Supporting Information for

Synthesis, Characterization of Titanium (IV) Complexes Bearing Monoanionic [O$^-$NX] (X=O, S, Se) Tridentate Ligands and Their Behavior in Ethylene Homo- and Co-polymerizaton with 1-Hexene

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General methods: All manipulations of air- and /or moisture- sensitive compounds were performed under an atmosphere of argon using standard Schlenk techniques. ^{1}H-NMR and ^{13}CNMR was recorded on a Varian XL-300MHz spectrometer with TMS as internal standard. Mass spectra were carried out with a HP5959A spectrometer. IR spectra were recorded using a Nicolet AV-360 spectrometer. Elemental analyse were performed by the Analytical Laboratory of Shanghai Institute of Organic Chemistry. M_n and M_w/M_n values of polymers were determined using a Waters alliance GPC 2000series at 150°C using polystyrene calibration. 1,2,4-trichlorobenzene was employed as a solvent at a flow rate of 1.0 mL/min. ^{13}C NMR data for polyethylene were obtained using *o*-dichlorobenzene-d^6 as a solvent at 110°C. Toluene, THF and hexane were refluxed over sodium/benzophenone ketyl, from which they were distilled prior to use. Dichloromethane was refluxed over CaH_2, from which it was distilled prior to use. Formylated phenol, 2-phenoxyl-aniline, appropriate 2-phenysulfanyl-aniline and 2-phenylselanyl-aniline was prepared according to published procedure.[1] Modified methylaluminoxane(MMAO) was purchased from Akzo Chemical as a 1.6M of a toluene solution. Polymerization-grade ethylene was purified before use.

(2-nitro-phenyl)-phenyl ether (3a)

To a stirred solution of phenol (9.4g, 0.1mol) in 30 mL DMSO, KOH (5.6 g, 0.1moL) was added. The mixture was stirred for 30 min. and then a solution of 1-chloro-2-nitro-benzene (15.7g, 0.1mol) in 10 mL DMSO was added drop wise during a period of 5 min. at room temperature. The resulted mixture was stirred for another 5 h at 90°C. After cooling to room temperature, the reaction mixture was poured into 200 mL water. The product was abstracted with ethyl ether (50mL×3). The combined ether was washed with water (50mL×5), dried with Na_2SO_4, and the solvent was removed in *vacuo* to give product as oil (20.3g) in 94% yield, which was used without further purification. ^{1}H NMR(300MHz, $CDCl_3$): δ 7.93 (dd, 1H, *J* = 1.5, 8.1 Hz, Ar-H); 7.49 (dt, 1H, *J* = 1.5, 7.5 Hz, Ar-H); 7.35-7.40 (m, 2H, Ph-H); 7.15-7.21 (m, 2H, Ph-H); 6.98-7.06 (m, 3H, Ph-H).

(2-nitro-phenyl)-(2,6-dichlorophenyl) ether (3b) Following above procedure, 2,6-dichloro phenol (1.63 g, 10mmol), KOH (0.56g, 10mmol) and 1-chloro-2-nitrobenzene(1.89g, 12 mmol) were used. **3b** (1.03g) was obtained as a yellow powder in 36% yield. ^{1}H NMR (300MHz,

$CDCl_3$): δ 7.87 (d, 1H, *J* = 8.1 Hz, Ar-H), 7.56-7.53 (m, 3H, Ar-H), 7.26 (d, *J* = 8.1 Hz, 2H, Ar-H), 6.83 (t, 1H, *J* = 8.1 Hz, Ar-H).

(2-nitro-phenyl)-(2,6-dimethylphenyl) ether (3c). Following above procedure, 2,6-dimethylphenol (14.6 g, 0.1 mol), KOH (5.6 g, 0.1mmol) and 1-chloro-2-nitro-benzene(18.9 g, 12mmol) were used. **3c** (18.4 g) was obtained as a yellow powder in 75 % yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.95 (dd, 1H, *J* = 1.5, 5.1 Hz, Ar-H), 7.37 (dt, 1H, *J* = 1.8, 9.0 Hz, Ar-H), 7.11-7.03 (m, 4H, Ar-H), 6.55 (d, 1H, *J* = 8.7 Hz, Ar-H); 2.14 (s, 6 H, -CH_3)

(2-nitro-phenyl)-(2,6-di-*iso*-proyllphenyl) ether (3d). Following above procedure, 2,6-di-*iso*-proyllphenol (3.56 g, 20mmol), KOH (1.12 g, 20mmol) and 1-chloro-2-nitro-benzene (3.15 g, 20 mmol) were used. **3d** (4.2 g) was obtained as a yellow powder in 70 % yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.95 (dd, 1H, *J* = 1.5, 8.1 Hz, Ar-H), 7.38-7.21 (m, 4H, Ar-H), 7.04 (t, 1H, *J* = 8.4 Hz, Ar-H), 6.54 (d, 1H, *J* = 8.4 Hz, Ar-H), 2.97 (hepta, 2H, *J* = 6.6 Hz, $CH(CH_3)_2$), 1.21 (d, 6H, *J* = 6.9 Hz, $CH(CH_3)_2$), 1.09 (d, 6H, *J* = 6.9 Hz, $CH(CH_3)_2$).

(2-nitro-phenyl)-phenyl sulfide (3e). Following above procedure, benzenethiol (11.0 g, 0.1mol), KOH (5.6 g, 0.1mmol) and 1-chloro-2-nitro-benzene(15.7g, 0.1mol) were used. **3e** (22.4g) was obtained as a yellow powder in 96% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.21 (dd, *J* = 1.2, 8.1Hz, 1H, Ar-H); 7.46-7.60 (m, 5H, Ar-H); 7.18-7.36 (m, 2H, Ar-H); 6.84 (d, 1H, *J* = 7.8 Hz, Ar-H).

(2-nitro-phenyl)-(4-trifluoromethylphenyl) sulfide (3f) . Following above procedure, 4-trifluoromethylbenzenethiol (4.45g, 25mmol), KOH (1.4g, 25mmol) and 1-chloro-2-nitrobenzene (3.94g, 25mmol) were used. **3f** (6.13g) was obtained as a yellow powder in 82% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.24(dd, 1H, *J* = 1.5, 8.1 Hz, Ar-H); 7.68-7.75 (m, 4H, Ar-H); 7.41 (dt, 1H, *J* = 1.5, 7.2 Hz, Ar-H); 7.30 (dt, 1H, *J* = 1.5, 7.2 Hz, Ar-H); 6.91 (dd, 1H, *J* = 1.5, 8.1 Hz, Ar-H).

(2-nitro-phenyl)-(3-chlorophenyl) sulfide (3g). Following above procedure, 3-chloro benzenethiol (4.33g, 30mmol), KOH (1.68g, 30mmol) and 1-chloro-2-nitro-benzene (4.72g, 30mmol) were used. **3g** (6.69g) was obtained as a yellow powder in 84% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.23 (d, 1H, *J* = 8.4 Hz, Ar-H); 7.59 (s, 1H, Ar-H); 7.38-7.51 (m, 4H, Ar-H); 7.28 (t, 1H, *J* = 7.5 Hz, Ar-H); 6.90 (d, 1H, *J* = 8.1 Hz, Ar-H).

(2-nitro-phenyl)-(4-methoxylphenyl) sulfide (3h). Following above procedure, 4-methoxyl benzenethiol (4.20g, 30mmol), KOH (1.68g, 30mmol) and 1-chloro-2-nitro-benzene (4.72g, 30mmol) were used. **3h** (7.12g) was obtained as a yellow powder in 91% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.24 (dd, *J* = 6.0, 8.1 Hz , 1H, Ar-H); 7.51 (d, 2H, *J* = 8.7 Hz, Ar-H); 7.34 (dt, 1H, *J* = 1.5, 7.5 Hz , Ar-H); 7.19 (dt, 1H, *J* = 1.5, 7.5 Hz, Ar-H); 7.01 (d, 2H, *J* = 7.8 Hz , Ar-H); 6.83 (d, *J* = 8.4 Hz , 1H, Ar-H); 3.88(s, 3H, OCH_3).

(2-nitro-phenyl)-(3-methoxylphenyl) sulfide (3i). Following above procedure, 3-methoxyl benzenethiol (4.20g, 30mmol), KOH (1.68 g, 30mmol) and 1-chloro-2-nitro-benzene (4.72g, 30mmol) were used. **3i** (6.97g) was obtained as a yellow powder in 89% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.22 (d, *J* = 8.1, 1H, Ar-H); 7.12-7.43 (m, 5H, Ar-H); 7.02 (d, 1H *J* = 8.1 Hz, Ar-H); 6.90 (d, 1H, *J* = 8.1 Hz, Ar-H); 3.83 (s, 3H, OCH_3).

(2-nitro-phenyl)-(2,6-dichlorophenyl) sulfide (3j). Following above procedure, 2,6-dichlorobenzenethiol (4.47g, 25mmol), KOH (1.40g, 25mmol) and 1-chloro-2-nitro-benzene (3.94g, 25mmol) were used. **3j** (7.47g) was obtained as a yellow powder in 83% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.31 (dd, 1H, *J* = 1.5, 8.4 Hz, Ar-H); 7.26-7.55(m, 5H, Ar-H); 6.68 (dd, 1H, *J* = 1.5, 8.4 Hz, Ar-H).

(2-nitro-phenyl)-(2,6-dimethylphenyl) sulfide (3k). Following above procedure, 2,6-dimethyl benzenethiol (4.14 g, 30mmol), KOH (1.68 g, 30 mmol) and 1-chloro-2-nitro-benzene (4.72 g, 30 mmol) were used. **3k** (6.14 g) was obtained as a yellow powder in 79% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.97 (dd, *J* = 1.5, 8.1 Hz, 1H, Ar-H); 7.38 (dt, *J* = 1.8, 7.5 Hz, 1H, Ar-H); 7.04-7.13 (m, 4H, Ar-H); 6.56 (dd, 1H, *J* = 6.0, 8.4 Hz, Ar-H); 2.15 (s, 6H, CH_3).

(2-nitro-phenyl)-(2,6-di-iso-propylphenyl) sulfide (3l). Following above procedure, 2,6-di-*iso*-propylbenzenethiol (4.85 g, 25 mmol), KOH (1.40 g, 25 mmol) and 1-chloro-2-nitro-benzene (3.94g, 25mmol) were used. **3l** (5.91 g) was obtained as a yellow powder in 75% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.31 (dd, *J* = 1.5, 8.4 Hz, 1H, Ar-H); 7.52 (t, *J* = 7.8, 1H, Ar-H); 7.29-7.35 (m, 3H, Ar-H); 7.19 (dt, 1H, *J* = 1.5, 7.2 Hz, Ar-H); 6.64 (dd, 1H, *J* = 1.2, 8.1 Hz, Ar-H); 3.56 (hepta, 2H, *J* =6.6 Hz, $CH(CH_3)_2$); 1.11 (d, 12H, *J* = 16.5 Hz , $CH(CH_3)_2$).

(2-nitro-phenyl)-phenyl selenide (3m). Following above procedure, benzeneselenol (4.71 g,

30 mmol), KOH(1.68 g, 30 mmol) and 1-chloro-2-nitro-benzene(4.72 g, 30 mmol) were used. **3m** (7.25 g) was obtained as a yellow powder in 87% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 8.24(d, *J* =8.1, 1H, Ar-H); 7.47-7.59 (m, 4H, Ar-H); 7.20-7.33(m, 3H, Ar-H); 6.85(d, *J* = 8.4 Hz, 1H, Ar-H).

2-phenoxyl-aniline (4a). To a slurry mixture of Zn powder (6.5 g, 100 mmoL) in 30 mL absolute ethanol and 0.5 mL AcOH, a solution of **3a** (4.3 g, 20 mmoL) in 10 mL ethanol was added dropwise during a period of 10 min. at 0 ^{o}C. The resulted mixture was allowed stirred for 3 h at room temperature. The reaction mixture was filtered and the solvent of the collected filtrate was removed in *vacuo* to give crude product. The crude product was purified by column chromagraphy on silica gel with petroleum ether-ethyl acetate (10:1) as the eluent. The product was afforded as a white powder in 94% yield (3.47g). ^{1}H NMR (300MHz, $CDCl_3$): δ 7.32-7.27 (m, 2H, Ar-H), 7.07-6.94(m, 4H, Ar-H); 6.88-6.79 (m, 2H, Ar-H), 6.71-6.68 (m, 1H, Ar-H),3.78 (brs, 2H, N-H).

2-(2,6-dichlorophenoxyl)-aniline (4b). Following above procedure, Zn powder (7.1 g, 126 mmol), and **3b** (6.0 g, 21 mmol) were used. **4b** (4.02 g) was obtained as a yellow powder in 76 % yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.37 (d, 2H, *J* = 8.1 Hz, Ar-H), 7.26-7.16 (m, 2H, Ar-H), 7.08 (t, 1H, *J* =7.2 Hz, Ar-H), 6.67 (q, 2H, *J* =7.5 Hz, Ar-H), 4.25 (brs, 2H, N-H).

2-(2,6-dimethylphenoxyl)-aniline (4c). Following above procedure, Zn powder (37.5 g, 670 mmol), and **3c** (24.3 g, 100 mmol) were used. **4c** (19.2 g) was obtained as a yellow powder in 90% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.11-7.08(m, 3H, Ar-H), 6.82(m, 2H, Ar-H), 6.58-6.55(m, 1H, Ar-H), 6.25(d, 1 H, *J* =7.5 Hz, Ar-H), 3.88(brs, 2H, NH), 2.16(s, 6H, -CH_3).

2-(2,6-di-*iso*-proylphenoxyl)-aniline (4d). Following above procedure, Zn powder (4.7 g, 84 mmol), and **3d** (4.2g, 14 mmol) were used. **4d** (3.2 g) was obtained as a yellow powder in 85 % yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.21(t, 3H, *J* = 4.5 Hz, Ar-H), 6.81-6.79(m, 2H, Ar-H), 6.57-6.51 (m, 1H, Ar-H), 6.22 (d, 1H, *J* = 6.0 Hz, Ar-H), 3.97 (brs, 2H, N-H), 3.02 (hepta, 2H, $CH(CH_3)_2$), 1.19(d, 6H, *J* = 6.9 Hz, $CH(CH_3)_2$), 1.08 (d, 6H, *J* = 7.2 Hz, $CH(CH_3)_2$).

2-phenysulfanyl-aniline (4e). Following above procedure, Zn powder (6.5 g, 20 mmol), and **3e** (4.62 g, 20 mmol) were used. **4e** (3.66 g) was obtained as a yellow powder in 91% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.47 (d, 1H, *J* = 6.0 Hz, Ar-H), 7.27-6.82 (m, 6H, Ar-H), 6.82-6.77 (m, 6H, Ar-H), 4.26 (brs, 2H, N-H).

2-(4-trifluoromethylphenysulfanyl) aniline (4f). Following above procedure, Zn powder (6.5 g, 100 mmol), and **3f** (5.98g, 20mmol) were used. **4f** (4.90 g) was obtained as a yellow powder in 91% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.46 (d, 3H, *J* = 7.5 Hz, Ar-H); 7.30 (t, 1H, *J* =7.2 Hz, Ar-H); 7.12 (d, *J* = 8.4 Hz, 2H, Ar-H); 6.77-6.84 (m, 2H, Ar-H); 4.29 (brs 2H, N-H).

2-(3-chlorophenysulfanyl)-aniline (4g). Following above procedure, Zn powder (6.5 g, 100 mmol), and **3g** (5.31 g, 20 mmol) were used. **4g** (4.00 g) was obtained as a yellow powder in 85% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.44-7.47 (m, 1H, Ar-H); 7.22-7.07 (m, 5H, Ar-H); 6.77-6.72 (m, 2H, Ar-H); 4.26 (brs, 2H, N-H).

2-(4-methoxylphenysulfanyl)-aniline (4h). Following above procedure, Zn powder (4.88 g, 75mmol), and **3h** (3.91 g, 15 mmol) were used. **4h** (3.01 g) was obtained as a yellow powder in 87% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.40 (dd, 1H, *J* = 1.5, 7.2 Hz, Ar-H); 7.11-7.25 (m, 3H, Ar-H); 6.70-6.82 (m, 4H, Ar-H); 4.26 (brs, 2H, N-H); 3.75 (s, 3H, O-CH_3).

2-(3-methoxylphenysulfanyl)-aniline (4i). Following above procedure, Zn powder (6.5 g, 100 mmol), and **3i** (5.22 g, 20 mmol) were used. **4i** (4.11 g) was obtained as a yellow powder in 89% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.52 (dd, 1H, *J* = 1.5, 7.8 Hz, Ar-H); 7.29 (dt, *J* = 1.5, 7.5 Hz, 1H, Ar-H); 7.19 (t, 1H, *J* =7.5 Hz, Ar-H); 6.71-6.84 (m, 5H, Ar-H); 4.34 (brs, 2H, N-H); 3.76 (s, 3H, OCH_3).

2-(2,6-dichlorophenysulfanyl)-aniline (4j). Following above procedure, Zn powder (6.5 g, 100 mmol), and **3j** (6.00 g, 20 mmol) were used. **4j** (4.91 g) was obtained as a yellow powder in 91% yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.37 (d, 2H *J* = 7.8 Hz, Ar-H); 7.25-7.07 (m, 3H, Ar-H); 6.65-6.70 (m, 2H, Ar-H); 4.29 (brs, 2H, N-H).

2-(2,6-di-methylphenysulfanyl)-aniline (4k). Following above procedure, Zn powder (6.5 g, 100 mmol), and **3k** (5.18 g, 20 mmol) were used. **4k** (3.98 g) was obtained as a yellow powder in 87% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.19-7.27 (m, 3H, Ar-H); 7.02 (t, 1H, *J* =7.2 Hz, Ar-H); 6.61-6.75 (m, 3H, Ar-H); 4.09 (brs, 2H, N-H); 2.48(s, 6H, -CH_3).

2-(2,6-di-*iso*-propylphenysulfanyl)-aniline (4l). Following above procedure, Zn powder (6.5 g, 100 mmol), and **3l** (6.30 g, 20 mmol) were used. **4l** (5.24 g) was obtained as a powder in 92% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.46 (t, 1H, *J* =7.5 Hz, Ar-H); 7.30 (d, *J* =7.8 Hz, 2H, Ar-H); 6.97 (t, 1H, *J* = 7.5 Hz, Ar-H); 6.72 (d, *J* = 7.8 Hz, 1H, Ar-H); 6.60 (t, 1H, *J* = 8.1

Hz, Ar-H); 6.48 (d, 1H, *J*=8.1 Hz, Ar-H); 4.09 (brs, 2H, N-H); 3.74 (hepta, 2H, *J*=6.6 Hz, $CH(CH_3)_2$); 1.18 (d, 12H, *J*=7.2 Hz, $CH(CH_3)_2$).

2-phenylselanyl-aniline (4m). Following above procedure, Zn powder (6.5 g, 100 mmol), and **3m** (5.88 g, 20 mmol) were used. **4m** (4.61 g) was obtained as a yellow powder in 91% yield. ^{1}H NMR (300MHz, $CDCl_3$): δ 7.49 (dd, 1H, *J* = 1.5, 7.2 Hz, Ar-H); 7.26-7.10 (m, 5H, Ar-H); 6.82-6.78 (m, 2H, Ar-H); 4.30 (brs, 2H, N-H).

N-(3,5-di-*tert*-butylsalicylidene)-2-phenoxylaniline (L1). A solution of 3,5-di-*tert*-butylsalicyl-aldehyde (5.62 g, 24 mmol), **4a** (3.65 g, 20 mmol) and glacial acetic acid (0.05 mL) in absolute ethanol (100 mL) was refluxed for 12 h and then concentrated to 50 mL. The resulting mixture was cooled to room temperature, and then left at –30 °C overnight. The yellow solid was collected and recrystallized from petroleum ether to give the product. Yield: 5.2 g (65%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 13.35 (s, 1H, Ar-OH); 8.67 (s, 1H, CH=N); 7.41-6.98 (m, 11H, Ar-H); 1.41 (s, 9H, *t*-Bu); 1.31 (s, 9H, *t*-Bu). ^{13}C NMR (75 MHz, $CDCl_3$): δ 164.5 (N=C), 158.4, 157.6, 149.4, 140.6, 140.1, 136.9, 129.6, 128.0, 127.3, 126.7, 124.6, 122.7, 121.0, 120.7, 118.2, 117.7, 35.0, 34.1, 31.4, 29.3. Anal. Calcd. for $C_{27}H_{31}NO_2$: C, 80.80; H, 7.73; N, 2.49. Found: C, 80.95; H, 7.93; N, 2.24. MS (EI), *m/z*: 401 [M^+].

N-(3,5-di-*tert*-butylsalicylidene)-2-(2,6-dichlorophenoxyl) aniline (L2). The same procedure as the preparations of **L1**. 3,5-Di-*tert*-butylsalicylaldehyde (3.83 g, 16.3 mmol), **4b** (3.46 g, 13.6 mmol) and glacial acetic acid (0.05 mL) were used. Yield: 5.5 g (86%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 13.69 (s, 1H, Ar-OH), 8.81 (s, 1H, CH=N), 7.48 (d, *J* = 2.1Hz, 1H, Ar-H), 7.42 (d, *J* = 8.1 Hz, 1H, Ar-H), 7.30-7.10 (m, 6H, Ar-H), 6.53 (t, *J* = 4.5 Hz, 1H, Ar-H), 1.47 (s, 9H, *t*-Bu), 1.30(s, 9H, *t*-Bu). ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.3 (CH=N), 158.5, 149.4, 147.6, 140.2, 137.9, 136.9, 129.8, 129.1, 128.0, 126.8, 126.3, 123.1, 121.4, 118.4, 114.2, 35.1, 34.1, 31.5, 29.4。 IR (KBr) ν: 1618, 1575, 1492, 1442, 1243, 1202, 1169, 1109, 775, 751. Anal. Calcd. for $C_{27}H_{29}Cl_2NO_2$: C, 68.94; H, 6.17; N, 2.98；Found: C, 68.92; H, 6.19; N, 2.70. MS (EI), *m/z*: 470[M^+].

N-(3,5-di-*tert*-butylsalicylidene)-2-(2,6-dimethylphenoxyl) aniline (L3). The same procedure as that for the preparations of **L1**. 3,5-Di-*tert*-butylsalicylaldehyde (7.02g, 30 mmol), **4c** (6.39 g, 30 mmol) and glacial acetic acid (0.05 mL) were used. Yield: 9.2 g (71%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 13.96 (s, 1 H, Ar-OH), 8.79 (s, 1H, CH=N), 7.39 (d, *J* = 2.4 Hz, 1H, Ar-H), 7.23-7.17 (m, 2H, Ar-H), 7.04-6.94 (m, 4H, Ar-H), 6.38 (d, *J* = 9.6 Hz, 1H, Ar-H), 2.10 (s, 6 H, Ar-CH_3), 1.41 (s, 9 H, *t*-Bu), 1.28 (s, 9 H, *t*-Bu). ^{13}C NMR (75 MHz, $CDCl_3$): δ 164.1 (CH=N), 158.6, 151.4, 150.7, 140.2, 137.2, 137.0, 131.5, 129.0, 127.8, 127.2, 126.7,

125.0, 121.7, 120.8, 118.5, 113.7, 35.1, 34.1, 31.5, 29.4, 16.4. IR (KBr) ν: 1617, 1575, 1473, 1357, 1230, 1172, 1106, 880, 744. Anal. Calcd. for $C_{29}H_{35}NO_2$: C, 81.06; H, 8.23; N,3.26. Found: C, 80.86; H, 8.13; N, 3.23。 MS (EI), *m/z*: 429[M^+].

N-(3,5-di-*tert*-butylsalicylidene)-2-(2,6-di-*iso*proylphenoxyl) aniline (L4). The same procedure as that for the preparation of **L1**. 3,5-Di-*tert*-butylsalicylaldehyde (2.19g, 9.4 mmol), **4d** (2.10 g, 8 mmol) and glacial acetic acid (0.05 mL) were used. Yield: 2.63 g (68 %). ^{1}H NMR (300 MHz, $CDCl_3$): δ 14.16 (s, 1 H, Ar-OH), 8.88 (s, 1H, CH=N), 7.46 (d, *J* = 2.1Hz, 1H, Ar-H), 7.30-7.34 (m, 1H, Ar-H), 7.24-7.26 (m, 4H, Ar-H), 7.00-7.05(m, 2H, Ar-H), 6.45(dd, *J* = 2.1, 7.5Hz, 1H, Ar-H), 3.06(hepta, *J* = 6.6 Hz, 1H, $CH(CH_3)_2$), 1.56(s, 9H, *t*-Bu), 1.46(s, 9H, *t*-Bu), 1.20 (d, *J* = 6.3 Hz, 6H, $CH(CH_3)_2$), 1.11(d, *J* = 6.9 Hz, 6H, $CH(CH_3)_2$). ^{13}C NMR (75 MHz, $CDCl_3$): δ 163.4 (CH=N), 158.7, 152.2, 148.8, 141.7, 140.1, 137.0, 136.5, 127.7, 127.1, 126.4, 125.7, 124.3, 121.5, 120.1, 118.4, 113.8, 35.1, 34.1, 31.4, 29.3, 27.0, 24.4, 22.2. IR (KBr) ν: 3061, 2961, 2906, 1618, 1879, 1492, 1441, 1392, 1361, 1242, 1203, 1168, 1113, 975, 883, 792. Anal. Calcd. for $C_{33}H_{43}NO_2$: C, 81.60; H, 8.92; N, 2.88. Found: C, 81.32; H, 8.89; N, 2.69. MS (EI), *m/z*: 485[M^+].

N-(3,5-di-*tert*-butylsalicylidene)-2-phenysulfanyl-aniline (L5). The same procedure as that for the preparation of **L1**. 3,5-Di-*tert*-butylsalicylaldehyde (2.34 g, 10 mmol), **4e** (2.01 g, 10 mmol) and glacial acetic acid (0.05 mL) were used. Yield: 3.9 g (95%). ^{1}H NMR (300MHz, $CDCl_3$): δ 13.31(s, 1H, Ar-OH); 8.56 (s, 1H, CH=N); 7.45-7.11 (m, 11H, Ar-H); 1.47 (s, 9H, *t*-Bu); 1.32 (s, 9H, *t*-Bu). ^{13}C NMR (75MHz, $CDCl_3$): δ 163.8(N=C), 158.3, 147.1, 140.4, 137.0, 133.8, 133.0, 132.6, 129.9, 129.3, 128.2, 127.7, 127.3, 126.9, 118.2, 35.1, 34.1, 31.4, 29.4. Anal. Calcd. for $C_{27}H_{31}NOS$: C, 77.70; H, 7.43; N, 3.36. Found: C, 77.98; H, 7.48; N, 2.99. MS (EI), *m/z*: 417[M^+]

N-(3,5-di-*tert*-butylsalicylidene)-2-(4-trifluoromethylphenysulfanyl)-aniline (L6). The same procedure as that for the preparations of **L1**. 3,5-Di-*tert*-butylsalicylaldehyde (0.8 g, 3.4 mmol), **4f** (0.9 g, 3.4 mmol) and glacial acetic acid (0.05 mL) were used. Yield: 1.15 g (67%). ^{1}H NMR (300MHz, $CDCl_3$): δ 13.07 (s, 1H, Ar-OH); 8.49 (s, 1H, CH=N); 7.49-7.41 (m, 5H, Ar-H); 7.34 (d, *J* = 8.1 Hz, 2H, Ar-H); 7.22 (q, *J* = 7.2 Hz, 2H, Ar-H); 7.16-7.14 (m, 1H, Ar-H); 1.43 (s, 9H, *t*-Bu); 1.32 (s, 9H, *t*-Bu). ^{19}F NMR (282.3 Hz, $CDCl_3$): δ 62.9. Anal. Calcd. for $C_{28}H_{30}NOF_3S$: C, 69.25; H, 6.23; N, 2.88. Found: C, 69.13; H, 6.21; N, 2.70. MS(EI), *m/z*: 485[M^+]

N-(3,5-di-*tert*-butylsalicylidene)-2-(3-chlorophenysulfanyl)-aniline (L7). The same procedure as that of the preparations of **L1**. 3,5-Di-*tert*-butylsalicylaldehyde (6.64 g, 28.4 mmol), **4g** (6.20 g, 28.4 mmol) and glacial acetic acid (0.05 mL) were used. Yield: 9.1 g (71%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 13.30 (s, 1H,

Ar-OH); 8.57 (s, 1H, CH=N); 7.51 (s, 1H), 7.38-7.22 (m, 9H, Ar-H); 1.52 (s, 9H, *t*-Bu); 1.37 (s, 9H, *t*-Bu). ^{13}C NMR (75MHz, $CDCl_3$): δ 164.00 (C=N), 158.3, 148.3, 140.4, 137.0, 134.7, 131.8, 130.9, 130.2,130.0, 129.4, 128.6, 128.4, 127.2, 127.0, 126.9, 118.6, 118.1, 35.1, 34.1, 31.4, 29.4. Anal. Calcd. for $C_{27}H_{30}NOSCl$: C, 71.76; H, 6.64; N, 3.10. Found: C, 71.52; H, 6.66; N, 2.81. MS (EI), *m/z*: 451[M^+]**.**

N-(3,5-di-*tert*-butylsalicylidene)-2-(4-methoxylphenysulfanyl)-aniline (L8). The same procedure as that of the preparation of **L1**. 3,5-Di-*tert*-butylsalicylaldehyde (3.5g, 15mmol), **4h** (3.5 g, 15 mmol) and glacial acetic acid (0.05 mL) were used. Yield: 4.4 g (66%). ^{1}H NMR (300MHz, $CDCl_3$): δ 13.41 (s, 1H, Ar-OH); 8.62 (s, 1H, CH=N); 7.50-7.47 (m, 3H, Ar-H), 7.24-7.08 (m, 4H, Ar-H); 6.94-6.87 (m, 3H, Ar-H); 3.84 (s, 3H, OCH_3); 1.52(s, 9H, *t*-Bu); 1.36(s, 9H, *t*-Bu). ^{13}C NMR (75 MHz, $CDCl_3$): δ 163.8 (C=N), 160.0, 158.3, 145.6, 140.4, 137.0, 136.5, 135.0, 128.2, 127.3, 126.8, 126.7, 126.0, 122.7, 118.3, 117.7, 115.0, 55.3, 35.1, 34.1, 31.4, 29.3. Anal. Calcd. for $C_{28}H_{33}NO_2S$: C, 75.13; H, 7.43; N, 3.13. Found: C, 74.88; H, 7.39; N, 2.96. MS (EI), *m/z*: 447[M^+].

