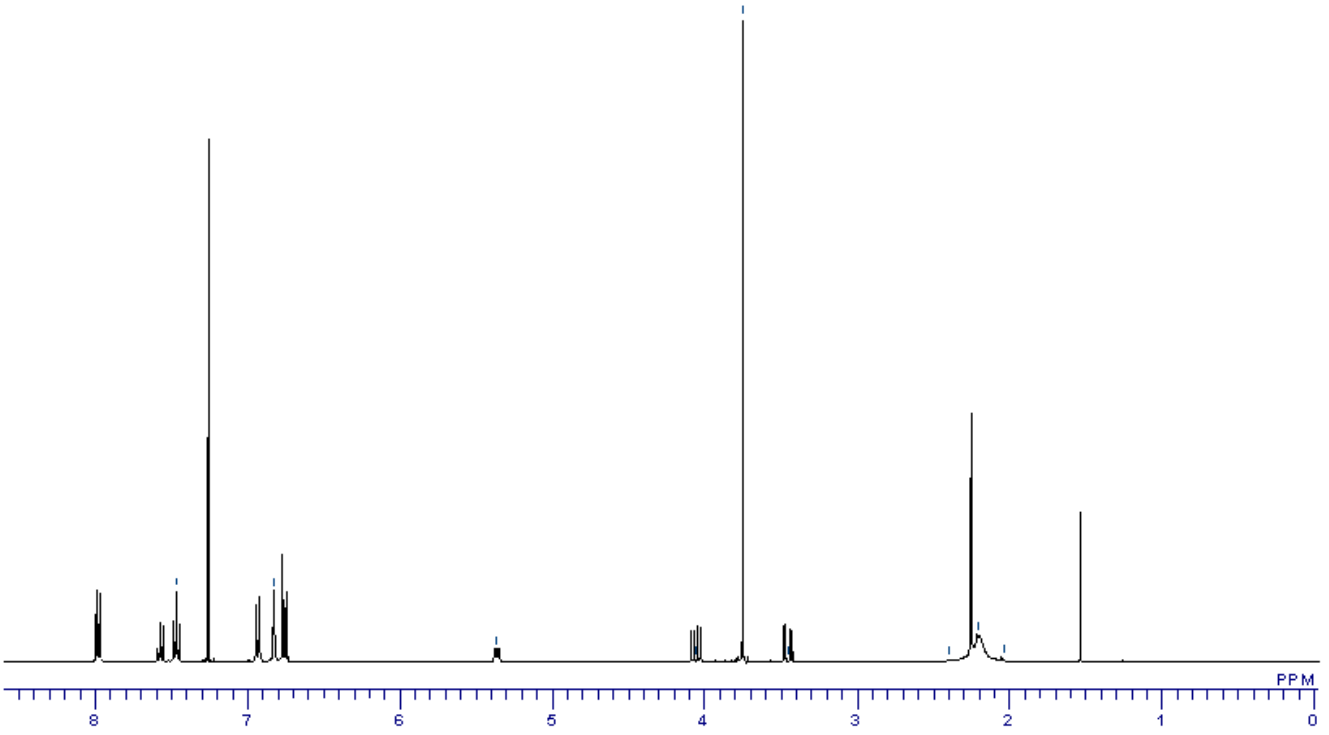
Figure S1. ^{1}H NMR spectrum of (TMEDA)Fe(-O-C(Ph)=CHCH(Mesityl)(Anisyl))$_2$ (**3**)

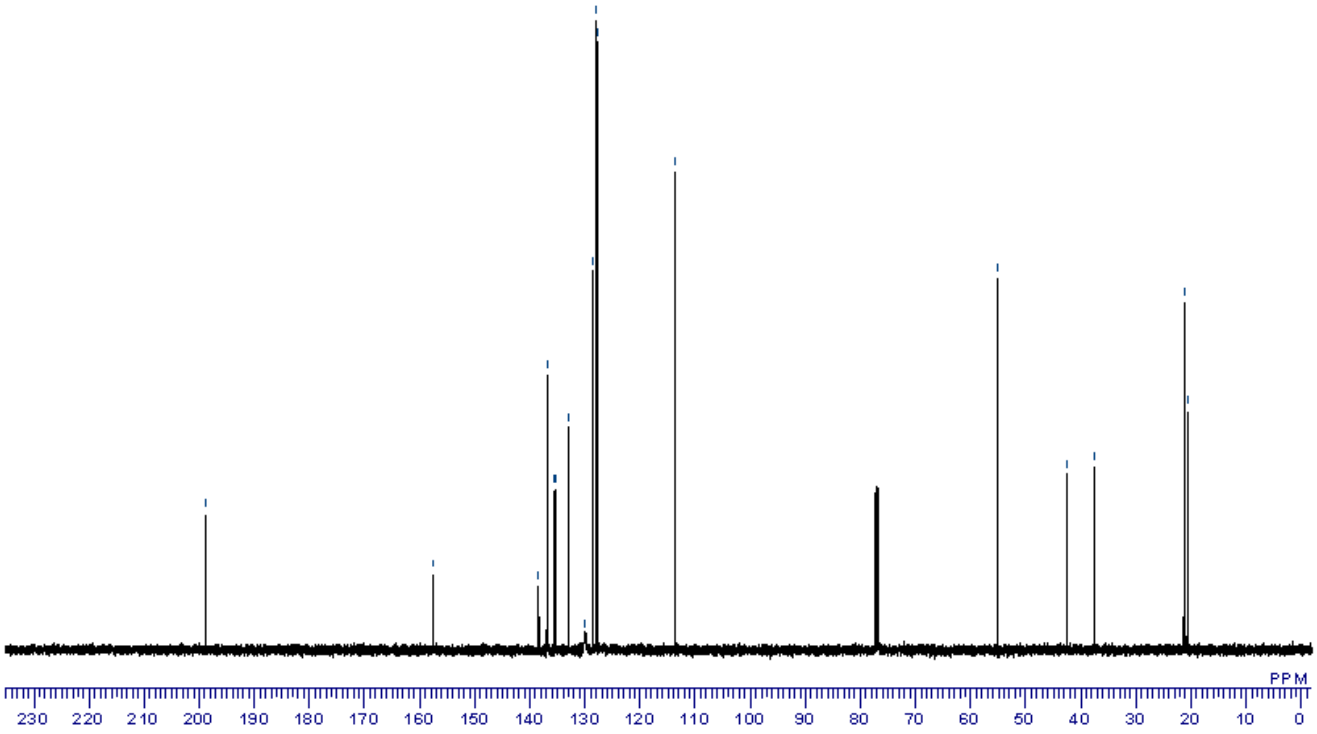


(^{1}H NMR in C_6D_6)

Figure S4. ^{1}H and ^{13}C NMR spectra of **4a**

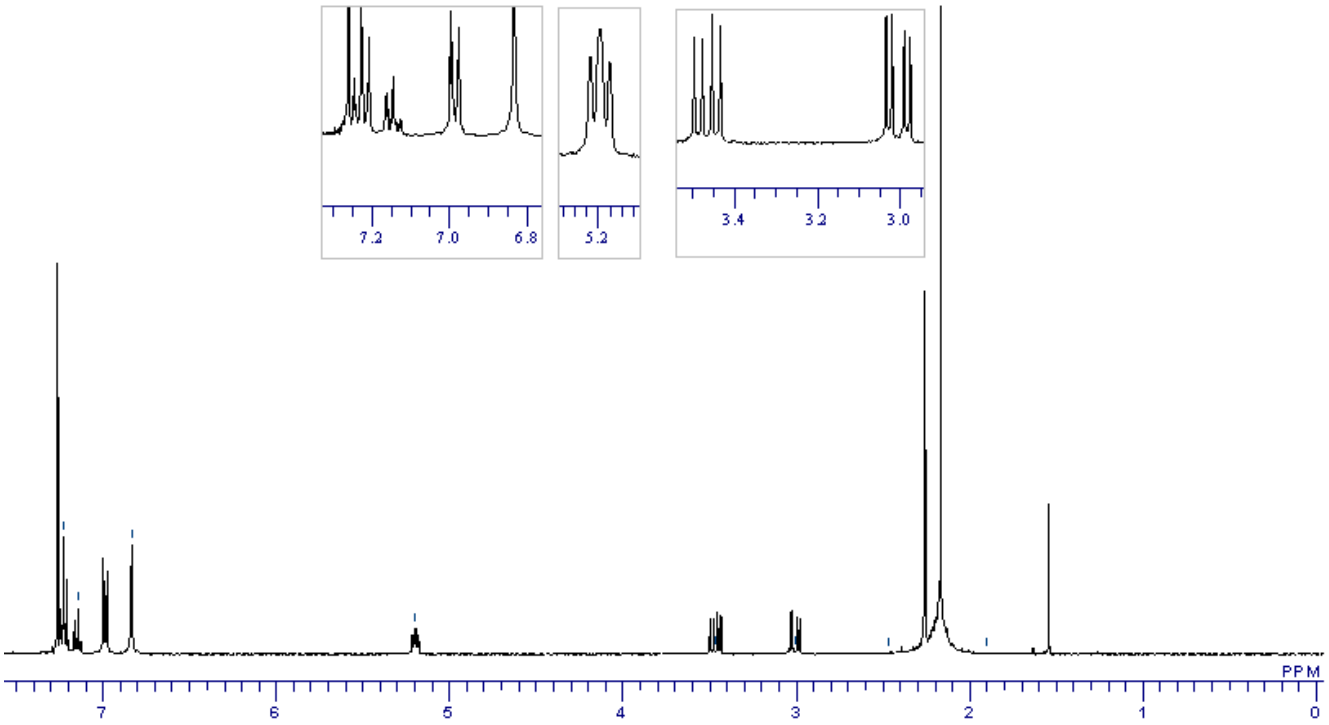


(^{1}H NMR in $CDCl_3$)

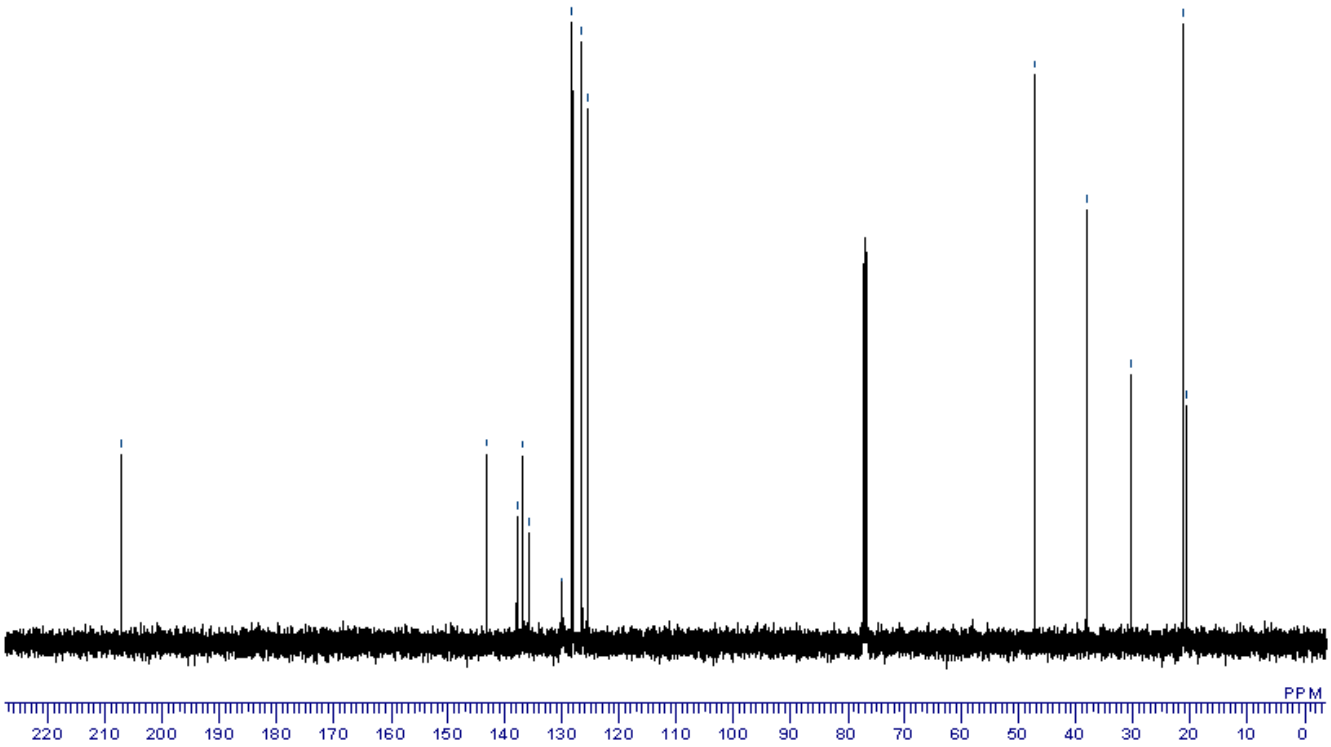


(^{13}C NMR in $CDCl_3$)

Figure S2. ^{1}H and ^{13}C NMR spectra of **4b**

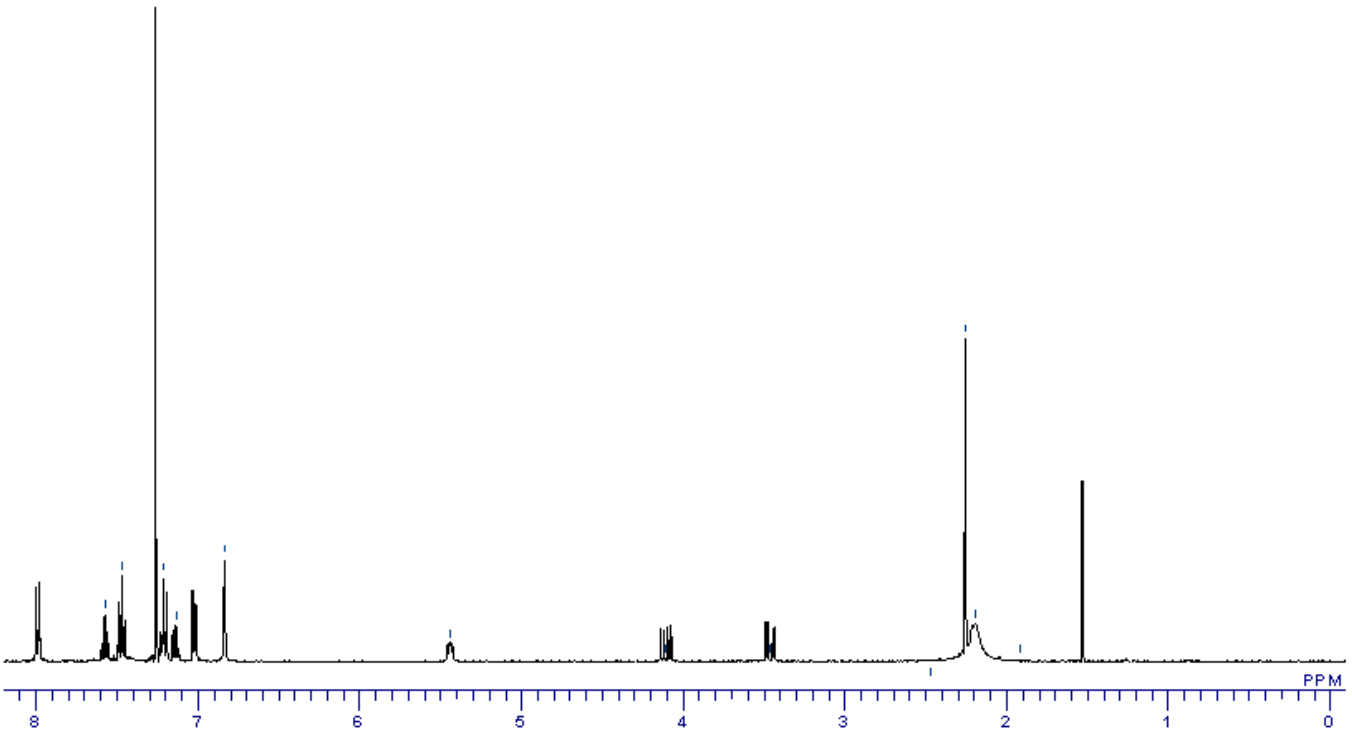


(^{1}H NMR in $CDCl_3$)