N-(3,5-di-*tert*-butylsalicylidene)-2-(3-methoxylphenysulfanyl)-aniline (L9). The same procedure as that for the preparation of **L1.** 3,5-Di-*tert*-butylsalicylaldehyde (5.4 g, 23 mmol), **4i** (5.3 g, 23 mmol) and glacial acetic acid (0.05 mL) were used. Yield: 7.5g (73%). ^{1}H NMR (300MHz, $CDCl_3$): δ 13.41 (s, 1H, Ar-OH); 8.62 (s, 1H, CH=N); 7.54 (d, J = 2.1 Hz, 1H, Ar-H); 7.32-7.18 (m, 6H, Ar-H), 7.08-7.04 (m, 2H, Ar-H), 6.85 (ddd, J = 0.9, 2.4, 7.2Hz, 1H, Ar-H); 3.78 (s, 3H, OCH_3); 1.55 (s, 9H, *t*-Bu); 1.40 (s, 9H, *t*-Bu). ^{13}C NMR (75MHz, $CDCl_3$): δ 163.8 (C=N), 160.0, 158.3, 147.4, 140.4, 137.0, 135.1, 132.0, 130.3, 130.0, 128.2, 127.6, 126.9, 126.8, 124.9, 118.3, 118.2, 117.5, 113.7, 55.2, 35.1, 34.1, 31.4, 29.4.Anal. Calcd. for $C_{28}H_{33}NO_2S$: C, 75.13; H, 7.43; N, 3.13. Found: C, 75.12; H, 7.51; N, 2.89. MS (EI), *m/z*: 447[M^+]

N-(3,5-di-*tert*-butylsalicylidene)-2-(2,6-di-chlorophenysulfanyl)aniline (L10). The same procedure as that for the preparations of **L1**. 3,5-Di-*tert*-butylsalicylaldehyde(3.6 g, 16 mmol), **4j** (3.5 g, 15 mmol) and glacial acetic acid (0.05 mL) were used. Yield: 5.8 g (92%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 13.24 (s, 1H, Ar-OH); 8.65 (s, 1H, CH=N); 7.50-7.45 (m, 3H, Ar-H); 7.30-7.07 (m, 5H, Ar-H); 6.66 (d, *J* = 7.8Hz, 1H, Ar-H); 1.51 (s, 9H, *t*-Bu); 1.36 (s, 9H, *t*-Bu). ^{13}C NMR (75 MHz, $CDCl_3$): δ 163.9 (C=N), 158.2, 145.9, 141.8, 140.4, 137.0, 131.3, 130.8, 130.6, 128.8, 128.3, 127.0, 126.9, 126.4, 126.0, 118.2, 118.1, 35.1, 34.1, 31.4, 29.4. Anal. Calcd. for $C_{27}H_{29}NOSCl_2$: C, 66.67; H, 6.01; N, 2.88. Found: C, 66.71; H, 5.97; N, 2.63. MS (EI), *m/z*: 486[M^+].

N-(3,5-di-*tert*-butylsalicylidene)-2-(2,6-di-methylphenysulfanyl)-aniline (L11). The same procedure as that for the preparation of **L1**. 3,5-Di-*tert*-butylsalicylaldehyde(3.37 g, 14 mmol), **4k** (2.75 g, 12 mmol) and

glacial acetic acid (0.05 mL) were used. Yield: 3.66 g (68%). ^{1}H NMR (300MHz, $CDCl_3$): δ 13.50 (s, 1H, Ar-OH); 8.70 (s, 1H, CH=N); 7.52 (d, *J* = 1.5Hz, 1H, Ar-H); 7.30-6.99 (m, 7H, Ar-H); 6.48 (d, *J* = 7.8 Hz, 1H, Ar-H); 2.46 (s, 6H, Ar-CH_3); 1.55 (s, 9H, *t*-Bu); 1.39 (s, 9H, *t*-Bu). ^{13}C NMR (75 MHz, $CDCl_3$): δ 163.3 (C=N), 158.3, 145.4, 144.1, 140.4, 137.1, 133.8, 130.1, 129.2, 128.4, 128.2, 126.9(3), 126.8(8), 125.1, 124.7, 118.4, 117.6, 35.1, 34.1, 31.4, 29.4, 21.7(Ar-C). Anal. Calcd. for $C_{29}H_{35}NOS$: C, 78.20; H, 7.86; N, 3.15. Found: C, 78.10; H, 7.87; N, 3.05. MS (EI), *m/z*: 445[M^+]

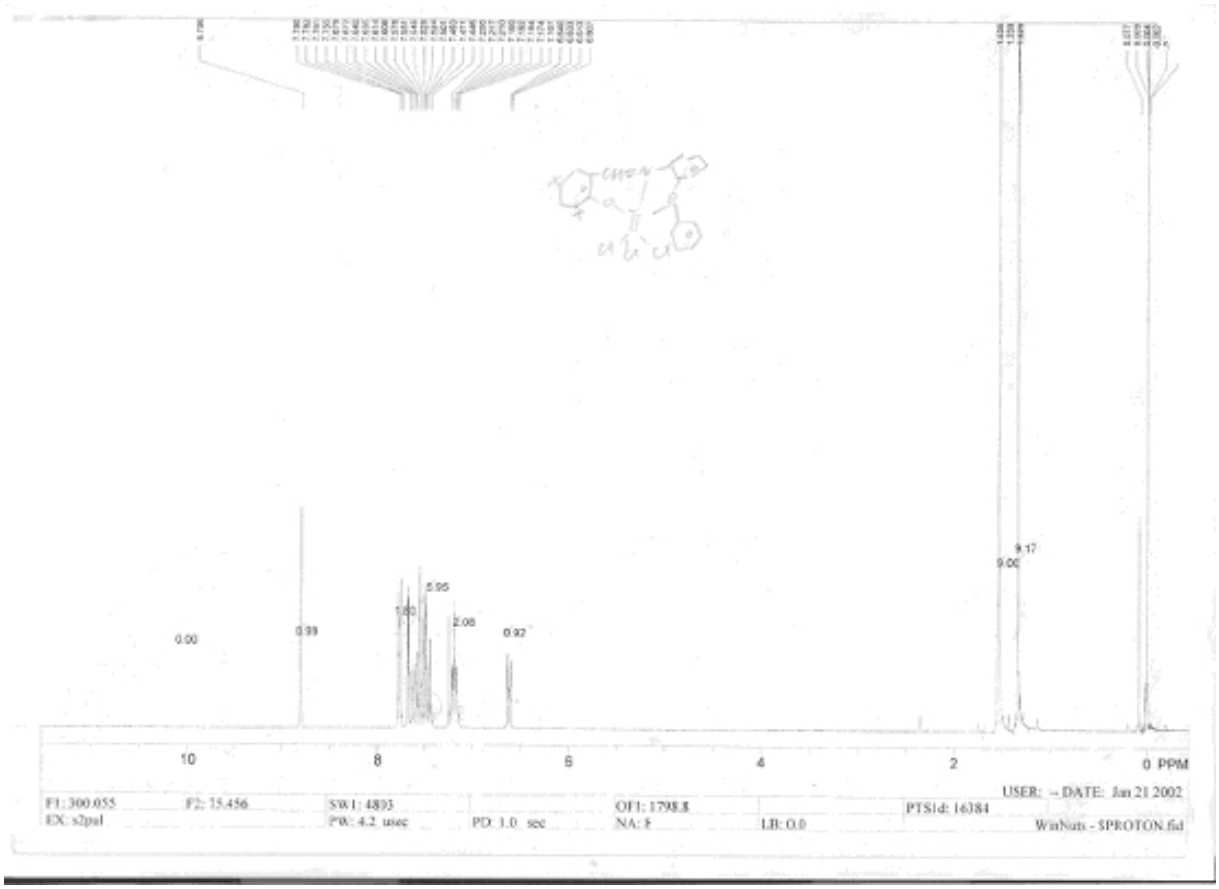
N-(3,5-di-*tert*-butylsalicylidene)-2-(2,6-di-*iso*-propylphenysulfanyl)aniline (L12). The same procedure as that for the preparation of **L1**. 3,5-Di-*tert*-butylsalicylaldehyde (3.80 g, 12 mmol), **4l** (2.82 g, 12 mmol) and glacial acetic acid (0.05 mL) were used. Yield: 4.5 g (75%). ^{1}H NMR (300MHz, $CDCl_3$): δ 13.48 (s, 1H, Ar-OH); 8.70 (s, 1H, CH=N); 7.49-7.42 (m, 2H, Ar-H); 7.29-7.26 (m, 3H, Ar-H); 7.15-6.95 (m, 3H, Ar-H), 6.43 (d, *J* = 7.8Hz, 1H, Ar-H); 3.71 (hepta, *J* = 6.9 Hz, 2H, $CH(CH_3)_2$); 1.51(s, 9H, *t*-Bu); 1.35 (s, 9H, *t*-Bu); 1.15 (d, *J* = 7.2, 12H, $CH(CH_3)_2$). ^{13}C NMR (75MHz, $CDCl_3$): δ 163.2 (C=N), 158.2, 154.1, 144.8, 140.3, 137.0, 135.7, 130.0, 128.1, 127.8, 126.8, 126.7, 125.4, 124.8, 124.0, 118.3, 117.4, 35.0, 34.0, 31.5, 31.3, 29.3, 24.1. Anal. Calcd. for $C_{33}H_{43}NOS$: C, 81.60; H, 8.92; N, 2.88. Found: C, 81.33; H, 8.84; N, 2.69. MS (EI), *m/z*: 501[M^+]

N-(3,5-di-*tert*-butylsalicylidene)-2-phenylselanylaniline (L13). The same procedure as that for the preparation of **L1**. 3,5-Di-*tert*-butylsalicylaldehyde (6.50 g, 28 mmol), **4m** (6.10 g, 24 mmol) and glacial acetic acid (0.05 mL) were used. Yield: 10.2 g (92%). ^{1}H NMR (300MHz, $CDCl_3$): δ 13.21 (s, 1H, Ar-OH); 8.57 (s, 1H, CH=N); 7.64-7.62 (m, 2H, Ar-H), 7.48 (s, 1H, Ar-H), 7.34-7.09 (m, 8H, Ar-H); 1.50 (s, 9H, *t*-Bu); 1.35 (s, 9H, *t*-Bu). ^{13}C NMR (75MHz, $CDCl_3$): δ 164.0, 158.3, 147.5, 140.5, 137.0, 135.7, 130.5, 130.3, 129.5, 128.6, 128.3, 128.2, 127.4, 127.1, 127.0, 118.0, 118.0, 35.1, 34.1, 31.4, 29.4. Anal. Calcd. for $C_{27}H_{31}NOSe$: C, 69.82; H, 6.68; N, 3.01. Found: C, 69.57; H, 6.40; N, 2.72. MS (EI), *m/z*: 464[M^+].

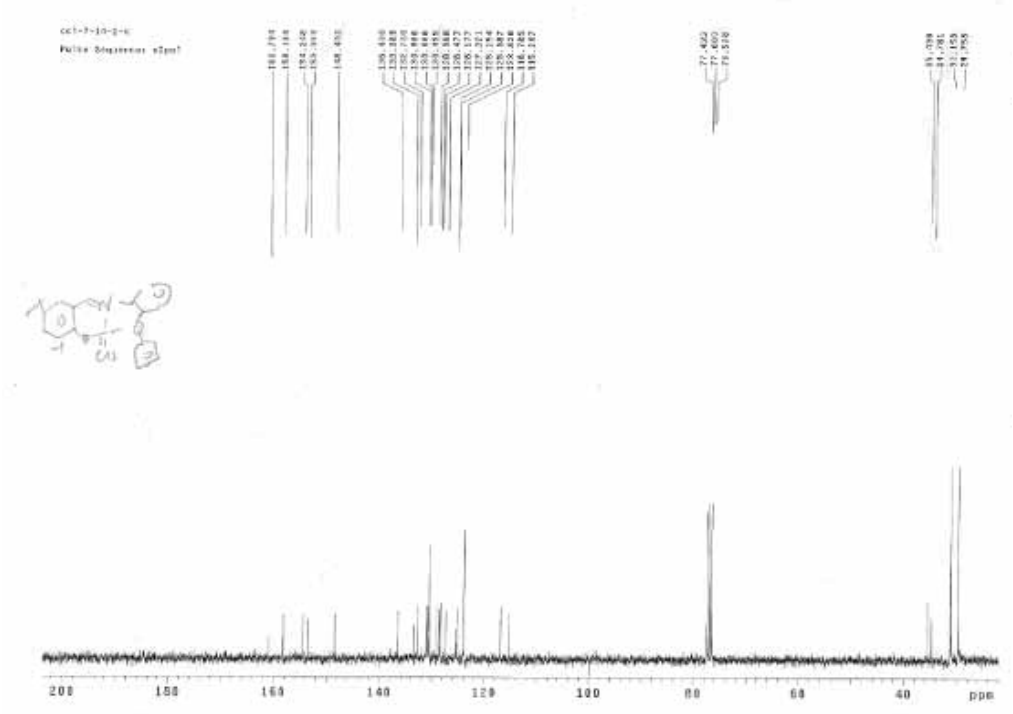
N-(3-*tert*-butylsalicylidene)-2-phenylsulfanylaniline (L14). The same procedures as that for the preparation of **L1**. 5-Di-*tert*-butylsalicylaldehyde (2.67 g, 15 mmol), **4e** (3.01 g, 15 mmol) and glacial acetic acid (0.05 mL) were used. Yield: 4.8 g (89%). ^{1}H NMR (300MHz, $CDCl_3$): δ 13.56 (s, 1H, Ar-OH); 8.55 (s, 1H, CH=N); 7.47-7.15 (m, 11H, Ar-H); 6.90 (t, *J* = 7.8Hz, 1H , Ar-H), 1.50 (s, 9H, *t*-Bu). ^{13}C NMR (75 MHz, $CDCl_3$): δ 163.3 (N=C), 160.5, 147.0, 137.7, 133.8, 132.8, , 132.5, 130.7, 130.5, 130.1, 129.3, 127.7, 127.5, 127.0, 118.9, 118.3, 118.2, 34.9, 29.3. Anal. Calcd. for $C_{23}H_{23}NOS$: C, 76.42; H, 6.41; N, 3.87. Found: C, 76.81; H, 6.42; N, 3.76. MS (EI), *m/z*: 361[M^+].

1. Moors, G. G. I.; Harrington, J. K. *J. Med. Chem.* **1975**, *18*, 386-391.

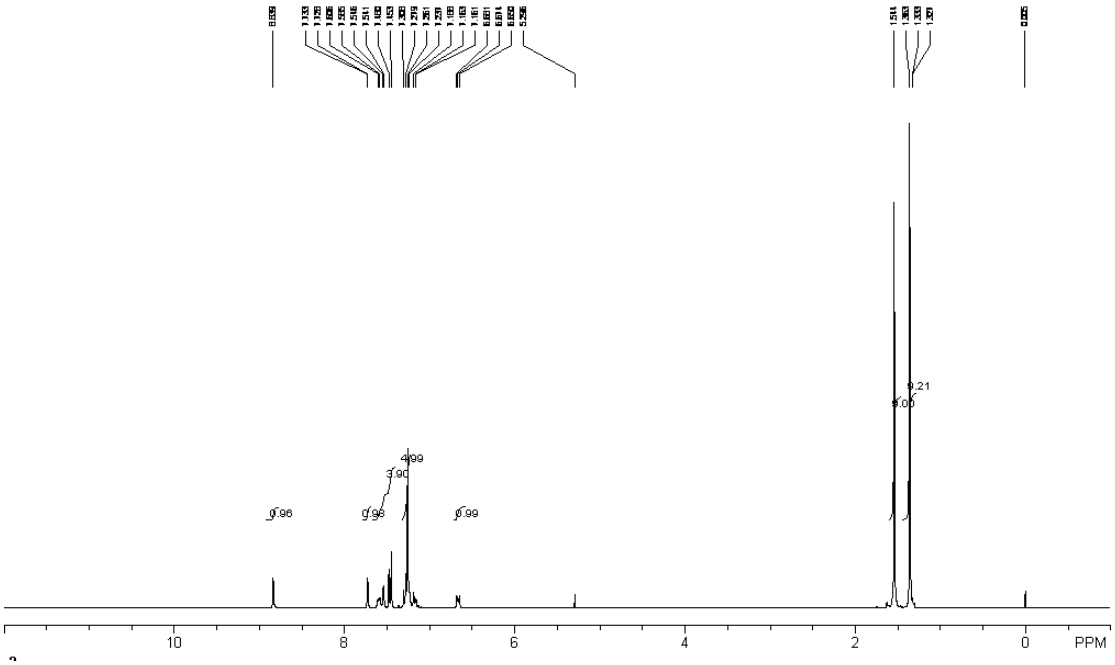
Part II. NMR Spectrum of Complexes.



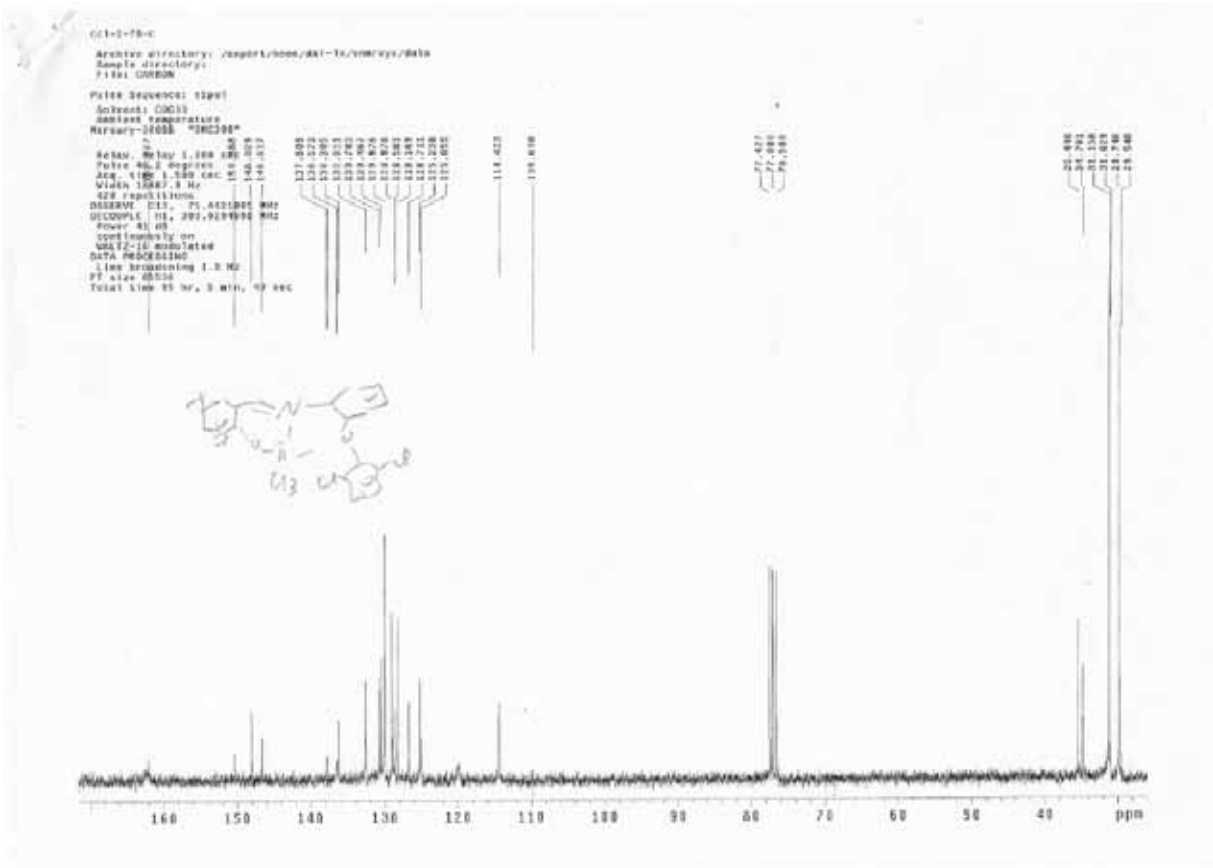
^{1}H NMR spectrum of 5a (recorded in $CDCl_3$)



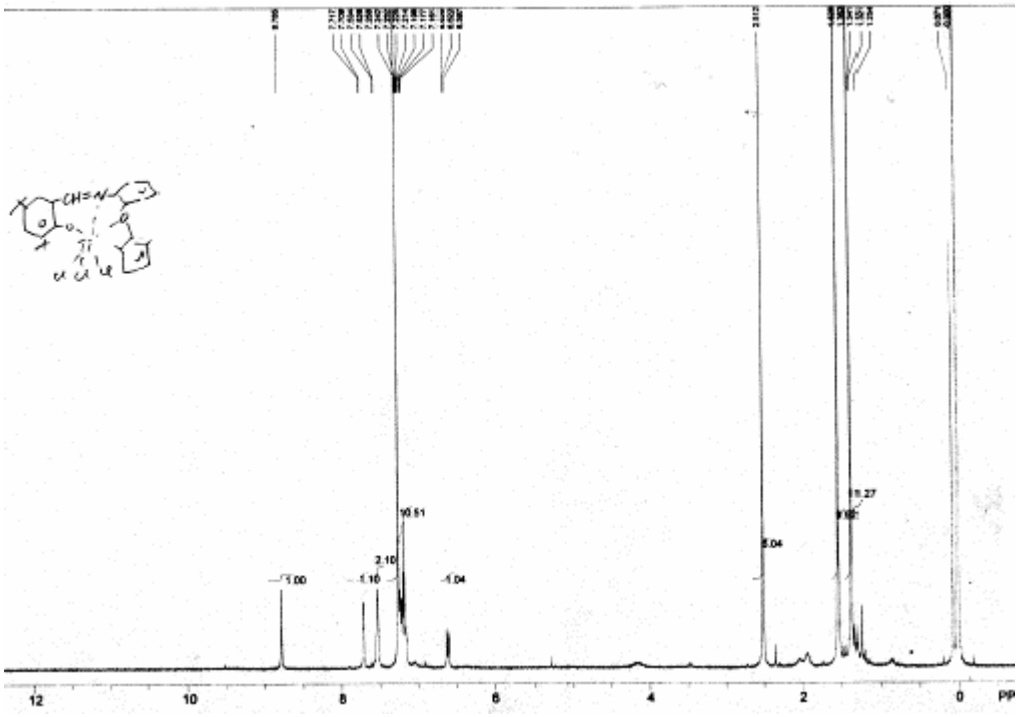
^{13}C NMR spectrum of 5a (recorded in $CDCl_3$)



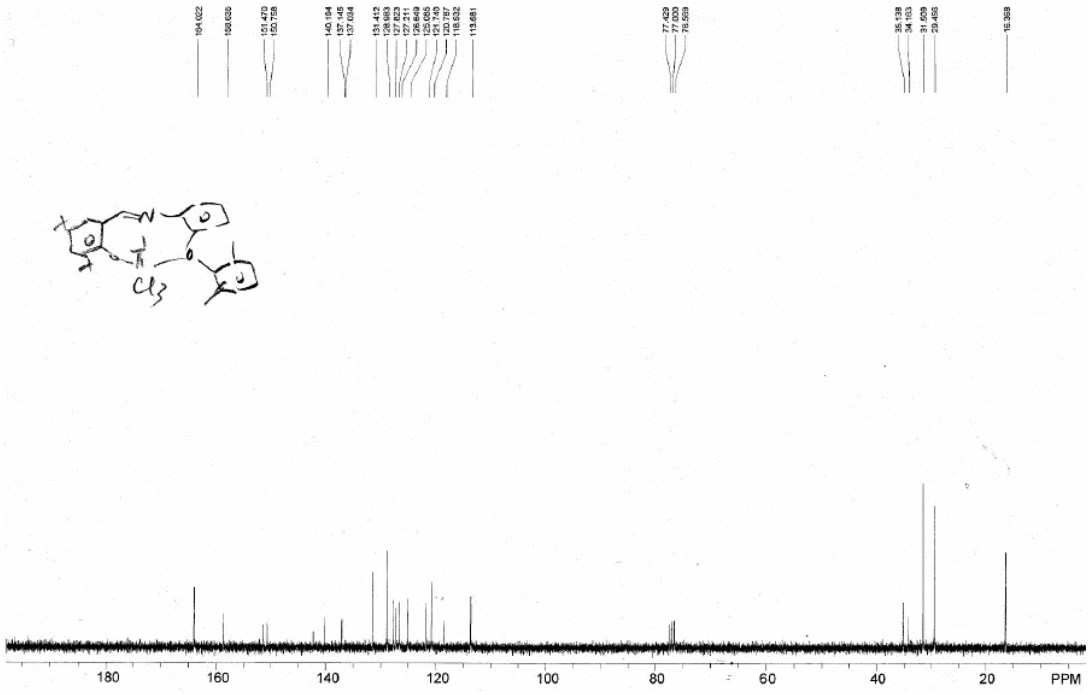
^{1}H NMR spectrum of 5b (recorded in $CDCl_3$)



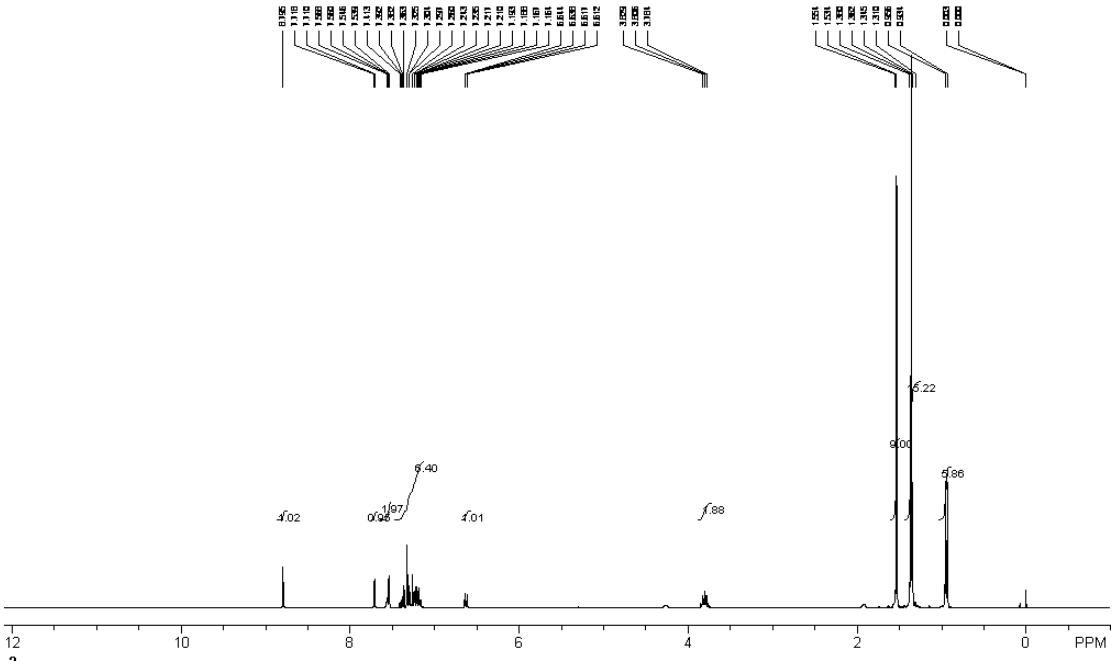
^{13}C NMR spectrum of 5b (recorded in $CDCl_3$)



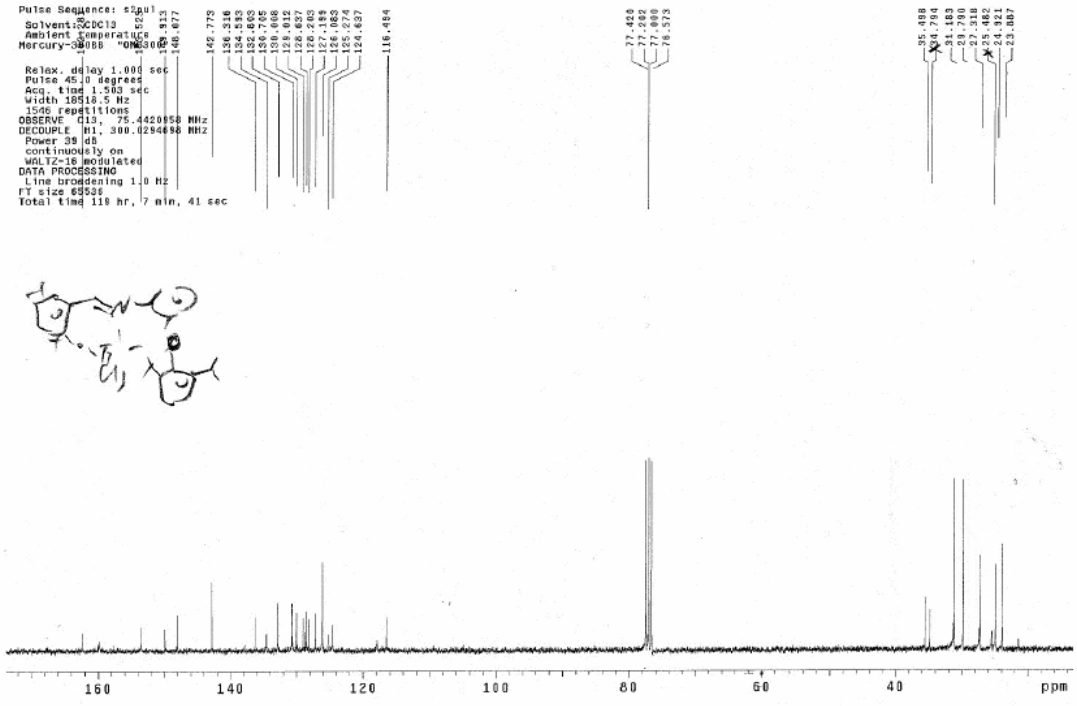
^{1}H NMR spectrum of 5c (recorded in $CDCl_3$)



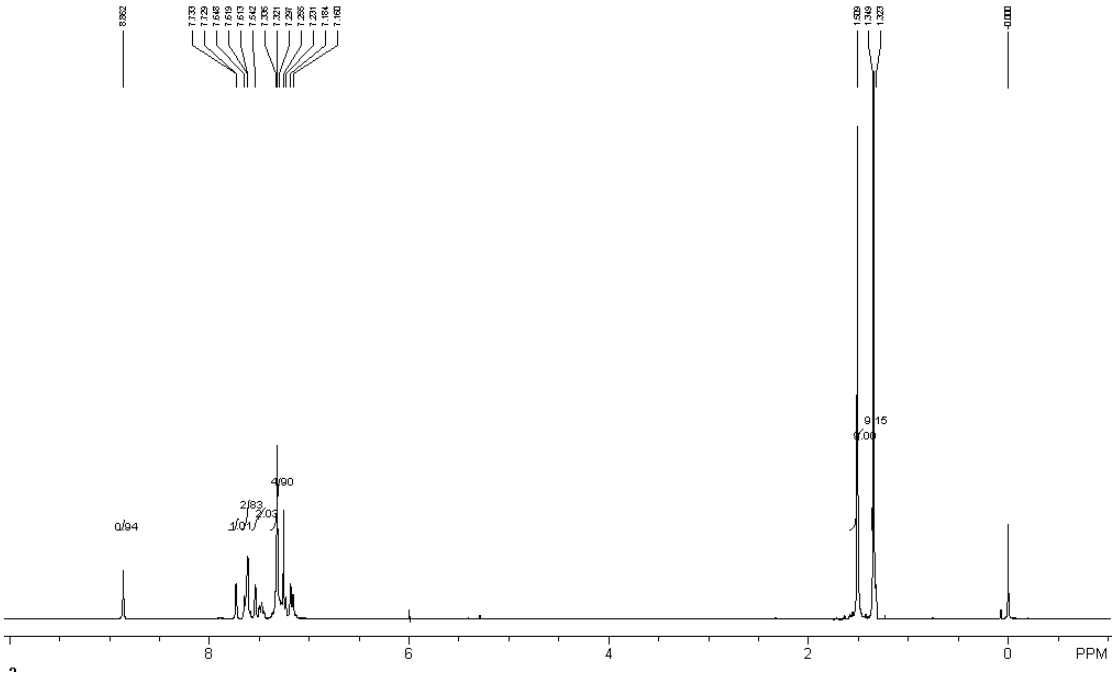
^{13}C NMR spectrum of 5c (recorded in $CDCl_3$)



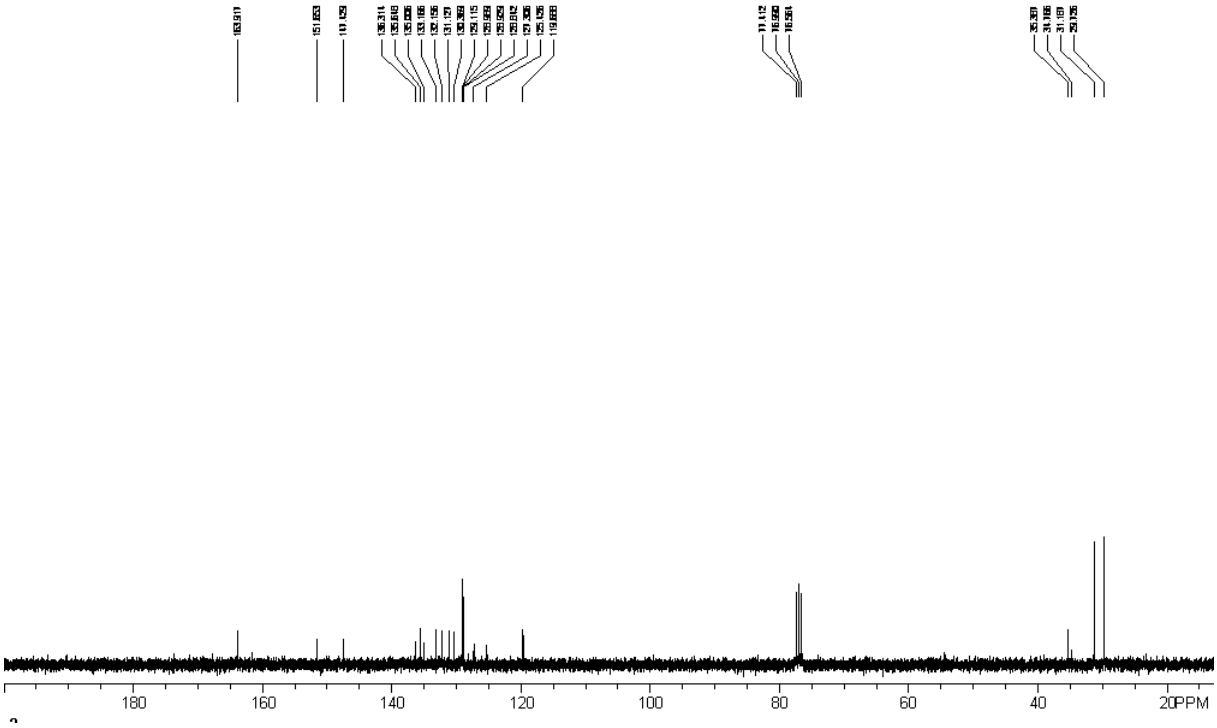
^{1}H NMR spectrum of 5d (recorded in $CDCl_3$)



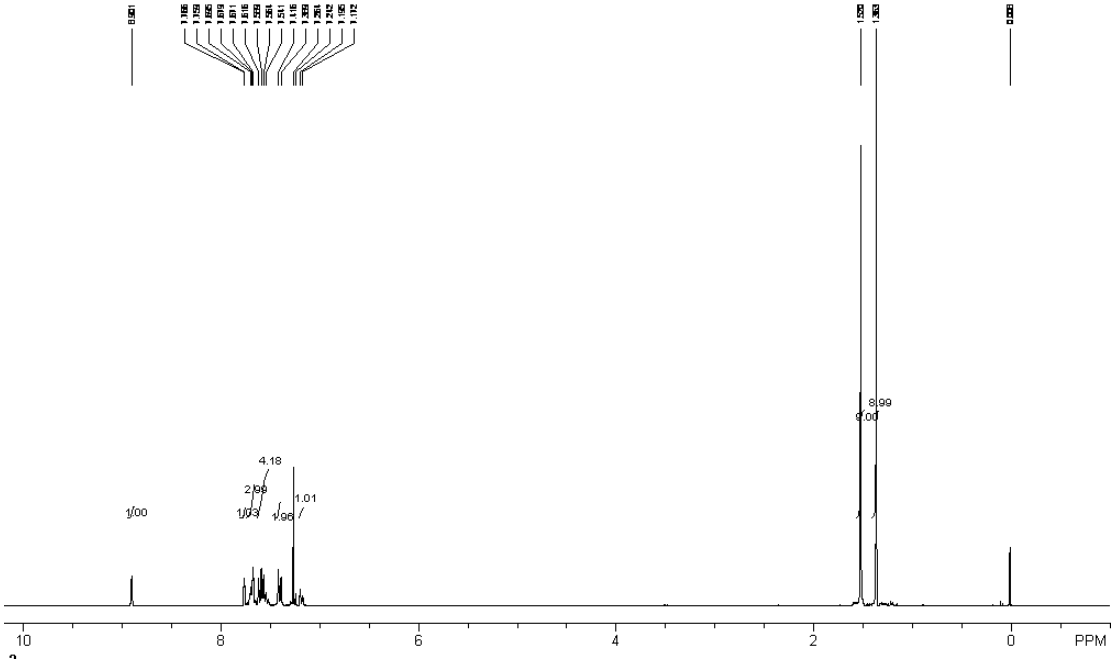
^{13}C NMR spectrum of 5d (recorded in $CDCl_3$)



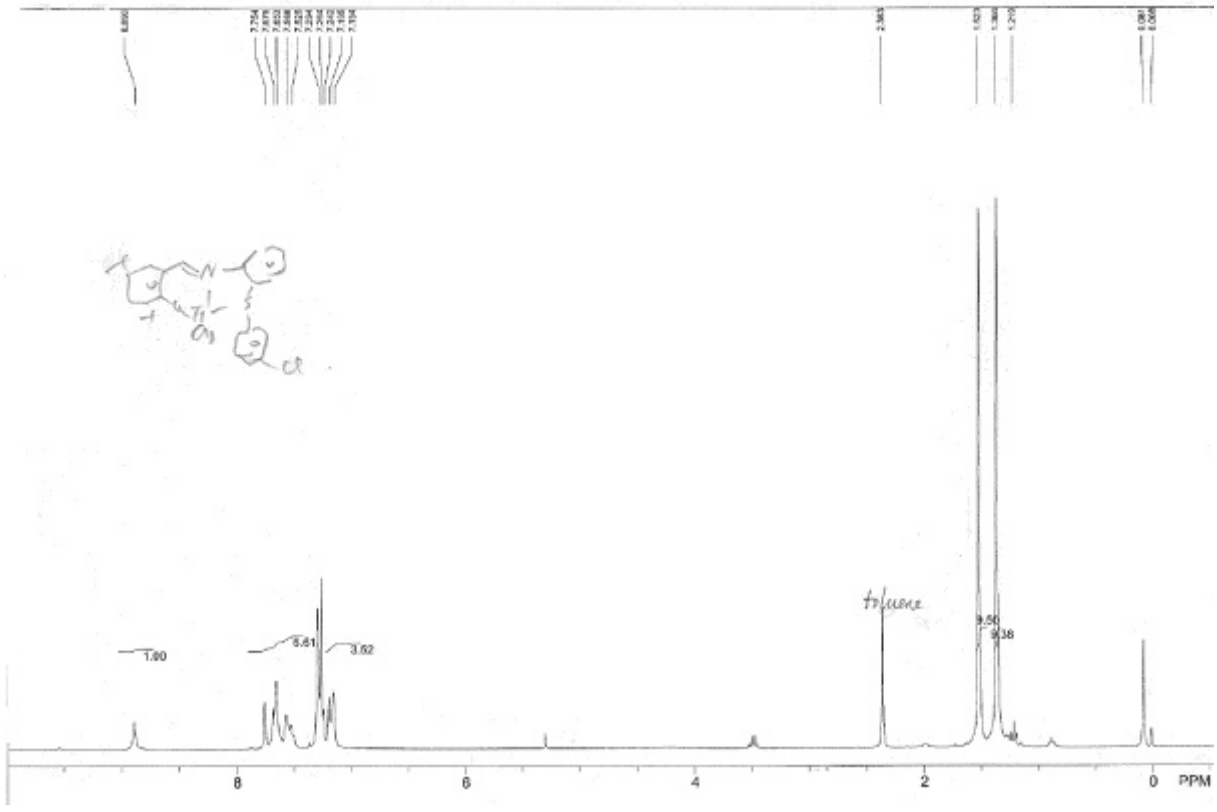
^{1}H NMR spectrum of 5e (recorded in $CDCl_3$).



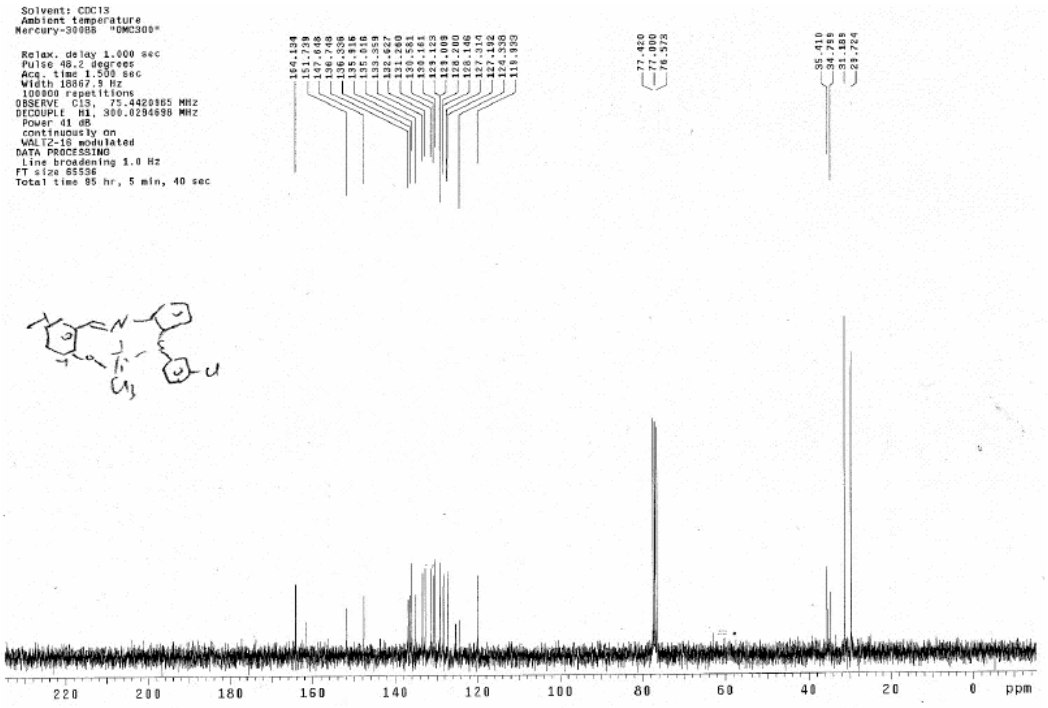
^{13}C NMR spectrum of 5e (recorded in $CDCl_3$)



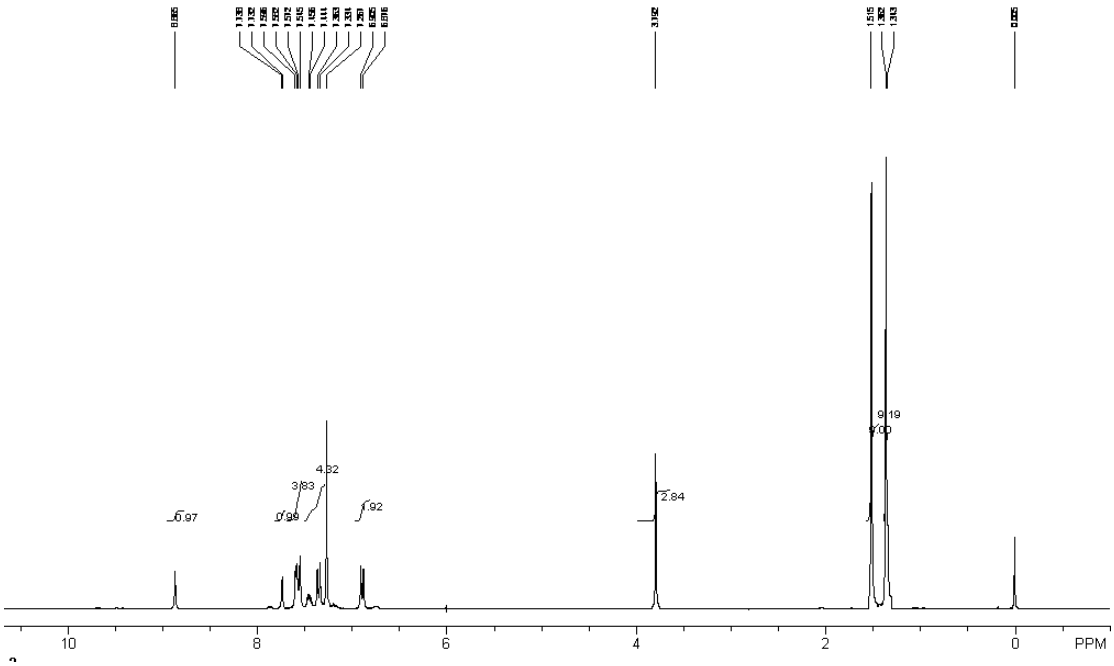
^{1}H NMR spectrum of 5f (recorded in $CDCl_3$).



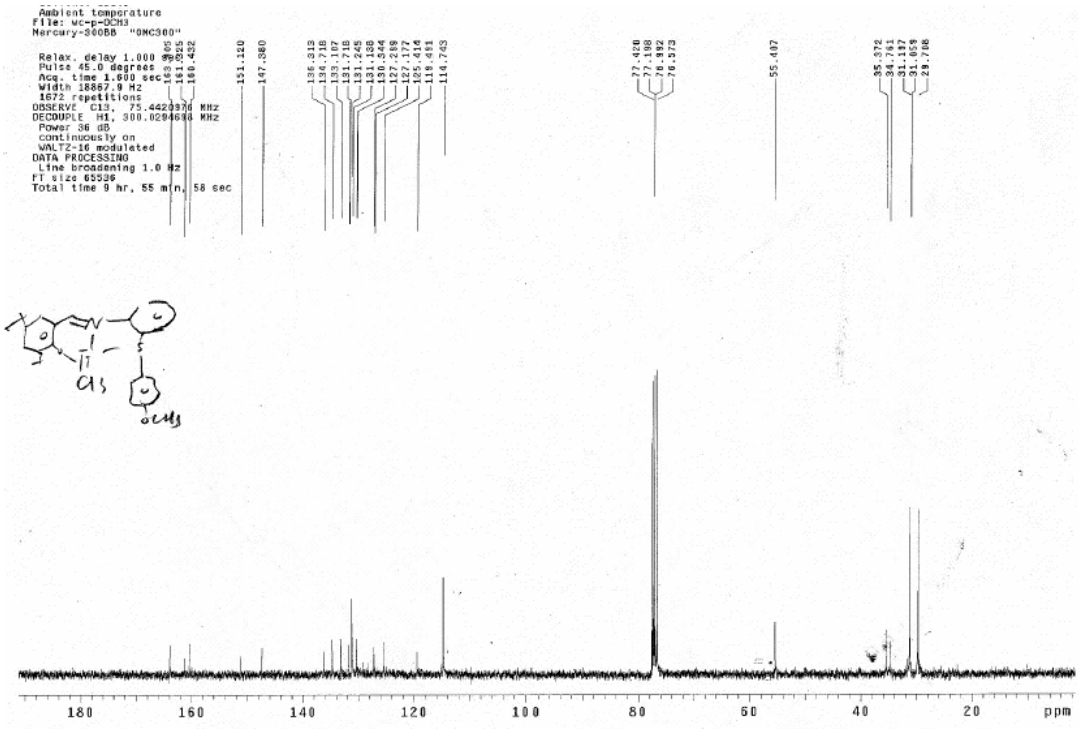
^{1}H NMR spectrum of 5g (recorded in $CDCl_3$).



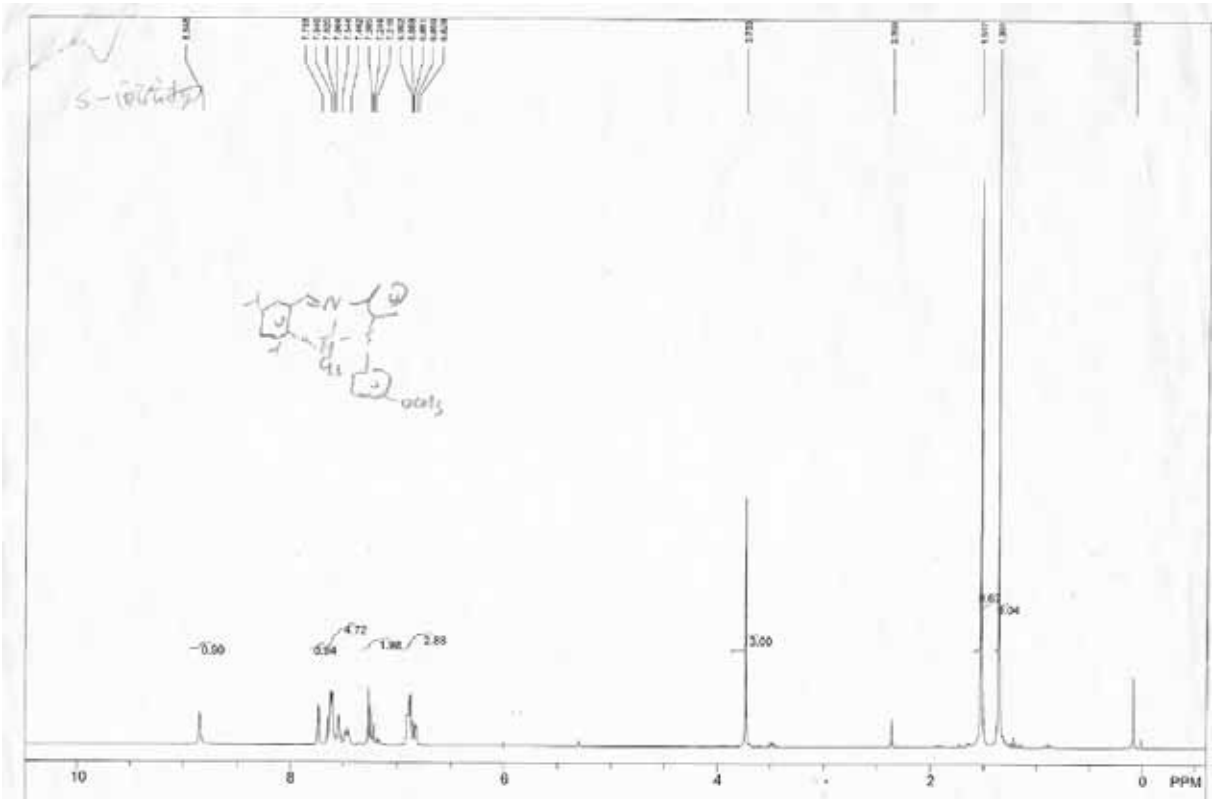
^{13}C NMR spectrum of 5g (recorded in $CDCl_3$)



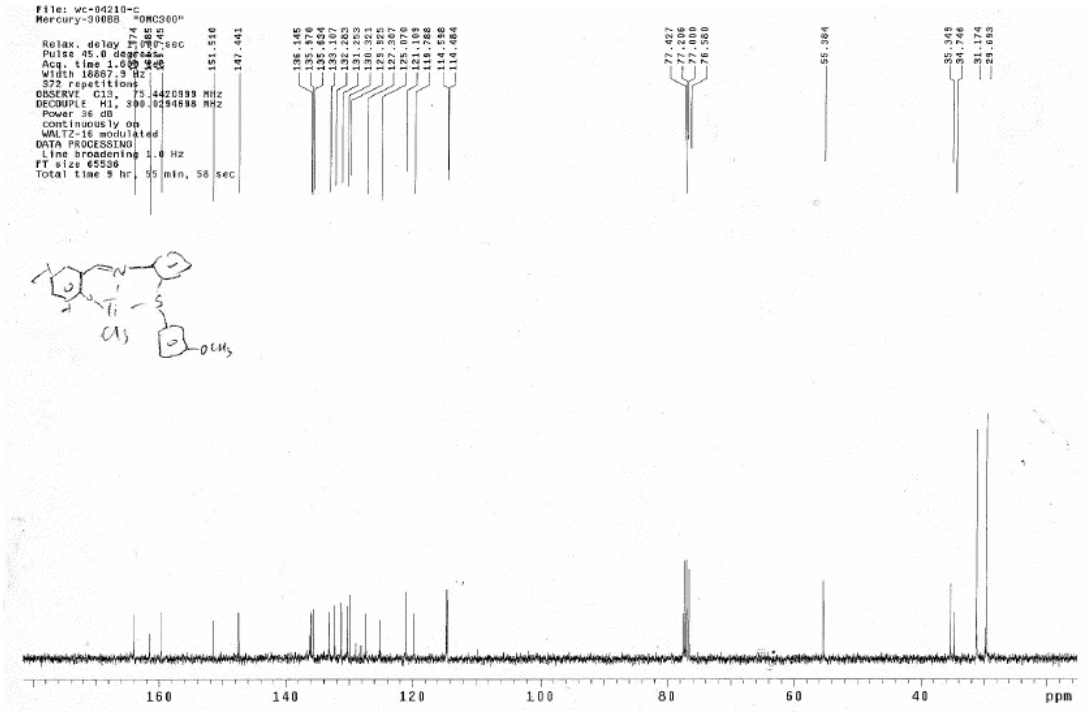
^{1}H NMR spectrum of 5h (recorded in $CDCl_3$).



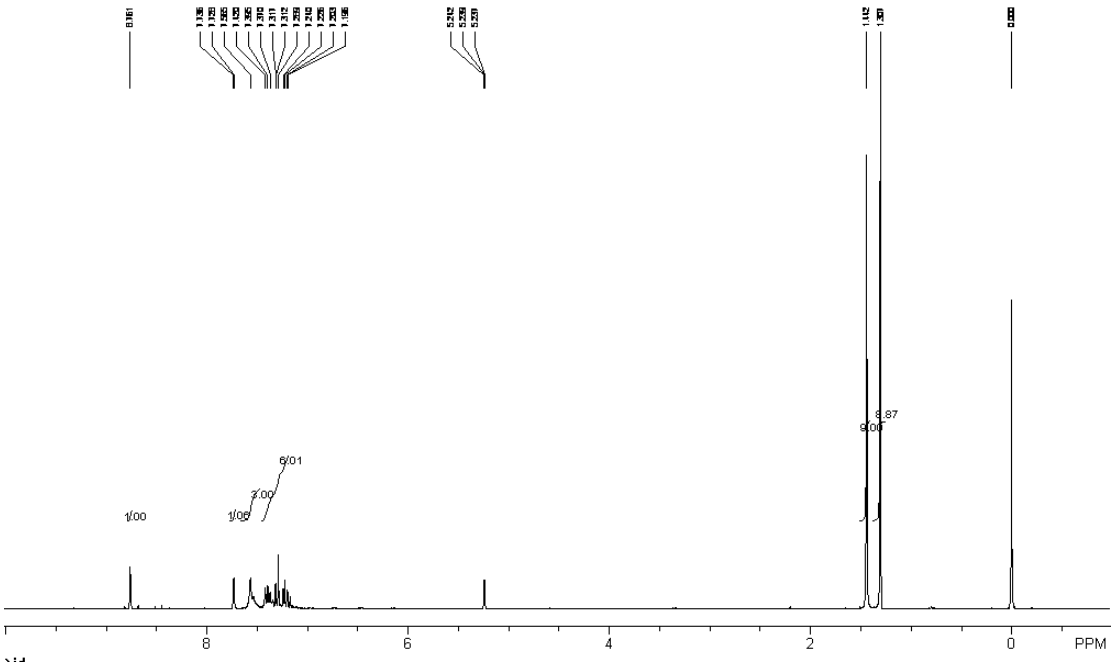
^{13}C NMR spectrum of 5h (recorded in $CDCl_3$)



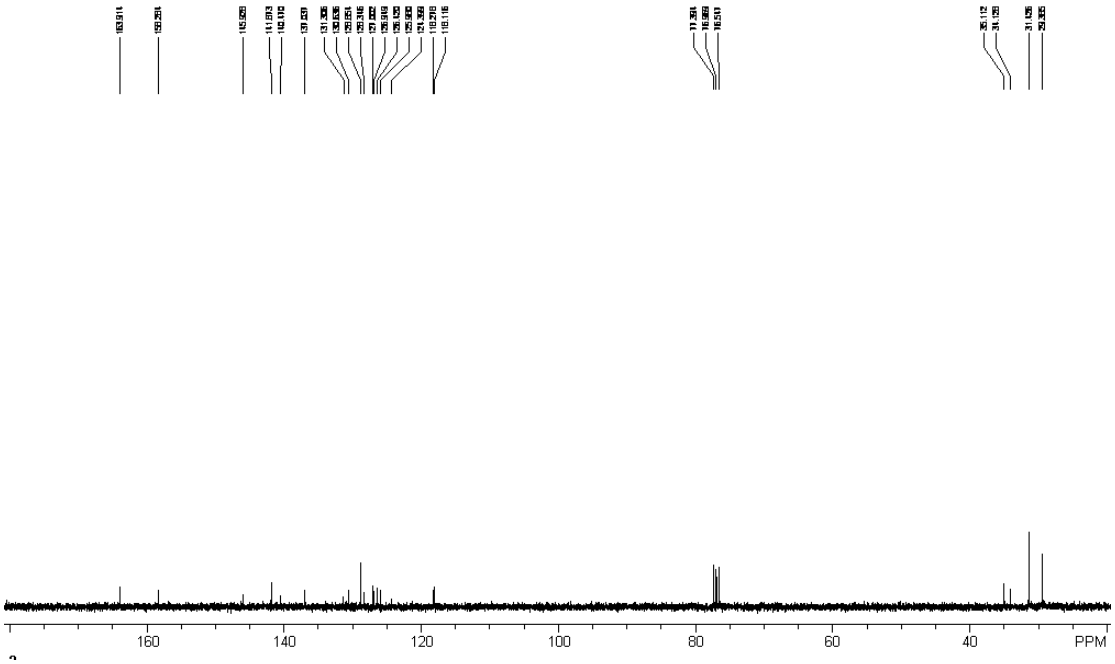
^{1}H NMR spectrum of 5i (recorded in $CDCl_3$).