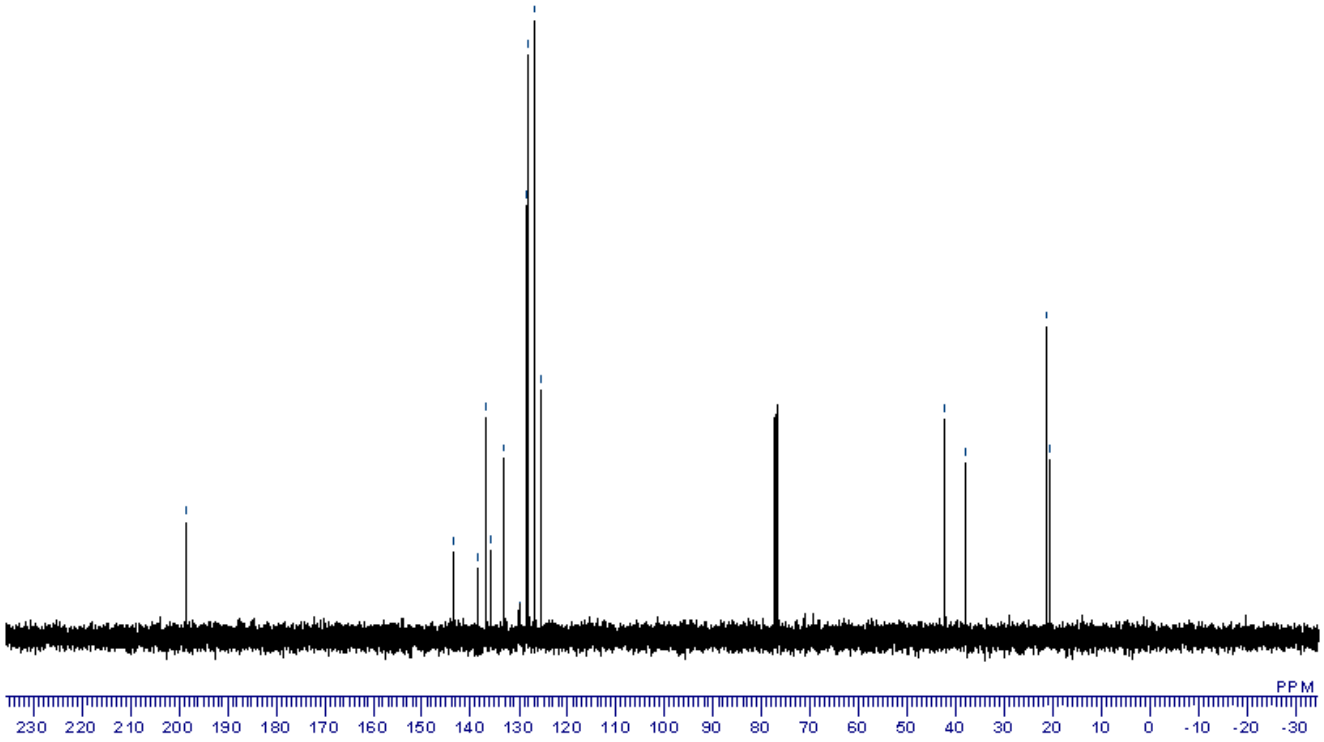


(^{13}C NMR in $CDCl_3$)

Figure S3. ^{1}H and ^{13}C NMR spectra of **4c**

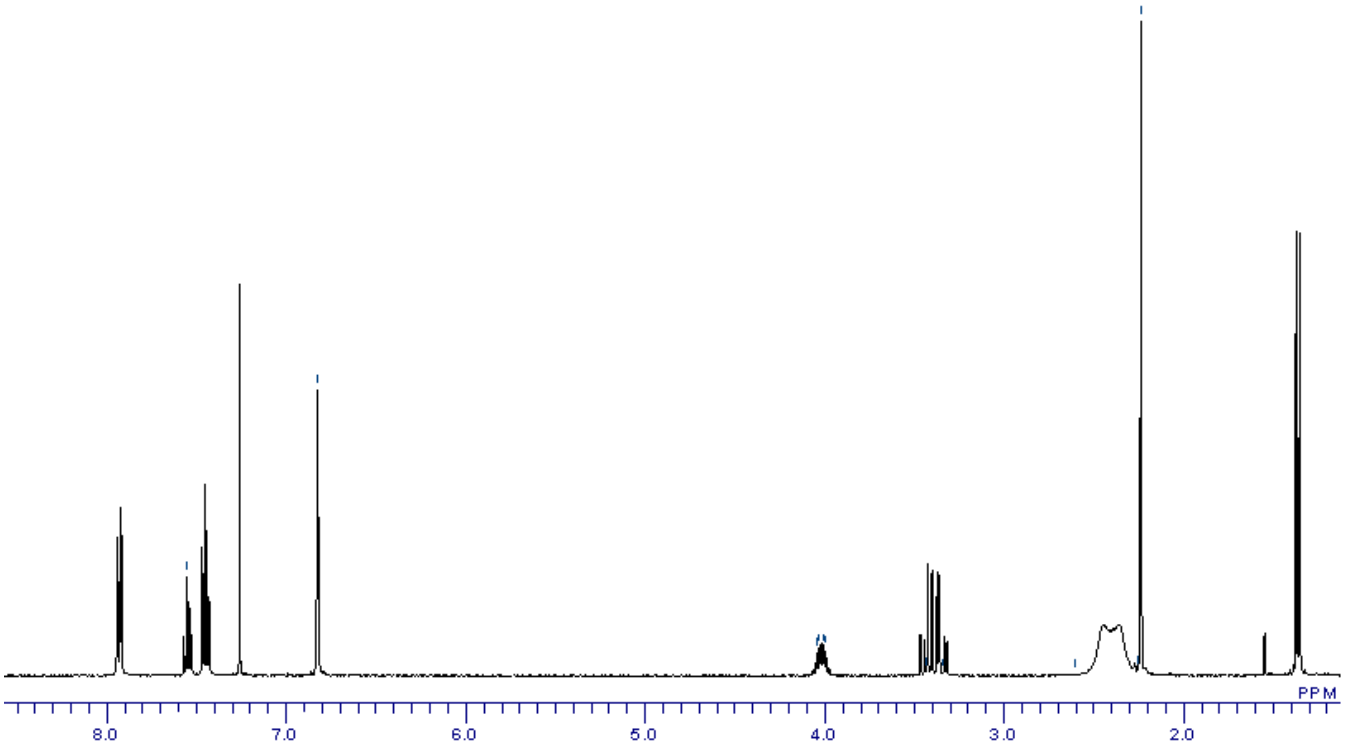


(^{1}H NMR in $CDCl_3$)

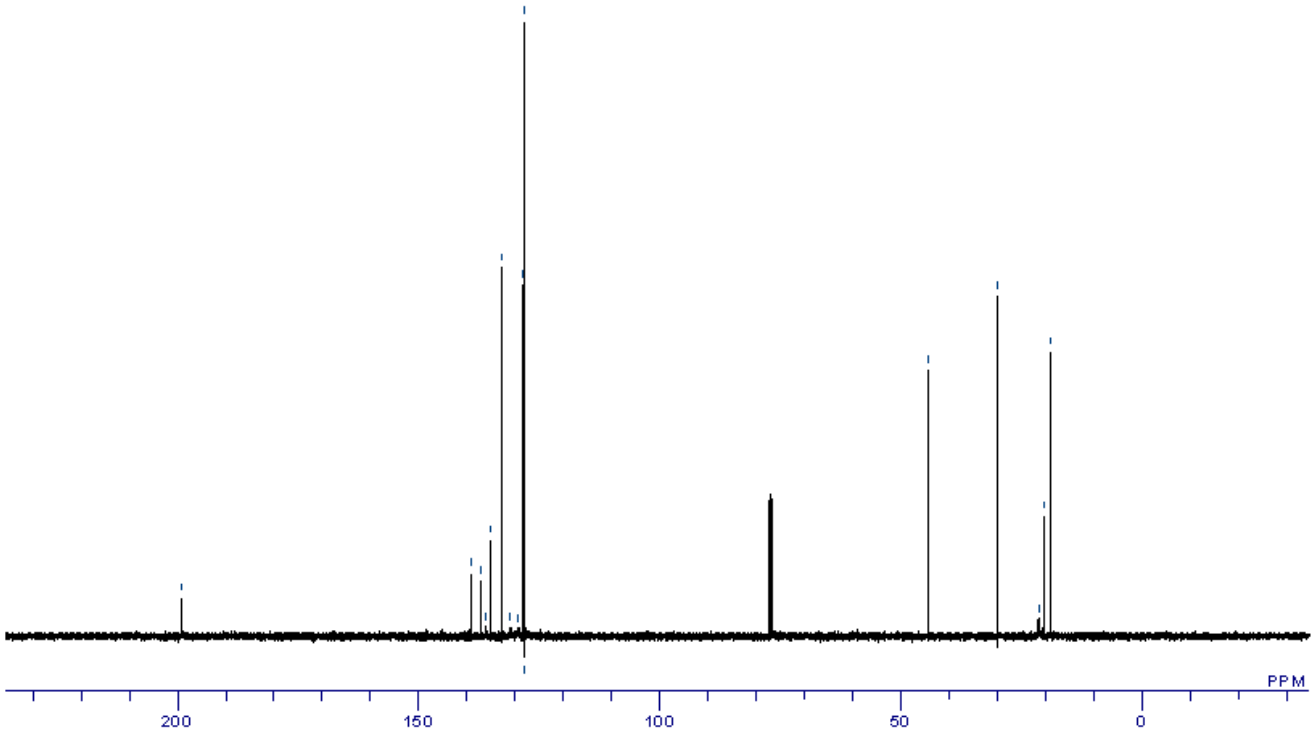


(^{13}C NMR in $CDCl_3$)

Figure S5. ^{1}H and ^{13}C NMR spectra of **4d**

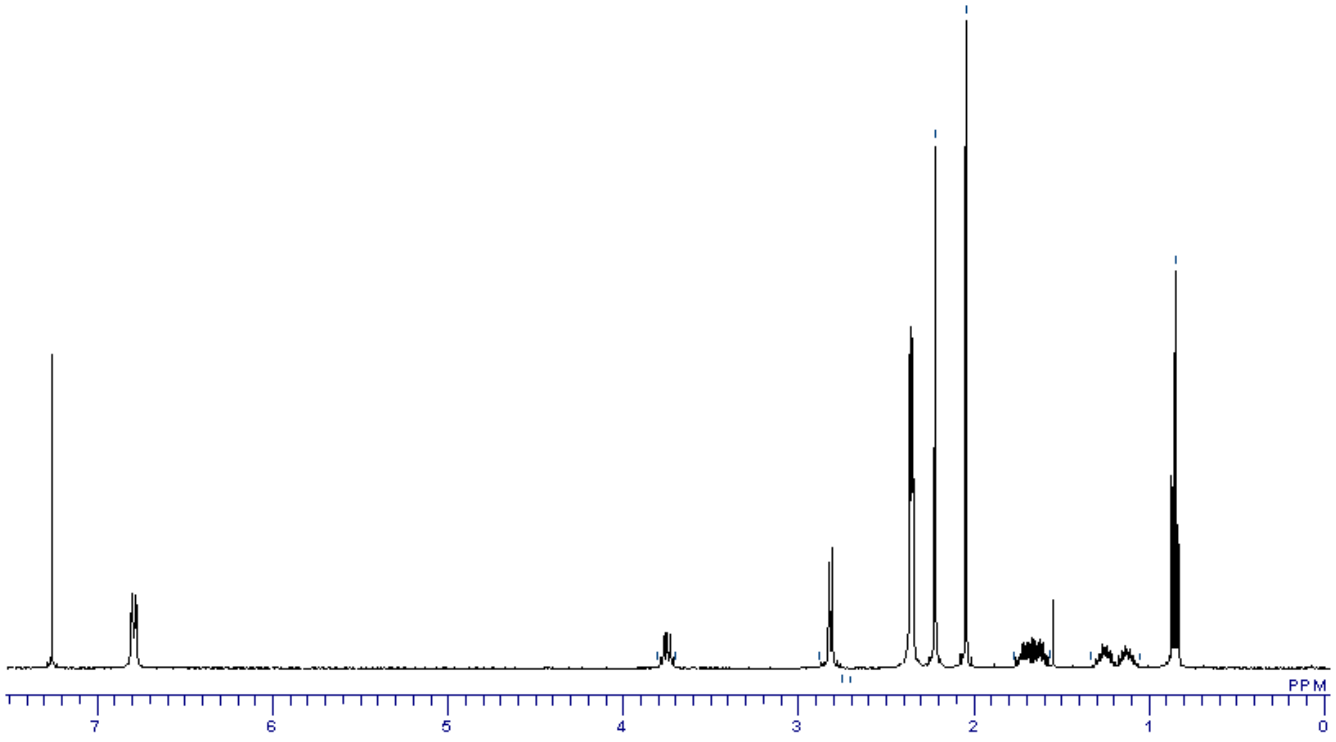


(^{1}H NMR in $CDCl_3$)

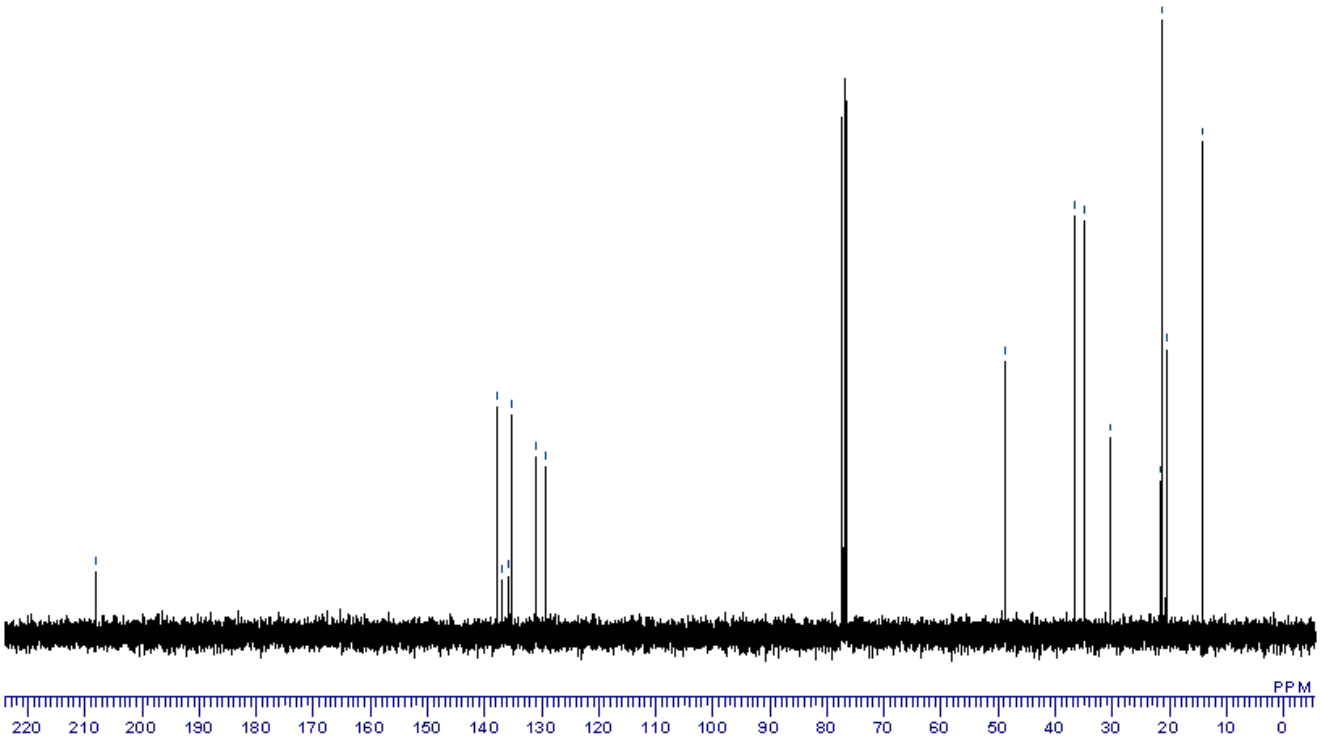


(^{13}C NMR in $CDCl_3$)