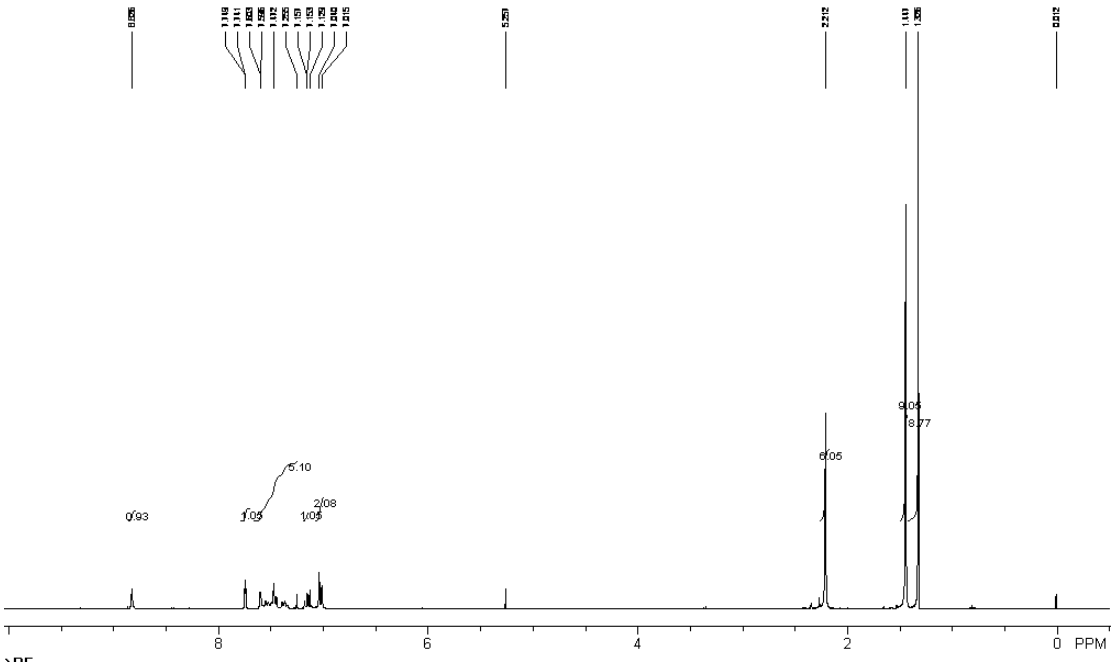
^{13}C NMR spectrum of 5i (recorded in $CDCl_3$)



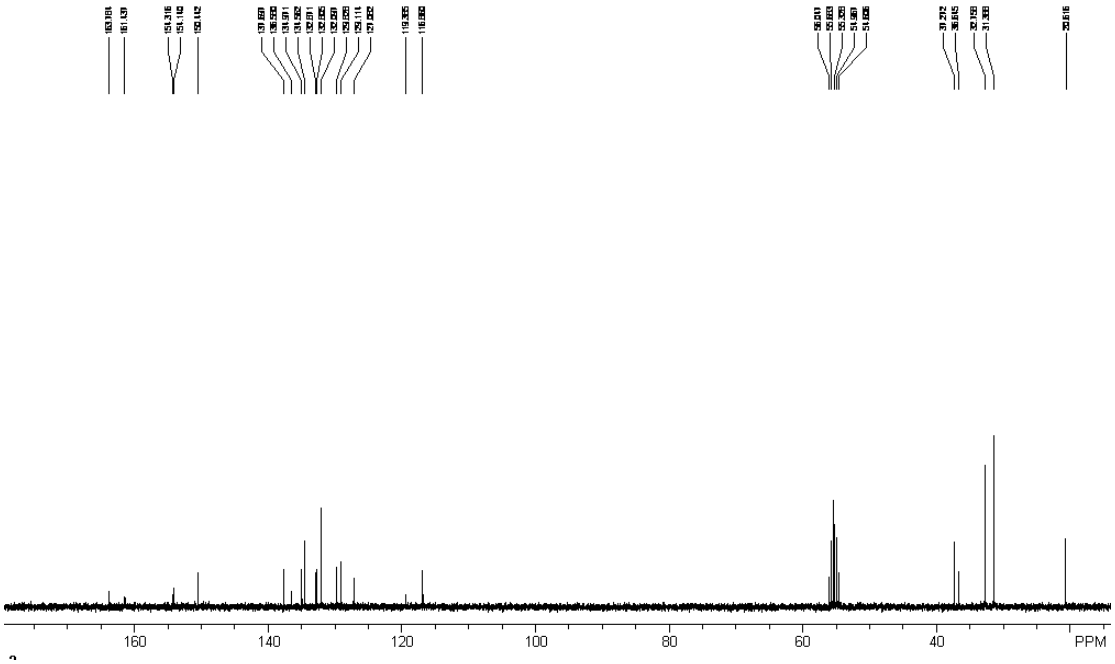
^{1}H NMR spectrum of 5j (recorded in CD_2Cl_2).



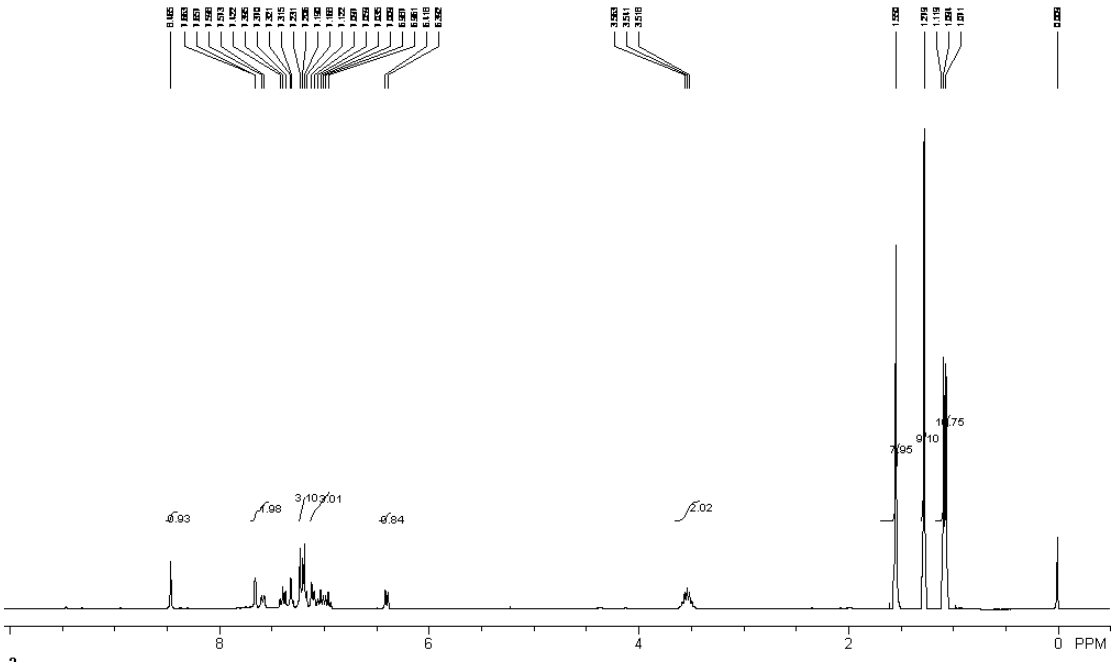
^{13}C NMR spectrum of 5j (recorded in $CDCl_3$)



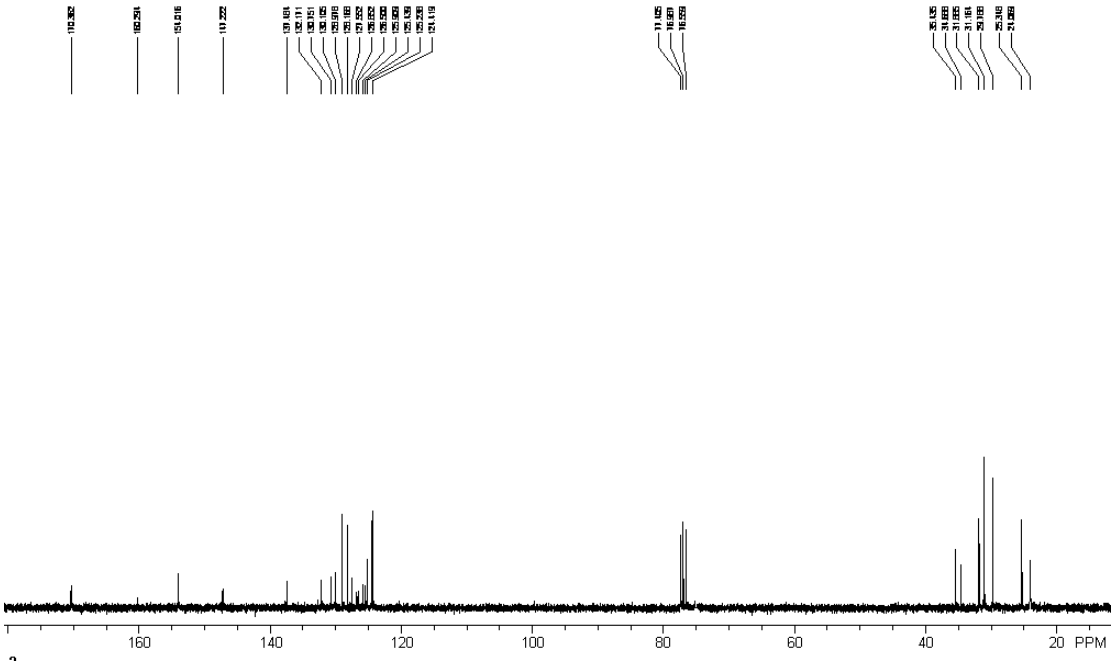
^{1}H NMR spectrum of 5k (recorded in CD_2Cl_2).



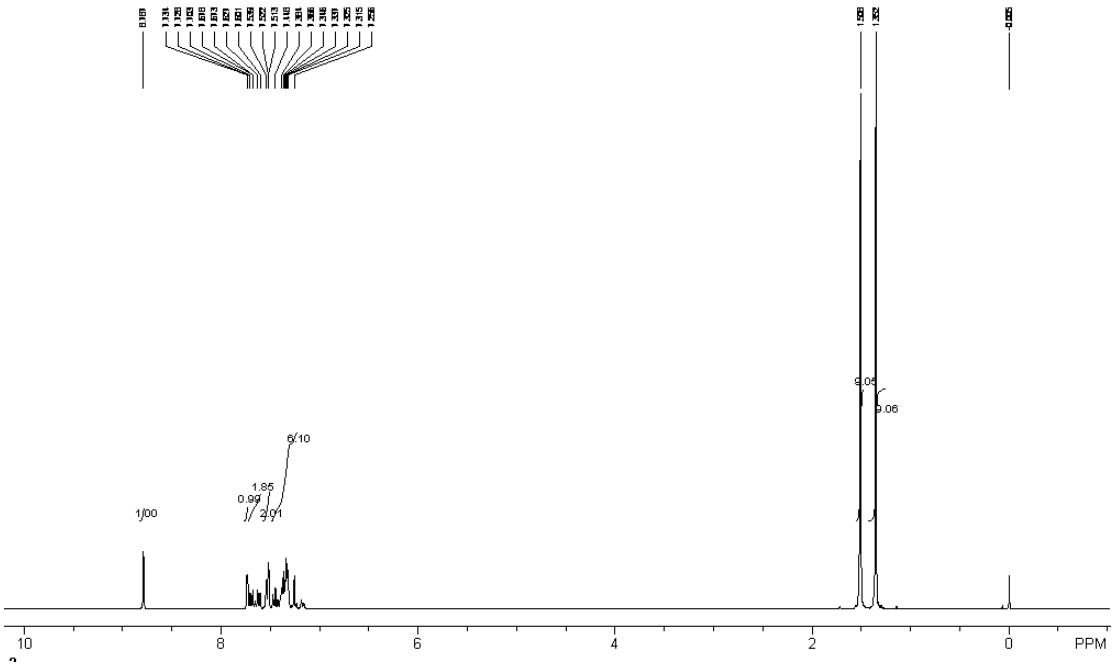
^{13}C NMR spectrum of 5k (recorded in CD_2Cl_2)



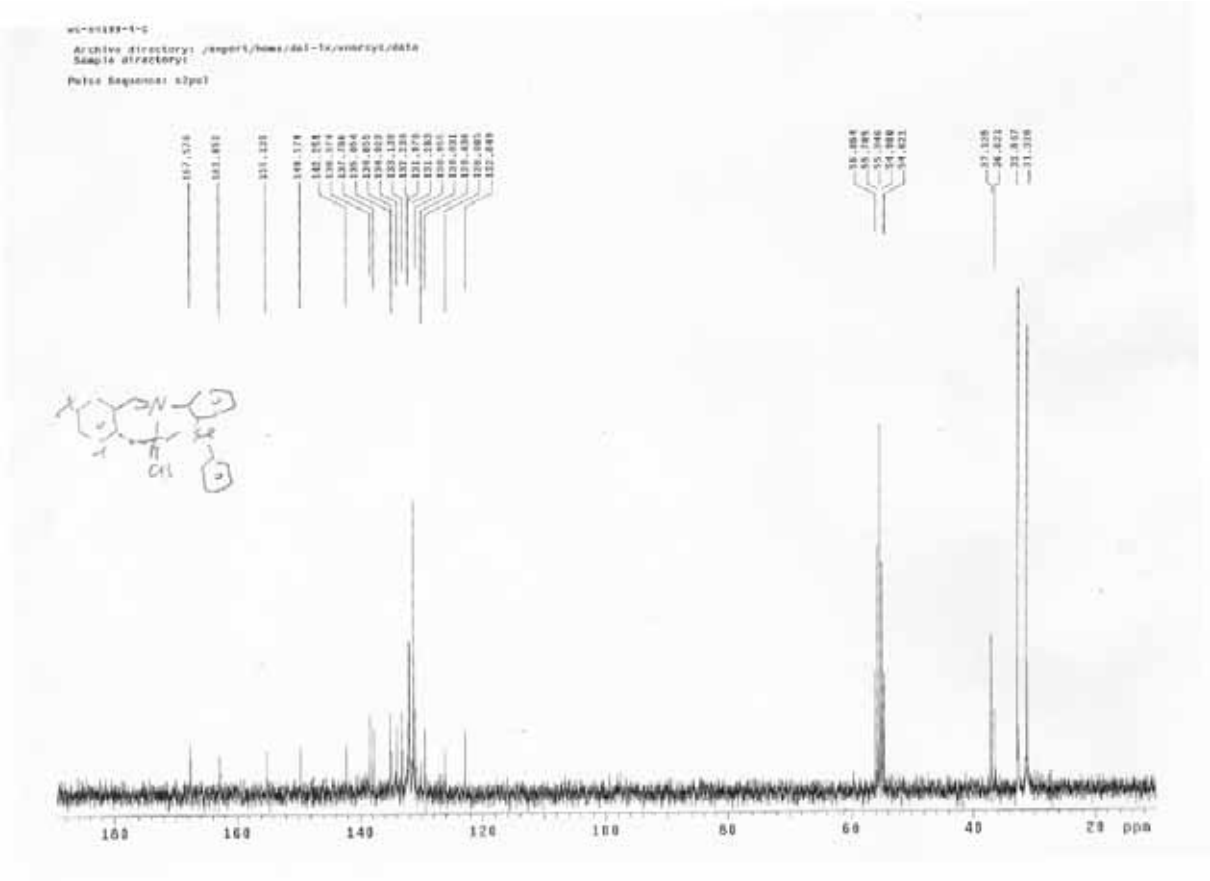
^{1}H NMR spectrum of 5l (recorded in $CDCl_3$).



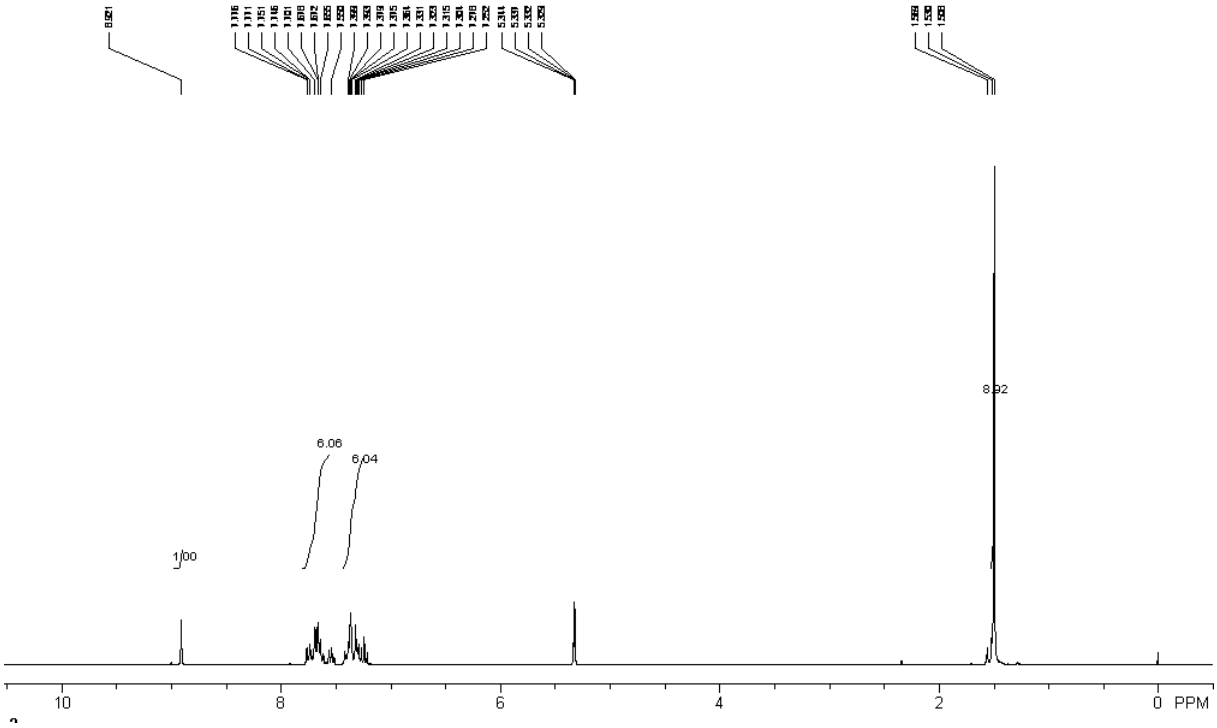
^{13}C NMR spectrum of 5l (recorded in $CDCl_3$).



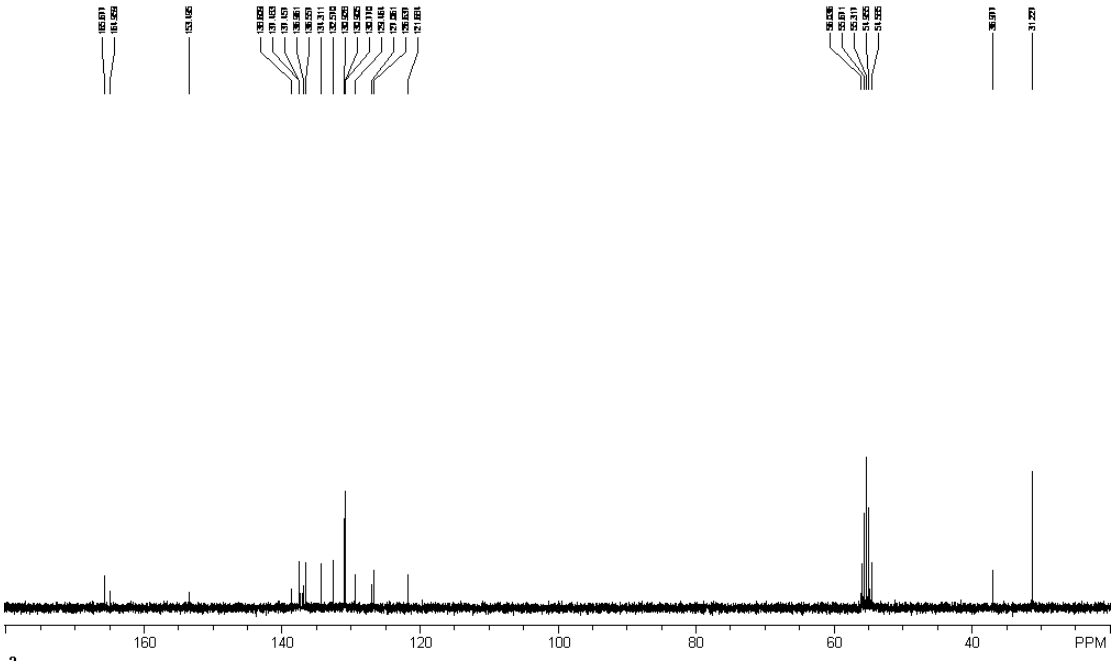
^{1}H NMR spectrum of 5m (recorded in $CDCl_3$).



^{13}C NMR spectrum of 5m (recorded in CD_2Cl_2)

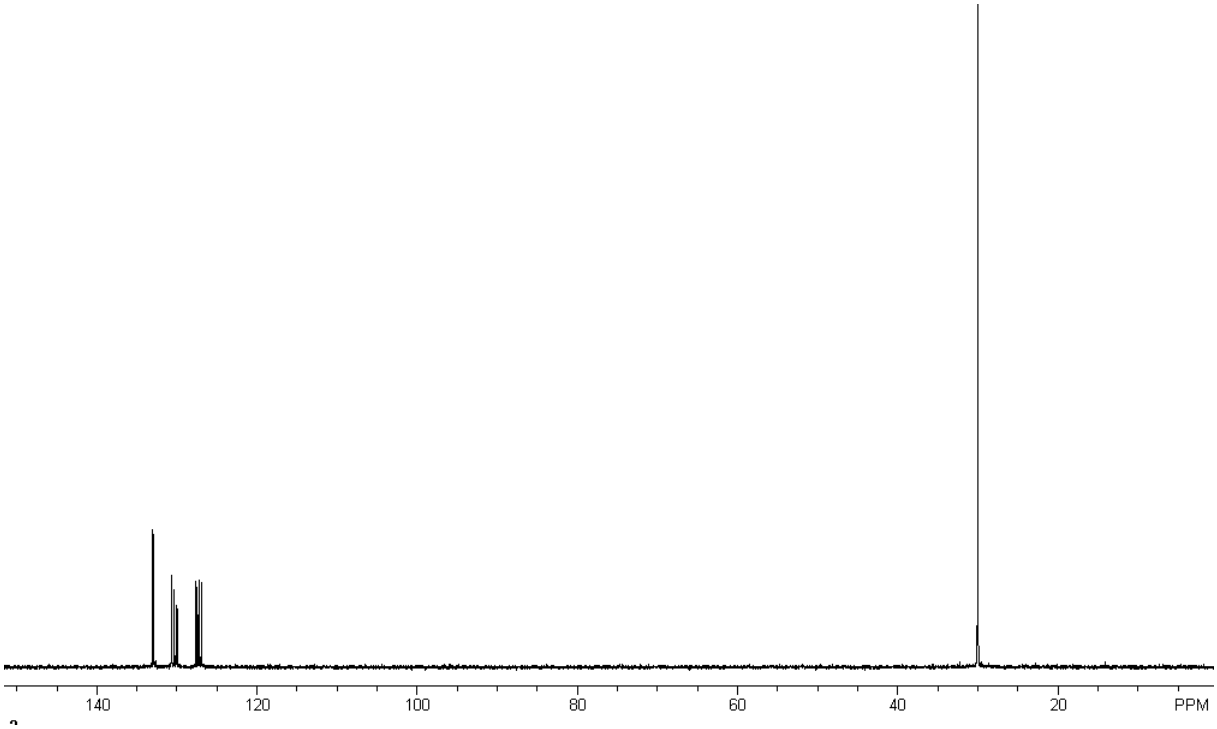


^{1}H NMR spectrum of 5n (recorded in CD_2Cl_2)

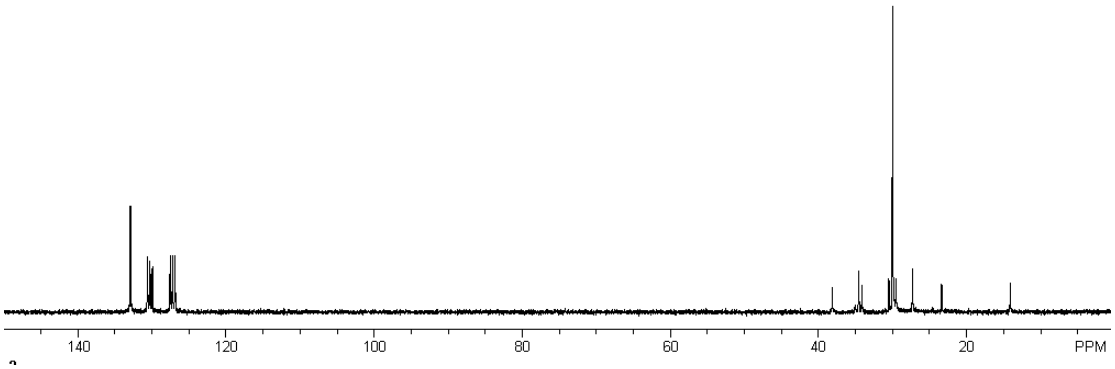


^{13}C NMR spectrum of 5n (recorded in CD_2Cl_2)

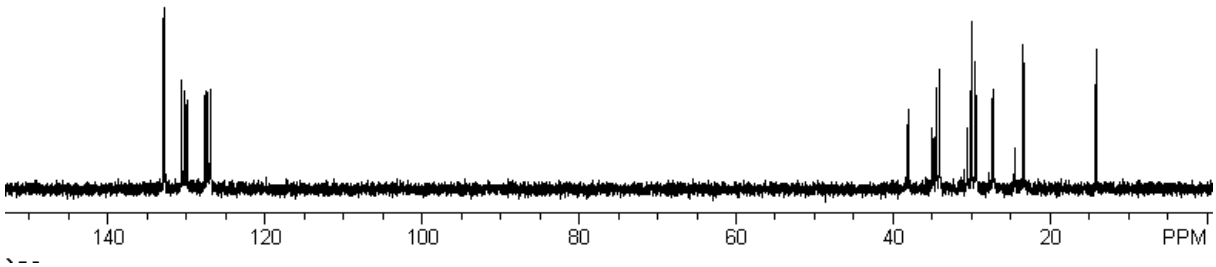
Part III. ^{13}C NMR Spectrum of Polymers



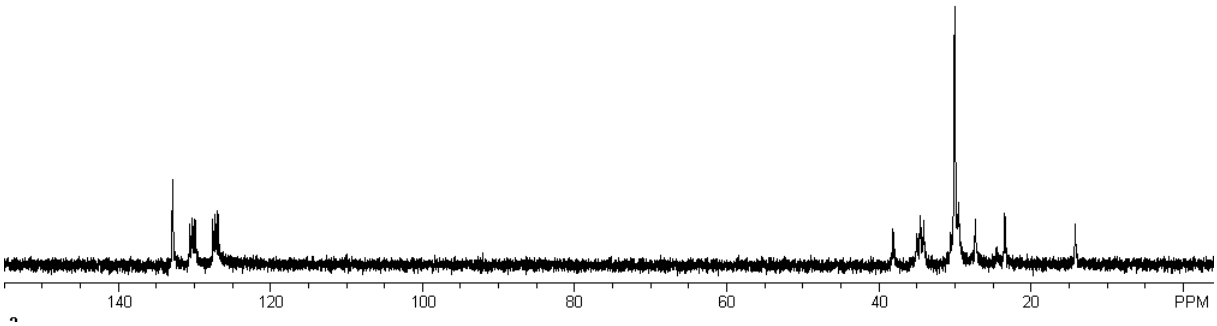
^{13}C NMR spectrum of polyethylene (recorded in *o*-$C_6D_4Cl_2$ at 110 °C)



^{13}C NMR spectrum of copolymer (table 4, entry 1, recorded in *o*-$C_6D_4Cl_2$ at 110 °C)



^{13}C NMR spectrum of copolymer (table 4, entry 4, recorded in *o*-$C_6D_4Cl_2$ at 110 °C)



^{13}C NMR spectrum of copolymer (table 4, entry 9, recorded in *o*-$C_6D_4Cl_2$ at 110 °C)

Part IV. Molecular Structure of Complexes.

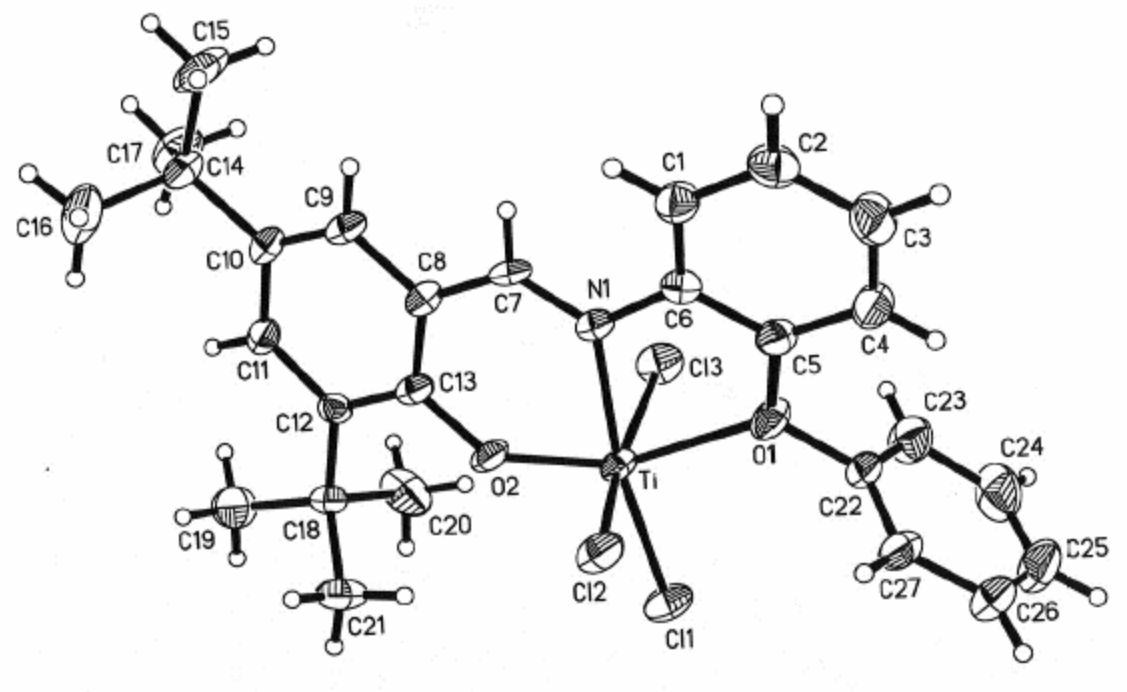


Figure 1. molecular structure of 5a

Table 1. Crystal data and structure refinement for **5a**

Identification code	cd22369
Empirical formula	C37.50 H42 N O2 Cl3 Ti
Formula weight	692.97
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 11.748(7) A alpha = 91.911(10) deg.
	b = 13.365(8) A beta = 91.691(10) deg.
	c = 13.646(8) A gamma = 112.738(10) deg.
Volume	1973(2) A^3
Z, Calculated density	2, 1.167 Mg/m^3
Absorption coefficient	0.450 mm^-1
F(000)	726
Crystal size	0.680 x 0.521 x 0.505 mm
Theta range for data collection	1.65 to 25.00 deg.
Limiting indices	13<=h<=6, -15<=k<=15, -16<=l<=16
Reflections collected / unique	9333 / 6746 [R(int) = 0.1545]
Completeness to theta = 25.00	97.2 %
Absorption correction	Sadabs
Max. and min. transmission	1.00000 and 0.27365
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6746 / 2 / 394
Goodness-of-fit on F^2	1.057
Final R indices [I>2sigma(I)]	R1 = 0.0959, wR2 = 0.2426
R indices (all data)	R1 = 0.1506, wR2 = 0.2956
Largest diff. peak and hole	0.865 and -0.835 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5a**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ti	193(1)	3171(1)	7025(1)	40(1)
Cl(1)	-543(2)	2324(2)	8445(1)	66(1)
Cl(2)	-962(2)	4293(2)	7143(1)	56(1)
Cl(3)	1745(2)	2480(2)	6899(1)	62(1)
O(1)	1737(4)	4633(3)	7726(3)	49(1)
O(2)	-763(4)	2244(3)	6058(3)	47(1)
N(1)	1102(5)	4239(4)	5828(3)	39(1)
C(1)	2504(7)	6169(5)	5476(5)	54(2)
C(2)	3378(7)	7188(6)	5833(5)	62(2)
C(3)	3734(8)	7357(6)	6835(6)	71(2)
C(4)	3210(7)	6532(6)	7489(5)	58(2)
C(5)	2336(6)	5525(5)	7119(4)	44(2)
C(6)	1990(6)	5325(5)	6114(4)	42(1)
C(7)	897(6)	3888(5)	4897(4)	41(1)
C(8)	57(6)	2843(5)	4491(4)	41(1)
C(9)	64(6)	2632(5)	3458(4)	45(2)
C(10)	-679(6)	1652(5)	3006(4)	44(2)
C(11)	-1499(6)	833(5)	3610(4)	44(2)
C(12)	-1564(5)	987(5)	4643(4)	37(1)
C(13)	-772(6)	2009(5)	5065(4)	39(1)
C(14)	-682(7)	1397(6)	1876(4)	53(2)
C(15)	300(10)	2374(8)	1371(6)	98(3)
C(16)	-1994(9)	1206(9)	1414(6)	91(3)
C(17)	-397(9)	374(7)	1693(6)	81(3)
C(18)	-2434(6)	57(5)	5272(4)	44(2)
C(19)	-3326(8)	-936(6)	4623(6)	72(2)
C(20)	-1611(8)	-339(7)	5938(7)	83(3)
C(21)	-3258(7)	454(6)	5926(6)	68(2)
C(22)	2079(6)	4797(5)	8757(4)	48(2)
C(23)	2951(8)	4407(7)	9117(6)	68(2)
C(24)	3239(9)	4578(8)	10156(7)	90(3)
C(25)	2740(10)	5117(8)	10741(6)	89(3)
C(26)	1877(9)	5494(8)	10357(6)	81(3)
C(27)	1515(7)	5317(6)	9351(5)	60(2)
C(28)	4778(14)	8527(12)	-10(15)	145(6)
C(29)	4019(18)	8337(17)	850(20)	224(12)
C(30)	4540(20)	8034(13)	1600(20)	232(14)
C(31)	5570(40)	7903(19)	1730(20)	250(20)
C(32)	6241(19)	8070(14)	876(17)	160(10)
C(33)	5819(17)	8415(14)	10(20)	191(9)
C(34)	6580(20)	8602(18)	-766(18)	267(16)

C(35)	5849(15)	5927(13)	4933(14)	149(5)
C(36)	5300(30)	5540(20)	4097(19)	228(10)
C(37)	4320(30)	4530(30)	4020(30)	303(15)
C(38)	3870(30)	4180(20)	3320(30)	270(30)

Table 3. Bond lengths [A] and angles [deg] for **5a**.

Ti-O(2)	1.806(4)
Ti-N(1)	2.219(5)
Ti-O(1)	2.249(5)
Ti-Cl(1)	2.296(2)
Ti-Cl(3)	2.348(2)
Ti-Cl(2)	2.385(2)
O(1)-C(5)	1.434(7)
O(1)-C(22)	1.437(7)
O(2)-C(13)	1.379(7)
N(1)-C(7)	1.321(7)
N(1)-C(6)	1.455(8)
C(1)-C(6)	1.402(8)
C(1)-C(2)	1.411(10)
C(1)-H(1)	0.9300
C(2)-C(3)	1.403(10)
C(2)-H(2)	0.9300
C(3)-C(4)	1.401(10)
C(3)-H(3)	0.9300
C(4)-C(5)	1.406(9)
C(4)-H(4)	0.9300
C(5)-C(6)	1.405(8)
C(7)-C(8)	1.443(9)
C(7)-H(7)	0.9300
C(8)-C(9)	1.429(8)
C(8)-C(13)	1.438(8)
C(9)-C(10)	1.374(9)
C(9)-H(9)	0.9300
C(10)-C(11)	1.447(9)
C(10)-C(14)	1.568(8)
C(11)-C(12)	1.426(8)
C(11)-H(11)	0.9300
C(12)-C(13)	1.413(9)
C(12)-C(18)	1.571(8)
C(14)-C(17)	1.543(10)
C(14)-C(15)	1.567(11)
C(14)-C(16)	1.570(11)
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600

C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-C(20)	1.555(9)
C(18)-C(21)	1.559(9)
C(18)-C(19)	1.560(10)
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-C(27)	1.389(9)
C(22)-C(23)	1.401(10)
C(23)-C(24)	1.438(11)
C(23)-H(24)	0.9300
C(24)-C(25)	1.347(14)
C(24)-H(25)	0.9300
C(25)-C(26)	1.392(14)
C(25)-H(26)	0.9300
C(26)-C(27)	1.409(10)
C(26)-H(6)	0.9300
C(27)-H(18)	0.9300
C(28)-C(33)	1.29(2)
C(28)-C(29)	1.46(3)
C(28)-H(29)	0.9300
C(29)-C(30)	1.33(3)
C(29)-H(28)	0.9300
C(30)-C(31)	1.29(4)
C(30)-H(27)	0.9300
C(31)-C(32)	1.40(4)
C(31)-H(35)	0.9300
C(32)-C(33)	1.42(3)
C(32)-H(32)	0.9300
C(33)-C(34)	1.38(3)
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600
C(35)-C(36)	1.28(2)
C(35)-C(37)#1	1.56(4)
C(36)-C(37)	1.40(2)
C(37)-C(38)	1.08(5)

C(37)-C(35)	1.56(4)
O(2)-Ti-N(1)	85.69(18)
O(2)-Ti-O(1)	158.32(17)
N(1)-Ti-O(1)	72.83(17)
O(2)-Ti-Cl(1)	104.35(15)
N(1)-Ti-Cl(1)	169.85(15)
O(1)-Ti-Cl(1)	97.21(12)
O(2)-Ti-Cl(3)	92.56(16)
N(1)-Ti-Cl(3)	86.33(14)
O(1)-Ti-Cl(3)	83.40(14)
Cl(1)-Ti-Cl(3)	94.58(8)
O(2)-Ti-Cl(2)	96.95(16)
N(1)-Ti-Cl(2)	83.91(14)
O(1)-Ti-Cl(2)	83.88(14)
Cl(1)-Ti-Cl(2)	93.26(8)
Cl(3)-Ti-Cl(2)	165.80(9)
C(5)-O(1)-C(22)	117.0(5)
C(5)-O(1)-Ti	117.4(3)
C(22)-O(1)-Ti	125.2(4)
C(13)-O(2)-Ti	140.8(4)
C(7)-N(1)-C(6)	121.2(5)
C(7)-N(1)-Ti	121.6(4)
C(6)-N(1)-Ti	117.1(4)
C(6)-C(1)-C(2)	120.5(6)
C(6)-C(1)-H(1)	119.7
C(2)-C(1)-H(1)	119.7
C(3)-C(2)-C(1)	119.7(6)
C(3)-C(2)-H(2)	120.2
C(1)-C(2)-H(2)	120.2
C(4)-C(3)-C(2)	120.7(7)
C(4)-C(3)-H(3)	119.7
C(2)-C(3)-H(3)	119.6
C(3)-C(4)-C(5)	118.7(6)
C(3)-C(4)-H(4)	120.7
C(5)-C(4)-H(4)	120.7
C(6)-C(5)-C(4)	121.7(6)
C(6)-C(5)-O(1)	115.2(5)
C(4)-C(5)-O(1)	123.1(5)
C(1)-C(6)-C(5)	118.6(6)
C(1)-C(6)-N(1)	125.4(6)
C(5)-C(6)-N(1)	116.0(5)
N(1)-C(7)-C(8)	128.2(5)
N(1)-C(7)-H(7)	115.9

C(8)-C(7)-H(7)	115.9
C(9)-C(8)-C(13)	118.6(6)
C(9)-C(8)-C(7)	117.5(5)
C(13)-C(8)-C(7)	123.8(5)
C(10)-C(9)-C(8)	121.9(6)
C(10)-C(9)-H(9)	119.1
C(8)-C(9)-H(9)	119.1
C(9)-C(10)-C(11)	117.8(5)
C(9)-C(10)-C(14)	122.9(6)
C(11)-C(10)-C(14)	119.3(6)
C(12)-C(11)-C(10)	123.6(6)
C(12)-C(11)-H(11)	118.2
C(10)-C(11)-H(11)	118.2
C(13)-C(12)-C(11)	116.0(5)
C(13)-C(12)-C(18)	122.4(5)
C(11)-C(12)-C(18)	121.6(5)
O(2)-C(13)-C(12)	120.7(5)
O(2)-C(13)-C(8)	117.1(5)
C(12)-C(13)-C(8)	122.2(5)
C(17)-C(14)-C(15)	109.1(7)
C(17)-C(14)-C(10)	110.2(5)
C(15)-C(14)-C(10)	111.0(6)
C(17)-C(14)-C(16)	109.9(7)
C(15)-C(14)-C(16)	108.3(7)
C(10)-C(14)-C(16)	108.3(6)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(20)-C(18)-C(21)	109.3(6)

C(20)-C(18)-C(19)	108.2(6)
C(21)-C(18)-C(19)	106.9(6)
C(20)-C(18)-C(12)	108.1(5)
C(21)-C(18)-C(12)	111.9(5)
C(19)-C(18)-C(12)	112.3(5)
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(27)-C(22)-C(23)	123.1(6)
C(27)-C(22)-O(1)	118.6(6)
C(23)-C(22)-O(1)	118.3(6)
C(22)-C(23)-C(24)	115.7(8)
C(22)-C(23)-H(24)	122.1
C(24)-C(23)-H(24)	122.1
C(25)-C(24)-C(23)	122.2(9)
C(25)-C(24)-H(25)	118.9
C(23)-C(24)-H(25)	118.9
C(24)-C(25)-C(26)	120.4(8)
C(24)-C(25)-H(26)	119.8
C(26)-C(25)-H(26)	119.8
C(25)-C(26)-C(27)	120.4(8)
C(25)-C(26)-H(6)	119.8
C(27)-C(26)-H(6)	119.8
C(22)-C(27)-C(26)	118.0(8)
C(22)-C(27)-H(18)	121.0
C(26)-C(27)-H(18)	121.0
C(33)-C(28)-C(29)	121(2)
C(33)-C(28)-H(29)	119.3
C(29)-C(28)-H(29)	119.3

C(30)-C(29)-C(28)	112(2)
C(30)-C(29)-H(28)	124.2
C(28)-C(29)-H(28)	124.2
C(31)-C(30)-C(29)	133(3)
C(31)-C(30)-H(27)	113.4
C(29)-C(30)-H(27)	113.4
C(30)-C(31)-C(32)	113(2)
C(30)-C(31)-H(35)	123.6
C(32)-C(31)-H(35)	123.6
C(31)-C(32)-C(33)	121(2)
C(31)-C(32)-H(32)	119.7
C(33)-C(32)-H(32)	119.7
C(28)-C(33)-C(34)	124(3)
C(28)-C(33)-C(32)	120(2)
C(34)-C(33)-C(32)	116(2)
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(36)-C(35)-C(37)#1	132.7(18)
C(35)-C(36)-C(37)	120(3)
C(38)-C(37)-C(36)	120(4)
C(38)-C(37)-C(35)#1	132(4)
C(36)-C(37)-C(35)#1	107(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **5a**.The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ti	49(1)	45(1)	26(1)	6(1)	8(1)	18(1)
Cl(1)	83(1)	79(1)	37(1)	22(1)	21(1)	30(1)
Cl(2)	68(1)	76(1)	39(1)	7(1)	9(1)	41(1)
Cl(3)	71(1)	64(1)	63(1)	9(1)	11(1)	38(1)
O(1)	68(3)	48(3)	27(2)	5(2)	0(2)	19(2)
O(2)	57(3)	54(3)	26(2)	2(2)	12(2)	16(2)
N(1)	44(3)	44(3)	31(3)	8(2)	10(2)	19(2)
C(1)	60(5)	50(4)	46(4)	9(3)	6(3)	14(3)
C(2)	60(5)	52(4)	62(5)	16(3)	9(4)	8(4)
C(3)	76(6)	47(4)	72(5)	1(4)	-1(4)	4(4)
C(4)	67(5)	60(5)	44(4)	-3(3)	-1(3)	23(4)
C(5)	48(4)	44(4)	39(3)	3(3)	6(3)	17(3)
C(6)	41(4)	42(4)	44(3)	7(3)	9(3)	15(3)
C(7)	45(4)	49(4)	31(3)	12(3)	20(3)	19(3)
C(8)	53(4)	42(3)	30(3)	5(2)	5(3)	22(3)
C(9)	57(4)	55(4)	29(3)	10(3)	11(3)	26(3)
C(10)	57(4)	52(4)	29(3)	1(3)	-1(3)	27(3)
C(11)	49(4)	50(4)	35(3)	-2(3)	-1(3)	22(3)
C(12)	32(3)	45(3)	40(3)	5(3)	6(2)	19(3)
C(13)	45(4)	50(4)	31(3)	8(3)	9(3)	26(3)
C(14)	70(5)	59(4)	31(3)	4(3)	5(3)	25(4)
C(15)	136(9)	98(7)	35(4)	10(4)	25(5)	18(6)
C(16)	102(8)	127(8)	59(5)	-12(5)	-24(5)	64(7)
C(17)	110(8)	97(6)	58(5)	3(4)	13(5)	64(6)
C(18)	40(4)	49(4)	43(3)	8(3)	13(3)	15(3)
C(19)	70(6)	60(5)	74(5)	-9(4)	11(4)	13(4)
C(20)	62(5)	75(6)	109(7)	49(5)	4(5)	19(4)
C(21)	63(5)	64(5)	72(5)	8(4)	36(4)	17(4)
C(22)	51(4)	55(4)	29(3)	2(3)	4(3)	11(3)
C(23)	68(5)	89(6)	57(5)	3(4)	-6(4)	41(5)
C(24)	80(7)	107(7)	78(6)	13(5)	-28(5)	34(6)
C(25)	106(8)	106(7)	41(4)	-6(4)	-6(5)	27(6)
C(26)	85(7)	99(7)	44(4)	-12(4)	13(4)	19(5)
C(27)	62(5)	81(5)	41(4)	-5(3)	10(3)	32(4)
C(28)	68(9)	149(12)	215(18)	-25(11)	-53(10)	45(9)
C(29)	90(12)	184(17)	400(40)	-40(20)	-77(17)	68(13)
C(30)	200(20)	103(11)	370(30)	-33(14)	-160(20)	43(12)
C(31)	350(50)	134(16)	260(30)	-50(20)	-200(30)	10(20)
C(32)	163(17)	103(10)	230(20)	-48(13)	-126(18)	83(11)
C(33)	95(12)	125(12)	320(30)	-85(16)	-14(16)	14(10)
C(34)	190(20)	240(20)	290(30)	-140(20)	100(20)	4(17)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5a**.

	x	y	z	U(eq)
H(1)	2266	6057	4812	65
H(2)	3718	7744	5406	74
H(3)	4323	8023	7068	86
H(4)	3437	6649	8155	69
H(7)	1350	4377	4447	49
H(9)	586	3174	3081	54
H(11)	-2011	171	3307	52
H(15A)	1099	2548	1688	146
H(15B)	80	2994	1424	146
H(15C)	324	2179	690	146
H(16A)	-2057	937	745	137
H(16B)	-2109	1879	1434	137
H(16C)	-2617	685	1781	137
H(17A)	386	482	2008	121
H(17B)	-367	243	1000	121
H(17C)	-1032	-240	1956	121
H(19A)	-3785	-1508	5036	108
H(19B)	-2854	-1189	4190	108
H(19C)	-3887	-721	4243	108
H(20A)	-1024	268	6318	124
H(20B)	-1179	-667	5537	124
H(20C)	-2120	-863	6371	124
H(21A)	-3742	728	5518	102
H(21B)	-2742	1021	6383	102
H(21C)	-3798	-142	6279	102
H(24)	3320	4060	8710	82
H(25)	3788	4308	10433	108
H(26)	2973	5237	11405	107
H(6)	1538	5865	10766	98
H(18)	916	5541	9093	72
H(29)	4503	8733	-585	175
H(28)	3269	8418	866	268
H(27)	4062	7886	2151	279
H(35)	5831	7718	2316	301
H(32)	6972	7954	874	193
H(34A)	7188	8296	-649	401
H(34B)	6990	9370	-837	401
H(34C)	6100	8269	-1357	401

Table 6. Torsion angles [deg] for **5a**.

O(2)-Ti-O(1)-C(5)	17.8(7)
N(1)-Ti-O(1)-C(5)	9.8(4)
Cl(1)-Ti-O(1)-C(5)	-168.2(4)
Cl(3)-Ti-O(1)-C(5)	98.0(4)
Cl(2)-Ti-O(1)-C(5)	-75.6(4)
O(2)-Ti-O(1)-C(22)	-169.7(5)
N(1)-Ti-O(1)-C(22)	-177.6(5)
Cl(1)-Ti-O(1)-C(22)	4.4(5)
Cl(3)-Ti-O(1)-C(22)	-89.5(5)
Cl(2)-Ti-O(1)-C(22)	96.9(5)
N(1)-Ti-O(2)-C(13)	21.0(6)
O(1)-Ti-O(2)-C(13)	13.4(9)
Cl(1)-Ti-O(2)-C(13)	-160.5(6)
Cl(3)-Ti-O(2)-C(13)	-65.1(6)
Cl(2)-Ti-O(2)-C(13)	104.3(6)
O(2)-Ti-N(1)-C(7)	-11.0(5)
O(1)-Ti-N(1)-C(7)	166.0(5)
Cl(1)-Ti-N(1)-C(7)	177.3(6)
Cl(3)-Ti-N(1)-C(7)	81.8(4)
Cl(2)-Ti-N(1)-C(7)	-108.5(4)
O(2)-Ti-N(1)-C(6)	172.4(4)
O(1)-Ti-N(1)-C(6)	-10.5(4)
Cl(1)-Ti-N(1)-C(6)	0.7(11)
Cl(3)-Ti-N(1)-C(6)	-94.7(4)
Cl(2)-Ti-N(1)-C(6)	75.0(4)
C(6)-C(1)-C(2)-C(3)	-0.2(11)
C(1)-C(2)-C(3)-C(4)	-1.3(13)
C(2)-C(3)-C(4)-C(5)	1.0(12)
C(3)-C(4)-C(5)-C(6)	0.8(11)
C(3)-C(4)-C(5)-O(1)	-179.4(6)
C(22)-O(1)-C(5)-C(6)	179.0(5)
Ti-O(1)-C(5)-C(6)	-7.9(7)
C(22)-O(1)-C(5)-C(4)	-0.8(9)
Ti-O(1)-C(5)-C(4)	172.3(5)
C(2)-C(1)-C(6)-C(5)	2.0(10)
C(2)-C(1)-C(6)-N(1)	-178.8(6)
C(4)-C(5)-C(6)-C(1)	-2.3(10)
O(1)-C(5)-C(6)-C(1)	177.9(5)
C(4)-C(5)-C(6)-N(1)	178.4(6)
O(1)-C(5)-C(6)-N(1)	-1.5(8)
C(7)-N(1)-C(6)-C(1)	14.4(9)
Ti-N(1)-C(6)-C(1)	-169.0(5)
C(7)-N(1)-C(6)-C(5)	-166.3(6)

Ti-N(1)-C(6)-C(5)	10.3(7)
C(6)-N(1)-C(7)-C(8)	179.8(6)
Ti-N(1)-C(7)-C(8)	3.4(8)
N(1)-C(7)-C(8)-C(9)	-175.8(6)
N(1)-C(7)-C(8)-C(13)	3.9(10)
C(13)-C(8)-C(9)-C(10)	-1.4(9)
C(7)-C(8)-C(9)-C(10)	178.3(6)
C(8)-C(9)-C(10)-C(11)	1.2(9)
C(8)-C(9)-C(10)-C(14)	-179.5(6)
C(9)-C(10)-C(11)-C(12)	-0.8(9)
C(14)-C(10)-C(11)-C(12)	180.0(6)
C(10)-C(11)-C(12)-C(13)	0.4(9)
C(10)-C(11)-C(12)-C(18)	-177.6(5)
Ti-O(2)-C(13)-C(12)	160.7(5)
Ti-O(2)-C(13)-C(8)	-19.0(9)
C(11)-C(12)-C(13)-O(2)	179.9(5)
C(18)-C(12)-C(13)-O(2)	-2.1(8)
C(11)-C(12)-C(13)-C(8)	-0.5(8)
C(18)-C(12)-C(13)-C(8)	177.5(5)
C(9)-C(8)-C(13)-O(2)	-179.4(5)
C(7)-C(8)-C(13)-O(2)	0.9(8)
C(9)-C(8)-C(13)-C(12)	0.9(9)
C(7)-C(8)-C(13)-C(12)	-178.7(5)
C(9)-C(10)-C(14)-C(17)	123.6(7)
C(11)-C(10)-C(14)-C(17)	-57.1(9)
C(9)-C(10)-C(14)-C(15)	2.7(9)
C(11)-C(10)-C(14)-C(15)	-178.1(7)
C(9)-C(10)-C(14)-C(16)	-116.1(7)
C(11)-C(10)-C(14)-C(16)	63.1(8)
C(13)-C(12)-C(18)-C(20)	-67.5(8)
C(11)-C(12)-C(18)-C(20)	110.4(7)
C(13)-C(12)-C(18)-C(21)	52.9(8)
C(11)-C(12)-C(18)-C(21)	-129.2(6)
C(13)-C(12)-C(18)-C(19)	173.2(6)
C(11)-C(12)-C(18)-C(19)	-9.0(8)
C(5)-O(1)-C(22)-C(27)	82.9(8)
Ti-O(1)-C(22)-C(27)	-89.7(7)
C(5)-O(1)-C(22)-C(23)	-98.2(7)
Ti-O(1)-C(22)-C(23)	89.2(7)
C(27)-C(22)-C(23)-C(24)	-0.1(12)
O(1)-C(22)-C(23)-C(24)	-178.9(7)
C(22)-C(23)-C(24)-C(25)	-2.5(14)
C(23)-C(24)-C(25)-C(26)	2.6(16)
C(24)-C(25)-C(26)-C(27)	0.0(15)

C(23)-C(22)-C(27)-C(26)	2.5(12)
O(1)-C(22)-C(27)-C(26)	-178.7(7)
C(25)-C(26)-C(27)-C(22)	-2.5(13)
C(33)-C(28)-C(29)-C(30)	-1(3)
C(28)-C(29)-C(30)-C(31)	2(3)
C(29)-C(30)-C(31)-C(32)	-3(4)
C(30)-C(31)-C(32)-C(33)	4(3)
C(29)-C(28)-C(33)-C(34)	-178.8(18)
C(29)-C(28)-C(33)-C(32)	2(3)
C(31)-C(32)-C(33)-C(28)	-3(3)
C(31)-C(32)-C(33)-C(34)	177(2)
C(37)#1-C(35)-C(36)-C(37)	2(6)
C(35)-C(36)-C(37)-C(38)	-178(4)
C(35)-C(36)-C(37)-C(35)#1	-2(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

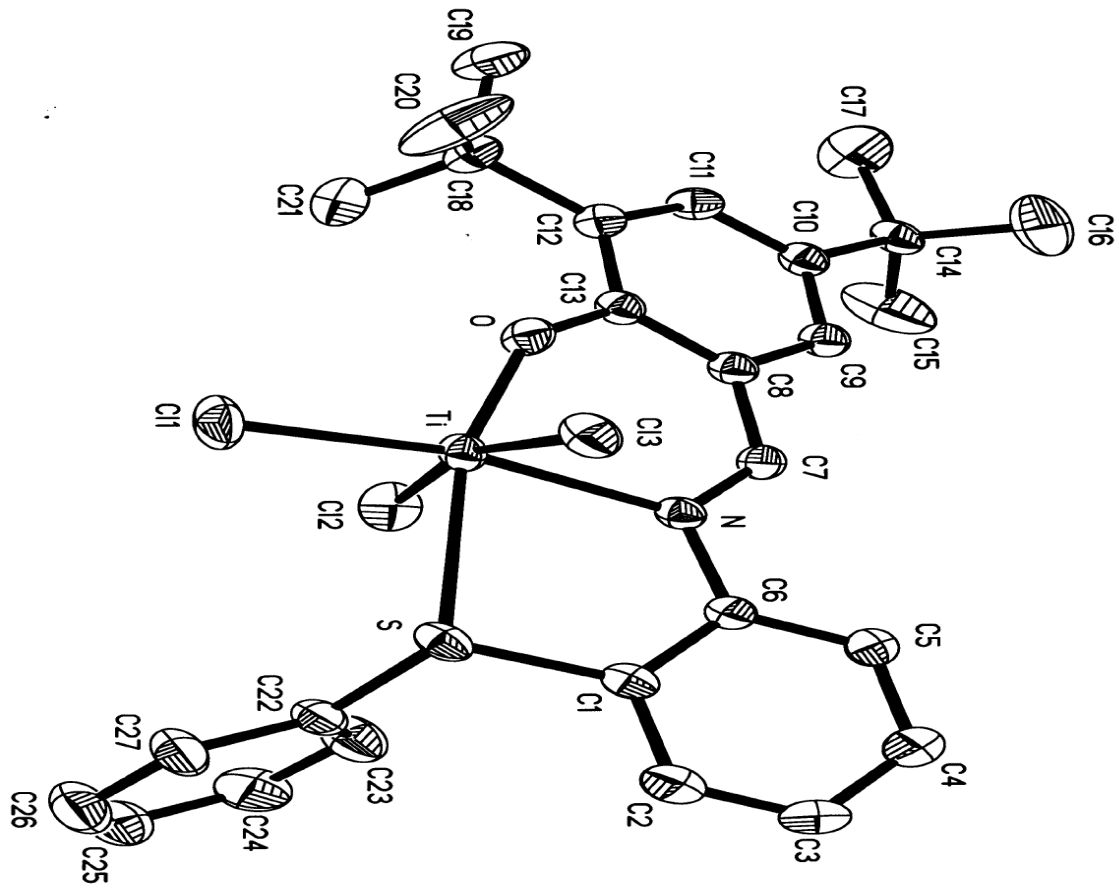


Figure 2. molecular structure of 5e

Table 7. Crystal data and structure refinement for **5e**

Identification code	cd22300
Empirical formula	C27 H30 N O S Cl3 Ti
Formula weight	570.83
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 12.663(2) A alpha = 90 deg.
	b = 17.026(3) A beta = 98.186(3) deg.
	c = 13.131(2) A gamma = 90 deg.
Volume	2802.4(7) A^3
Z, Calculated density	4, 1.353 Mg/m^3
Absorption coefficient	0.686 mm^-1
F(000)	1184
Crystal size	0.945 x 0.459 x 0.176 mm
Theta range for data collection	1.97 to 28.29 deg.
Limiting indices	-16<=h<=16, -22<=k<=16, -17<=l<=16
Reflections collected / unique	16260 / 6408 [R(int) = 0.1188]
Completeness to theta = 28.29	92.0 %
Absorption correction	Sadabs
Max. and min. transmission	1.00000 and 0.46335
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6408 / 0 / 361
Goodness-of-fit on F^2	0.904
Final R indices [I>2sigma(I)]	R1 = 0.0530, wR2 = 0.1228
R indices (all data)	R1 = 0.0899, wR2 = 0.1353
Largest diff. peak and hole	0.564 and -0.385 e.A^-3