Figure S6. ^{1}H and ^{13}C NMR spectra of **4e**

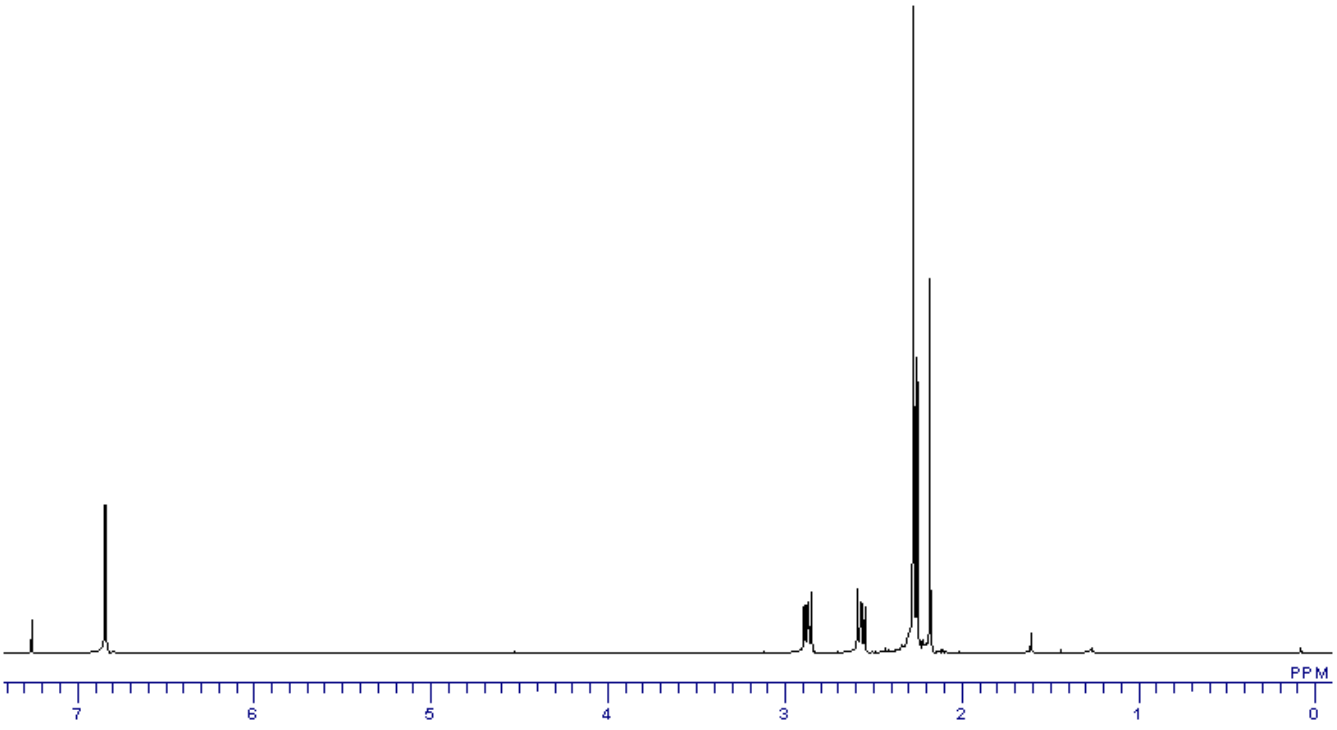


(^{1}H NMR in $CDCl_3$)

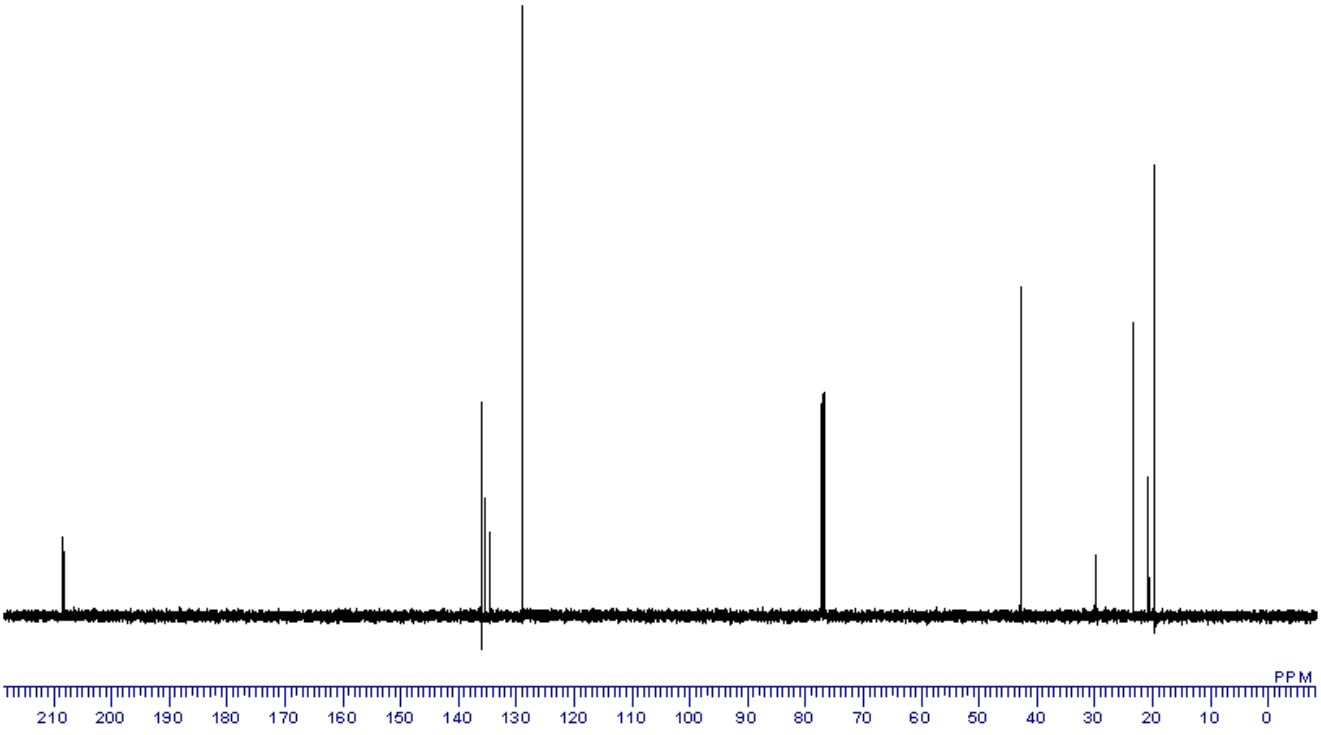


(^{13}C NMR in $CDCl_3$)

Figure S7. ^{1}H and ^{13}C NMR spectra of **4f**

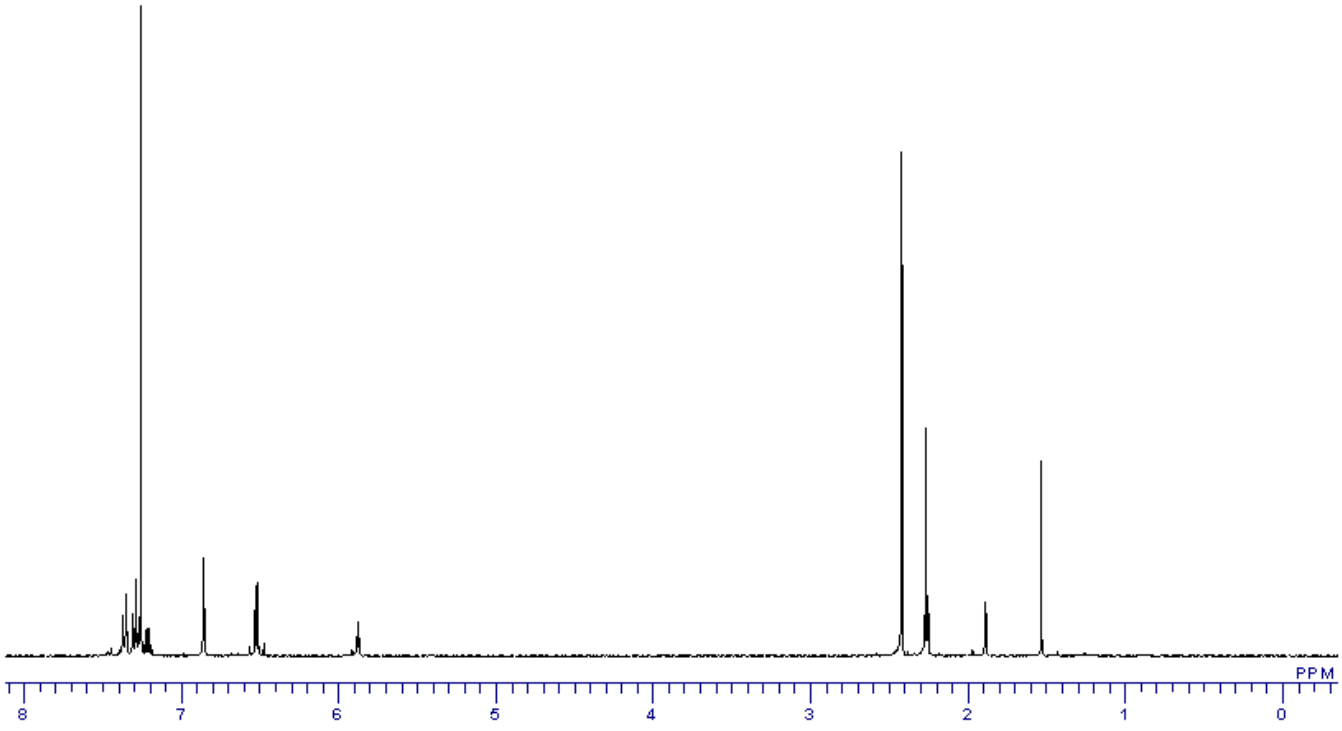


(^{1}H NMR in $CDCl_3$)

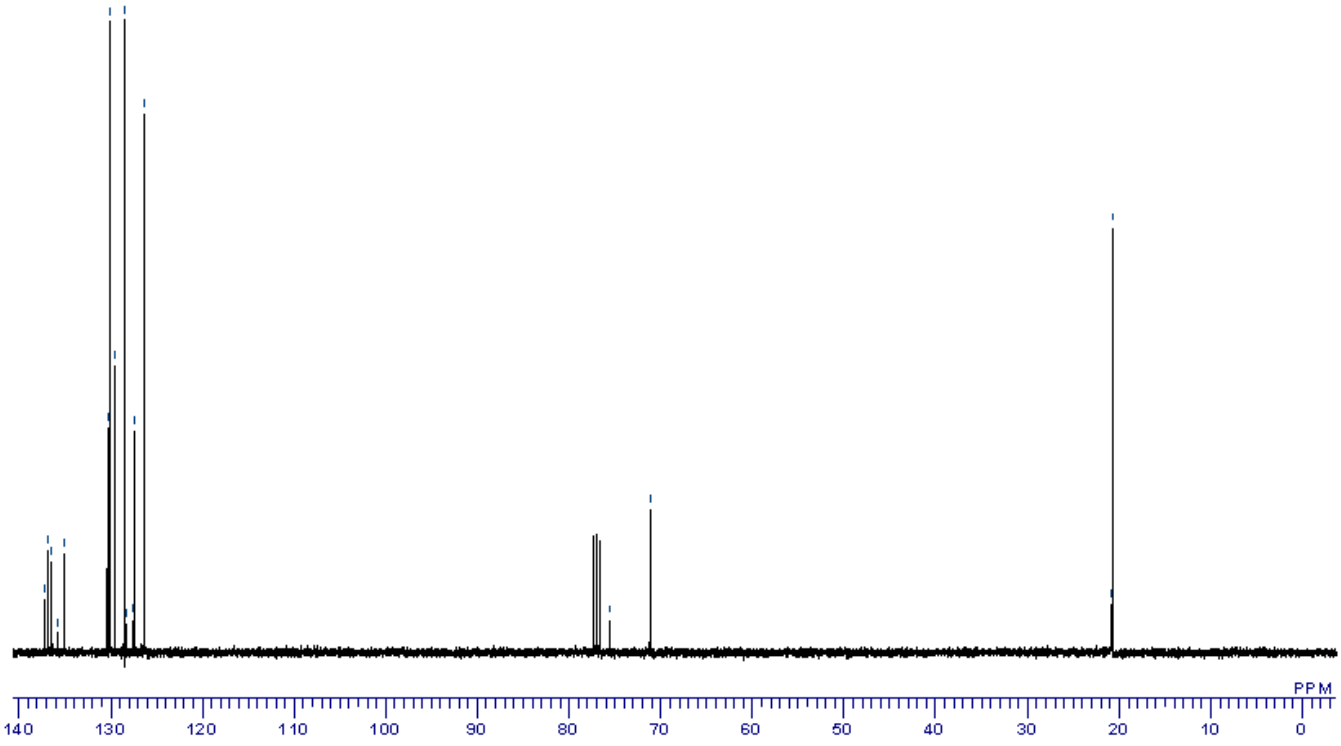


(^{13}C NMR in $CDCl_3$)

Figure S8. ^{1}H and ^{13}C NMR spectra of **4g**

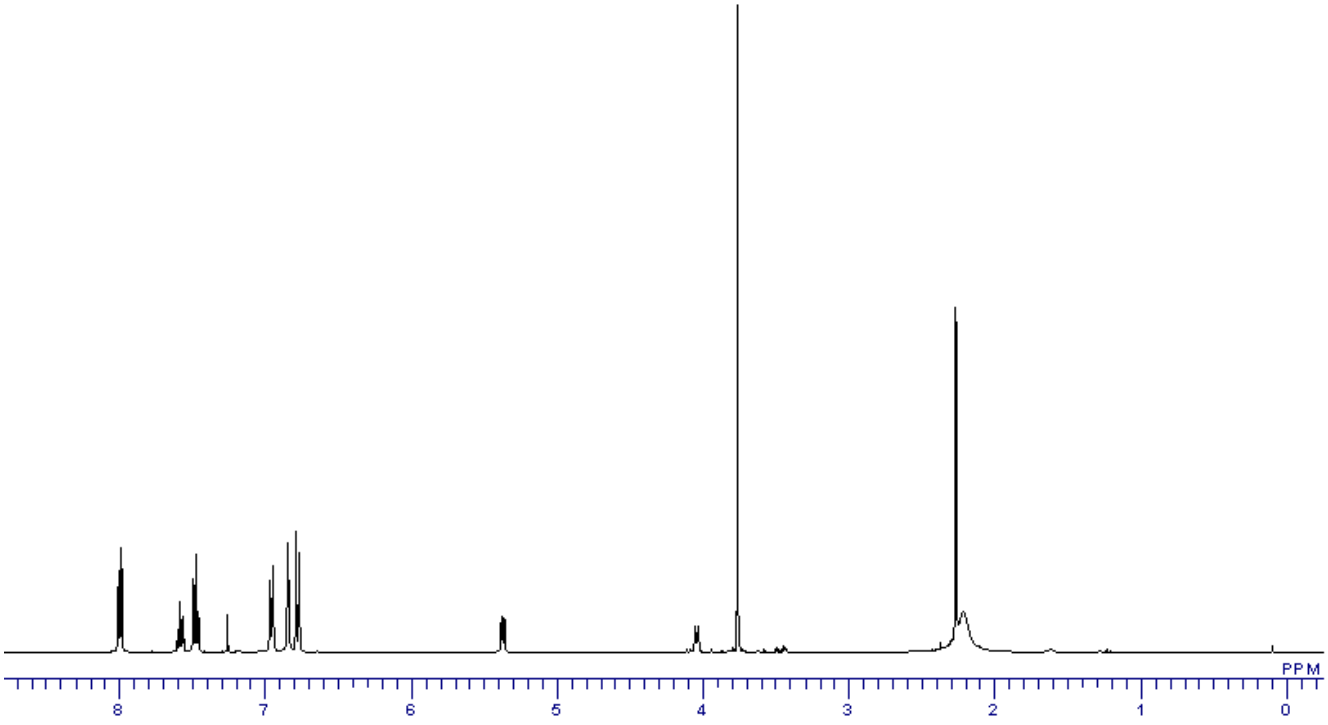


(^{1}H NMR in $CDCl_3$)

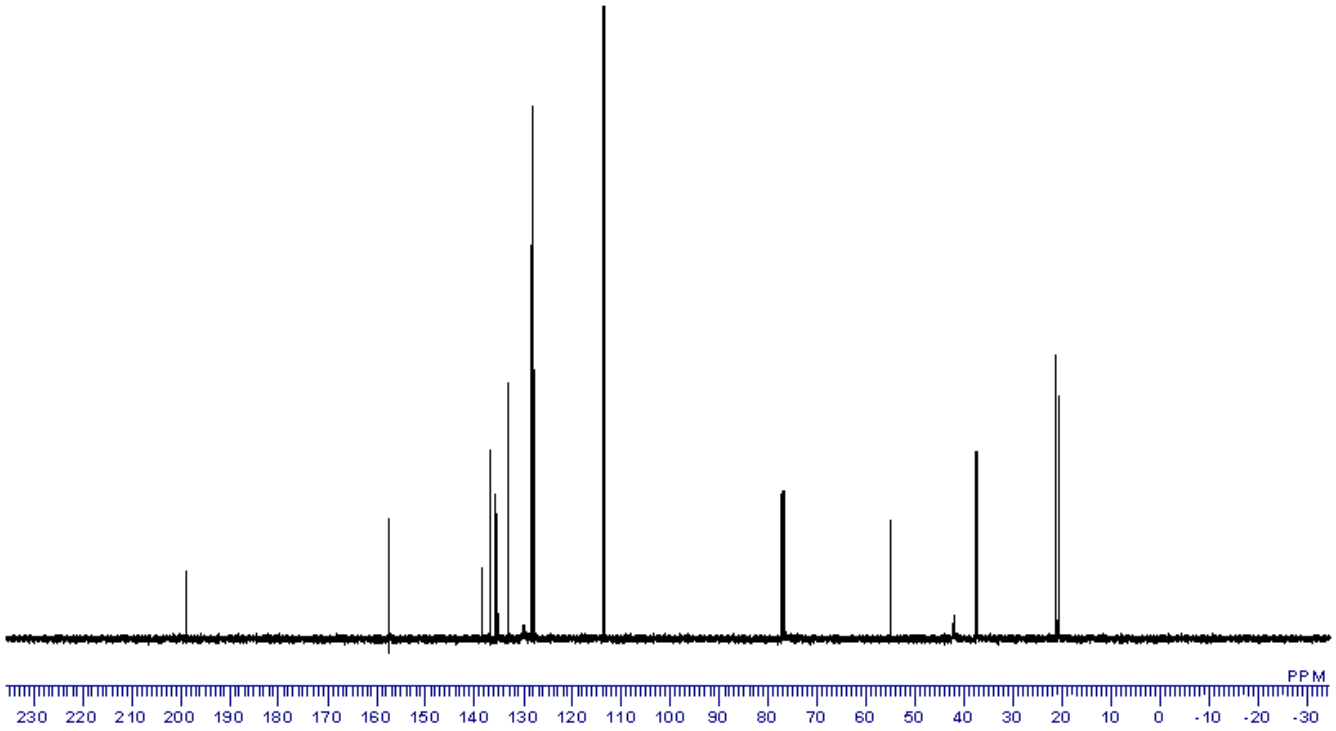


(^{13}C NMR in $CDCl_3$)

Figure S9. ^{1}H and ^{13}C NMR spectra of **4a-*d*$_1$**

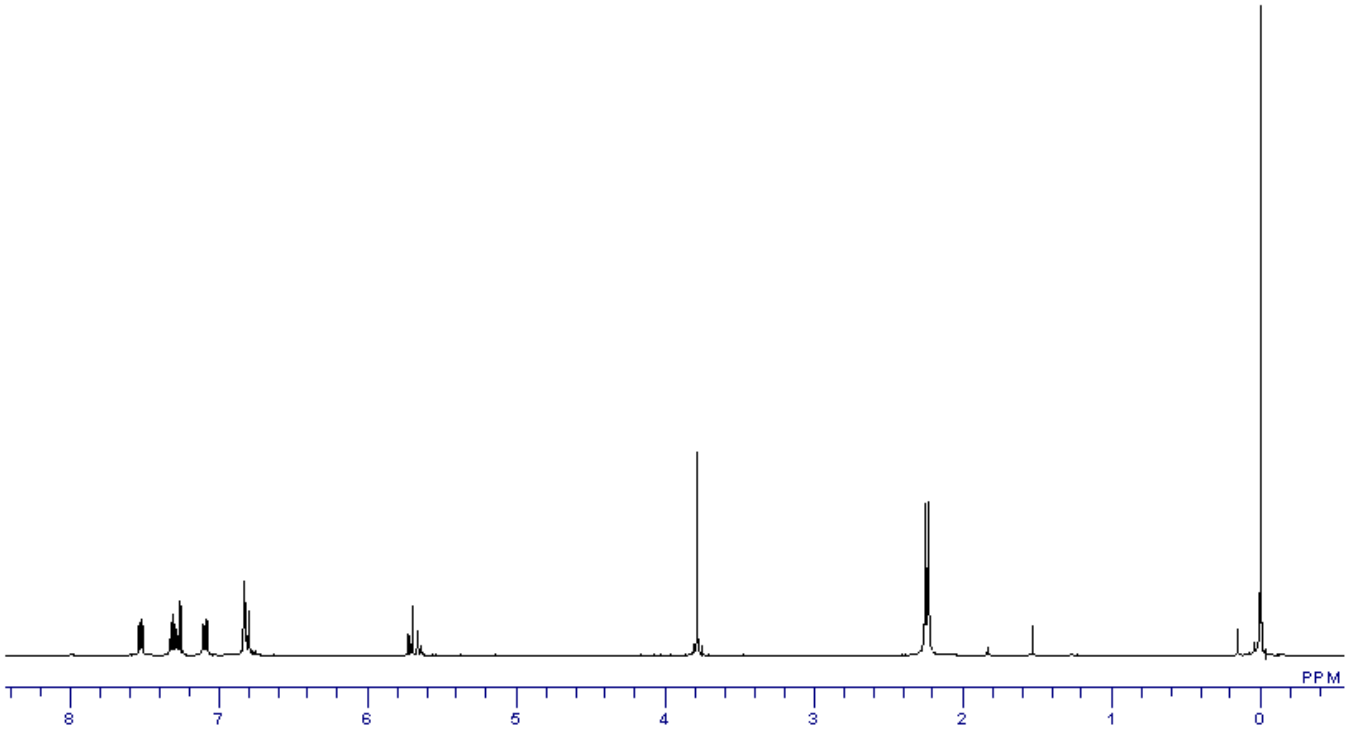


(^{1}H NMR in $CDCl_3$)

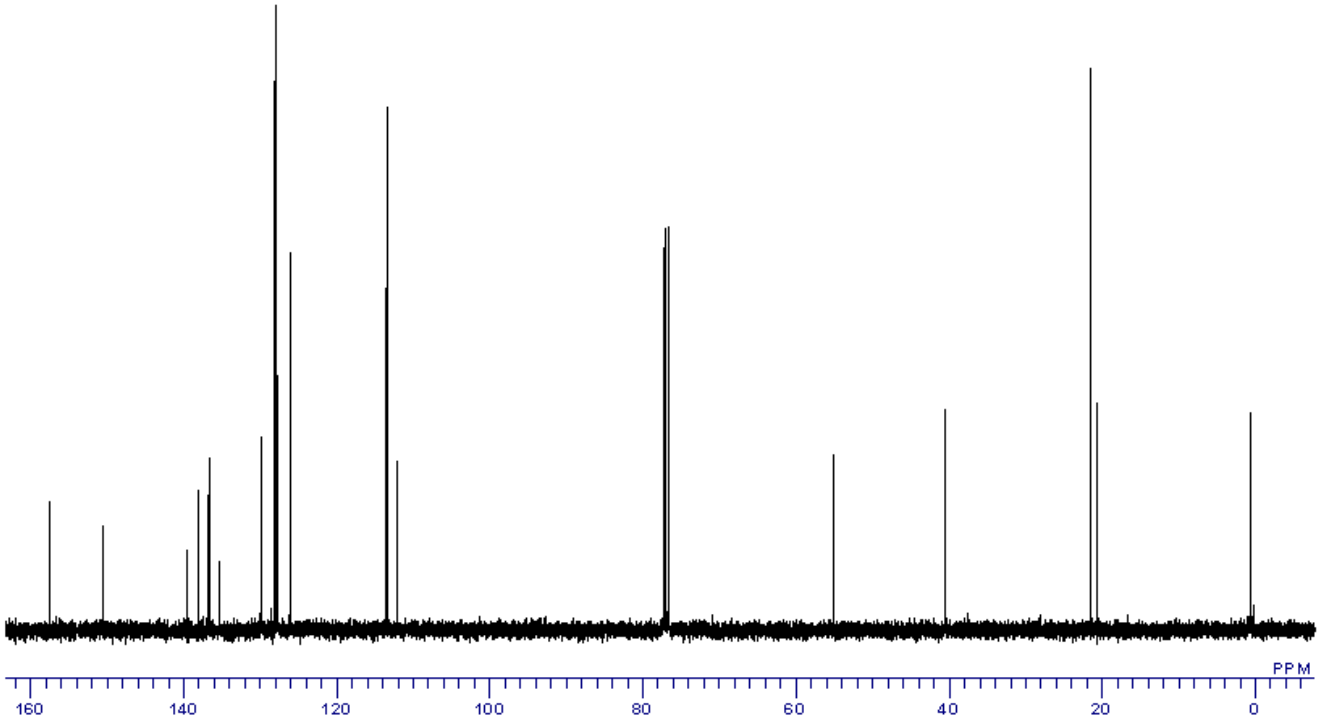


(^{13}C NMR in $CDCl_3$)

Figure S10. ^{1}H and ^{13}C NMR spectra of **5**

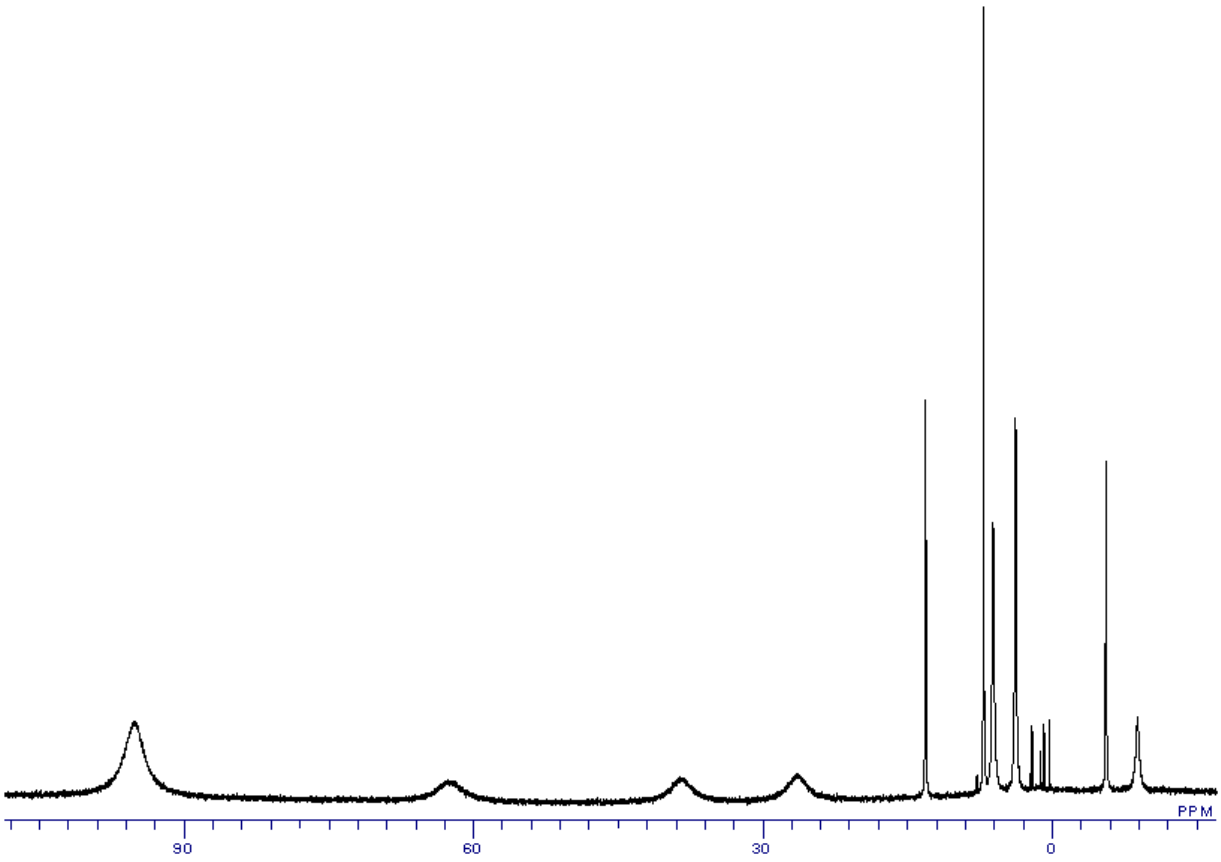


(^{1}H NMR in $CDCl_3$)



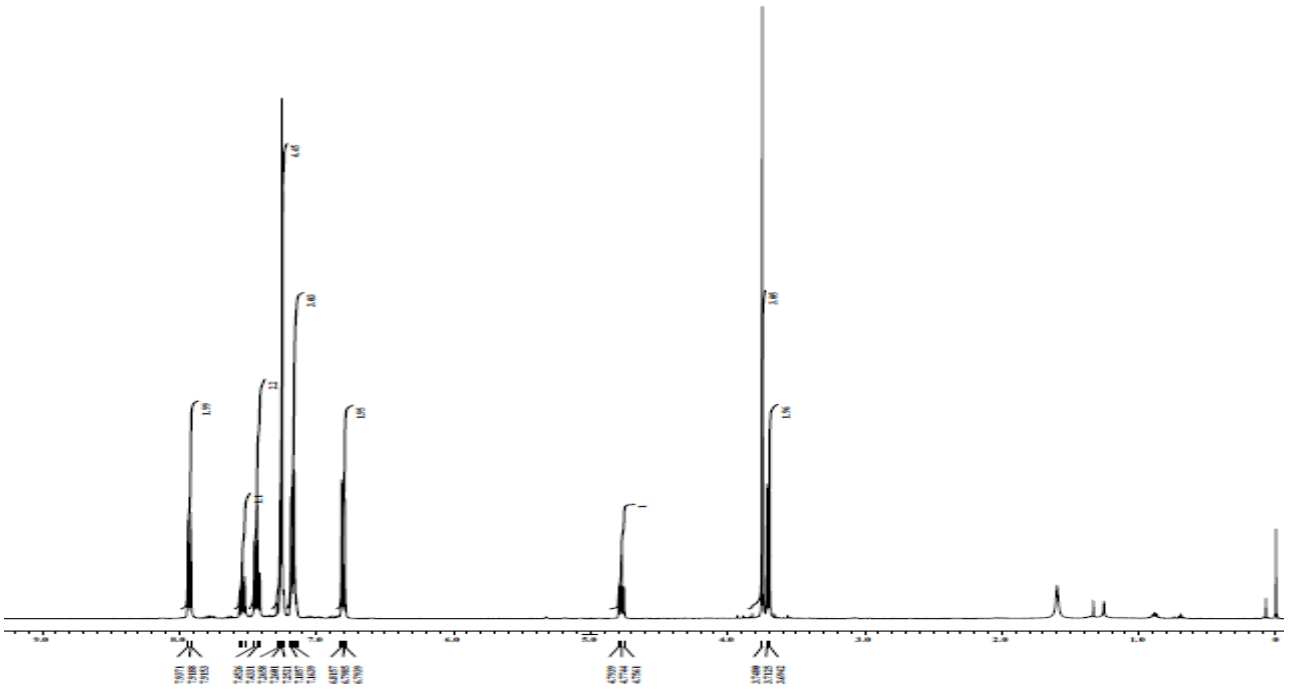
(^{13}C NMR in $CDCl_3$)

Figure S11. ^{1}H NMR spectrum of (TMEDA)Fe(-O-C(Ph)=CHPh)$_2$ (**7**)