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5e**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ti	1707(1)	10222(1)	7853(1)	38(1)
S	457(1)	9295(1)	6669(1)	43(1)
Cl(1)	2198(1)	10800(1)	6452(1)	66(1)
Cl(2	2971(1)	9253(1)	7977(1)	62(1)
Cl(3)	88(1)	10902(1)	7763(1)	47(1)
O	2384(2)	10741(1)	8940(1)	43(1)
N	1007(2)	9497(1)	8970(2)	34(1)
C(1)	-99(2)	8766(2)	7624(2)	40(1)
C(2)	-861(3)	8197(2)	7308(3)	58(1)
C(3)	-1348(3)	7790(2)	8004(3)	60(1)
C(4)	-1104(3)	7962(2)	9031(3)	56(1)
C(5)	-354(3)	8530(2)	9360(3)	47(1)
C(6)	180(2)	8931(2)	8668(2)	36(1)
C(7)	1381(2)	9540(2)	9946(2)	38(1)
C(8)	2246(2)	10028(2)	10443(2)	36(1)
C(9)	2572(2)	9886(2)	11491(2)	40(1)
C(10)	3409(2)	10301(2)	12026(2)	39(1)
C(11)	3888(3)	10868(2)	11498(2)	42(1)
C(12)	3582(2)	11061(2)	10464(2)	38(1)
C(13)	2748(2)	10612(2)	9945(2)	37(1)
C(14)	3765(3)	10109(2)	13168(2)	45(1)
C(15)	4080(5)	9262(2)	13285(3)	117(2)
C(16)	2880(3)	10272(3)	13774(3)	97(2)
C(17)	4727(3)	10617(3)	13617(3)	98(2)
C(18)	4182(2)	11683(2)	9926(2)	49(1)
C(19)	4921(3)	12186(2)	10686(3)	76(1)
C(20)	3393(3)	12263(3)	9335(4)	117(2)
C(21)	4856(4)	11278(3)	9222(4)	111(2)
C(22)	1107(2)	8556(2)	6031(2)	44(1)
C(23)	1636(3)	7924(2)	6529(3)	65(1)
C(24)	2161(3)	7398(2)	5967(4)	70(1)
C(25)	2133(3)	7495(3)	4924(3)	70(1)
C(26)	1591(4)	8099(3)	4442(3)	74(1)
C(27)	1077(3)	8645(2)	4988(2)	59(1)

Table 9. Bond lengths [A] and angles [deg] for **5e**

Ti-O	1.7910(19)
Ti-N	2.198(2)
Ti-Cl(1)	2.2509(10)
Ti-Cl(2)	2.2887(10)
Ti-Cl(3)	2.5908(9)
S-C(1)	1.769(3)
S-C(22)	1.777(3)
O-C(13)	1.352(3)
N-C(7)	1.304(3)
N-C(6)	1.438(3)
C(1)-C(2)	1.389(4)
C(1)-C(6)	1.394(4)
C(2)-C(3)	1.362(5)
C(2)-H(2)	0.90(3)
C(3)-C(4)	1.371(5)
C(3)-H(3)	0.91(3)
C(4)-C(5)	1.381(4)
C(4)-H(4)	1.00(4)
C(5)-C(6)	1.387(4)
C(5)-H(5)	0.90(3)
C(7)-C(8)	1.453(4)
C(7)-H(7)	0.95(3)
C(8)-C(13)	1.392(4)
C(8)-C(9)	1.401(4)
C(9)-C(10)	1.379(4)
C(9)-H(9)	0.98(3)
C(10)-C(11)	1.379(4)
C(10)-C(14)	1.538(4)
C(11)-C(12)	1.398(4)
C(11)-H(11)	0.87(3)
C(12)-C(13)	1.400(4)
C(12)-C(18)	1.534(4)
C(14)-C(16)	1.490(5)
C(14)-C(15)	1.497(5)
C(14)-C(17)	1.541(5)
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600

C(17)-H(17C)	0.9600
C(18)-C(21)	1.511(5)
C(18)-C(19)	1.529(4)
C(18)-C(20)	1.535(5)
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-C(27)	1.373(4)
C(22)-C(23)	1.381(5)
C(23)-C(24)	1.390(5)
C(23)-H(23)	0.86(3)
C(24)-C(25)	1.375(6)
C(24)-H(24)	0.92(4)
C(25)-C(26)	1.345(6)
C(25)-H(25)	0.96(4)
C(26)-C(27)	1.391(5)
C(26)-H(26)	1.08(5)
C(27)-H(27)	1.00(4)

O-Ti-N	86.44(8)
O-Ti-Cl(1)	106.21(7)
N-Ti-Cl(1)	167.35(7)
O-Ti-Cl(2)	92.76(7)
N-Ti-Cl(2)	83.81(7)
Cl(1)-Ti-Cl(2)	95.79(4)
O-Ti-Cl(3)	96.48(7)
N-Ti-Cl(3)	83.01(6)
Cl(1)-Ti-Cl(3)	94.84(4)
Cl(2)-Ti-Cl(3)	163.38(4)
O-Ti-S	164.04(7)
N-Ti-S	77.79(6)
Cl(1)-Ti-S	89.55(4)
Cl(2)-Ti-S	87.99(4)
Cl(3)-Ti-S	79.36(3)
C(1)-S-C(22)	103.38(14)
C(1)-S-Ti	98.94(10)
C(22)-S-Ti	115.43(10)
C(13)-O-Ti	139.06(18)

C(7)-N-C(6)	117.2(2)
C(7)-N-Ti	120.0(2)
C(6)-N-Ti	122.65(16)
C(2)-C(1)-C(6)	120.1(3)
C(2)-C(1)-S	118.2(2)
C(6)-C(1)-S	121.6(2)
C(3)-C(2)-C(1)	121.1(3)
C(3)-C(2)-H(2)	122(2)
C(1)-C(2)-H(2)	117(2)
C(2)-C(3)-C(4)	119.4(4)
C(2)-C(3)-H(3)	122(2)
C(4)-C(3)-H(3)	118(2)
C(3)-C(4)-C(5)	120.4(4)
C(3)-C(4)-H(4)	124(2)
C(5)-C(4)-H(4)	115.3(19)
C(4)-C(5)-C(6)	121.1(3)
C(4)-C(5)-H(5)	121(2)
C(6)-C(5)-H(5)	118(2)
C(5)-C(6)-C(1)	117.8(3)
C(5)-C(6)-N	123.6(3)
C(1)-C(6)-N	118.6(3)
N-C(7)-C(8)	128.2(3)
N-C(7)-H(7)	117.6(17)
C(8)-C(7)-H(7)	114.1(17)
C(13)-C(8)-C(9)	119.6(3)
C(13)-C(8)-C(7)	124.3(2)
C(9)-C(8)-C(7)	116.1(3)
C(10)-C(9)-C(8)	120.7(3)
C(10)-C(9)-H(9)	121.2(16)
C(8)-C(9)-H(9)	118.1(16)
C(9)-C(10)-C(11)	117.6(3)
C(9)-C(10)-C(14)	119.0(3)
C(11)-C(10)-C(14)	123.4(3)
C(10)-C(11)-C(12)	124.9(3)
C(10)-C(11)-H(11)	119(2)
C(12)-C(11)-H(11)	116(2)
C(11)-C(12)-C(13)	115.5(3)
C(11)-C(12)-C(18)	121.5(3)
C(13)-C(12)-C(18)	122.8(2)
O-C(13)-C(8)	117.4(2)
O-C(13)-C(12)	121.0(3)
C(8)-C(13)-C(12)	121.6(2)
C(16)-C(14)-C(15)	109.6(4)
C(16)-C(14)-C(10)	110.0(3)

C(15)-C(14)-C(10)	110.0(3)
C(16)-C(14)-C(17)	107.7(3)
C(15)-C(14)-C(17)	108.4(3)
C(10)-C(14)-C(17)	111.1(3)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(21)-C(18)-C(19)	108.0(3)
C(21)-C(18)-C(12)	109.1(3)
C(19)-C(18)-C(12)	112.6(3)
C(21)-C(18)-C(20)	111.6(4)
C(19)-C(18)-C(20)	105.2(3)
C(12)-C(18)-C(20)	110.4(3)
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5

H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(27)-C(22)-C(23)	120.1(3)
C(27)-C(22)-S	116.3(3)
C(23)-C(22)-S	123.7(3)
C(22)-C(23)-C(24)	119.2(4)
C(22)-C(23)-H(23)	118(2)
C(24)-C(23)-H(23)	123(2)
C(25)-C(24)-C(23)	120.4(4)
C(25)-C(24)-H(24)	120(2)
C(23)-C(24)-H(24)	120(2)
C(26)-C(25)-C(24)	120.0(4)
C(26)-C(25)-H(25)	120(2)
C(24)-C(25)-H(25)	120(2)
C(25)-C(26)-C(27)	120.9(4)
C(25)-C(26)-H(26)	127(3)
C(27)-C(26)-H(26)	111(3)
C(22)-C(27)-C(26)	119.5(4)
C(22)-C(27)-H(27)	119(3)
C(26)-C(27)-H(27)	122(3)

Table 10. Anisotropic displacement parameters (A^2 x 10^3) for **5e.** The anisotropic displacement factor exponent takes the form:-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ti	49(1)	40(1)	25(1)	5(1)	5(1)	1(1)
S	58(1)	41(1)	28(1)	-2(1)	1(1)	7(1)
Cl(1)	96(1)	68(1)	40(1)	15(1)	29(1)	5(1)
Cl(2)	52(1)	69(1)	65(1)	11(1)	9(1)	16(1)
Cl(3)	59(1)	45(1)	37(1)	3(1)	6(1)	11(1)
O	53(1)	45(1)	28(1)	10(1)	-1(1)	-9(1)
N	41(1)	35(1)	26(1)	0(1)	0(1)	0(1)
C(1)	46(2)	40(2)	34(2)	-5(1)	0(1)	3(1)
C(2)	68(2)	61(2)	43(2)	-13(2)	5(2)	-9(2)
C(3)	60(2)	54(2)	63(2)	-14(2)	2(2)	18(2)
C(4)	59(2)	54(2)	57(2)	-2(2)	13(2)	12(2)
C(5)	52(2)	53(2)	37(2)	-3(2)	9(2)	-7(2)
C(6)	39(2)	34(2)	34(2)	-2(1)	4(1)	1(1)
C(7)	47(2)	37(2)	29(2)	5(1)	5(1)	-2(1)
C(8)	45(2)	33(2)	27(1)	1(1)	0(1)	1(1)
C(9)	52(2)	39(2)	29(2)	4(1)	2(1)	0(2)
C(10)	49(2)	40(2)	29(2)	2(1)	1(1)	6(1)
C(11)	41(2)	41(2)	40(2)	-2(1)	-7(1)	-2(2)
C(12)	38(2)	36(2)	38(2)	4(1)	0(1)	3(1)
C(13)	44(2)	37(2)	28(1)	2(1)	2(1)	4(1)
C(14)	62(2)	48(2)	23(1)	-2(1)	-2(1)	5(2)
C(15)	221(6)	75(3)	43(2)	6(2)	-20(3)	51(4)
C(16)	108(4)	144(5)	38(2)	6(3)	14(2)	20(3)
C(17)	105(3)	138(4)	43(2)	15(2)	-21(2)	36(3)
C(18)	47(2)	49(2)	49(2)	8(2)	0(2)	12(2)
C(19)	83(3)	57(2)	83(3)	7(2)	-2(2)	28(2)
C(20)	87(3)	89(3)	156(5)	88(3)	-45(3)	35(3)
C(21)	133(4)	107(4)	110(4)	-25(3)	75(3)	51(3)
C(22)	59(2)	39(2)	33(2)	-4(1)	6(1)	-1(2)
C(23)	98(3)	52(2)	45(2)	3(2)	9(2)	16(2)
C(24)	84(3)	47(2)	78(3)	-7(2)	4(2)	14(2)
C(25)	70(3)	69(3)	76(3)	-23(2)	29(2)	4(2)
C(26)	106(3)	69(3)	52(2)	-8(2)	30(2)	7(2)
C(27)	84(3)	56(2)	38(2)	-2(2)	18(2)	7(2)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5e**.

	x	y	z	U(eq)
H(15A)	4209	9129	14003	175
H(15B)	4717	9176	12983	175
H(15C)	3516	8940	12945	175
H(16A)	2296	9923	13559	145
H(16B)	2646	10806	13662	145
H(16C)	3127	10194	14492	145
H(17A)	4547	11162	13522	147
H(17B)	5325	10497	13270	147
H(17C)	4908	10508	14338	147
H(19A)	4517	12421	11172	113
H(19B)	5235	12591	10318	113
H(19C)	5473	11862	11044	113
H(20A)	2678	12123	9428	175
H(20B)	3460	12245	8617	175
H(20C)	3546	12785	9592	175
H(21A)	5356	10934	9618	167
H(21B)	5236	11665	8884	167
H(21C)	4404	10979	8715	167
H(4)	-1430(20)	7700(20)	9590(30)	69(11)
H(3)	-1870(20)	7430(20)	7810(20)	53(9)
H(2)	-990(20)	8090(19)	6630(30)	62(10)
H(5)	-190(20)	8650(20)	10030(20)	59(10)
H(7)	1030(20)	9243(16)	10410(20)	40(8)
H(9)	2170(20)	9499(17)	11840(20)	40(8)
H(11)	4430(20)	1127(18)	11820(20)	48(9)
H(27)	720(30)	9120(30)	4650(30)	15(16)
H(23)	1580(30)	7850(20)	7170(30)	65(11)
H(24)	2590(30)	7010(20)	6310(30)	79(13)
H(25)	2530(30)	7140(20)	4540(30)	67(11)
H(26)	1560(40)	8270(30)	3640(40)	50(20)

Table 12. Torsion angles [deg] for **5e**

O-Ti-S-C(1)	-6.9(3)
N-Ti-S-C(1)	2.01(12)
Cl(1)-Ti-S-C(1)	-178.07(10)
Cl(2)-Ti-S-C(1)	86.11(10)
Cl(3)-Ti-S-C(1)	-83.06(10)
O-Ti-S-C(22)	-116.4(3)
N-Ti-S-C(22)	-107.51(13)
Cl(1)-Ti-S-C(22)	72.41(12)
Cl(2)-Ti-S-C(22)	-23.41(12)
Cl(3)-Ti-S-C(22)	167.42(11)
N-Ti-O-C(13)	27.1(3)
Cl(1)-Ti-O-C(13)	-153.3(3)
Cl(2)-Ti-O-C(13)	-56.5(3)
Cl(3)-Ti-O-C(13)	109.7(3)
S-Ti-O-C(13)	35.9(5)
O-Ti-N-C(7)	-11.7(2)
Cl(1)-Ti-N-C(7)	170.3(2)
Cl(2)-Ti-N-C(7)	81.4(2)
Cl(3)-Ti-N-C(7)	-108.7(2)
S-Ti-N-C(7)	170.7(2)
O-Ti-N-C(6)	172.1(2)
Cl(1)-Ti-N-C(6)	-5.8(4)
Cl(2)-Ti-N-C(6)	-94.7(2)
Cl(3)-Ti-N-C(6)	75.11(19)
S-Ti-N-C(6)	-5.46(19)
C(22)-S-C(1)-C(2)	-62.6(3)
Ti-S-C(1)-C(2)	178.5(2)
C(22)-S-C(1)-C(6)	120.0(3)
Ti-S-C(1)-C(6)	1.1(3)
C(6)-C(1)-C(2)-C(3)	-0.1(5)
S-C(1)-C(2)-C(3)	-177.5(3)
C(1)-C(2)-C(3)-C(4)	1.9(6)
C(2)-C(3)-C(4)-C(5)	-1.4(6)
C(3)-C(4)-C(5)-C(6)	-0.9(5)
C(4)-C(5)-C(6)-C(1)	2.7(5)
C(4)-C(5)-C(6)-N	-176.6(3)
C(2)-C(1)-C(6)-C(5)	-2.2(4)
S-C(1)-C(6)-C(5)	175.1(2)
C(2)-C(1)-C(6)-N	177.2(3)
S-C(1)-C(6)-N	-5.5(4)
C(7)-N-C(6)-C(5)	11.1(4)
Ti-N-C(6)-C(5)	-172.6(2)
C(7)-N-C(6)-C(1)	-168.3(3)

Ti-N-C(6)-C(1)	8.0(3)
C(6)-N-C(7)-C(8)	176.6(3)
Ti-N-C(7)-C(8)	0.3(4)
N-C(7)-C(8)-C(13)	7.7(5)
N-C(7)-C(8)-C(9)	-172.3(3)
C(13)-C(8)-C(9)-C(10)	-2.1(5)
C(7)-C(8)-C(9)-C(10)	177.9(3)
C(8)-C(9)-C(10)-C(11)	1.6(4)
C(8)-C(9)-C(10)-C(14)	-178.1(3)
C(9)-C(10)-C(11)-C(12)	0.8(5)
C(14)-C(10)-C(11)-C(12)	-179.6(3)
C(10)-C(11)-C(12)-C(13)	-2.4(5)
C(10)-C(11)-C(12)-C(18)	-178.0(3)
Ti-O-C(13)-C(8)	-25.8(4)
Ti-O-C(13)-C(12)	155.6(2)
C(9)-C(8)-C(13)-O	-178.2(3)
C(7)-C(8)-C(13)-O	1.8(4)
C(9)-C(8)-C(13)-C(12)	0.4(4)
C(7)-C(8)-C(13)-C(12)	-179.7(3)
C(11)-C(12)-C(13)-O	-179.8(3)
C(18)-C(12)-C(13)-O	-4.2(4)
C(11)-C(12)-C(13)-C(8)	1.7(4)
C(18)-C(12)-C(13)-C(8)	177.3(3)
C(9)-C(10)-C(14)-C(16)	-62.4(4)
C(11)-C(10)-C(14)-C(16)	117.9(4)
C(9)-C(10)-C(14)-C(15)	58.3(4)
C(11)-C(10)-C(14)-C(15)	-121.3(4)
C(9)-C(10)-C(14)-C(17)	178.4(3)
C(11)-C(10)-C(14)-C(17)	-1.3(4)
C(11)-C(12)-C(18)-C(21)	105.4(4)
C(13)-C(12)-C(18)-C(21)	-69.9(4)
C(11)-C(12)-C(18)-C(19)	-14.4(4)
C(13)-C(12)-C(18)-C(19)	170.2(3)
C(11)-C(12)-C(18)-C(20)	-131.7(4)
C(13)-C(12)-C(18)-C(20)	53.0(4)
C(1)-S-C(22)-C(27)	143.7(3)
Ti-S-C(22)-C(27)	-109.4(3)
C(1)-S-C(22)-C(23)	-37.2(3)
Ti-S-C(22)-C(23)	69.7(3)
C(27)-C(22)-C(23)-C(24)	2.0(6)
S-C(22)-C(23)-C(24)	-177.1(3)
C(22)-C(23)-C(24)-C(25)	-1.5(6)
C(23)-C(24)-C(25)-C(26)	-0.3(7)
C(24)-C(25)-C(26)-C(27)	1.7(7)

C(23)-C(22)-C(27)-C(26)	-0.7(6)
S-C(22)-C(27)-C(26)	178.5(3)
C(25)-C(26)-C(27)-C(22)	-1.2(6)

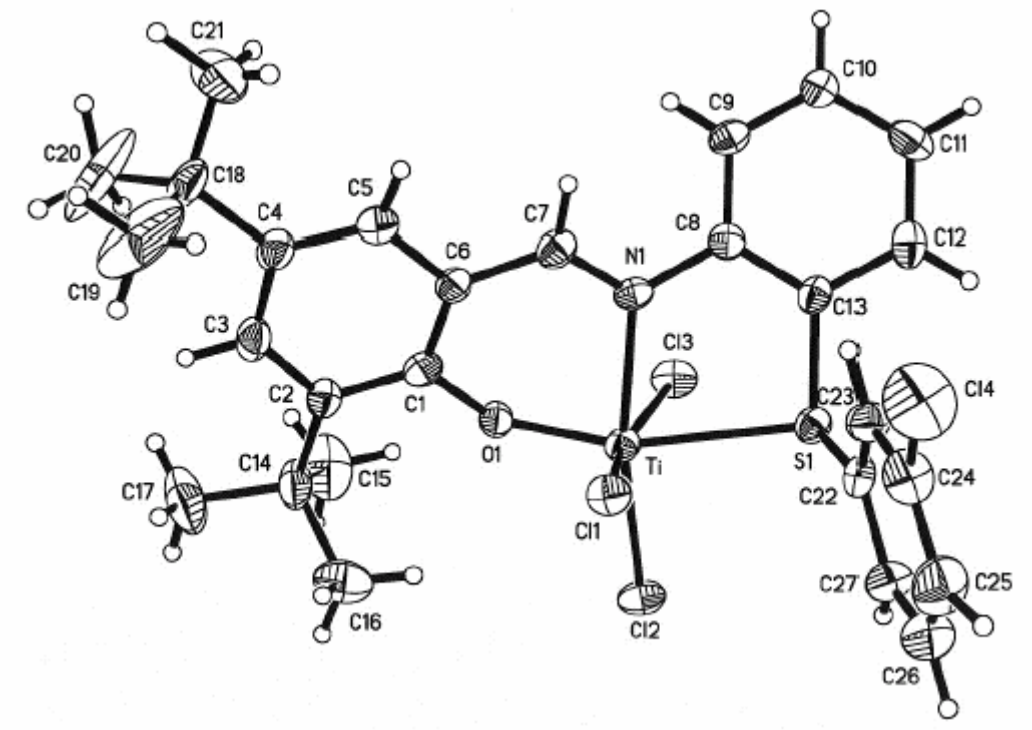


Figure 3. Molecular structure of 5g

Table 13. Crystal data and structure refinement for **5g.**

Identification code	cd2551
Empirical formula	C28 H30 N O Cl7 S Ti
Formula weight	724.64
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 12.846(5) A alpha = 90 deg. b = 14.395(5) A beta = 102.623(8) deg. c = 19.068(6) A gamma = 90 deg.
Volume	3441(2) A^3
Z, Calculated density	4, 1.399 Mg/m^3
Absorption coefficient	0.875 mm^-1
F(000)	1480
Crystal size	0.283 x 0.207 x 0.125 mm
Theta range for data collection	1.75 to 27.00 deg.
Limiting indices	-10<=h<=16, -18<=k<=18, -23<=l<=24
Reflections collected / unique	19948 / 7475 [R(int) = 0.1417]
Completeness to theta = 27.00	99.3 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.76945
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7475 / 0 / 355
Goodness-of-fit on F^2	0.748
Final R indices [I>2sigma(I)]	R1 = 0.0688, wR2 = 0.1433
R indices (all data)	R1 = 0.1863, wR2 = 0.1736
Largest diff. peak and hole	0.725 and -0.518 e.A^-3

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5g**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ti	2312(1)	1878(1)	1255(1)	38(1)
S(1)	306(1)	2019(1)	1334(1)	42(1)
Cl(1)	1859(1)	2758(1)	234(1)	49(1)
Cl(2)	2028(2)	500(1)	661(1)	58(1)
Cl(3)	2335(2)	1196(1)	2361(1)	55(1)
Cl(4)	-1536(2)	4883(2)	-369(1)	103(1)
Cl(5)	9831(2)	9488(2)	1457(1)	125(1)
Cl(6)	9574(4)	7637(3)	1811(2)	216(2)
Cl(7)	7783(3)	8765(4)	1457(3)	324(4)
N(1)	2278(4)	3181(3)	1834(2)	36(1)
O(1)	3701(3)	2131(3)	1349(2)	43(1)
C(1)	4324(5)	2899(4)	1327(3)	42(2)
C(2)	5287(5)	2835(4)	1106(3)	45(2)
C(3)	5844(5)	3658(5)	1119(3)	52(2)
C(4)	5526(6)	4517(5)	1349(3)	49(2)
C(5)	4568(6)	4546(5)	1555(3)	46(2)
C(6)	3948(5)	3735(4)	1549(3)	39(2)
C(7)	2991(5)	3818(4)	1820(3)	41(2)
C(8)	1422(5)	3364(4)	2192(3)	37(2)
C(9)	1587(5)	3975(4)	2778(3)	45(2)
C(10)	749(6)	4167(5)	3102(4)	58(2)
C(11)	-223(6)	3741(5)	2876(4)	68(2)
C(12)	-379(5)	3111(5)	2308(3)	55(2)
C(13)	468(5)	2928(4)	1977(3)	39(2)
C(14)	5696(6)	1905(5)	876(5)	70(2)
C(15)	5849(6)	1205(6)	1481(5)	100(3)
C(16)	4891(7)	1512(6)	217(4)	97(3)
C(17)	6755(7)	2017(6)	667(6)	134(4)
C(18)	6208(6)	5384(5)	1335(4)	167(2)
C(19)	6149(8)	5684(7)	588(5)	146(4)
C(20)	7396(9)	5178(8)	1603(6)	160(5)
C(21)	5988(9)	6109(9)	1804(6)	162(5)
C(22)	-506(5)	2502(5)	543(3)	42(2)
C(23)	-699(5)	3425(5)	430(4)	47(2)
C(24)	-1319(6)	3696(6)	-211(4)	67(2)
C(25)	-1760(7)	3076(8)	-737(5)	82(3)
C(26)	-1555(7)	2154(7)	-610(4)	80(3)
C(27)	-927(6)	1830(6)	28(4)	58(2)
C(28)	8970(7)	8575(6)	1278(4)	95(3)

Table 15. Bond lengths [A] and angles [deg] for **5g**.