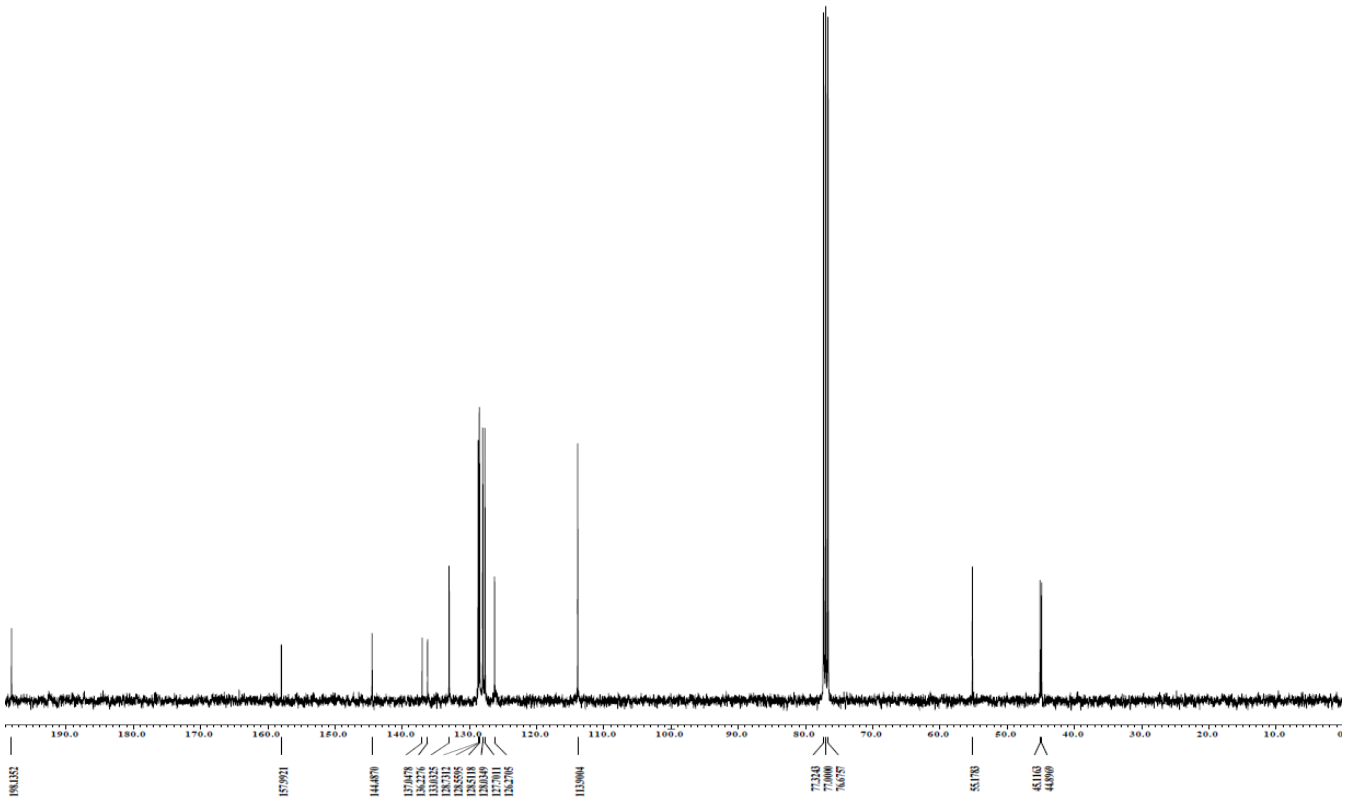


(^{1}H NMR in C_6D_6)

Figure S12. ^{1}H and ^{13}C NMR spectra of **9**



(^{1}H NMR in $CDCl_3$)



(^{13}C NMR in $CDCl_3$)

Figure S13. The Molecular Structure of (TMEDA)Fe(-O-C(Ph)=CHCH(Mesityl)(Anisyl))$_2$ (**3**).

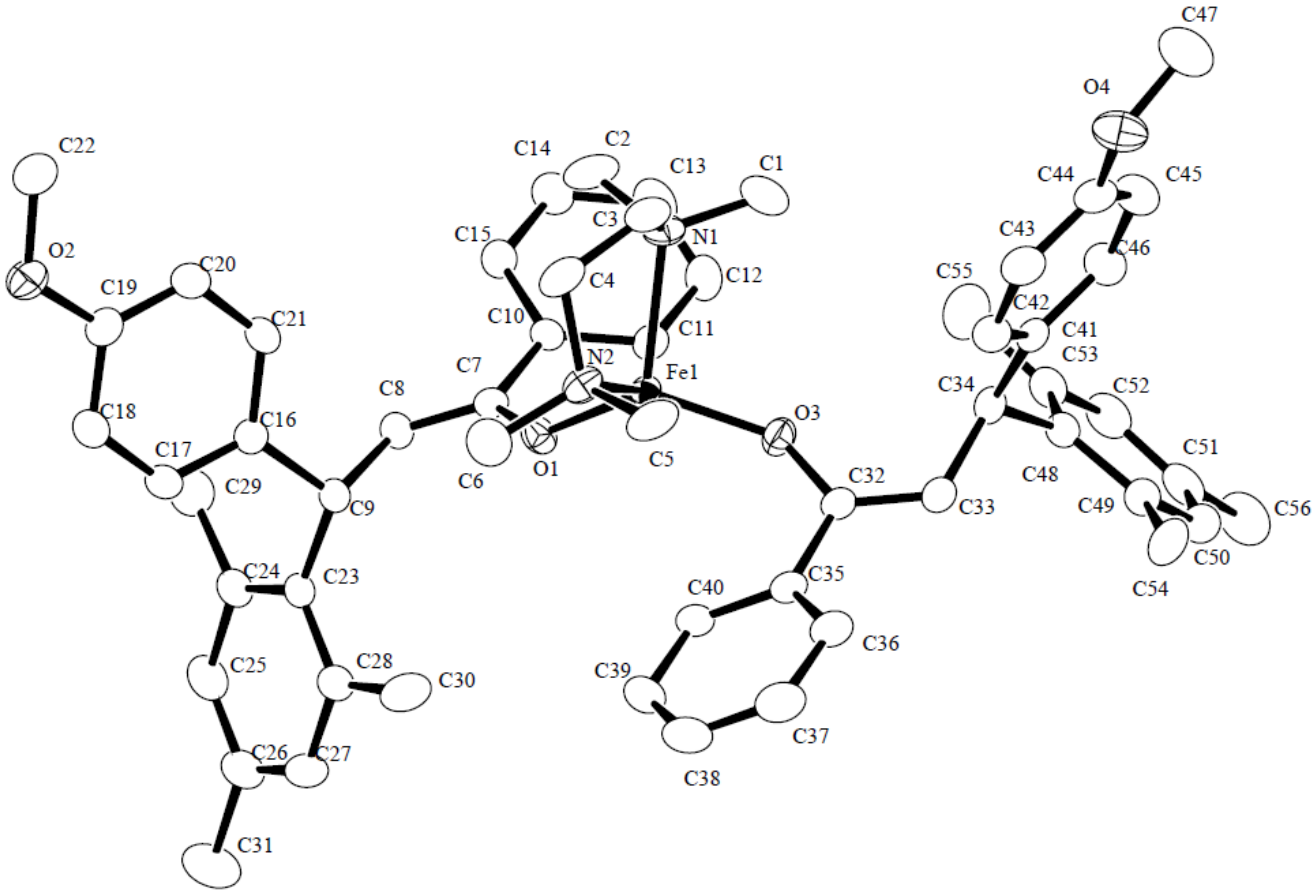


Table S1. X-ray Crystallographic Data of (TMEDA)Fe(-O-C(Ph)=CHCH(Mesityl)(Anisyl))$_2$ (**3**).

Empirical Formula	$C_{56}H_{66}FeN_2O_4$
Formula Weight	887.00
Crystal Color, Habit	colorless, block
Crystal Dimensions	0.200 X 0.200 X 0.100 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 11.523(2) Å b = 31.766(5) Å c = 14.061(3) Å β = 105.738(3) ° V = 4954(2) Å^3
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.189 g/cm^3
F_{000}	1896.00
μ(MoKα)	3.504 cm^{-1}
Detector	Rigaku Saturn
Radiation	MoKα (λ = 0.71070 Å) graphite monochromated
Voltage, Current	50kV, 16mA
Temperature	-150.0°C
Detector Aperture	70 mm x 70 mm
Data Images	720 exposures
ω oscillation Range (χ=45.0, ϕ=90.0)	-110.0 - 70.0°
Exposure Rate	80.0 sec./°
Detector Swing Angle	-20.11 °
Detector Position	45.04 mm
Pixel Size	0.137 mm
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 38564 Unique: 11203 (R_{int} = 0.0575)
Structure Solution	Direct Methods (SIR97)
No. Observations (All reflections)	11203
No. Variables	634
Reflection/Parameter Ratio	17.67
Residuals: R1 (I>2.00σ(I))	0.0586
Residuals: R (All reflections)	0.0705
Residuals: wR2 (All reflections)	0.1934
Goodness of Fit Indicator	1.002
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	1.44 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.61 e$^-$/Å^3

Table S1-1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Fe(1)	0.65083(3)	0.253820(10)	0.49463(2)	1.384(7)
O(1)	0.55016(13)	0.29394(5)	0.53284(12)	1.99(3)
O(2)	0.3043(2)	0.46395(6)	0.16097(12)	2.73(4)
O(3)	0.74720(13)	0.21365(5)	0.58025(12)	2.04(3)
O(4)	0.9890(2)	0.05614(7)	0.3089(2)	3.38(5)
N(1)	0.5725(2)	0.21736(6)	0.36092(13)	1.99(4)
N(2)	0.7383(2)	0.28883(6)	0.40026(13)	2.01(4)
C(1)	0.5830(3)	0.17150(8)	0.3789(2)	3.06(6)
C(2)	0.4452(3)	0.22712(10)	0.3162(2)	2.91(6)
C(3)	0.6458(2)	0.22990(8)	0.2929(2)	2.26(5)
C(4)	0.6690(2)	0.27645(9)	0.2987(2)	2.41(5)
C(5)	0.8665(2)	0.27751(10)	0.4162(2)	2.72(6)
C(6)	0.7298(3)	0.33487(8)	0.4125(2)	3.05(6)
C(7)	0.4339(2)	0.29774(7)	0.5282(2)	1.54(4)
C(8)	0.3805(2)	0.33535(7)	0.5299(2)	1.79(4)
C(9)	0.4456(2)	0.37678(7)	0.5308(2)	1.74(4)
C(10)	0.3635(2)	0.25779(7)	0.5223(2)	1.54(4)
C(11)	0.4202(2)	0.22113(7)	0.5660(2)	1.84(4)
C(12)	0.3561(3)	0.18380(8)	0.5593(2)	2.54(5)
C(13)	0.2353(3)	0.18199(8)	0.5070(3)	2.92(6)
C(14)	0.1787(3)	0.21789(8)	0.4618(2)	2.65(5)
C(15)	0.2415(2)	0.25557(7)	0.4699(2)	2.03(5)
C(16)	0.4040(2)	0.40010(7)	0.4315(2)	1.72(4)
C(17)	0.4136(2)	0.44368(7)	0.4241(2)	1.95(5)
C(18)	0.3807(2)	0.46410(7)	0.3338(2)	2.20(5)
C(19)	0.3372(2)	0.44097(8)	0.2472(2)	2.04(5)
C(20)	0.3287(2)	0.39771(8)	0.2525(2)	2.11(5)
C(21)	0.3621(2)	0.37785(7)	0.3438(2)	1.99(5)
C(22)	0.2506(3)	0.44142(9)	0.0722(2)	2.97(6)
C(23)	0.4437(2)	0.40358(6)	0.6204(2)	1.84(4)
C(24)	0.3355(3)	0.41911(7)	0.6353(2)	2.32(5)
C(25)	0.3396(3)	0.44249(8)	0.7206(2)	2.92(6)
C(26)	0.4467(3)	0.45067(8)	0.7915(2)	3.03(6)
C(27)	0.5522(3)	0.43515(8)	0.7760(2)	2.85(6)
C(28)	0.5532(3)	0.41171(7)	0.6918(2)	2.30(5)
C(29)	0.2140(3)	0.41218(9)	0.5628(2)	3.01(6)
C(30)	0.6720(3)	0.39587(10)	0.6826(2)	3.31(6)
C(31)	0.4492(4)	0.47652(11)	0.8829(3)	4.59(8)
C(32)	0.8607(2)	0.20905(7)	0.6342(2)	1.57(4)
C(33)	0.9082(2)	0.17053(7)	0.6619(2)	1.89(4)
C(34)	0.8405(2)	0.13036(7)	0.6267(2)	1.77(4)
C(35)	0.9330(2)	0.24842(7)	0.6609(2)	1.72(5)
C(36)	1.0569(3)	0.24871(8)	0.6696(2)	2.30(5)
C(37)	1.1216(3)	0.28655(9)	0.6876(2)	2.98(6)
C(38)	1.0641(3)	0.32390(9)	0.6980(2)	2.96(6)
C(39)	0.9426(3)	0.32390(8)	0.6900(2)	2.42(5)
C(40)	0.8770(2)	0.28621(7)	0.6709(2)	1.83(4)
C(41)	0.8866(2)	0.10825(7)	0.5470(2)	1.74(4)
C(42)	0.9443(2)	0.13137(8)	0.4882(2)	2.21(5)

C(43)	0.9775(3)	0.11302(8)	0.4108(2)	2.61(5)
C(44)	0.9534(3)	0.07090(8)	0.3879(2)	2.39(5)
C(45)	0.8958(3)	0.04738(8)	0.4442(2)	2.80(6)
C(46)	0.8627(3)	0.06609(8)	0.5229(2)	2.50(5)
C(47)	0.9549(4)	0.01461(11)	0.2764(3)	4.26(8)
C(48)	0.8258(2)	0.10133(7)	0.7092(2)	1.81(4)
C(49)	0.9257(2)	0.08680(7)	0.7841(2)	1.96(5)
C(50)	0.9065(3)	0.06354(8)	0.8623(2)	2.41(5)
C(51)	0.7913(3)	0.05373(8)	0.8688(2)	2.54(5)
C(52)	0.6945(3)	0.06631(8)	0.7932(2)	2.62(5)
C(53)	0.7095(2)	0.08972(7)	0.7136(2)	2.14(5)
C(54)	1.0536(2)	0.09520(9)	0.7832(2)	2.75(6)
C(55)	0.5988(3)	0.10289(10)	0.6336(3)	3.59(7)
C(56)	0.7722(4)	0.03045(9)	0.9571(3)	3.72(7)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S1-2. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	0.0194(2)	0.0198(2)	0.0137(2)	0.00188(10)	0.00505(12)	0.00059(10)
O(1)	0.0210(8)	0.0216(8)	0.0339(9)	-0.0003(6)	0.0093(7)	-0.0036(7)
O(2)	0.0449(11)	0.0347(10)	0.0219(8)	0.0006(8)	0.0056(7)	0.0043(7)
O(3)	0.0208(8)	0.0248(8)	0.0289(8)	0.0002(6)	0.0016(6)	0.0054(7)
O(4)	0.0493(12)	0.0496(12)	0.0328(10)	-0.0071(9)	0.0170(9)	-0.0119(9)
N(1)	0.0255(10)	0.0342(11)	0.0170(9)	-0.0014(8)	0.0076(7)	-0.0059(8)
N(2)	0.0245(10)	0.0338(11)	0.0190(9)	-0.0011(8)	0.0071(7)	0.0040(8)
C(1)	0.055(2)	0.0314(13)	0.0327(13)	-0.0049(12)	0.0159(12)	-0.0110(11)
C(2)	0.0270(12)	0.063(2)	0.0199(11)	-0.0044(12)	0.0050(9)	-0.0081(11)
C(3)	0.0264(12)	0.046(2)	0.0155(10)	0.0024(10)	0.0086(9)	-0.0049(10)
C(4)	0.0269(12)	0.049(2)	0.0165(10)	0.0011(10)	0.0070(9)	0.0057(10)
C(5)	0.0253(12)	0.059(2)	0.0204(11)	-0.0023(11)	0.0087(9)	0.0016(11)
C(6)	0.052(2)	0.0314(13)	0.0350(13)	-0.0083(12)	0.0168(12)	0.0084(11)
C(7)	0.0211(10)	0.0219(10)	0.0158(9)	-0.0028(8)	0.0051(8)	0.0001(8)
C(8)	0.0204(10)	0.0208(10)	0.0276(11)	0.0010(8)	0.0076(8)	-0.0010(8)
C(9)	0.0219(10)	0.0186(10)	0.0245(11)	0.0011(8)	0.0041(8)	-0.0003(8)
C(10)	0.0240(11)	0.0202(10)	0.0161(9)	-0.0000(8)	0.0087(8)	-0.0020(8)
C(11)	0.0225(10)	0.0263(11)	0.0212(10)	-0.0006(8)	0.0058(8)	0.0020(9)
C(12)	0.0315(13)	0.0246(12)	0.041(2)	-0.0010(9)	0.0101(10)	0.0069(10)
C(13)	0.0291(13)	0.0266(12)	0.058(2)	-0.0081(10)	0.0165(12)	0.0004(11)
C(14)	0.0224(12)	0.0314(13)	0.046(2)	-0.0034(9)	0.0073(10)	-0.0045(11)
C(15)	0.0213(11)	0.0264(11)	0.0299(12)	0.0030(8)	0.0076(9)	-0.0010(9)
C(16)	0.0211(10)	0.0243(11)	0.0211(10)	0.0027(8)	0.0078(8)	-0.0005(8)
C(17)	0.0271(11)	0.0239(11)	0.0235(11)	-0.0022(9)	0.0073(9)	-0.0031(9)
C(18)	0.0311(12)	0.0227(11)	0.0298(12)	-0.0022(9)	0.0080(9)	-0.0003(9)
C(19)	0.0240(11)	0.0320(12)	0.0227(11)	0.0036(9)	0.0081(9)	0.0020(9)
C(20)	0.0282(11)	0.0306(12)	0.0225(11)	0.0019(9)	0.0088(9)	-0.0049(9)
C(21)	0.0289(12)	0.0215(11)	0.0266(11)	0.0021(8)	0.0096(9)	-0.0038(9)
C(22)	0.045(2)	0.043(2)	0.0233(12)	0.0052(12)	0.0069(10)	0.0005(11)