Ti-O(1)	1.791(4)
Ti-N(1)	2.181(5)
Ti-Cl(2)	2.273(2)
Ti-Cl(1)	2.2889(19)
Ti-Cl(3)	2.321(2)
Ti-S(1)	2.622(2)
S(1)-C(13)	1.775(6)
S(1)-C(22)	1.777(6)
Cl(4)-C(24)	1.747(8)
Cl(5)-C(28)	1.703(8)
Cl(6)-C(28)	1.764(9)
Cl(7)-C(28)	1.657(9)
N(1)-C(7)	1.301(7)
N(1)-C(8)	1.441(7)
O(1)-C(1)	1.371(7)
C(1)-C(2)	1.394(8)
C(1)-C(6)	1.396(8)
C(2)-C(3)	1.381(8)
C(2)-C(14)	1.537(9)
C(3)-C(4)	1.402(8)
C(3)-H(3)	0.9300
C(4)-C(5)	1.372(8)
C(4)-C(18)	1.528(9)
C(5)-C(6)	1.413(8)
C(5)-H(5)	1.07(7)
C(6)-C(7)	1.438(8)
C(7)-H(7)	0.9300
C(8)-C(13)	1.357(8)
C(8)-C(9)	1.402(8)
C(9)-C(10)	1.380(8)
C(9)-H(9)	0.9300
C(10)-C(11)	1.373(9)
C(10)-H(10)	0.9300
C(11)-C(12)	1.393(9)
C(11)-H(11)	0.9300
C(12)-C(13)	1.396(8)
C(12)-H(12)	0.9300
C(14)-C(17)	1.508(9)
C(14)-C(15)	1.511(10)
C(14)-C(16)	1.550(10)
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600

C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-C(21)	1.441(12)
C(18)-C(19)	1.474(10)
C(18)-C(20)	1.529(12)
C(19)-H(19A	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-C(23)	1.360(8)
C(22)-C(27)	1.401(9)
C(23)-C(24)	1.361(9)
C(23)-H(23)	0.9300
C(24)-C(25)	1.370(11)
C(25)-C(26)	1.365(11)
C(25)-H(25)	0.94(6)
C(26)-C(27)	1.385(10)
C(26)-H(26)	0.9300
C(27)-H(27)	0.93(6)
C(28)-H(28)	0.9800
O(1)-Ti-N(1)	84.49(18)
O(1)-Ti-Cl(2)	105.98(14)
N(1)-Ti-Cl(2)	169.52(15)
O(1)-Ti-Cl(1)	92.03(14)
N(1)-Ti-Cl(1)	85.70(13)
Cl(2)-Ti-Cl(1)	94.36(8)
O(1)-Ti-Cl(3)	100.40(14)
N(1)-Ti-Cl(3)	84.32(13)
Cl(2)-Ti-Cl(3)	93.02(7)
Cl(1)-Ti-Cl(3)	163.22(8)
O(1)-Ti-S(1)	161.51(14)
N(1)-Ti-S(1)	77.02(14)
Cl(2)-Ti-S(1)	92.51(7)
Cl(1)-Ti-S(1)	86.31(6)

Cl(3)-Ti-S(1)	78.32(7)
C(13)-S(1)-C(22	104.9(3)
C(13)-S(1)-Ti	97.4(2)
C(22)-S(1)-Ti	112.6(2)
C(7)-N(1)-C(8)	119.6(5)
C(7)-N(1)-Ti	120.3(4)
C(8)-N(1)-Ti	120.0(4)
C(1)-O(1)-Ti	137.4(4)
O(1)-C(1)-C(2)	121.2(6)
O(1)-C(1)-C(6)	116.3(6)
C(2)-C(1)-C(6)	122.5(6)
C(3)-C(2)-C(1)	115.4(6)
C(3)-C(2)-C(14)	123.0(6)
C(1)-C(2)-C(14)	121.7(6)
C(2)-C(3)-C(4)	125.2(7)
C(2)-C(3)-H(3)	117.4
C(4)-C(3)-H(3)	117.4
C(5)-C(4)-C(3)	117.2(6)
C(5)-C(4)-C(18)	122.2(7)
C(3)-C(4)-C(18)	120.5(6)
C(4)-C(5)-C(6)	120.8(7)
C(4)-C(5)-H(5)	124(4)
C(6)-C(5)-H(5)	113(4)
C(1)-C(6)-C(5)	118.8(6)
C(1)-C(6)-C(7)	124.1(6)
C(5)-C(6)-C(7)	117.0(6)
N(1)-C(7)-C(6)	127.5(6)
N(1)-C(7)-H(7)	116.2
C(6)-C(7)-H(7)	116.2
C(13)-C(8)-C(9)	120.0(6)
C(13)-C(8)-N(1)	120.3(5)
C(9)-C(8)-N(1)	119.7(6)
C(10)-C(9)-C(8)	119.1(6)
C(10)-C(9)-H(9)	120.5
C(8)-C(9)-H(9)	120.5
C(11)-C(10)-C(9)	120.9(7)
C(11)-C(10)-H(10)	119.5
C(9)-C(10)-H(10)	119.5
C(10)-C(11)-C(12)	120.1(7)
C(10)-C(11)-H(11)	120.0
C(12)-C(11)-H(11)	120.0
C(11)-C(12)-C(13)	118.7(6)
C(11)-C(12)-H(12)	120.7
C(13)-C(12)-H(12)	120.7

C(8)-C(13)-C(12)	121.2(6)
C(8)-C(13)-S(1)	120.7(5)
C(12)-C(13)-S(1)	117.8(5)
C(17)-C(14)-C(15)	107.4(7)
C(17)-C(14)-C(2)	111.5(6)
C(15)-C(14)-C(2)	111.0(7)
C(17)-C(14)-C(16)	107.7(7)
C(15)-C(14)-C(16)	109.1(7)
C(2)-C(14)-C(16)	109.9(6)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(21)-C(18)-C(19)	114.3(8)
C(21)-C(18)-C(4)	113.0(8)
C(19)-C(18)-C(4)	110.3(7)
C(21)-C(18)-C(20)	104.5(8)
C(19)-C(18)-C(20)	102.5(7)
C(4)-C(18)-C(20)	111.7(8)
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5

H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(23)-C(22)-C(27)	122.3(7)
C(23)-C(22)-S(1)	124.8(5)
C(27)-C(22)-S(1)	113.0(5)
C(22)-C(23)-C(24)	118.3(7)
C(22)-C(23)-H(23)	120.9
C(24)-C(23)-H(23)	120.9
C(23)-C(24)-C(25)	122.5(8)
C(23)-C(24)-Cl(4)	118.4(7)
C(25)-C(24)-Cl(4)	119.1(7)
C(26)-C(25)-C(24)	118.0(8)
C(26)-C(25)-H(25)	121(4)
C(24)-C(25)-H(25)	120(4)
C(25)-C(26)-C(27)	122.4(9)
C(25)-C(26)-H(26)	118.8
C(27)-C(26)-H(26)	118.8
C(26)-C(27)-C(22)	116.5(8)
C(26)-C(27)-H(27)	120(4)
C(22)-C(27)-H(27)	123(4)
Cl(7)-C(28)-Cl(5)	114.7(5)
Cl(7)-C(28)-Cl(6)	108.5(5)
Cl(5)-C(28)-Cl(6)	106.8(5)
Cl(7)-C(28)-H(28)	108.9
Cl(5)-C(28)-H(28)	108.9
Cl(6)-C(28)-H(28)	108.9

Symmetry transformations used to generate equivalent atoms:

Table 16. Anisotropic displacement parameters (A^2 x 10^3) for **5g**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ti	41(1)	27(1)	45(1)	-1(1)	8(1)	-2(1)
S(1)	44(1)	34(1)	47(1)	0(1)	8(1)	-4(1)
Cl(1)	58(1)	46(1)	43(1)	5(1)	10(1)	-2(1)
Cl(2)	74(1)	33(1)	65(1)	-13(1)	10(1)	-5(1)
Cl(3)	73(1)	39(1)	51(1)	7(1)	9(1)	5(1)
Cl(4)	115(2)	79(2)	110(2)	42(1)	14(2)	33(2)
Cl(5)	163(3)	107(2)	103(2)	-14(2)	29(2)	-55(2)
Cl(6)	372(6)	147(3)	103(2)	14(2)	-2(3)	-110(4)
Cl(7)	173(4)	454(9)	406(7)	243(7)	196(5)	-107(5)
N(1)	42(3)	29(3)	35(3)	1(2)	3(3)	1(3)
O(1)	41(3)	34(3)	58(3)	-5(2)	16(2)	-1(2)
C(1)	45(4)	41(4)	39(4)	2(3)	3(3)	-3(3)
C(2)	40(4)	42(4)	54(4)	4(3)	1(4)	-2(3)
C(3)	49(5)	56(5)	53(4)	6(4)	8(4)	-13(4)
C(4)	54(5)	44(4)	50(4)	0(4)	4(4)	-11(4)
C(5)	49(5)	43(4)	46(4)	1(3)	9(4)	-6(4)
C(6)	41(4)	36(4)	39(4)	2(3)	7(3)	-2(3)
C(7)	44(4)	27(4)	49(4)	-1(3)	5(4)	1(3)
C(8)	41(4)	27(3)	43(4)	2(3)	1(3)	1(3)
C(9)	51(5)	34(4)	48(4)	1(3)	9(4)	-2(3)
C(10)	50(5)	59(5)	68(5)	-19(4)	18(4)	-9(4)
C(11)	72(6)	64(5)	81(6)	-18(5)	43(5)	5(5)
C(12)	45(5)	59(5)	63(5)	1(4)	18(4)	-6(4)
C(13)	35(4)	32(4)	49(4)	1(3)	6(3)	-1(3)
C(14)	49(5)	48(5)	125(7)	-10(5)	42(5)	-4(4)
C(15)	84(7)	65(6)	158(9)	33(6)	39(6)	29(5)
C(16)	106(8)	84(7)	106(7)	-43(6)	35(6)	-4(6)
C(17)	126(8)	68(7)	254(13)	-25(7)	139(9)	-12(6)
C(18)	76(6)	59(5)	110(5)	-6(4)	25(5)	-32(4)
C(22)	28(4)	50(4)	47(4)	1(3)	6(3)	-3(3)
C(23)	47(5)	45(4)	48(4)	-1(3)	3(4)	3(3)
C(24)	62(6)	72(6)	66(6)	15(5)	11(5)	10(5)
C(25)	69(7)	110(9)	58(6)	15(6)	-6(5)	11(6)
C(26)	78(7)	94(7)	65(6)	-13(5)	10(5)	-6(6)
C(27)	62(6)	56(5)	52(5)	-13(5)	2(4)	-7(5)
C(28)	124(8)	101(7)	65(6)	-27(5)	32(6)	-38(6)

Table 17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5g**

	x	y	z	U(eq)
H(3)	6480	3641	962	62
H(7)	2867	4395	2006	49
H(9)	2251	4247	2947	54
H(10)	845	4591	3479	70
H(11)	-778	3874	3102	82
H(12)	1033	2818	2152	66
H(15A)	6342	1447	1892	150
H(15B)	6125	637	1329	150
H(15C)	5176	1086	1605	150
H(16A)	4210	1429	337	145
H(16B)	5144	925	82	145
H(16C)	4822	1939	-178	145
H(17A)	6678	2439	269	201
H(17B)	6991	1424	531	201
H(17C)	7271	2259	1067	201
H(19A)	5581	6125	451	219
H(19B)	6016	5155	275	219
H(19C)	6812	5967	553	219
H(20A)	7772	5747	1748	235
H(20B)	7669	4897	1224	235
H(20C)	7493	4761	2005	235
H(21A)	6458	6624	1790	232
H(21B)	6099	5877	2286	232
H(21C)	5262	6310	1647	232
H(23)	-416	3860	781	57
H(26)	1847	1727	-964	96
H(28)	8876	8406	770	114
H(5)	4140(50)	5170(50)	1610(30)	90(20)
H(25)	2270(50)	3280(40)	-1140(30	70(20)
H(27)	-770(50)	1200(40)	90(30)	50(20)

Table 18. Torsion angles [deg] for **5g**.

O(1)-Ti-S(1)-C(13)	-13.8(5)
N(1)-Ti-S(1)-C(13)	-12.7(2)
Cl(2)-Ti-S(1)-C(13)	166.6(2)
Cl(1)-Ti-S(1)-C(13)	-99.2(2)
Cl(3)-Ti-S(1)-C(13)	74.1(2)
O(1)-Ti-S(1)-C(22)	95.7(5)
N(1)-Ti-S(1)-C(22)	96.8(3)
Cl(2)-Ti-S(1)-C(22)	-83.9(2)
Cl(1)-Ti-S(1)-C(22)	10.4(2)
Cl(3)-Ti-S(1)-C(22)	-176.4(2)
O(1)-Ti-N(1)-C(7)	24.4(4)
Cl(2)-Ti-N(1)-C(7)	-158.9(6)
Cl(1)-Ti-N(1)-C(7)	-68.1(4)
Cl(3)-Ti-N(1)-C(7)	125.4(4)
S(1)-Ti-N(1)-C(7)	-155.3(5)
O(1)-Ti-N(1)-C(8)	-160.0(4)
Cl(2)-Ti-N(1)-C(8)	16.8(10)
Cl(1)-Ti-N(1)-C(8)	107.5(4)
Cl(3)-Ti-N(1)-C(8)	-58.9(4)
S(1)-Ti-N(1)-C(8)	20.3(4)
N(1)-Ti-O(1)-C(1)	-38.0(5)
Cl(2)-Ti-O(1)-C(1)	142.7(5)
Cl(1)-Ti-O(1)-C(1)	47.5(5)
Cl(3)-Ti-O(1)-C(1)	-121.1(5)
S(1)-Ti-O(1)-C(1)	-36.9(8)
Ti-O(1)-C(1)-C(2)	-150.7(5)
Ti-O(1)-C(1)-C(6)	30.3(8)
O(1)-C(1)-C(2)-C(3)	-179.1(5)
C(6)-C(1)-C(2)-C(3)	-0.3(9)
O(1)-C(1)-C(2)-C(14)	0.1(9)
C(6)-C(1)-C(2)-C(14)	178.9(6)
C(1)-C(2)-C(3)-C(4)	1.7(10)
C(14)-C(2)-C(3)-C(4)	-177.5(7)
C(2)-C(3)-C(4)-C(5)	-2.4(10)
C(2)-C(3)-C(4)-C(18)	-179.7(6)
C(3)-C(4)-C(5)-C(6)	1.6(9)
C(18)-C(4)-C(5)-C(6)	178.8(6)
O(1)-C(1)-C(6)-C(5)	178.5(5)
C(2)-C(1)-C(6)-C(5)	-0.3(9)
O(1)-C(1)-C(6)-C(7)	2.7(9)
C(2)-C(1)-C(6)-C(7)	-176.2(6)
C(4)-C(5)-C(6)-C(1)	-0.4(9)
C(4)-C(5)-C(6)-C(7)	175.8(6)

C(8)-N(1)-C(7)-C(6)	173.8(5)
Ti-N(1)-C(7)-C(6)	-10.5(8)
C(1)-C(6)-C(7)-N(1)	-7.6(10)
C(5)-C(6)-C(7)-N(1)	176.4(6)
C(7)-N(1)-C(8)-C(13)	152.1(6)
Ti-N(1)-C(8)-C(13)	-23.6(7)
C(7)-N(1)-C(8)-C(9)	-29.8(8)
Ti-N(1)-C(8)-C(9)	154.5(4)
C(13)-C(8)-C(9)-C(10	-3.9(9)
N(1)-C(8)-C(9)-C(10)	178.0(5)
C(8)-C(9)-C(10)-C(11)	2.6(10)
C(9)-C(10)-C(11)-C(12)	-0.5(11
C(10)-C(11)-C(12)-C(13)	-0.2(11
C(9)-C(8)-C(13)-C(12)	3.3(9)
N(1)-C(8)-C(13)-C(12)	-178.7(5)
C(9)-C(8)-C(13)-S(1)	-169.9(4)
N(1)-C(8)-C(13)-S(1)	8.1(8)
C(11)-C(12)-C(13)-C(8)	-1.2(10
C(11)-C(12)-C(13)-S(1)	172.2(5)
C(22)-S(1)-C(13)-C(8)	-108.8(5)
Ti-S(1)-C(13)-C(8)	7.0(5)
C(22)-S(1)-C(13)-C(12)	77.8(5)
Ti-S(1)-C(13)-C(12)	-166.5(5)
C(3)-C(2)-C(14)-C(17)	-0.5(11)
C(1)-C(2)-C(14)-C(17)	-179.6(7)
C(3)-C(2)-C(14)-C(15)	119.3(7)
C(1)-C(2)-C(14)-C(15)	-59.9(9)
C(3)-C(2)-C(14)-C(16)	-119.9(7)
C(1)-C(2)-C(14)-C(16)	61.0(9)
C(5)-C(4)-C(18)-C(21)	23.1(11)
C(3)-C(4)-C(18)-C(21)	-159.8(8)
C(5)-C(4)-C(18)-C(19)	-106.2(8)
C(3)-C(4)-C(18)-C(19)	70.9(9)
C(5)-C(4)-C(18)-C(20)	140.5(8)
C(3)-C(4)-C(18)-C(20)	-42.3(10
C(13)-S(1)-C(22)-C(23)	15.1(6)
Ti-S(1)-C(22)-C(23)	-89.7(6)
C(13)-S(1)-C(22)-C(27)	-165.9(5)
Ti-S(1)-C(22)-C(27)	89.3(5)
C(27)-C(22)-C(23)-C(24)	-0.5(10
S(1)-C(22)-C(23)-C(24)	178.5(5)
C(22)-C(23)-C(24)-C(25)	0.7(11
C(22)-C(23)-C(24)-Cl(4)	-178.1(5)
C(23)-C(24)-C(25)-C(26)	-0.7(13

Cl(4)-C(24)-C(25)-C(26)	178.1(7)
C(24)-C(25)-C(26)-C(27)	0.3(13
C(25)-C(26)-C(27)-C(22)	-0.1(12
C(23)-C(22)-C(27)-C(26)	0.2(10
S(1)-C(22)-C(27)-C(26)	-178.9(5)

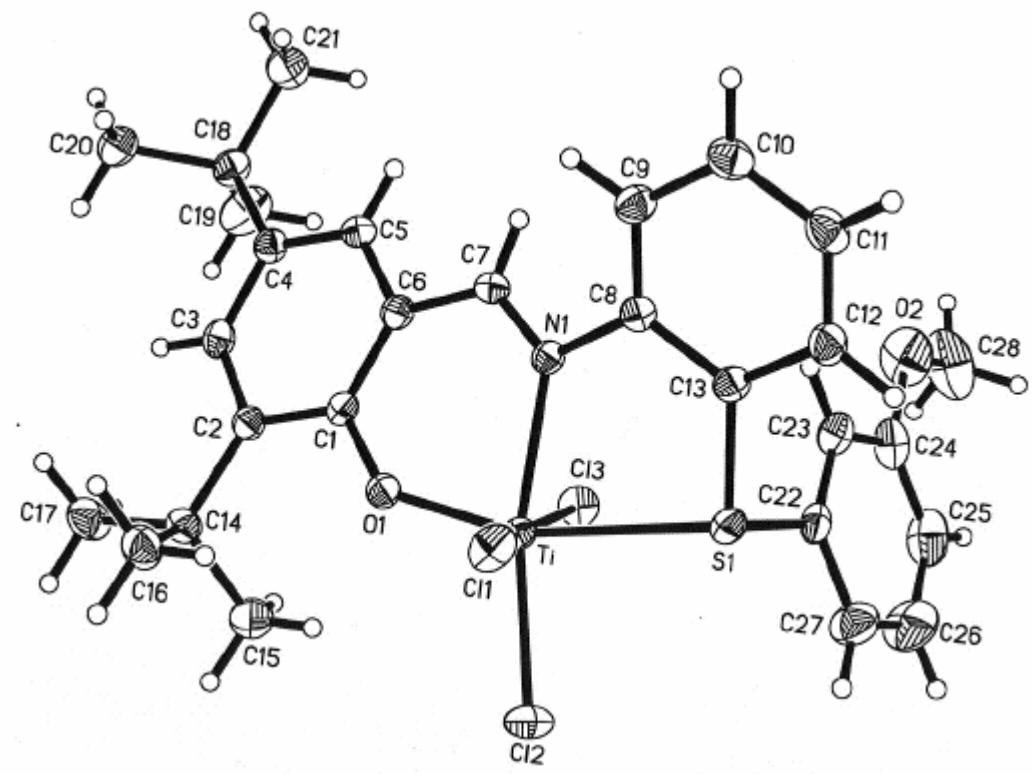


Figure 4. Molecular structure of 5i

Table 19. Crystal data and structure refinement for **5i**.

Identification code	cd2566
Empirical formula	C29 H33 N O2 Cl6 S Ti
Formula weight	720.22
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 14.8394(12) A alpha = 90 deg. b = 13.6848(11) A beta = 111.990(2) deg. c = 17.5778(14) A gamma = 90 deg.
Volume	3309.9(5) A^3
Z, Calculated density	4, 1.445 Mg/m^3
Absorption coefficient	0.834 mm^-1
F(000)	1480
Crystal size	0.345 x 0.317 x 0.127 mm
Theta range for data collection	1.48 to 27.00 deg.
Limiting indices	-18<=h<=18, -17<=k<=17, -19<=l<=22
Reflections collected / unique	19232 / 7211 [R(int) = 0.0662]
Completeness to theta = 27.00	99.7 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.85934
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7211 / 0 / 388
Goodness-of-fit on F^2	0.938
Final R indices [I>2sigma(I)]	R1 = 0.0493, wR2 = 0.1041
R indices (all data)	R1 = 0.0744, wR2 = 0.1214
Largest diff. peak and hole	0.720 and -0.403 e.A^-3

Table 20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5i**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ti	3624(1)	2431(1)	4831(1)	29(1)
S(1)	3794(1)	619(1)	4452(1)	33(1)
Cl(1)	5289(1)	2248(1)	5437(1)	45(1)
Cl(2)	3423(1)	1947(1)	6005(1)	48(1)
Cl(3)	1992(1)	2310(1	4063(1)	41(1)
Cl(4)	776(1)	3748(1)	416(1)	95(1)
Cl(5)	25(1)	1810(1)	198(1)	103(1)
Cl(6)	1324(1)	2435(1	1789(1)	99(1)
N(1)	3822(2)	2549(2)	3676(1)	27(1)
O(1)	3576(1)	3747(1)	4787(1)	34(1)
O(2)	743(2)	-173(2)	1958(2)	82(1)
C(1)	3200(2)	4424(2)	4195(2)	29(1)
C(2)	2932(2)	5345(2)	4392(2)	31(1)
C(3)	2531(2)	5983(2)	3735(2)	36(1)
C(4)	2393(2)	5776(2)	2921(2)	34(1)
C(5)	2695(2)	4875(2)	2764(2)	34(1)
C(6)	3099(2)	4188(2)	3395(2)	30(1)
C(7)	3474(2)	3288(2)	3190(2)	32(1)
C(8)	4273(2)	1784(2)	3388(2)	29(1)
C(9)	4753(2)	1953(2)	2863(2)	37(1)
C(10)	5172(2)	1194(2	2593(2)	44(1)
C(11)	5154(2)	264(2)	2886(2)	44(1)
C(12)	4705(2)	81(2)	3423(2)	39(1)
C(13)	4274(2)	839(2)	3686(2)	31(1)
C(14)	3112(2)	5633(2)	5281(2)	37(1)
C(15)	2557(3)	4946(3)	5649(2)	60(1)
C(16)	4199(2)	5580(2)	5781(2)	51(1)
C(17)	2774(3)	6678(2)	5338(2)	55(1)
C(18)	1903(2)	6533(2)	2251(2)	41(1)
C(19)	840(3)	6654(3)	2169(3)	70(1)
C(20)	2427(3)	7521(2)	2494(2)	53(1)
C(21)	1939(3)	6233(2)	1424(2)	60(1)
C(22)	2656(2)	32(2)	3934(2)	36(1)
C(23)	2123(2)	133(2)	3114(2)	44(1)
C(24)	1216(2)	-300(2)	2779(2)	51(1)
C(25)	863(3)	-834(3)	3269(3)	65(1)
C(26)	1418(3)	-931(3)	4085(3)	77(1)
C(27)	2322(3)	-507(3)	4439(2)	60(1)
C(28)	-228(3)	-510(4)	1586(3)	97(2)
C(29)	1022(3)	2542(3)	725(3)	69(1)

Table 21. Bond lengths [A] and angles [deg] for **5i**

Ti-O(1)	1.8030(18)
Ti-N(1)	2.164(2)
Ti-Cl(2)	2.2901(9)
Ti-Cl(3)	2.2952(9)
Ti-Cl(1)	2.3088(9)
Ti-S(1)	2.6044(9)
S(1)-C(13)	1.770(3)
S(1)-C(22)	1.782(3)
Cl(4)-C(29)	1.733(4)
Cl(5)-C(29)	1.739(4)
Cl(6)-C(29)	1.758(5)
N(1)-C(7)	1.300(3)
N(1)-C(8)	1.433(3)
O(1)-C(1)	1.349(3)
O(2)-C(24)	1.360(4)
O(2)-C(28)	1.418(4)
C(1)-C(6)	1.394(4)
C(1)-C(2)	1.403(4)
C(2)-C(3)	1.391(4)
C(2)-C(14)	1.535(4)
C(3)-C(4)	1.396(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.375(4)
C(4)-C(18)	1.533(4)
C(5)-C(6)	1.406(4)
C(5)-H(5)	0.9300
C(6)-C(7)	1.452(4)
C(7)-H(7)	0.91(3)
C(8)-C(9)	1.379(4)
C(8)-C(13)	1.396(4)
C(9)-C(10)	1.384(4)
C(9)-H(9)	0.9300
C(10)-C(11)	1.377(4)
C(10)-H(10)	0.9300
C(11)-C(12)	1.366(4)
C(11)-H(11)	0.93(3)
C(12)-C(13)	1.385(4)
C(12)-H(12)	0.96(3)
C(14)-C(16)	1.523(4)
C(14)-C(17)	1.531(4)
C(14)-C(15)	1.543(4)
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600

C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-C(21)	1.529(4)
C(18)-C(20)	1.538(4)
C(18)-C(19)	1.539(5)
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-C(23)	1.367(4)
C(22)-C(27)	1.380(4)
C(23)-C(24)	1.385(4)
C(23)-H(23)	0.9300
C(24)-C(25)	1.374(5)
C(25)-C(26)	1.368(6)
C(25)-H(25)	0.92(4)
C(26)-C(27)	1.378(5)
C(26)-H(26)	0.9300
C(27)-H(27)	0.9300
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-H(29)	0.97(3)
O(1)-Ti-N(1)	84.40(8)
O(1)-Ti-Cl(2)	108.12(7)
N(1)-Ti-Cl(2)	167.47(6)
O(1)-Ti-Cl(3)	91.73(7)
N(1)-Ti-Cl(3)	86.39(6)
Cl(2)-Ti-Cl(3)	92.52(3)
O(1)-Ti-Cl(1)	98.43(7)
N(1)-Ti-Cl(1)	86.75(6)
Cl(2)-Ti-Cl(1)	91.82(3)
Cl(3)-Ti-Cl(1)	167.12(4)

O(1)-Ti-S(1)	161.15(7)
N(1)-Ti-S(1)	76.77(6)
Cl(2)-Ti-S(1)	90.72(3)
Cl(3)-Ti-S(1)	87.88(3)
Cl(1)-Ti-S(1)	79.94(3)
C(13)-S(1)-C(22)	105.18(14)
C(13)-S(1)-Ti	97.91(9)
C(22)-S(1)-Ti	113.32(9)
C(7)-N(1)-C(8)	117.4(2)
C(7)-N(1)-Ti	121.00(18)
C(8)-N(1)-Ti	121.48(17)
C(1)-O(1)-Ti	135.85(18)
C(24)-O(2)-C(28)	118.6(4)
O(1)-C(1)-C(6)	118.5(2)
O(1)-C(1)-C(2)	120.0(3)
C(6)-C(1)-C(2)	121.5(3)
C(3)-C(2)-C(1)	115.6(3)
C(3)-C(2)-C(14)	122.8(2)
C(1)-C(2)-C(14)	121.6(3)
C(2)-C(3)-C(4)	125.2(3)
C(2)-C(3)-H(3)	117.4
C(4)-C(3)-H(3)	117.4
C(5)-C(4)-C(3)	117.0(3)
C(5)-C(4)-C(18)	123.2(3)
C(3)-C(4)-C(18)	119.7(2)
C(4)-C(5)-C(6)	121.0(3)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
C(1)-C(6)-C(5)	119.6(2)
C(1)-C(6)-C(7)	122.7(3)
C(5)-C(6)-C(7)	117.4(3)
N(1)-C(7)-C(6)	126.3(3)
N(1)-C(7)-H(7)	115.9(17)
C(6)-C(7)-H(7)	117.8(17)
C(9)-C(8)-C(13)	118.6(2)
C(9)-C(8)-N(1)	122.7(2)
C(13)-C(8)-N(1)	118.6(2)
C(8)-C(9)-C(10)	121.0(3)
C(8)-C(9)-H(9)	119.5
C(10)-C(9)-H(9)	119.5
C(11)-C(10)-C(9)	119.4(3)
C(11)-C(10)-H(10)	120.3
C(9)-C(10)-H(10)	120.3
C(12)-C(11)-C(10)	120.7(3)

C(12)-C(11)-H(11)	120.9(19)
C(10)-C(11)-H(11)	118.1(19)
C(11)-C(12)-C(13)	119.9(3)
C(11)-C(12)-H(12)	122.9(16)
C(13)-C(12)-H(12)	117.2(16)
C(12)-C(13)-C(8)	120.3(3)
C(12)-C(13)-S(1)	119.6(2)
C(8)-C(13)-S(1)	119.9(2)
C(16)-C(14)-C(17)	108.0(3)
C(16)-C(14)-C(2)	108.5(2)
C(17)-C(14)-C(2)	111.7(2)
C(16)-C(14)-C(15)	110.2(3)
C(17)-C(14)-C(15)	107.6(3)
C(2)-C(14)-C(15)	110.8(3)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(21)-C(18)-C(4)	111.9(2)
C(21)-C(18)-C(20)	107.9(3)
C(4)-C(18)-C(20)	109.6(3)
C(21)-C(18)-C(19)	109.8(3)
C(4)-C(18)-C(19)	108.6(3)
C(20)-C(18)-C(19)	109.0(3)
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(23)-C(22)-C(27)	121.8(3)
C(23)-C(22)-S(1)	123.8(2)
C(27)-C(22)-S(1)	114.3(3)
C(22)-C(23)-C(24)	119.4(3)
C(22)-C(23)-H(23)	120.3
C(24)-C(23)-H(23)	120.3
O(2)-C(24)-C(25)	124.6(4)
O(2)-C(24)-C(23)	115.4(3)
C(25)-C(24)-C(23)	120.0(4)
C(26)-C(25)-C(24)	119.2(4)
C(26)-C(25)-H(25)	125(3)
C(24)-C(25)-H(25)	115(3)
C(25)-C(26)-C(27)	122.3(4)
C(25)-C(26)-H(26)	118.9
C(27)-C(26)-H(26)	118.9
C(26)-C(27)-C(22)	117.3(4)
C(26)-C(27)-H(27)	121.4
C(22)-C(27)-H(27)	121.4
O(2)-C(28)-H(28A)	109.5
O(2)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
O(2)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
Cl(4)-C(29)-Cl(5)	110.1(3)
Cl(4)-C(29)-Cl(6)	110.7(2)
Cl(5)-C(29)-Cl(6)	110.3(2)
Cl(4)-C(29)-H(29)	106(2)
Cl(5)-C(29)-H(29)	108(2)
Cl(6)-C(29)-H(29)	112(2)

Symmetry transformations used to generate equivalent atoms:

Table 22. Anisotropic displacement parameters (A^2 x 10^3) for **5i**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ti	32(1)	27(1)	26(1)	4(1)	9(1)	3(1)
S(1)	35(1)	28(1)	34(1)	5(1)	12(1)	2(1)
Cl(1	32(1)	47(1)	48(1)	11(1)	4(1)	-2(1)
Cl(2	55(1)	60(1)	34(1)	11(1)	20(1)	7(1)
Cl(3	31(1)	47(1)	44(1)	2(1)	11(1)	4(1)
Cl(4	90(1)	78(1)	126(1)	4(1)	52(1)	6(1)
Cl(5	73(1)	103(1)	114(1)	-21(1)	14(1)	-22(1)
Cl(6	83(1)	122(1)	81(1)	0(1)	20(1)	-6(1)
N(1)	27(1)	24(1)	30(1)	2(1)	10(1)	3(1)
O(1)	42(1)	27(1)	29(1)	3(1)	9(1)	3(1)
O(2)	56(2)	89(2)	73(2)	-7(2)	-9(2)	-16(2)
C(1)	29(2)	26(1)	31(2)	3(1)	10(1)	-1(1)
C(2)	29(2)	31(1)	33(2)	1(1)	12(1)	-1(1)
C(3)	36(2)	26(1)	45(2)	0(1)	15(1)	4(1)
C(4)	34(2)	30(2)	34(2)	4(1)	10(1)	4(1)
C(5)	39(2)	33(2)	29(2)	3(1)	13(1)	0(1)
C(6)	30(2)	26(1)	33(2)	2(1)	11(1)	3(1)
C(7)	36(2)	32(2)	26(2)	1(1)	12(1)	0(1)
C(8)	27(1)	30(1)	29(2)	1(1)	8(1)	3(1)
C(9)	39(2)	35(2)	38(2)	6(1)	15(1)	3(1)
C(10	42(2)	49(2)	45(2)	-2(2)	23(2)	6(2)
C(11	46(2)	43(2)	44(2)	-3(2)	17(2)	13(2)
C(12	45(2)	31(2)	37(2)	2(1)	12(2)	7(1)
C(13	29(2)	30(1)	32(2)	3(1)	10(1)	3(1)
C(14	43(2)	35(2)	34(2)	-2(1)	17(1)	2(1)
C(15	75(3)	59(2)	58(2)	-4(2)	41(2)	-9(2)
C(16	56(2)	46(2)	39(2)	-3(2)	5(2)	-4(2)
C(17	72(2)	48(2)	49(2)	-5(2)	27(2)	15(2)
C(18	47(2)	32(2)	41(2)	10(1)	11(2)	9(1)
C(19	52(2)	66(2)	83(3)	31(2)	15(2)	20(2)
C(20	72(3)	35(2)	54(2)	10(2)	25(2)	6(2)
C(21	90(3)	41(2)	40(2)	13(2)	14(2)	14(2)
C(22	38(2)	26(1)	47(2)	-3(1)	19(2)	-3(1)
C(23	41(2)	36(2)	52(2)	1(2)	15(2)	-5(1)
C(24	41(2)	41(2)	64(3)	-11(2)	10(2)	1(2)
C(25	44(2)	55(2)	100(4)	-15(2)	29(2)	-16(2)
C(26	69(3)	81(3)	93(4)	6(3)	44(3)	-27(2)
C(27	63(2)	63(2)	57(2)	7(2)	25(2)	-16(2)
C(28	50(2)	102(4)	102(4)	-39(3)	-15(2)	5(2)
C(29	46(2)	76(3)	85(3)	-11(2)	26(2)	-3(2)