C(23)	0.0310(12)	0.0167(10)	0.0209(10)	0.0011(8)	0.0048(9)	0.0017(8)
C(24)	0.0391(13)	0.0226(11)	0.0263(11)	0.0023(9)	0.0086(10)	-0.0010(9)
C(25)	0.055(2)	0.0301(13)	0.0296(13)	0.0082(12)	0.0177(12)	-0.0030(10)
C(26)	0.066(2)	0.0266(12)	0.0214(11)	-0.0025(12)	0.0103(11)	-0.0008(9)
C(27)	0.054(2)	0.0280(12)	0.0203(11)	-0.0096(11)	0.0001(11)	0.0016(9)
C(28)	0.0386(13)	0.0193(11)	0.0261(12)	-0.0057(9)	0.0031(10)	0.0025(9)
C(29)	0.033(2)	0.044(2)	0.039(2)	0.0100(11)	0.0143(11)	-0.0061(12)
C(30)	0.0303(13)	0.050(2)	0.038(2)	-0.0066(12)	-0.0031(11)	-0.0042(12)
C(31)	0.099(3)	0.047(2)	0.029(2)	-0.007(2)	0.020(2)	-0.0116(13)
C(32)	0.0195(10)	0.0259(11)	0.0151(9)	0.0010(8)	0.0064(8)	-0.0001(8)
C(33)	0.0199(10)	0.0268(11)	0.0238(11)	0.0024(8)	0.0036(8)	0.0006(9)
C(34)	0.0185(10)	0.0234(10)	0.0253(11)	0.0028(8)	0.0056(8)	0.0029(8)
C(35)	0.0227(11)	0.0285(11)	0.0145(10)	-0.0006(8)	0.0055(8)	-0.0001(8)
C(36)	0.0223(12)	0.037(2)	0.0266(12)	-0.0021(9)	0.0044(9)	-0.0020(9)
C(37)	0.0251(12)	0.048(2)	0.038(2)	-0.0088(11)	0.0043(10)	-0.0028(12)
C(38)	0.041(2)	0.036(2)	0.0323(13)	-0.0154(11)	0.0057(11)	-0.0054(11)
C(39)	0.039(2)	0.0260(12)	0.0275(12)	-0.0038(10)	0.0105(10)	-0.0045(9)
C(40)	0.0256(11)	0.0264(11)	0.0178(10)	-0.0027(8)	0.0065(8)	-0.0019(8)
C(41)	0.0188(10)	0.0245(11)	0.0209(10)	0.0032(8)	0.0018(8)	0.0017(8)
C(42)	0.0310(12)	0.0276(12)	0.0245(11)	-0.0027(9)	0.0058(9)	0.0017(9)
C(43)	0.0330(13)	0.038(2)	0.0265(12)	-0.0046(10)	0.0053(9)	0.0028(10)
C(44)	0.0285(12)	0.0388(13)	0.0215(11)	-0.0006(10)	0.0035(9)	-0.0032(10)
C(45)	0.046(2)	0.0297(13)	0.0324(13)	-0.0053(11)	0.0135(11)	-0.0034(10)
C(46)	0.0375(13)	0.0285(12)	0.0317(12)	-0.0049(10)	0.0141(10)	0.0020(10)
C(47)	0.071(3)	0.046(2)	0.049(2)	0.003(2)	0.024(2)	-0.017(2)
C(48)	0.0222(10)	0.0224(10)	0.0248(11)	0.0019(8)	0.0073(8)	-0.0020(8)
C(49)	0.0248(11)	0.0269(11)	0.0242(11)	0.0029(9)	0.0091(9)	-0.0010(9)
C(50)	0.0364(13)	0.0306(12)	0.0244(11)	0.0019(10)	0.0078(10)	0.0011(9)
C(51)	0.046(2)	0.0228(11)	0.0344(13)	-0.0031(10)	0.0213(11)	-0.0052(10)
C(52)	0.0336(13)	0.0292(12)	0.043(2)	-0.0062(10)	0.0211(11)	-0.0040(11)
C(53)	0.0232(11)	0.0245(11)	0.0358(13)	-0.0005(8)	0.0114(9)	-0.0020(9)
C(54)	0.0226(12)	0.044(2)	0.0363(13)	0.0063(10)	0.0052(10)	0.0089(11)
C(55)	0.0220(13)	0.047(2)	0.066(2)	-0.0038(11)	0.0093(12)	0.011(2)
C(56)	0.072(2)	0.037(2)	0.041(2)	-0.007(2)	0.030(2)	0.0032(12)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S1-3. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Fe(1)	O(1)	1.8965(18)	Fe(1)	O(3)	1.8936(16)
Fe(1)	N(1)	2.1841(18)	Fe(1)	N(2)	2.177(2)
O(1)	C(7)	1.329(3)	O(2)	C(19)	1.378(3)
O(2)	C(22)	1.426(3)	O(3)	C(32)	1.330(3)
O(4)	C(44)	1.367(4)	O(4)	C(47)	1.416(4)
N(1)	C(1)	1.478(4)	N(1)	C(2)	1.463(3)
N(1)	C(3)	1.492(4)	N(2)	C(4)	1.487(3)
N(2)	C(5)	1.478(4)	N(2)	C(6)	1.479(4)
C(3)	C(4)	1.501(4)	C(7)	C(8)	1.347(4)

C(7)	C(10)	1.497(4)	C(8)	C(9)	1.513(4)
C(9)	C(16)	1.538(3)	C(9)	C(23)	1.525(4)
C(10)	C(11)	1.394(3)	C(10)	C(15)	1.400(3)
C(11)	C(12)	1.387(4)	C(12)	C(13)	1.388(4)
C(13)	C(14)	1.380(4)	C(14)	C(15)	1.387(4)
C(16)	C(17)	1.395(4)	C(16)	C(21)	1.389(3)
C(17)	C(18)	1.383(4)	C(18)	C(19)	1.394(4)
C(19)	C(20)	1.381(4)	C(20)	C(21)	1.388(4)
C(23)	C(24)	1.409(4)	C(23)	C(28)	1.408(3)
C(24)	C(25)	1.401(4)	C(24)	C(29)	1.507(4)
C(25)	C(26)	1.384(4)	C(26)	C(27)	1.383(5)
C(26)	C(31)	1.519(5)	C(27)	C(28)	1.401(4)
C(28)	C(30)	1.496(4)	C(32)	C(33)	1.354(3)
C(32)	C(35)	1.493(3)	C(33)	C(34)	1.507(3)
C(34)	C(41)	1.535(4)	C(34)	C(48)	1.527(4)
C(35)	C(36)	1.399(4)	C(35)	C(40)	1.388(4)
C(36)	C(37)	1.401(4)	C(37)	C(38)	1.386(4)
C(38)	C(39)	1.374(4)	C(39)	C(40)	1.403(4)
C(41)	C(42)	1.400(4)	C(41)	C(46)	1.390(4)
C(42)	C(43)	1.378(4)	C(43)	C(44)	1.386(4)
C(44)	C(45)	1.383(4)	C(45)	C(46)	1.397(4)
C(48)	C(49)	1.410(3)	C(48)	C(53)	1.408(4)
C(49)	C(50)	1.392(4)	C(49)	C(54)	1.501(4)
C(50)	C(51)	1.390(4)	C(51)	C(52)	1.376(4)
C(51)	C(56)	1.511(5)	C(52)	C(53)	1.393(4)
C(53)	C(55)	1.513(4)			

Table S1-4. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Fe(1)	O(3)	124.82(8)	O(1)	Fe(1)	N(1)	117.28(7)
O(1)	Fe(1)	N(2)	104.43(8)	O(3)	Fe(1)	N(1)	102.95(7)
O(3)	Fe(1)	N(2)	116.32(8)	N(1)	Fe(1)	N(2)	84.14(8)
Fe(1)	O(1)	C(7)	137.15(14)	C(19)	O(2)	C(22)	117.1(2)
Fe(1)	O(3)	C(32)	138.87(15)	C(44)	O(4)	C(47)	117.6(3)
Fe(1)	N(1)	C(1)	112.32(14)	Fe(1)	N(1)	C(2)	112.92(16)
Fe(1)	N(1)	C(3)	103.68(13)	C(1)	N(1)	C(2)	108.0(2)
C(1)	N(1)	C(3)	109.8(2)	C(2)	N(1)	C(3)	110.11(18)
Fe(1)	N(2)	C(4)	103.51(15)	Fe(1)	N(2)	C(5)	113.09(15)
Fe(1)	N(2)	C(6)	112.25(18)	C(4)	N(2)	C(5)	109.60(19)
C(4)	N(2)	C(6)	109.74(19)	C(5)	N(2)	C(6)	108.5(2)
N(1)	C(3)	C(4)	110.6(2)	N(2)	C(4)	C(3)	110.75(19)
O(1)	C(7)	C(8)	122.6(2)	O(1)	C(7)	C(10)	116.75(19)
C(8)	C(7)	C(10)	120.7(2)	C(7)	C(8)	C(9)	122.9(2)
C(8)	C(9)	C(16)	112.28(16)	C(8)	C(9)	C(23)	112.0(2)
C(16)	C(9)	C(23)	114.20(18)	C(7)	C(10)	C(11)	120.09(18)
C(7)	C(10)	C(15)	121.56(19)	C(11)	C(10)	C(15)	118.3(2)
C(10)	C(11)	C(12)	120.4(2)	C(11)	C(12)	C(13)	120.7(3)
C(12)	C(13)	C(14)	119.4(3)	C(13)	C(14)	C(15)	120.3(3)
C(10)	C(15)	C(14)	120.9(2)	C(9)	C(16)	C(17)	122.30(18)
C(9)	C(16)	C(21)	120.6(2)	C(17)	C(16)	C(21)	117.0(2)

C(16)	C(17)	C(18)	121.8(2)	C(17)	C(18)	C(19)	119.9(2)
O(2)	C(19)	C(18)	116.0(3)	O(2)	C(19)	C(20)	124.6(2)
C(18)	C(19)	C(20)	119.4(2)	C(19)	C(20)	C(21)	119.8(2)
C(16)	C(21)	C(20)	122.1(2)	C(9)	C(23)	C(24)	122.03(18)
C(9)	C(23)	C(28)	118.7(2)	C(24)	C(23)	C(28)	119.2(2)
C(23)	C(24)	C(25)	119.2(3)	C(23)	C(24)	C(29)	123.1(3)
C(25)	C(24)	C(29)	117.8(3)	C(24)	C(25)	C(26)	122.2(3)
C(25)	C(26)	C(27)	118.0(3)	C(25)	C(26)	C(31)	121.3(3)
C(27)	C(26)	C(31)	120.7(3)	C(26)	C(27)	C(28)	122.1(3)
C(23)	C(28)	C(27)	119.3(3)	C(23)	C(28)	C(30)	122.7(3)
C(27)	C(28)	C(30)	118.0(3)	O(3)	C(32)	C(33)	121.4(2)
O(3)	C(32)	C(35)	116.53(19)	C(33)	C(32)	C(35)	122.01(18)
C(32)	C(33)	C(34)	122.53(18)	C(33)	C(34)	C(41)	112.1(2)
C(33)	C(34)	C(48)	114.55(18)	C(41)	C(34)	C(48)	114.21(19)
C(32)	C(35)	C(36)	121.0(2)	C(32)	C(35)	C(40)	120.4(2)
C(36)	C(35)	C(40)	118.5(2)	C(35)	C(36)	C(37)	120.1(3)
C(36)	C(37)	C(38)	120.5(3)	C(37)	C(38)	C(39)	119.8(3)
C(38)	C(39)	C(40)	120.0(3)	C(35)	C(40)	C(39)	121.1(3)
C(34)	C(41)	C(42)	120.3(2)	C(34)	C(41)	C(46)	122.2(3)
C(42)	C(41)	C(46)	117.2(3)	C(41)	C(42)	C(43)	121.5(3)
C(42)	C(43)	C(44)	120.7(3)	O(4)	C(44)	C(43)	115.7(3)
O(4)	C(44)	C(45)	125.2(3)	C(43)	C(44)	C(45)	119.0(3)
C(44)	C(45)	C(46)	120.0(3)	C(41)	C(46)	C(45)	121.6(3)
C(34)	C(48)	C(49)	122.0(2)	C(34)	C(48)	C(53)	119.65(18)
C(49)	C(48)	C(53)	118.4(3)	C(48)	C(49)	C(50)	119.4(3)
C(48)	C(49)	C(54)	122.7(3)	C(50)	C(49)	C(54)	117.9(2)
C(49)	C(50)	C(51)	122.0(2)	C(50)	C(51)	C(52)	118.2(3)
C(50)	C(51)	C(56)	121.2(3)	C(52)	C(51)	C(56)	120.6(3)
C(51)	C(52)	C(53)	121.6(3)	C(48)	C(53)	C(52)	120.2(2)
C(48)	C(53)	C(55)	121.0(3)	C(52)	C(53)	C(55)	118.8(3)

Table S1-5. Torsion Angles(°) (Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
O(1)	Fe(1)	O(3)	C(32)	-96.83(19)	O(3)	Fe(1)	O(1)	C(7)	-98.56(17)
O(1)	Fe(1)	N(1)	C(1)	-124.69(12)	O(1)	Fe(1)	N(1)	C(2)	-2.30(15)
O(1)	Fe(1)	N(1)	C(3)	116.85(10)	N(1)	Fe(1)	O(1)	C(7)	33.2(2)
O(1)	Fe(1)	N(2)	C(4)	-101.11(10)	O(1)	Fe(1)	N(2)	C(5)	140.37(10)
O(1)	Fe(1)	N(2)	C(6)	17.17(11)	N(2)	Fe(1)	O(1)	C(7)	124.00(16)
O(3)	Fe(1)	N(1)	C(1)	16.38(14)	O(3)	Fe(1)	N(1)	C(2)	138.78(12)
O(3)	Fe(1)	N(1)	C(3)	-102.08(10)	N(1)	Fe(1)	O(3)	C(32)	126.03(18)
O(3)	Fe(1)	N(2)	C(4)	117.17(10)	O(3)	Fe(1)	N(2)	C(5)	-1.36(14)
O(3)	Fe(1)	N(2)	C(6)	-124.56(10)	N(2)	Fe(1)	O(3)	C(32)	36.2(2)
N(1)	Fe(1)	N(2)	C(4)	15.60(10)	N(1)	Fe(1)	N(2)	C(5)	-102.93(11)
N(1)	Fe(1)	N(2)	C(6)	133.87(11)	N(2)	Fe(1)	N(1)	C(1)	132.08(13)
N(2)	Fe(1)	N(1)	C(2)	-105.52(12)	N(2)	Fe(1)	N(1)	C(3)	13.62(10)
Fe(1)	O(1)	C(7)	C(8)	-155.98(14)	Fe(1)	O(1)	C(7)	C(10)	24.8(3)
C(22)	O(2)	C(19)	C(18)	-175.1(2)	C(22)	O(2)	C(19)	C(20)	4.3(4)
Fe(1)	O(3)	C(32)	C(33)	-158.09(15)	Fe(1)	O(3)	C(32)	C(35)	20.8(4)
C(47)	O(4)	C(44)	C(43)	-173.4(2)	C(47)	O(4)	C(44)	C(45)	6.0(4)
Fe(1)	N(1)	C(3)	C(4)	-41.75(16)	C(1)	N(1)	C(3)	C(4)	-161.95(16)

C(2)	N(1)	C(3)	C(4)	79.3(2)	Fe(1)	N(2)	C(4)	C(3)	-43.64(19)
C(5)	N(2)	C(4)	C(3)	77.3(3)	C(6)	N(2)	C(4)	C(3)	-163.6(2)
N(1)	C(3)	C(4)	N(2)	61.3(3)	O(1)	C(7)	C(8)	C(9)	3.8(3)
O(1)	C(7)	C(10)	C(11)	30.0(3)	O(1)	C(7)	C(10)	C(15)	-147.20(19)
C(8)	C(7)	C(10)	C(11)	-149.3(2)	C(8)	C(7)	C(10)	C(15)	33.6(3)
C(10)	C(7)	C(8)	C(9)	-176.98(17)	C(7)	C(8)	C(9)	C(16)	107.7(3)
C(7)	C(8)	C(9)	C(23)	-122.2(2)	C(8)	C(9)	C(16)	C(17)	154.98(19)
C(8)	C(9)	C(16)	C(21)	-29.2(3)	C(8)	C(9)	C(23)	C(24)	-63.6(3)
C(8)	C(9)	C(23)	C(28)	114.13(19)	C(16)	C(9)	C(23)	C(24)	65.4(3)
C(16)	C(9)	C(23)	C(28)	-116.84(19)	C(23)	C(9)	C(16)	C(17)	26.1(3)
C(23)	C(9)	C(16)	C(21)	-158.11(18)	C(7)	C(10)	C(11)	C(12)	-178.77(19)
C(7)	C(10)	C(15)	C(14)	177.4(2)	C(11)	C(10)	C(15)	C(14)	0.2(4)
C(15)	C(10)	C(11)	C(12)	-1.5(4)	C(10)	C(11)	C(12)	C(13)	1.6(4)
C(11)	C(12)	C(13)	C(14)	-0.4(5)	C(12)	C(13)	C(14)	C(15)	-1.0(5)
C(13)	C(14)	C(15)	C(10)	1.1(5)	C(9)	C(16)	C(17)	C(18)	177.17(19)
C(9)	C(16)	C(21)	C(20)	-177.22(19)	C(17)	C(16)	C(21)	C(20)	-1.2(4)
C(21)	C(16)	C(17)	C(18)	1.3(4)	C(16)	C(17)	C(18)	C(19)	-0.3(4)
C(17)	C(18)	C(19)	O(2)	178.7(2)	C(17)	C(18)	C(19)	C(20)	-0.7(4)
O(2)	C(19)	C(20)	C(21)	-178.6(2)	C(18)	C(19)	C(20)	C(21)	0.7(4)
C(19)	C(20)	C(21)	C(16)	0.3(4)	C(9)	C(23)	C(24)	C(25)	178.10(18)
C(9)	C(23)	C(24)	C(29)	-2.5(4)	C(9)	C(23)	C(28)	C(27)	-177.97(18)
C(9)	C(23)	C(28)	C(30)	1.3(3)	C(24)	C(23)	C(28)	C(27)	-0.2(3)
C(24)	C(23)	C(28)	C(30)	179.08(19)	C(28)	C(23)	C(24)	C(25)	0.4(3)
C(28)	C(23)	C(24)	C(29)	179.75(19)	C(23)	C(24)	C(25)	C(26)	-0.5(4)
C(29)	C(24)	C(25)	C(26)	-179.9(2)	C(24)	C(25)	C(26)	C(27)	0.3(4)
C(24)	C(25)	C(26)	C(31)	179.3(2)	C(25)	C(26)	C(27)	C(28)	-0.1(4)
C(31)	C(26)	C(27)	C(28)	-179.1(3)	C(26)	C(27)	C(28)	C(23)	0.0(4)
C(26)	C(27)	C(28)	C(30)	-179.3(2)	O(3)	C(32)	C(33)	C(34)	5.5(4)
O(3)	C(32)	C(35)	C(36)	-146.69(19)	O(3)	C(32)	C(35)	C(40)	28.9(3)
C(33)	C(32)	C(35)	C(36)	32.2(4)	C(33)	C(32)	C(35)	C(40)	-152.2(2)
C(35)	C(32)	C(33)	C(34)	-173.39(19)	C(32)	C(33)	C(34)	C(41)	104.4(3)
C(32)	C(33)	C(34)	C(48)	-123.4(3)	C(33)	C(34)	C(41)	C(42)	-24.8(3)
C(33)	C(34)	C(41)	C(46)	161.94(15)	C(33)	C(34)	C(48)	C(49)	-55.9(3)
C(33)	C(34)	C(48)	C(53)	121.7(2)	C(41)	C(34)	C(48)	C(49)	75.4(3)
C(41)	C(34)	C(48)	C(53)	-107.0(2)	C(48)	C(34)	C(41)	C(42)	-157.21(15)
C(48)	C(34)	C(41)	C(46)	29.5(3)	C(32)	C(35)	C(36)	C(37)	175.38(19)
C(32)	C(35)	C(40)	C(39)	-176.08(17)	C(36)	C(35)	C(40)	C(39)	-0.4(4)
C(40)	C(35)	C(36)	C(37)	-0.3(4)	C(35)	C(36)	C(37)	C(38)	0.7(4)
C(36)	C(37)	C(38)	C(39)	-0.4(4)	C(37)	C(38)	C(39)	C(40)	-0.3(4)
C(38)	C(39)	C(40)	C(35)	0.7(4)	C(34)	C(41)	C(42)	C(43)	-174.48(16)
C(34)	C(41)	C(46)	C(45)	174.09(16)	C(42)	C(41)	C(46)	C(45)	0.6(3)
C(46)	C(41)	C(42)	C(43)	-0.9(3)	C(41)	C(42)	C(43)	C(44)	0.7(4)
C(42)	C(43)	C(44)	O(4)	179.25(19)	C(42)	C(43)	C(44)	C(45)	-0.2(4)
O(4)	C(44)	C(45)	C(46)	-179.45(19)	C(43)	C(44)	C(45)	C(46)	-0.1(4)
C(44)	C(45)	C(46)	C(41)	-0.2(4)	C(34)	C(48)	C(49)	C(50)	174.22(18)
C(34)	C(48)	C(49)	C(54)	-6.0(4)	C(34)	C(48)	C(53)	C(52)	-174.37(18)
C(34)	C(48)	C(53)	C(55)	4.6(4)	C(49)	C(48)	C(53)	C(52)	3.3(4)
C(49)	C(48)	C(53)	C(55)	-177.71(19)	C(53)	C(48)	C(49)	C(50)	-3.4(4)
C(53)	C(48)	C(49)	C(54)	176.34(19)	C(48)	C(49)	C(50)	C(51)	0.6(4)
C(54)	C(49)	C(50)	C(51)	-179.2(2)	C(49)	C(50)	C(51)	C(52)	2.4(4)
C(49)	C(50)	C(51)	C(56)	-176.7(2)	C(50)	C(51)	C(52)	C(53)	-2.6(4)
C(56)	C(51)	C(52)	C(53)	176.6(3)	C(51)	C(52)	C(53)	C(48)	-0.3(4)

C(51) C(52) C(53) C(55) -179.3(2)

Figure S14. The Molecular Structure of (TMEDA)Fe(-O-C(Ph)=CHPh)$_2$ (7**)**.

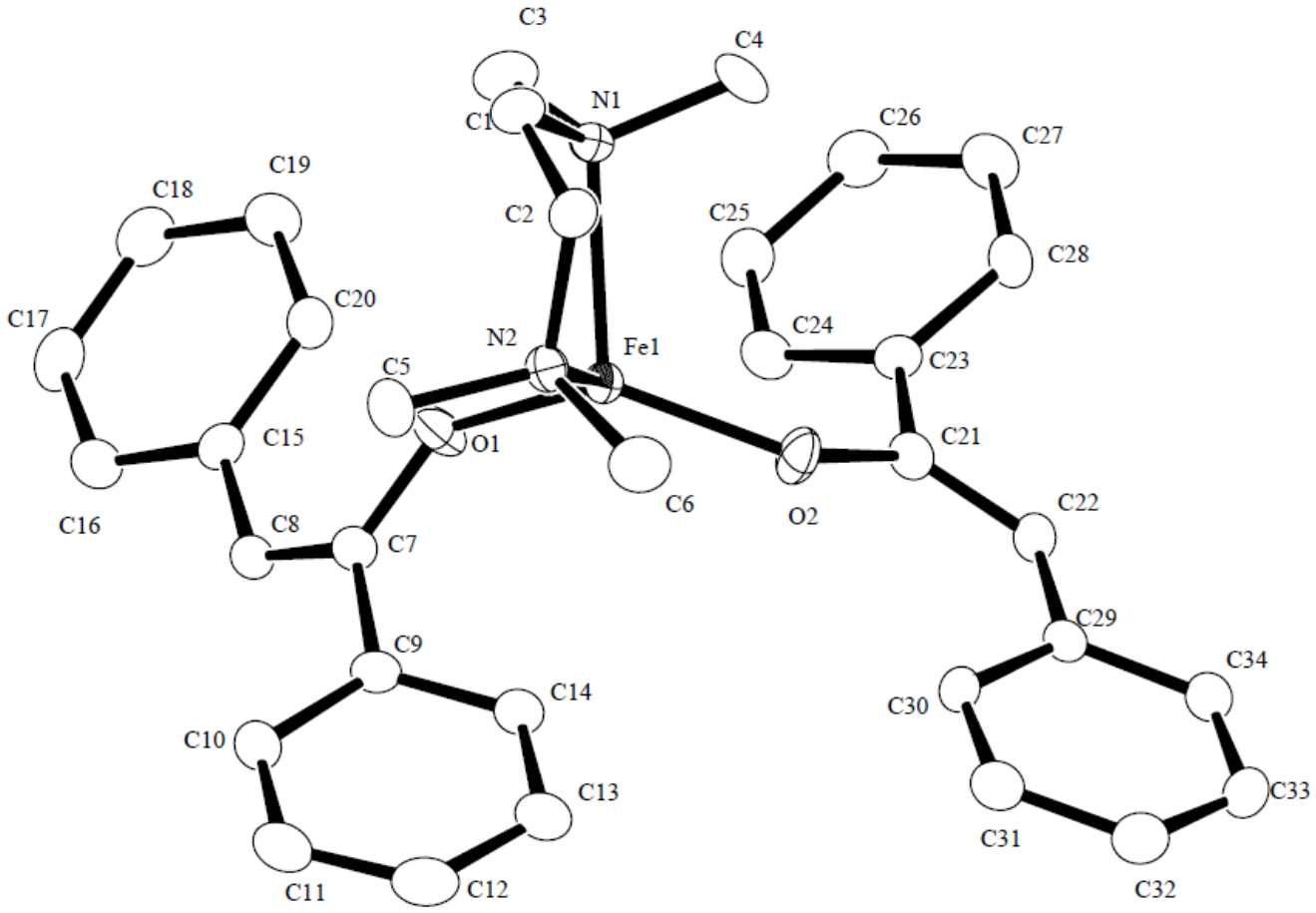


Table S2. X-ray Crystallographic Data of (TMEDA)Fe(-O-C(Ph)=CHPh)$_2$ (**7**).

Empirical Formula	$C_{34}H_{38}FeN_2O_2$
Formula Weight	562.53
Crystal Color, Habit	brown, block
Crystal Dimensions	0.160 X 0.140 X 0.120 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 11.09(2) Å b = 11.68(2) Å c = 13.261(6) Å α = 59.84(9) ^{o} β = 75.33(9) ^{o} γ = 84.57(13) ^{o} V = 1435(4) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.301 g/cm^3
F_{000}	596.00
μ(MoKα)	5.580cm^{-1}
Detector	Rigaku Saturn
Radiation	MoKα (λ = 0.71070 Å) graphite monochromated
Detector Aperture	70 mm x 70 mm
Data Images	720 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	-110.0 - 70.0^o
Exposure Rate	72.0 sec./^{o}
Detector Swing Angle	-20.10^o
Detector Position	45.04 mm
Pixel Size	0.137 mm
$2\theta_{max}$	54.9^o
No. of Reflections Measured	Total: 11342 Unique: 6279 (R_{int} = 0.0325)
Structure Solution	Direct Methods (SIR97)
No. Observations (All reflections)	6279
No. Variables	390
Reflection/Parameter Ratio	16.10
Residuals: R1 (I>2.00σ(I))	0.0616
Residuals: R (All reflections)	0.0655
Residuals: wR2 (All reflections)	0.1988
Goodness of Fit Indicator	1.001
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	2.30 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.61 e$^-$/Å^3

Table S2-1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Fe(1)	0.35046(2)	0.20389(3)	0.76412(2)	1.157(9)
O(1)	0.2948(2)	0.3013(2)	0.6202(2)	1.93(4)
O(2)	0.2693(2)	0.0750(2)	0.9213(2)	1.86(4)
N(1)	0.5382(2)	0.1507(2)	0.7022(2)	1.36(4)
N(2)	0.4525(2)	0.3294(2)	0.7963(2)	1.31(4)
C(1)	0.6236(2)	0.2513(3)	0.6882(2)	1.77(5)
C(2)	0.5806(2)	0.2806(3)	0.7909(2)	1.63(4)
C(3)	0.5574(3)	0.1551(3)	0.5858(3)	2.26(5)
C(4)	0.5648(3)	0.0162(3)	0.7925(3)	2.03(5)
C(5)	0.4535(3)	0.4698(3)	0.7029(3)	2.03(5)
C(6)	0.4006(3)	0.3184(3)	0.9158(3)	2.07(5)
C(7)	0.2108(2)	0.3924(2)	0.5818(2)	1.44(4)
C(8)	0.1799(2)	0.4342(2)	0.4759(2)	1.49(4)
C(9)	0.1525(2)	0.4487(2)	0.6612(2)	1.47(4)
C(10)	0.1374(2)	0.5856(2)	0.6168(2)	1.73(5)
C(11)	0.0965(3)	0.6348(3)	0.6946(3)	2.15(5)
C(12)	0.0656(3)	0.5498(3)	0.8181(3)	2.21(5)
C(13)	0.0724(3)	0.4135(3)	0.8628(2)	2.00(5)
C(14)	0.1163(2)	0.3639(3)	0.7853(2)	1.63(4)
C(15)	0.2279(2)	0.3867(2)	0.3906(2)	1.45(4)
C(16)	0.2006(2)	0.4554(3)	0.2779(3)	1.76(5)
C(17)	0.2472(3)	0.4167(3)	0.1922(2)	2.04(5)
C(18)	0.3200(3)	0.3076(3)	0.2172(2)	2.14(5)
C(19)	0.3448(3)	0.2349(3)	0.3305(3)	1.97(5)
C(20)	0.2995(2)	0.2738(2)	0.4159(2)	1.67(4)
C(21)	0.2202(2)	-0.0467(2)	0.9713(2)	1.53(4)
C(22)	0.1481(2)	-0.1122(2)	1.0850(2)	1.57(4)
C(23)	0.2499(2)	-0.1115(2)	0.8957(2)	1.49(4)
C(24)	0.2417(3)	-0.0401(3)	0.7761(3)	1.68(5)
C(25)	0.2764(3)	-0.0945(3)	0.7016(2)	1.95(5)
C(26)	0.3222(3)	-0.2214(3)	0.7445(3)	2.13(5)
C(27)	0.3290(3)	-0.2942(3)	0.8637(3)	2.27(5)
C(28)	0.2925(3)	-0.2407(2)	0.9392(2)	1.79(5)
C(29)	0.1079(2)	-0.0642(2)	1.1700(2)	1.45(4)
C(30)	0.1227(2)	0.0688(2)	1.1398(2)	1.62(4)
C(31)	0.0842(3)	0.1068(3)	1.2258(3)	1.94(5)
C(32)	0.0286(3)	0.0154(3)	1.3440(2)	2.19(5)
C(33)	0.0120(3)	-0.1162(3)	1.3750(2)	2.09(5)
C(34)	0.0503(2)	-0.1544(3)	1.2900(3)	1.82(5)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S2-2. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	0.0146(2)	0.0137(3)	0.0147(3)	-0.00002(13)	-0.0031(2)	-0.0064(2)

O(1)	0.0298(9)	0.0241(8)	0.0240(9)	0.0135(7)	-0.0144(7)	-0.0138(7)
O(2)	0.0297(9)	0.0159(8)	0.0203(8)	-0.0071(7)	0.0031(7)	-0.0082(7)
N(1)	0.0154(8)	0.0158(8)	0.0187(9)	0.0022(7)	-0.0022(7)	-0.0083(8)
N(2)	0.0185(9)	0.0143(8)	0.0180(9)	-0.0006(7)	-0.0048(7)	-0.0083(8)
C(1)	0.0142(10)	0.0267(11)	0.0259(12)	-0.0011(8)	-0.0031(9)	-0.0131(10)
C(2)	0.0160(10)	0.0213(10)	0.0226(11)	-0.0033(8)	-0.0042(8)	-0.0090(9)
C(3)	0.0278(12)	0.0371(13)	0.0282(12)	0.0039(10)	-0.0029(10)	-0.0237(11)
C(4)	0.0232(12)	0.0186(11)	0.033(2)	0.0097(9)	-0.0135(10)	-0.0099(10)
C(5)	0.0281(12)	0.0141(10)	0.0293(13)	-0.0018(9)	-0.0067(10)	-0.0063(10)
C(6)	0.0289(12)	0.0314(12)	0.0281(12)	0.0018(10)	-0.0088(10)	-0.0212(11)
C(7)	0.0166(10)	0.0163(10)	0.0206(10)	0.0004(8)	-0.0038(8)	-0.0086(9)
C(8)	0.0185(10)	0.0164(10)	0.0186(10)	0.0023(8)	-0.0039(8)	-0.0070(9)
C(9)	0.0155(10)	0.0190(10)	0.0234(11)	0.0015(8)	-0.0043(8)	-0.0124(9)
C(10)	0.0212(11)	0.0166(10)	0.0243(12)	0.0005(8)	-0.0046(9)	-0.0080(10)
C(11)	0.0256(12)	0.0199(11)	0.039(2)	0.0044(9)	-0.0073(10)	-0.0170(11)
C(12)	0.0264(12)	0.037(2)	0.0324(13)	0.0079(10)	-0.0080(10)	-0.0260(12)
C(13)	0.0256(12)	0.0307(12)	0.0226(11)	0.0097(10)	-0.0093(9)	-0.0152(10)
C(14)	0.0203(11)	0.0201(10)	0.0220(11)	0.0030(8)	-0.0046(9)	-0.0114(10)
C(15)	0.0160(10)	0.0170(10)	0.0206(11)	-0.0043(8)	-0.0005(8)	-0.0093(9)
C(16)	0.0196(11)	0.0193(10)	0.0276(12)	0.0004(8)	-0.0066(9)	-0.0110(10)
C(17)	0.0315(13)	0.0265(12)	0.0187(11)	-0.0062(10)	-0.0051(10)	-0.0099(10)
C(18)	0.0318(13)	0.0304(12)	0.0234(12)	-0.0026(10)	-0.0030(10)	-0.0175(11)
C(19)	0.0293(12)	0.0231(11)	0.0273(12)	0.0039(9)	-0.0069(10)	-0.0165(10)
C(20)	0.0242(11)	0.0184(10)	0.0193(11)	0.0000(9)	-0.0048(9)	-0.0083(9)
C(21)	0.0201(10)	0.0146(9)	0.0221(11)	0.0002(8)	-0.0051(8)	-0.0080(9)
C(22)	0.0191(10)	0.0143(9)	0.0212(11)	-0.0018(8)	-0.0029(8)	-0.0055(9)
C(23)	0.0164(10)	0.0174(10)	0.0226(11)	-0.0010(8)	-0.0019(8)	-0.0109(9)
C(24)	0.0225(11)	0.0211(11)	0.0238(12)	0.0037(9)	-0.0090(9)	-0.0127(10)
C(25)	0.0282(12)	0.0251(12)	0.0226(12)	-0.0012(9)	-0.0075(9)	-0.0123(10)
C(26)	0.0315(13)	0.0290(12)	0.0283(12)	0.0007(10)	-0.0057(10)	-0.0205(11)
C(27)	0.035(2)	0.0184(11)	0.035(2)	0.0040(9)	-0.0060(11)	-0.0163(11)
C(28)	0.0273(12)	0.0153(10)	0.0216(11)	0.0003(9)	-0.0055(9)	-0.0065(9)
C(29)	0.0154(10)	0.0164(10)	0.0203(11)	0.0026(8)	-0.0052(8)	-0.0069(9)
C(30)	0.0190(10)	0.0169(10)	0.0176(11)	0.0003(8)	-0.0001(8)	-0.0047(9)
C(31)	0.0246(12)	0.0219(11)	0.0277(13)	0.0036(9)	-0.0056(10)	-0.0134(10)
C(32)	0.0298(13)	0.0340(13)	0.0209(12)	0.0081(10)	-0.0060(10)	-0.0159(11)
C(33)	0.0223(11)	0.0283(12)	0.0179(11)	0.0025(9)	-0.0020(9)	-0.0052(10)
C(34)	0.0194(11)	0.0192(10)	0.0244(12)	0.0007(8)	-0.0044(9)	-0.0068(10)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S2-3. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Fe(1)	O(1)	1.897(3)	Fe(1)	O(2)	1.891(4)
Fe(1)	N(1)	2.189(4)	Fe(1)	N(2)	2.190(4)
O(1)	C(7)	1.329(4)	O(2)	C(21)	1.331(4)
N(1)	C(1)	1.488(5)	N(1)	C(3)	1.479(4)
N(1)	C(4)	1.481(4)	N(2)	C(2)	1.477(4)
N(2)	C(5)	1.476(4)	N(2)	C(6)	1.486(4)

C(1)	C(2)	1.519(5)	C(7)	C(8)	1.361(4)
C(7)	C(9)	1.493(5)	C(8)	C(15)	1.463(5)
C(9)	C(10)	1.408(5)	C(9)	C(14)	1.398(4)
C(10)	C(11)	1.382(5)	C(11)	C(12)	1.389(4)
C(12)	C(13)	1.394(5)	C(13)	C(14)	1.385(5)
C(15)	C(16)	1.396(4)	C(15)	C(20)	1.405(4)
C(16)	C(17)	1.391(5)	C(17)	C(18)	1.380(5)
C(18)	C(19)	1.392(4)	C(19)	C(20)	1.388(5)
C(21)	C(22)	1.358(4)	C(21)	C(23)	1.494(5)
C(22)	C(29)	1.455(5)	C(23)	C(24)	1.397(4)
C(23)	C(28)	1.401(5)	C(24)	C(25)	1.387(5)
C(25)	C(26)	1.391(5)	C(26)	C(27)	1.388(5)
C(27)	C(28)	1.390(5)	C(29)	C(30)	1.411(5)
C(29)	C(34)	1.407(4)	C(30)	C(31)	1.381(5)
C(31)	C(32)	1.389(4)	C(32)	C(33)	1.394(5)
C(33)	C(34)	1.370(5)			

Table S2-4. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Fe(1)	O(2)	131.99(11)	O(1)	Fe(1)	N(1)	102.75(14)
O(1)	Fe(1)	N(2)	112.39(14)	O(2)	Fe(1)	N(1)	113.27(15)
O(2)	Fe(1)	N(2)	102.70(15)	N(1)	Fe(1)	N(2)	83.20(14)
Fe(1)	O(1)	C(7)	136.0(2)	Fe(1)	O(2)	C(21)	135.1(2)
Fe(1)	N(1)	C(1)	105.1(2)	Fe(1)	N(1)	C(3)	113.26(18)
Fe(1)	N(1)	C(4)	110.3(2)	C(1)	N(1)	C(3)	109.1(2)
C(1)	N(1)	C(4)	110.5(3)	C(3)	N(1)	C(4)	108.6(3)
Fe(1)	N(2)	C(2)	104.9(2)	Fe(1)	N(2)	C(5)	110.9(3)
Fe(1)	N(2)	C(6)	113.07(19)	C(2)	N(2)	C(5)	110.4(3)
C(2)	N(2)	C(6)	108.9(3)	C(5)	N(2)	C(6)	108.6(3)
N(1)	C(1)	C(2)	110.6(2)	N(2)	C(2)	C(1)	110.9(3)
O(1)	C(7)	C(8)	122.7(3)	O(1)	C(7)	C(9)	116.1(3)
C(8)	C(7)	C(9)	121.3(3)	C(7)	C(8)	C(15)	127.1(3)
C(7)	C(9)	C(10)	122.7(3)	C(7)	C(9)	C(14)	119.2(3)
C(10)	C(9)	C(14)	118.0(3)	C(9)	C(10)	C(11)	120.7(3)
C(10)	C(11)	C(12)	120.6(3)	C(11)	C(12)	C(13)	119.2(4)
C(12)	C(13)	C(14)	120.3(3)	C(9)	C(14)	C(13)	121.0(3)
C(8)	C(15)	C(16)	118.9(3)	C(8)	C(15)	C(20)	123.7(3)
C(16)	C(15)	C(20)	117.4(3)	C(15)	C(16)	C(17)	121.2(3)
C(16)	C(17)	C(18)	120.8(3)	C(17)	C(18)	C(19)	119.0(3)
C(18)	C(19)	C(20)	120.5(3)	C(15)	C(20)	C(19)	121.1(3)
O(2)	C(21)	C(22)	123.4(3)	O(2)	C(21)	C(23)	116.4(3)
C(22)	C(21)	C(23)	120.2(3)	C(21)	C(22)	C(29)	127.8(3)
C(21)	C(23)	C(24)	119.7(3)	C(21)	C(23)	C(28)	122.0(3)
C(24)	C(23)	C(28)	118.3(3)	C(23)	C(24)	C(25)	121.0(3)
C(24)	C(25)	C(26)	120.3(3)	C(25)	C(26)	C(27)	119.2(4)
C(26)	C(27)	C(28)	120.7(3)	C(23)	C(28)	C(27)	120.5(3)
C(22)	C(29)	C(30)	124.1(2)	C(22)	C(29)	C(34)	118.9(3)
C(30)	C(29)	C(34)	117.1(3)	C(29)	C(30)	C(31)	120.9(3)
C(30)	C(31)	C(32)	120.8(3)	C(31)	C(32)	C(33)	119.0(4)
C(32)	C(33)	C(34)	120.3(3)	C(29)	C(34)	C(33)	121.8(3)

Table S2-5. Torsion Angles(°) (Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle
O(1)	Fe(1)	O(2)	C(21)	64.3(3)
O(1)	Fe(1)	N(1)	C(1)	97.76(16)
O(1)	Fe(1)	N(1)	C(4)	-143.13(15)
O(1)	Fe(1)	N(2)	C(2)	-116.01(16)
O(1)	Fe(1)	N(2)	C(6)	125.43(15)
O(2)	Fe(1)	N(1)	C(1)	-114.67(16)
O(2)	Fe(1)	N(1)	C(4)	4.44(18)
O(2)	Fe(1)	N(2)	C(2)	97.42(16)
O(2)	Fe(1)	N(2)	C(6)	-21.14(13)
N(1)	Fe(1)	N(2)	C(2)	-14.98(9)
N(1)	Fe(1)	N(2)	C(6)	-133.54(14)
N(2)	Fe(1)	N(1)	C(3)	-132.71(14)
Fe(1)	O(1)	C(7)	C(8)	-171.67(14)
Fe(1)	O(2)	C(21)	C(22)	-168.86(14)
Fe(1)	N(1)	C(1)	C(2)	40.63(18)
C(4)	N(1)	C(1)	C(2)	-78.4(3)
C(5)	N(2)	C(2)	C(1)	-77.6(3)
N(1)	C(1)	C(2)	N(2)	-58.7(3)
O(1)	C(7)	C(9)	C(10)	134.4(3)
C(8)	C(7)	C(9)	C(10)	-44.8(4)
C(9)	C(7)	C(8)	C(15)	-178.98(18)
C(7)	C(8)	C(15)	C(20)	10.7(4)
C(7)	C(9)	C(14)	C(13)	174.1(2)
C(14)	C(9)	C(10)	C(11)	4.5(4)
C(10)	C(11)	C(12)	C(13)	-2.1(4)
C(12)	C(13)	C(14)	C(9)	-1.1(4)
C(8)	C(15)	C(20)	C(19)	-178.62(19)
C(20)	C(15)	C(16)	C(17)	-2.6(4)
C(16)	C(17)	C(18)	C(19)	1.1(4)
C(18)	C(19)	C(20)	C(15)	0.1(4)
O(2)	C(21)	C(23)	C(24)	-45.5(3)
C(22)	C(21)	C(23)	C(24)	135.3(3)
C(23)	C(21)	C(22)	C(29)	-178.7(2)
C(21)	C(22)	C(29)	C(34)	-169.8(3)
C(21)	C(23)	C(28)	C(27)	-174.72(19)
C(28)	C(23)	C(24)	C(25)	-1.0(4)
C(24)	C(25)	C(26)	C(27)	1.9(4)
C(26)	C(27)	C(28)	C(23)	-1.0(4)
C(22)	C(29)	C(34)	C(33)	178.9(2)
C(34)	C(29)	C(30)	C(31)	1.3(4)
C(30)	C(31)	C(32)	C(33)	-0.0(4)
C(32)	C(33)	C(34)	C(29)	0.5(4)

atom1	atom2	atom3	atom4	angle
O(2)	Fe(1)	O(1)	C(7)	65.0(3)
O(1)	Fe(1)	N(1)	C(3)	-21.22(14)
N(1)	Fe(1)	O(1)	C(7)	-156.53(18)
O(1)	Fe(1)	N(2)	C(5)	3.20(13)
N(2)	Fe(1)	O(1)	C(7)	-68.7(3)
O(2)	Fe(1)	N(1)	C(3)	126.35(15)
N(1)	Fe(1)	O(2)	C(21)	-71.0(3)
O(2)	Fe(1)	N(2)	C(5)	-143.38(13)
N(2)	Fe(1)	O(2)	C(21)	-158.97(17)
N(1)	Fe(1)	N(2)	C(5)	104.23(18)
N(2)	Fe(1)	N(1)	C(1)	-13.74(10)
N(2)	Fe(1)	N(1)	C(4)	105.38(19)
Fe(1)	O(1)	C(7)	C(9)	9.1(3)
Fe(1)	O(2)	C(21)	C(23)	12.0(4)
C(3)	N(1)	C(1)	C(2)	162.37(17)
Fe(1)	N(2)	C(2)	C(1)	41.92(17)
C(6)	N(2)	C(2)	C(1)	163.26(17)
O(1)	C(7)	C(8)	C(15)	1.8(4)
O(1)	C(7)	C(9)	C(14)	-42.4(3)
C(8)	C(7)	C(9)	C(14)	138.3(3)
C(7)	C(8)	C(15)	C(16)	-169.9(2)
C(7)	C(9)	C(10)	C(11)	-172.4(2)
C(10)	C(9)	C(14)	C(13)	-3.0(4)
C(9)	C(10)	C(11)	C(12)	-2.1(4)
C(11)	C(12)	C(13)	C(14)	3.6(4)
C(8)	C(15)	C(16)	C(17)	177.98(19)
C(16)	C(15)	C(20)	C(19)	2.0(4)
C(15)	C(16)	C(17)	C(18)	1.1(4)
C(17)	C(18)	C(19)	C(20)	-1.6(4)
O(2)	C(21)	C(22)	C(29)	2.2(4)
O(2)	C(21)	C(23)	C(28)	131.1(3)
C(22)	C(21)	C(23)	C(28)	-48.1(4)
C(21)	C(22)	C(29)	C(30)	10.3(4)
C(21)	C(23)	C(24)	C(25)	175.74(19)
C(24)	C(23)	C(28)	C(27)	1.9(4)
C(23)	C(24)	C(25)	C(26)	-0.9(4)
C(25)	C(26)	C(27)	C(28)	-1.0(4)
C(22)	C(29)	C(30)	C(31)	-178.9(2)
C(30)	C(29)	C(34)	C(33)	-1.2(4)
C(29)	C(30)	C(31)	C(32)	-0.7(4)
C(31)	C(32)	C(33)	C(34)	0.1(4)