Table 23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5i**.

	x	y	z	U(eq)
H(3)	2339	6595	3847	43
H(5)	2630	4717	2231	41
H(9)	4795	2587	2688	44
H(10)	5464	1310	2216	52
H(15A)	2774	4286	5642	89
H(15B)	1873	4986	5330	89
H(15C)	2678	5137	6204	89
H(16A)	4422	4923	5776	76
H(16B)	4324	5775	6336	76
H(16C)	4536	6010	5546	76
H(17A)	2911	6838	5902	82
H(17B)	2088	6727	5031	82
H(17C)	3113	7123	5116	82
H(19A)	503	6044	2001	105
H(19B)	531	7146	1766	105
H(19C)	822	6846	2688	105
H(20A)	2377	7747	2994	80
H(20B)	2132	7989	2066	80
H(20C)	3100	7444	2575	80
H(21A)	2602	6129	1485	90
H(21B)	1661	6741	1030	90
H(21C)	1577	5640	1240	90
H(23)	2368	489	2784	52
H(26)	1177	-1296	4414	92
H(27)	2693	-581	4995	72
H(28A)	-238	-1211	1607	146
H(28B)	-495	-299	1024	146
H(28C)	-610	-247	1874	146
H(7)	3454(19)	3220(19)	2670(18)	33(8)
H(11)	5500(20)	-220(20)	2744(19)	49(9)
H(12)	4668(19)	-560(20)	3632(17)	31(7)
H(25)	260(30)	-1110(30)	3000(30)	102(16)
H(29)	1550(20)	2350(20)	570(20)	55(10)

Table 24. Torsion angles [deg] for **5i.**

O(1)-Ti-S(1)-C(13)	12.9(2)
N(1)-Ti-S(1)-C(13)	15.25(11)
Cl(2)-Ti-S(1)-C(13)	-165.47(9)
Cl(3)-Ti-S(1)-C(13)	102.04(9)
Cl(1)-Ti-S(1)-C(13)	-73.75(9)
O(1)-Ti-S(1)-C(22)	-97.5(2)
N(1)-Ti-S(1)-C(22)	-95.10(13)
Cl(2)-Ti-S(1)-C(22)	84.18(11)
Cl(3)-Ti-S(1)-C(22)	-8.31(11)
Cl(1)-Ti-S(1)-C(22)	175.90(11)
O(1)-Ti-N(1)-C(7)	-27.7(2)
Cl(2)-Ti-N(1)-C(7)	149.7(2)
Cl(3)-Ti-N(1)-C(7)	64.4(2)
Cl(1)-Ti-N(1)-C(7)	-126.5(2)
S(1)-Ti-N(1)-C(7)	153.0(2)
O(1)-Ti-N(1)-C(8)	157.0(2)
Cl(2)-Ti-N(1)-C(8)	-25.5(4)
Cl(3)-Ti-N(1)-C(8)	-110.86(19)
Cl(1)-Ti-N(1)-C(8)	58.23(19)
S(1)-Ti-N(1)-C(8)	-22.20(18)
N(1)-Ti-O(1)-C(1)	38.3(2)
Cl(2)-Ti-O(1)-C(1)	-141.1(2)
Cl(3)-Ti-O(1)-C(1)	-47.9(2)
Cl(1)-Ti-O(1)-C(1)	124.2(2)
S(1)-Ti-O(1)-C(1)	40.6(4)
Ti-O(1)-C(1)-C(6)	-27.6(4)
Ti-O(1)-C(1)-C(2)	153.2(2)
O(1)-C(1)-C(2)-C(3)	-178.6(2)
C(6)-C(1)-C(2)-C(3)	2.3(4)
O(1)-C(1)-C(2)-C(14)	3.7(4)
C(6)-C(1)-C(2)-C(14)	-175.5(3)
C(1)-C(2)-C(3)-C(4)	-0.9(4)
C(14)-C(2)-C(3)-C(4)	176.8(3)
C(2)-C(3)-C(4)-C(5)	-1.1(4)
C(2)-C(3)-C(4)-C(18)	177.5(3)
C(3)-C(4)-C(5)-C(6)	1.6(4)
C(18)-C(4)-C(5)-C(6)	-176.9(3)
O(1)-C(1)-C(6)-C(5)	179.0(2)
C(2)-C(1)-C(6)-C(5)	-1.8(4)
O(1)-C(1)-C(6)-C(7)	-6.7(4)
C(2)-C(1)-C(6)-C(7)	172.5(3)
C(4)-C(5)-C(6)-C(1)	-0.3(4)
C(4)-C(5)-C(6)-C(7)	-174.9(3)

C(8)-N(1)-C(7)-C(6)	-171.9(3)
Ti-N(1)-C(7)-C(6)	12.7(4)
C(1)-C(6)-C(7)-N(1)	9.7(4)
C(5)-C(6)-C(7)-N(1)	-175.9(3)
C(7)-N(1)-C(8)-C(9)	30.9(4)
Ti-N(1)-C(8)-C(9)	-153.7(2)
C(7)-N(1)-C(8)-C(13)	-152.6(3)
Ti-N(1)-C(8)-C(13)	22.8(3)
C(13)-C(8)-C(9)-C(10)	4.2(4)
N(1)-C(8)-C(9)-C(10)	-179.4(3)
C(8)-C(9)-C(10)-C(11)	-3.4(5)
C(9)-C(10)-C(11)-C(12)	1.7(5)
C(10)-C(11)-C(12)-C(13)	-0.9(5)
C(11)-C(12)-C(13)-C(8)	1.7(5)
C(11)-C(12)-C(13)-S(1)	-174.1(2)
C(9)-C(8)-C(13)-C(12)	-3.3(4)
N(1)-C(8)-C(13)-C(12)	-179.9(3)
C(9)-C(8)-C(13)-S(1)	172.5(2)
N(1)-C(8)-C(13)-S(1)	-4.1(4)
C(22)-S(1)-C(13)-C(12)	-78.3(3)
Ti-S(1)-C(13)-C(12)	164.8(2)
C(22)-S(1)-C(13)-C(8)	105.8(2)
Ti-S(1)-C(13)-C(8)	-11.1(2)
C(3)-C(2)-C(14)-C(16)	-117.5(3)
C(1)-C(2)-C(14)-C(16)	60.0(3)
C(3)-C(2)-C(14)-C(17)	1.4(4)
C(1)-C(2)-C(14)-C(17)	178.9(3)
C(3)-C(2)-C(14)-C(15)	121.3(3)
C(1)-C(2)-C(14)-C(15)	-61.1(3)
C(5)-C(4)-C(18)-C(21)	-9.0(4)
C(3)-C(4)-C(18)-C(21)	172.5(3)
C(5)-C(4)-C(18)-C(20)	-128.7(3)
C(3)-C(4)-C(18)-C(20)	52.8(4)
C(5)-C(4)-C(18)-C(19)	112.4(3)
C(3)-C(4)-C(18)-C(19)	-66.2(4)
C(13)-S(1)-C(22)-C(23)	-24.9(3)
Ti-S(1)-C(22)-C(23)	80.9(3)
C(13)-S(1)-C(22)-C(27)	158.1(2)
Ti-S(1)-C(22)-C(27)	-96.1(2)
C(27)-C(22)-C(23)-C(24)	1.2(5)
S(1)-C(22)-C(23)-C(24)	-175.6(2)
C(28)-O(2)-C(24)-C(25)	7.9(5)
C(28)-O(2)-C(24)-C(23)	-173.7(3)
C(22)-C(23)-C(24)-O(2)	-179.2(3)

C(22)-C(23)-C(24)-C(25)	-0.6(5)
O(2)-C(24)-C(25)-C(26)	178.2(4)
C(23)-C(24)-C(25)-C(26)	-0.2(6)
C(24)-C(25)-C(26)-C(27)	0.4(7)
C(25)-C(26)-C(27)-C(22)	0.2(6)
C(23)-C(22)-C(27)-C(26)	-1.0(5)
S(1)-C(22)-C(27)-C(26)	176.1(3)

Symmetry transformations used to generate equivalent atoms:

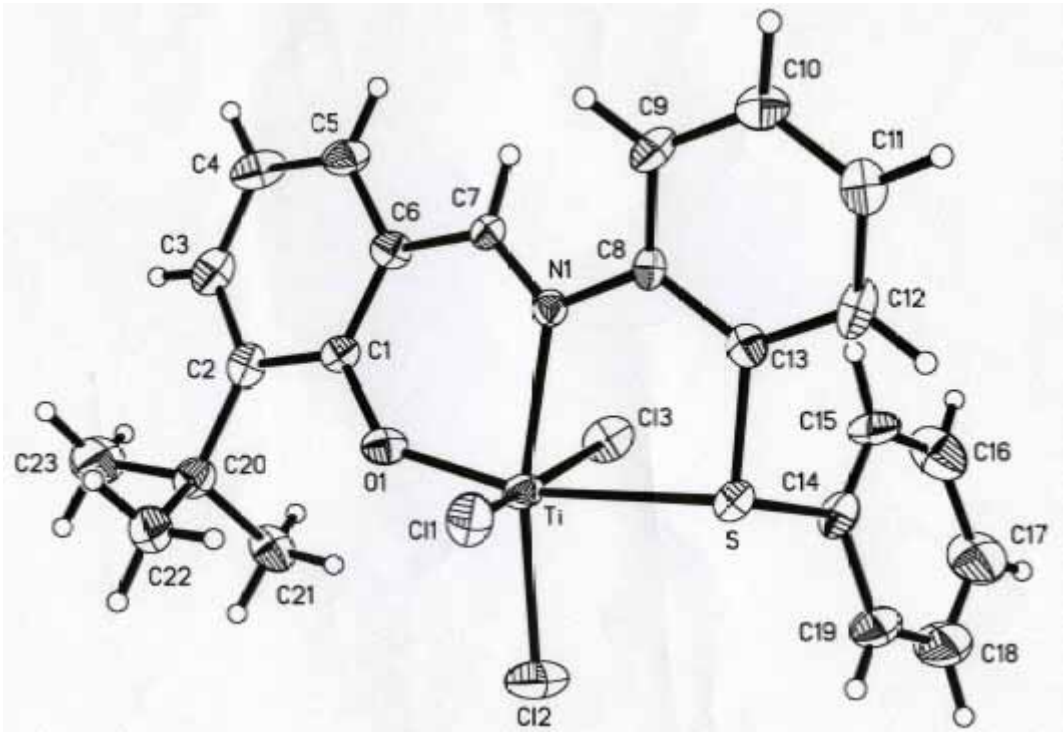


Figure 5. Molecular structure of 5n

Table 25. Crystal data and structure refinement for **5n**.

Identification code	cd23347
Empirical formula	C23 H22 N O S Cl3 Ti
Formula weight	514.73
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 8.758(4) A alpha = 90 deg. b = 11.801(6) A beta = 105.016(8) deg. c = 11.899(6) A gamma = 90 deg.
Volume	1187.8(10) A^3
Z, Calculated density	2, 1.439 Mg/m^3
Absorption coefficient	0.801 mm^-1
F(000)	528
Crystal size	0.499 x 0.424 x 0.287 mm
Theta range for data collection	1.77 to 27.95 deg.
Limiting indices	-10<=h<=11, -14<=k<=13, -8<=l<=13
Reflections collected / unique	2539 / 2227 [R(int) = 0.0978]
Completeness to theta = 27.95	60.1 %
Absorption correction	Sadabs
Max. and min. transmission	1.00000 and 0.32039
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2227 / 1 / 274
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0763, wR2 = 0.1932
R indices (all data)	R1 = 0.0872, wR2 = 0.2025
Absolute structure parameter	0.01(10)
Largest diff. peak and hole	0.858 and -0.720 e.A^-3

Table 26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5n**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ti	8224(2)	8775(2)	3077(2)	36(1)
S	10581(3)	7422(2)	3893(3)	36(1)
Cl(1)	8061(3)	8574(3)	4994(3)	49(1)
Cl(2)	6688(4)	7262(3)	2398(3)	65(1)
Cl(3)	9128(4)	8941(3)	1447(3)	51(1)
N(1)	10118(9)	9964(8)	3814(8)	30(2)
O(1)	6968(8)	10000(7)	2742(7)	39(2)
C(1)	7100(12)	11084(9)	2452(10)	31(3)
C(2)	5740(13)	11689(10)	1831(10)	36(3)
C(3)	6018(14)	12798(11)	1560(12)	47(3)
C(4)	7495(14)	13324(11)	1898(11)	47(3)
C(5)	8772(13)	12729(10)	2508(12)	45(3)
C(6)	8615(11)	11579(10)	2819(11)	34(3)
C(7)	9982(12)	11003(9)	3517(12)	38(3)
C(8)	11612(11)	9588(9)	4554(10)	31(3)
C(9)	12676(13)	10340(10)	5285(11	43(3
C(10)	14142(13)	9948(11)	5883(11	43(3
C(11)	14528(12)	8835(12)	5856(10	43(3
C(12)	13492(13)	8057(11)	5229(10	39(3
C(13)	12019(11)	8448(10)	4580(10	35(3
C(14)	11342(13)	6819(10)	2767(11	41(3
C(15)	12345(13)	7358(12)	2241(13	53(4
C(16)	12707(15)	6846(16)	1306(15	72(5
C(17)	12198(18)	5753(17)	962(17)	83(6)
C(18)	11195(19)	5233(16)	1530(19	88(6
C(19)	10789(15)	5733(12)	2470(15	60(4
C(20)	4112(13)	11116(11)	1498(12	43(3
C(21)	4084(13)	10178(13)	652(12)	53(4)
C(22)	3709(14)	10702(12)	2615(15	60(4
C(23)	2854(15)	12008(15)	890(16)	76(5)

Table 27. Bond lengths [A] and angles [deg] for **5n**

Ti-O(1)	1.798(8)
Ti-N(1)	2.177(8)
Ti-Cl(2)	2.256(4)
Ti-Cl(3)	2.285(4)
Ti-Cl(1)	2.334(4)
Ti-S	2.591(3)
S-C(13)	1.786(11)
S-C(14)	1.792(12)
N(1)-C(7)	1.273(15)
N(1)-C(8)	1.445(13)
O(1)-C(1)	1.337(13)
C(1)-C(6)	1.412(14)
C(1)-C(2)	1.421(14)
C(2)-C(3)	1.384(18)
C(2)-C(20)	1.534(16)
C(3)-C(4)	1.397(17)
C(3)-H(3)	0.9300
C(4)-C(5)	1.360(16)
C(4)-H(4)	0.9300
C(5)-C(6)	1.422(17)
C(5)-H(5)	0.9300
C(6)-C(7)	1.439(15)
C(7)-H(7)	0.9300
C(8)-C(13)	1.390(16)
C(8)-C(9)	1.412(16)
C(9)-C(10)	1.376(16)
C(9)-H(9)	0.9300
C(10)-C(11)	1.360(18)
C(10)-H(10)	0.9300
C(11)-C(12)	1.367(17)
C(11)-H(11)	0.9300
C(12)-C(13)	1.399(14)
C(12)-H(12)	0.9300
C(14)-C(15)	1.361(17)
C(14)-C(19)	1.383(17)
C(15)-C(16)	1.37(2)
C(15)-H(15)	0.9300
C(16)-C(17)	1.39(2)
C(16)-H(16)	0.9300
C(17)-C(18)	1.38(3)
C(17)-H(17)	0.9300
C(18)-C(19)	1.39(2)
C(18)-H(18)	0.9300

C(19)-H(19)	0.9300
C(20)-C(21)	1.49(2)
C(20)-C(22)	1.54(2)
C(20)-C(23)	1.559(19)
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
O(1)-Ti-N(1)	85.9(3)
O(1)-Ti-Cl(2)	106.5(2)
N(1)-Ti-Cl(2)	167.5(3)
O(1)-Ti-Cl(3)	94.0(3)
N(1)-Ti-Cl(3)	83.7(3)
Cl(2)-Ti-Cl(3)	94.00(16)
O(1)-Ti-Cl(1)	96.3(3)
N(1)-Ti-Cl(1)	84.5(3)
Cl(2)-Ti-Cl(1)	95.04(15)
Cl(3)-Ti-Cl(1)	163.82(12)
O(1)-Ti-S	163.9(2)
N(1)-Ti-S	78.3(2)
Cl(2)-Ti-S	89.40(14)
Cl(3)-Ti-S	87.33(13)
Cl(1)-Ti-S	79.38(11)
C(13)-S-C(14)	104.9(5)
C(13)-S-Ti	98.8(4)
C(14)-S-Ti	112.3(4)
C(7)-N(1)-C(8)	118.0(9)
C(7)-N(1)-Ti	120.2(7)
C(8)-N(1)-Ti	121.5(7)
C(1)-O(1)-Ti	137.5(7)
O(1)-C(1)-C(6)	117.0(9)
O(1)-C(1)-C(2)	119.9(9)
C(6)-C(1)-C(2)	123.1(10)
C(3)-C(2)-C(1)	115.0(10)
C(3)-C(2)-C(20)	124.4(10)
C(1)-C(2)-C(20)	120.7(10)
C(2)-C(3)-C(4)	124.0(11)
C(2)-C(3)-H(3)	118.0

C(4)-C(3)-H(3)	118.0
C(5)-C(4)-C(3)	119.8(11)
C(5)-C(4)-H(4)	120.1
C(3)-C(4)-H(4)	120.1
C(4)-C(5)-C(6)	120.6(10)
C(4)-C(5)-H(5)	119.7
C(6)-C(5)-H(5)	119.7
C(1)-C(6)-C(5)	117.5(9)
C(1)-C(6)-C(7)	123.9(10)
C(5)-C(6)-C(7)	118.6(10)
N(1)-C(7)-C(6)	128.2(10)
N(1)-C(7)-H(7)	115.9
C(6)-C(7)-H(7)	115.9
C(13)-C(8)-C(9)	118.0(9)
C(13)-C(8)-N(1)	119.8(10)
C(9)-C(8)-N(1)	122.1(9)
C(10)-C(9)-C(8)	119.1(11)
C(10)-C(9)-H(9)	120.5
C(8)-C(9)-H(9)	120.5
C(11)-C(10)-C(9)	121.1(11)
C(11)-C(10)-H(10	119.4
C(9)-C(10)-H(10)	119.4
C(10)-C(11)-C(12)	121.8(10)
C(10)-C(11)-H(11)	119.1
C(12)-C(11)-H(11)	119.1
C(11)-C(12)-C(13)	117.8(11)
C(11)-C(12)-H(12)	121.1
C(13)-C(12)-H(12)	121.1
C(8)-C(13)-C(12)	121.7(11)
C(8)-C(13)-S	120.0(8)
C(12)-C(13)-S	118.0(10)
C(15)-C(14)-C(19)	122.7(12)
C(15)-C(14)-S	124.6(10)
C(19)-C(14)-S	112.7(10)
C(14)-C(15)-C(16)	118.6(13)
C(14)-C(15)-H(15)	120.7
C(16)-C(15)-H(15)	120.7
C(15)-C(16)-C(17)	121.5(16)
C(15)-C(16)-H(16)	119.2
C(17)-C(16)-H(16)	119.2
C(18)-C(17)-C(16)	117.6(17)
C(18)-C(17)-H(17)	121.2
C(16)-C(17)-H(17)	121.2
C(17)-C(18)-C(19)	122.2(15)

C(17)-C(18)-H(18)	118.9
C(19)-C(18)-H(18)	118.9
C(14)-C(19)-C(18)	117.0(14)
C(14)-C(19)-H(19)	121.5
C(18)-C(19)-H(19)	121.5
C(21)-C(20)-C(2)	110.7(10)
C(21)-C(20)-C(22)	112.3(12)
C(2)-C(20)-C(22)	108.8(10)
C(21)-C(20)-C(23)	107.6(11)
C(2)-C(20)-C(23)	108.6(11)
C(22)-C(20)-C(23)	108.8(11)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(20)-C(23)-H(23A)	109.5
C(20)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(20)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 28. Anisotropic displacement parameters (A^2 x 10^3) for **5n**. The anisotropic displacement factor exponent takes the form:-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ti	38(1)	27(1)	41(1)	5(1)	5(1)	-1(1)
S	46(1)	29(2)	35(2)	0(1)	12(1)	3(1)
Cl(1)	56(2)	48(2)	46(2)	9(2)	21(1)	9(1)
Cl(2)	71(2)	49(2)	65(3)	6(2)	-4(2)	-24(2)
Cl(3)	74(2)	48(2)	29(2)	2(2)	8(1)	-1(1)
N(1)	28(4)	31(6)	30(6)	-5(4)	6(3)	2(3)
O(1)	41(4)	39(5)	31(5)	2(4)	-2(3)	-6(3)
C(1)	42(5)	29(7)	22(7)	6(5)	11(4)	-1(4)
C(2)	48(6)	40(7)	20(7)	7(5)	7(5)	9(5)
C(3)	61(7)	43(8)	30(8)	5(6)	0(6)	13(5)
C(4)	76(8)	32(8)	26(8)	15(5)	-2(6)	-8(5)
C(5)	50(6)	38(8)	41(8)	-5(6)	-2(5)	-8(5)
C(6)	39(5)	33(7)	30(8)	14(5)	8(5)	-1(4)
C(7)	34(5)	24(7)	57(10)	-1(5)	16(5)	1(4)
C(8)	32(5)	33(7)	30(8)	-1(5)	10(4)	9(4)
C(9)	59(7)	27(7)	41(9)	-6(5)	11(6)	4(5)
C(10)	53(6)	49(9)	22(7)	-16(6)	2(5)	-7(5)
C(11)	47(5)	57(9)	25(7)	5(6)	10(5)	9(6)
C(12)	64(7)	43(8)	11(7)	6(5)	14(5)	25(5)
C(13)	36(5)	44(7)	27(8)	-5(5)	10(4)	1(4)
C(14)	57(6)	38(8)	28(8)	-13(5)	15(5)	8(5)
C(15)	61(7)	36(8)	59(10)	-15(7)	12(6)	-19(6)
C(16)	60(8)	106(14	55(12)	-21(10)	25(7)	-14(8)
C(17)	72(10)	94(14	77(15)	-50(11)	9(9)	-18(9)
C(18)	79(10)	60(11	128(18)	-47(11	34(10	-22(8)
C(19)	65(7)	39(8)	76(12)	-21(8)	18(7)	-11(6)
C(20)	54(7)	36(7)	41(9)	9(6)	15(6)	1(5)
C(21)	41(6)	78(10)	35(9)	-11(7)	1(5)	-5(6)
C(22)	46(7)	58(10)	75(12)	-13(8)	16(6)	0(6)
C(23)	55(8)	71(12)	86(14)	-3(9)	-10(8)	-1(7)

Table 29. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5n**.

	x	y	z	U(eq)
H(3)	5170	13218	1125	56
H(4)	7605	14078	1708	57
H(5)	9757	13077	2724	55
H(7)	10881	11447	3785	45
H(9)	12391	11090	5361	51
H(10)	14880	10454	6313	52
H(11)	15524	8595	6276	51
H(12)	13759	7294	5234	46
H(15)	12776	8058	2510	63
H(16)	13306	7239	893	86
H(17)	12521	5385	371	100
H(18)	10778	4526	1275	105
H(19)	10173	5355	2880	72
H(21A)	4386	10466	-13	79
H(21B)	3036	9868	410	79
H(21C)	4811	9596	1017	79
H(22A)	2696	10335	2416	89
H(22B)	3678	11337	3113	89
H(22C)	4501	10176	3014	89
H(23A)	3079	12257	182	114
H(23B)	2888	12644	1398	114
H(23C)	1822	11671	716	114

Table 30. Torsion angles [deg] for **5n**

O(1)-Ti-S-C(13)	-6.3(12)
N(1)-Ti-S-C(13)	4.6(5)
Cl(2)-Ti-S-C(13)	-177.2(4)
Cl(3)-Ti-S-C(13)	88.8(4)
Cl(1)-Ti-S-C(13)	-81.9(4)
O(1)-Ti-S-C(14)	-116.5(11)
N(1)-Ti-S-C(14)	-105.5(5)
Cl(2)-Ti-S-C(14)	72.7(5)
Cl(3)-Ti-S-C(14)	-21.3(5)
Cl(1)-Ti-S-C(14)	167.9(5)
O(1)-Ti-N(1)-C(7)	-20.4(9)
Cl(2)-Ti-N(1)-C(7)	154.2(11)
Cl(3)-Ti-N(1)-C(7)	74.1(9)
Cl(1)-Ti-N(1)-C(7)	-117.1(9)
S-Ti-N(1)-C(7)	162.7(9)
O(1)-Ti-N(1)-C(8)	165.9(9)
Cl(2)-Ti-N(1)-C(8)	-19.5(19)
Cl(3)-Ti-N(1)-C(8)	-99.7(8)
Cl(1)-Ti-N(1)-C(8)	69.2(8)
S-Ti-N(1)-C(8)	-11.1(7)
N(1)-Ti-O(1)-C(1)	32.4(11)
Cl(2)-Ti-O(1)-C(1)	-146.4(11)
Cl(3)-Ti-O(1)-C(1)	-51.0(11)
Cl(1)-Ti-O(1)-C(1)	116.5(11)
S-Ti-O(1)-C(1)	43.2(19)
Ti-O(1)-C(1)-C(6)	-25.7(17)
Ti-O(1)-C(1)-C(2)	155.9(9)
O(1)-C(1)-C(2)-C(3)	-178.9(12)
C(6)-C(1)-C(2)-C(3)	2.9(18)
O(1)-C(1)-C(2)-C(20)	0.6(17)
C(6)-C(1)-C(2)-C(20)	-177.6(11)
C(1)-C(2)-C(3)-C(4)	-2.6(19)
C(20)-C(2)-C(3)-C(4)	177.9(13)
C(2)-C(3)-C(4)-C(5)	2(2)
C(3)-C(4)-C(5)-C(6)	-1(2)
O(1)-C(1)-C(6)-C(5)	179.5(12)
C(2)-C(1)-C(6)-C(5)	-2.2(18)
O(1)-C(1)-C(6)-C(7)	-2.7(17)
C(2)-C(1)-C(6)-C(7)	175.5(12)
C(4)-C(5)-C(6)-C(1)	1.1(19)
C(4)-C(5)-C(6)-C(7)	-176.8(13)
C(8)-N(1)-C(7)-C(6)	-178.2(12)
Ti-N(1)-C(7)-C(6)	7.8(18)

C(1)-C(6)-C(7)-N(1)	8(2)
C(5)-C(6)-C(7)-N(1)	-174.4(13)
C(7)-N(1)-C(8)-C(13)	-158.0(12)
Ti-N(1)-C(8)-C(13)	15.9(14)
C(7)-N(1)-C(8)-C(9)	23.7(16)
Ti-N(1)-C(8)-C(9)	-162.4(10)
C(13)-C(8)-C(9)-C(10)	7.7(18)
N(1)-C(8)-C(9)-C(10)	-173.9(11)
C(8)-C(9)-C(10)-C(11)	-5(2)
C(9)-C(10)-C(11)-C(12)	1(2)
C(10)-C(11)-C(12)-C(13	1.7(18)
C(9)-C(8)-C(13)-C(12)	-5.5(18)
N(1)-C(8)-C(13)-C(12)	176.1(10)
C(9)-C(8)-C(13)-S	168.2(10)
N(1)-C(8)-C(13)-S	-10.2(16)
C(11)-C(12)-C(13)-C(8)	0.8(18)
C(11)-C(12)-C(13)-S	-173.1(10)
C(14)-S-C(13)-C(8)	117.2(10)
Ti-S-C(13)-C(8)	1.2(11)
C(14)-S-C(13)-C(12)	-68.9(10)
Ti-S-C(13)-C(12)	175.1(9)
C(13)-S-C(14)-C(15)	-26.0(13)
Ti-S-C(14)-C(15)	80.2(11)
C(13)-S-C(14)-C(19)	154.6(10)
Ti-S-C(14)-C(19)	-99.2(9)
C(19)-C(14)-C(15)-C(16	6(2)
S-C(14)-C(15)-C(16)	-173.2(10)
C(14)-C(15)-C(16)-C(17	-6(2)
C(15)-C(16)-C(17)-C(18	6(2)
C(16)-C(17)-C(18)-C(19	-5(3)
C(15)-C(14)-C(19)-C(18	-5(2)
S-C(14)-C(19)-C(18)	174.2(13)
C(17)-C(18)-C(19)-C(14	5(3)
C(3)-C(2)-C(20)-C(21)	114.3(15)
C(1)-C(2)-C(20)-C(21)	-65.2(15)
C(3)-C(2)-C(20)-C(22)	-121.9(14)
C(1)-C(2)-C(20)-C(22)	58.6(15)
C(3)-C(2)-C(20)-C(23)	-3.6(18)
C(1)-C(2)-C(20)-C(23)	176.9(12)

Symmetry transformations used to generate equivalent atoms: