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# Selenothiocarbonate complexes of iron: Structure of CpFe(CO)<sub>2</sub>SeC(S)O-4-C<sub>6</sub>H<sub>4</sub>Cl

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#### Abstract

Stable complexes of general formula CpFe(CO)<sub>2</sub>SeC(S)OR, where R = Ph(1a), 4-C<sub>6</sub>H<sub>4</sub>Cl (1b), 4-C<sub>6</sub>H<sub>4</sub>F (1c), C<sub>6</sub>F<sub>5</sub> (1d), 4-C<sub>6</sub>H<sub>4</sub>CH<sub>3</sub> (1e), were prepared by the reaction of ( $\mu$ -Se)[CpFe(CO)<sub>2</sub>]<sub>2</sub> with ROC(S)Cl at room temperature. When a THF solution of 1 was photo-lyzed the chelate complexes CpFe(CO)( $\kappa^2 Se$ , S-SeC(S)OR) (2) were obtained in good yields. All of these complexes have been characterized by elemental analyses, IR and <sup>1</sup>H NMR spectroscopy. The structure of CpFe(CO)<sub>2</sub>SeC(S)O-4-C<sub>6</sub>H<sub>4</sub>Cl (1b) is reported. © 2005 Elsevier Ltd. All rights reserved.

Keywords: Complexes; Iron; Selenium; Selenothiocarbonate; Structure; Chlorothionoformates

#### 1. Introduction

Considerable interest in organometallic complexes containing selenium ligands is promoted by their potential applications in areas such as material science [1–6], catalysis [7–10], electronic industry [11–13], and biochemistry [14–18]. Recently, some of these complexes have been used as precursors for the synthesis of metal selenides which are used in electronic devices [7–13]. Moreover, selenium has been found in a number of proteins and enzymes [14–18]. One class of hydrogenases is known to contain iron, nickel and selenium atoms. The enzyme isolated from *Desulfourbno baculatus* is a representative of this class of enzymes. X-ray absorption spectroscopy and EPR studies of this enzyme indicated that the Ni-atom is bonded to 3–4 nitrogen or oxygen atoms, 1–2 sulfur or chlorine atoms and one selenium atom of a selenocysteine residue [19–22].

Several transition metal polyselenide complexes have been reported in the literature. Insertion of elemental selenium into metal-metal bonds represents a successful route for the synthesis of such complexes. In this context, insertion of elemental selenium into the M–M bonds of the dimers  $[CpM(CO)_2]_2$  gave  $(\mu$ -Se<sub>x</sub>) $[CpM(CO)_2]_2$  (M = Fe, x = 1; M = Ru, x = 5) [23–25]. The Cp-substituted Cr-dimers  $[Cp'Cr(CO)_3]_2$  (Cp' = C<sub>5</sub>H<sub>4</sub>Me, C<sub>5</sub>H<sub>4</sub>COMe, C<sub>5</sub>H<sub>4</sub>CO<sub>2</sub>Me) react with one equivalent of selenium to give the linear complexes ( $\mu$ -Se) $[Cp'Cr(CO)_2]_2$  which contain two Cr–Se triple bonds. These linear complexes react with another equivalent of selenium to give the butterfly complexes ( $\mu$ , $\kappa^2Se$ , Se-Se<sub>2</sub>) $[Cp'Cr(CO)_2]_2$  [26,27]. Tungsten selenides ( $\mu$ -Se<sub>m</sub>)- $[CpW(CO)_3]_2$  (m = 2, 3, 4) have been prepared by the reaction of the anion CpW(CO)<sub>3</sub>Li with elemental selenium followed by oxidation of the resulting inserted products (CpW(CO)<sub>3</sub>Se<sub>n</sub>Li) [28].

Our investigation showed that the iron selenide complex,  $(\mu$ -Se)[CpFe(CO)<sub>2</sub>]<sub>2</sub>, which contains two lone pairs of electrons around the selenium atom, is useful in the syntheses of several iron selenium complexes. Selenocarboxylates (CpFe(CO)<sub>2</sub>SeCOR)[23] and selenosulfonates (CpFe(CO)<sub>2</sub>-SeSO<sub>2</sub>R) [29] have been synthesized by the reaction of this iron selenide with acid- or sulfonyl-chlorides, respectively. Photolytic reactions of the selenocarboxylate complexes with EPh<sub>3</sub> ligands (E = P, As, Sb) gave the CO-substituted products of the general formula CpFe(CO)(EPh<sub>3</sub>)SeCOR [30]. More recently, iron selenocarbonate complexes, CpFe(CO)<sub>2</sub>SeCO<sub>2</sub>R, have also been prepared by treatment

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of  $(\mu$ -Se)[CpFe(CO)<sub>2</sub>]<sub>2</sub> with alkyl or aryl chloroformates [31].

Based on our previous reactions of the iron selenide with electrophiles [29–31] this paper describes its reaction with chlorothionoformates (ROC(S)Cl). This reaction was found to give the expected selenothiocarbonates, CpFe(CO)<sub>2</sub>SeC-(S)OR. These complexes can be converted to the chelated complexes CpFe(CO)( $\kappa^2 Se$ , S-SeC(S)OR) upon photolysis.

#### 2. Experimental

All manipulations were performed under an inert atmosphere of nitrogen using standard Schlenk line techniques. Diethyl ether, hexane and benzene were distilled from sodium/benzophenone ketyl under nitrogen. Dichloromethane was refluxed over  $P_2O_5$  and distilled under nitrogen. The complex ( $\mu$ -Se)[CpFe(CO)<sub>2</sub>]<sub>2</sub> was prepared by literature method [23]. The reagents: chlorothionoformates, iron dimer [CpFe(CO)<sub>2</sub>]<sub>2</sub>, and selenium were obtained from Acros and were used as received.

Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker 200 MHz spectrometer. Chemical shifts are in ppm relative to TMS at 0 ppm. Infrared (IR) spectra were recorded on a Nicolat Nexus FT-IR spectrometer using NaCl solvent cells. Elemental analyses were done in Laboratoire d'Analyse Elémentaire, Université de Montréal, Montréal, Que., Canada. Melting points were reported on a Staurt Melting point apparatus (SMP3) and are uncorrected. The photolytic reactions were carried out in a medium pressure mercury lamp (150 W) with a quartz immersion cell.

# 2.1. General procedure for the preparation of $CpFe(CO)_2SeC(S)OR(1)$

The complex ( $\mu$ -Se)[CpFe(CO)<sub>2</sub>]<sub>2</sub> (0.22 g, 0.50 mmol) dissolved in diethyl ether (70 mL) was stirred under N<sub>2</sub> and chlorothionoformate (0.55 mmol) was added. After stirring overnight, the volatiles were removed under reduced pressure and the resulting solid was redissolved in a minimum amount of CH<sub>2</sub>Cl<sub>2</sub> and introduced to a silica gel column made up in hexane. Elution with hexane removes the unreacted chlorothionoformates. Elution with hexane/dichloromethane solution (1:1 v:v ratio) gave a red-brown band which was collected and identified as CpFe(CO)<sub>2</sub>SeC(S)OR, followed by a red band which was also collected and identified as CpFe(CO)<sub>2</sub>Cl. The CpFe(CO)<sub>2</sub>SeC(S)OR were recrystallized from dichloromethane/hexane.

# 2.1.1. $[CpFe(CO)_2SeC(S)OC_6H_5]$ (1a)

Yield: 72%. m.p. 159–160 °C. <sup>1</sup>H NMR (CDCl<sub>3</sub>)  $\delta$  4.95 (s, 5H, C<sub>5</sub>H<sub>5</sub>); 7.41 (m, 5H, C<sub>6</sub>H<sub>5</sub>). IR (CH<sub>2</sub>Cl<sub>2</sub>, cm<sup>-1</sup>)  $\nu_{CO}$  2035s, 1985s. Calc. for C<sub>14</sub>H<sub>10</sub>FeO<sub>3</sub>SSe: C, 42.78; H, 2.56; S, 8.16. Found: C, 42.70; H, 2.44; S, 7.88%.

# 2.1.2. $[CpFe(CO)_2SeC(S)O-4-C_6H_4Cl]$ (1b)

Yield: 82%. m.p. 99–100 °C. <sup>1</sup>H NMR (CDCl<sub>3</sub>)  $\delta$  5.06 (s, 5H, C<sub>5</sub>H<sub>5</sub>); 7.02 (d, 2H, C<sub>6</sub>H<sub>4</sub>); 7.37 (d, 2H, C<sub>6</sub>H<sub>4</sub>). IR

 $(CH_2Cl_2, cm^{-1}) v_{CO}$  2037s, 1992s. Calc. for  $C_{14}H_9ClFeO_3$  SSe: C, 39.33; H, 2.12; S, 7.50. Found: C, 39.02; H, 1.96; S, 7.00%.

#### 2.1.3. $[CpFe(CO)_2SeC(S)O-4-C_6H_4F]$ (1c)

Yield: 80%. m.p. 136–137 °C. <sup>1</sup>H NMR (CDCl<sub>3</sub>)  $\delta$  5.06 (s, 5H, C<sub>5</sub>H<sub>5</sub>); 7.06 (d, 2H, C<sub>6</sub>H<sub>4</sub>); 7.20 (d, 2H, C<sub>6</sub>H<sub>4</sub>). IR (CH<sub>2</sub>Cl<sub>2</sub>, cm<sup>-1</sup>)  $\nu_{CO}$  2036s, 1991s. Calc. for C<sub>14</sub>H<sub>9</sub>FFeO<sub>3</sub> SSe: C, 40.90; H, 2.21; S, 7.80. Found: C, 39.98; H, 2.18; S, 7.11%.

#### 2.1.4. $[CpFe(CO)_2SeC(S)OC_6F_5]$ (1d)

Yield: 87%. m.p. 133–134 °C. <sup>1</sup>H NMR (CDCl<sub>3</sub>)  $\delta$  5.08 (s, H's, C<sub>5</sub>H<sub>5</sub>). IR (CH<sub>2</sub>Cl<sub>2</sub>, cm<sup>-1</sup>)  $v_{CO}$  2041s, 1997s. Calc. for C<sub>14</sub>H<sub>5</sub>F<sub>5</sub>FeO<sub>3</sub>SSe: C, 34.81; H, 1.04; S 6.64. Found: C, 34.34; H, 1.08; S, 5.98%.

# 2.1.5. $[CpFe(CO)_2SeC(S)O-4-C_6H_4Me]$ (1e)

Yield: 89%. m.p. 148–149 °C. <sup>1</sup>H NMR (CDCl<sub>3</sub>)  $\delta$  2.33 (s, 3H, CH<sub>3</sub>); 5.03 (s, 5H, C<sub>5</sub>H<sub>5</sub>); 6.93 (d, 2H, C<sub>6</sub>H<sub>4</sub>); 7.22 (d, 2H, C<sub>6</sub>H<sub>4</sub>). IR (CH<sub>2</sub>Cl<sub>2</sub>, cm<sup>-1</sup>)  $\nu$ <sub>CO</sub> 2036s, 1991s. Calc. for C<sub>15</sub>H<sub>12</sub>FeO<sub>3</sub>SSe: C, 44.25; H, 2.97; S, 7.88. Found: C, 44.46; H, 2.77; S, 7.50%.

# 2.2. General procedure for the preparation of $CpFe(CO)(\kappa^2Se,S-SeC(S)OR)$ (2)

A THF solution (30 mL) of CpFe(CO)<sub>2</sub>SeC(S)OR (0.25 mmol) was irradiated under a stream of N<sub>2</sub> for 30 min. The volatiles were removed by vacuum and the resulting solid was dissolved in a minimum amount of dichloromethane and transferred to a silica gel column. The column was eluted with CH<sub>2</sub>Cl<sub>2</sub>/hexane (1:2 v:v ratio) to separate the products as an orange-brown band which were recrystallized from hexane.

# 2.2.1. $[CpFe(CO)(\kappa^2 Se, S-SeC(S)OC_6H_5)]$ (2a)

Yield: 85%. m.p. 102–103 °C. <sup>1</sup>H NMR (CDCl<sub>3</sub>)  $\delta$  4.65 (s, 5H, C<sub>5</sub>H<sub>5</sub>); 7.10 (m, 5H, C<sub>6</sub>H<sub>5</sub>). IR (CH<sub>2</sub>Cl<sub>2</sub>, cm<sup>-1</sup>)  $\nu_{CO}$  1954s. Calc. for C<sub>13</sub>H<sub>10</sub>FeO<sub>2</sub>SSe: C, 42.77; H, 2.76; S 8.78. Found: C, 42.54; H, 2.66; S, 8.47%.

# 2.2.2. $[CpFe(CO)(\kappa^2 Se, S-SeC(S)O-4-C_6H_4Cl)]$ (2b)

Yield: 90%. m.p. 79–80 °C. <sup>1</sup>H NMR (CDCl<sub>3</sub>)  $\delta$  4.65 (s, 5H, C<sub>5</sub>H<sub>5</sub>); 7.07 (d, 2H, C<sub>6</sub>H<sub>4</sub>); 7.35 (d, 2H, C<sub>6</sub>H<sub>4</sub>). IR (CH<sub>2</sub>Cl<sub>2</sub>, cm<sup>-1</sup>)  $\nu$ <sub>CO</sub> 1947s. Calc. for C<sub>13</sub>H<sub>9</sub>ClFeO<sub>2</sub>SSe: C, 39.08; H, 2.27; S, 8.03. Found: C, 39.60; H, 2.47; S, 7.38%.

#### 2.2.3. $[CpFe(CO)(\kappa^2 Se, S-SeC(S)O-4-C_6H_4F)]$ (2c)

Yield: 78%. m.p. 95–96 °C. <sup>1</sup>H NMR (CDCl<sub>3</sub>)  $\delta$  4.65 (s, 5H, C<sub>5</sub>H<sub>5</sub>); 7.11 (d, 2H, C<sub>6</sub>H<sub>4</sub>); 7.25 (d, 2H, C<sub>6</sub>H<sub>4</sub>). IR (CH<sub>2</sub>Cl<sub>2</sub>, cm<sup>-1</sup>)  $\nu$ <sub>CO</sub> 1952s. Calc. for C<sub>13</sub>H<sub>9</sub>FFeO<sub>2</sub>SSe: C, 40.77; H, 2.37; S, 8.37. Found: C, 40.34; H, 2.09; S, 7.95%.

#### 2.2.4. $[CpFe(CO)(\kappa^2Se, S-SeC(S)OC_6F_5)]$ (2d)

Yield: 65%. m.p. 72–73 °C. <sup>1</sup>H NMR (CDCl<sub>3</sub>)  $\delta$  4.69 (s, H's, C<sub>5</sub>H<sub>5</sub>). IR (CH<sub>2</sub>Cl<sub>2</sub>, cm<sup>-1</sup>)  $v_{CO}$  1959s. Calc. for

Table 1

Selected crystal data and refinement parameters for  $\mbox{CpFe}(\mbox{CO})_2 \mbox{SeC}(\mbox{S}) \mbox{O-4-C}_6 \mbox{H}_4 \mbox{Cl}~(\mbox{1b})$ 

Empirical formula	C14H9ClFeO2SSe	
Formula weight	427.53	
Crystal size (mm)	$0.13 \times 0.10 \times 0.08$	
Crystal system	monoclinic	
Space group	$P2_{1}/c$	
Unit cell dimensions		
a (Å)	6.9410(10)	
$b(\mathbf{A})$	13.4830(10)	
c (Å)	16.5320(10)	
α (°)	90.00	
β(°)	98.27(5)	
γ (°)	90.00	
$V(\dot{A}^3)$	1531.1(3)	
Z	4	
Index ranges	-9 < h < 9, 0 < k < 18, 0 < l < 23	
$D_{\rm calc} ({\rm Mg}{\rm m}^{-3})$	1.855	
Radiation type	Μο Κα	
$\mu (\mathrm{mm}^{-1})$	3.677	
$\lambda$ (Å)	0.71069	
$\theta$ Range (°)	1.96-30.04	
$R[F^2 \ge 2\sigma(F^2)]$	0.0621	
$wR(F^2)^{a}$	0.036	
3 + (5)(-2) + (2)(-2)(-2)(-2)(-2)(-2)(-2)(-2)(-2)(-2)(		

<sup>a</sup>  $w = 1/[\sigma^2(F_o^2) + (0.0426P)^2]$ , where  $P = (F_o^2 + 2F_o^2)/3$ .

C<sub>13</sub>H<sub>5</sub>F<sub>5</sub>FeO<sub>2</sub>SSe: C, 34.32; H, 1.11; S, 7.05. Found: C, 33.71; H, 1.00; S 6.77%.

# 2.2.5. $[CpFe(CO)(\kappa^2 Se, S-SeC(S)O-4-C_6H_4Me)]$ (2e)

Yield: 92%. m.p. 88–89 °C. <sup>1</sup>H NMR (CDCl<sub>3</sub>)  $\delta$  2.36 (s, 3H, CH<sub>3</sub>); 4.66 (s, 5H, C<sub>5</sub>H<sub>5</sub>); 7.02 (d, 2H, C<sub>6</sub>H<sub>4</sub>); 7.20 (d, 2H, C<sub>6</sub>H<sub>4</sub>). IR (CH<sub>2</sub>Cl<sub>2</sub>, cm<sup>-1</sup>)  $v_{CO}$  1950s. Calc. for C<sub>14</sub>H<sub>12</sub>FeO<sub>2</sub>SSe: C, 44.35; H, 3.19; S, 8.46. Found: C, 44.85; H, 3.07; S, 8.46%.

#### 2.3. X-ray structure analysis

Single crystal of **1b** was obtained from CH<sub>2</sub>Cl<sub>2</sub>/hexane mixture. Intensity data were collected on a KappaCCD dif-

fractometer with graphite monochromated Mo K $\alpha$  radiation at 173 K. The crystallographic data are shown in Table 1. The cell parameters were determined from 5095 reflections collected in the range  $1.96 \le \theta \le 30.04^\circ$ . There were 4473 independent reflections with 3717 observed reflections (>2 $\sigma(I)$ ). The structure was solved by direct method using SHELXS-97 [32] and DIFMAP synthesis using SHELXTL-96 [33].

#### 3. Results and discussion

#### 3.1. Synthesis and characterization of 1

The selenothiocarbonate complexes  $CpFe(CO)_2SeC$ (S)OR [R = Ph (1a), 4-C<sub>6</sub>H<sub>4</sub>Cl (1b), 4-C<sub>6</sub>H<sub>4</sub>F (1c), C<sub>6</sub>F<sub>5</sub> (1d), 4-C<sub>6</sub>H<sub>4</sub>Me (1e)] were readily synthesized by stirring a diethylether solution of chlorothionoformates and ( $\mu$ -Se)[CpFe(CO)<sub>2</sub>]<sub>2</sub> (Scheme 1) at room temperature.

To the best of my knowledge, complexes 1 are the first selenothiocarbonate of iron to be reported. The analogues ethyl-dithiocarbonate complexes, Cp'Fe(CO)<sub>2</sub>SC(S)OEt  $(Cp' = C_5H_5, C_5Me_5)$  are reported by the reaction of  $[Cp'Fe(CO)_2]_2$  and  $[EtOC(S)S]_2$ . Substitution reactions of these dicarbonyl complexes with phosphine or phosphite ligands gave Cp'Fe(CO)(L)SC(S)OEt (L = PPh<sub>3</sub>, PBu<sub>3</sub>,  $P(OEt)_3$ ,  $P(OPh)_3$  [34,35]. Complexes 1 are air stable as solids and in solutions. They are soluble in most common organic solvents such as THF, CH<sub>2</sub>Cl<sub>2</sub> but sparingly soluble in hydrocarbons. These complexes were isolated as redbrown solids and characterized by elemental analysis, IR and <sup>1</sup>H NMR spectroscopy. The solution IR spectra of 1 (in CH<sub>2</sub>Cl<sub>2</sub>) exhibited two strong absorbances in the carbonyl region at 2035–2041 and 1985–1997  $\text{cm}^{-1}$ . These  $v_{CO}$  stretches are comparable to those of CpFe(CO)<sub>2</sub>-SeSO<sub>2</sub>R (2038–2043 and 1993–1999 cm<sup>-1</sup>) [29] and of CpFe- $(CO)_2SeCO_2R$  (2036–2043 and 1988–1993 cm<sup>-1</sup>) [31] but higher than those of selenocarboxylates, CpFe(CO)<sub>2</sub>SeCOR



R= Ph (a), 4-C<sub>6</sub>H<sub>4</sub>Cl (b), 4-C<sub>6</sub>H<sub>4</sub>F (c), C<sub>6</sub>F<sub>5</sub> (d), 4-C<sub>6</sub>H<sub>4</sub>Me (e)

 $(2030-2035 \text{ and } 1965-1973 \text{ cm}^{-1})$  [23]. These results show that the ligands: selenosulfonates, selenocarbonates and selenothiocarbonates are of comparable basicity, and they all have higher basicity than the selenocarbxylate ligands.

The <sup>1</sup>H NMR spectra for complexes **1** are in accordance with their formulation. Their spectra display a singlet in the range 4.95–5.08 ppm for their cyclopentadienyl ring protons. This peak falls within the same range observed for selenocarbonates CpFe(CO)<sub>2</sub>SeCO<sub>2</sub>R (4.98–5.09 ppm) [12]. However, this peak is lower than that observed for selenosulfonate, CpFe(CO)<sub>2</sub>SeSO<sub>2</sub>R (5.19–5.24 ppm) [29] and of selenocarboxylate complexes, CpFe(CO)<sub>2</sub>SeCOR (5.08–5.11 ppm) [23]. The resonances for the protons of the R-groups are observed in the expected values and multiplicity.

#### 3.2. Synthesis and characterization of 2

Photolytic reaction of a THF solution of complexes 1 in the absence of added ligand leads to the generation of the chelate complexes CpFe(CO)( $\kappa^2 Se, S$ -SeC(S)OR) (2). The selenocarbonate ligands in 2 are bonded to the metal through both the sulfur and the selenium atoms. These dark red complexes are soluble in most organic solvents including hydrocarbons. Solutions of 2 are quite air sensitive even under inert atmosphere. Upon exposure to air, they decompose within few minutes.

Complexes 2 are characterised by IR, <sup>1</sup>H NMR spectroscopy as well as elemental analysis. The IR spectra of 2 show the characteristic  $v_{CO}$  absorption in the range 1947–1959 cm<sup>-1</sup>. This absorption is similar to those of CpFe(CO)(EPh<sub>3</sub>)SeCOR (1941–1957 cm<sup>-1</sup>) and are lower than those of the starting complexes 1. These differences might be attributed to the weak  $\pi$ -acid character of the chelate selenothiocarbonate ligand compared to that of carbonyl ligand. The <sup>1</sup>H NMR spectra of 2 show the Cppeak in the range 4.65–4.69 ppm. This peak is lower than that of the corresponding Cp-peak of complexes 1 and

within the same range observed for CpFe(CO)(EPh<sub>3</sub>)-SeCOR (4.61–4.77 ppm).

# 3.3. Crystal structure

The structure of  $CpFe(CO)_2SeC(S)O-4-C_6H_4Cl$  (1b) was determined crystallographically and is shown in Fig. 1. The relevant bond parameters are listed in Table 2. The complex adopts the geometry of a three-legged pianostool, with Cp as the base and the two carbonyls and the Se-coordinated selenothiocarbonate ligand as the legs. The Cp ligand is bound to the metal in an  $\eta^5$ -fashion with Fe–C bond distances ranging between 2.081(3) and 2.112(3) Å. The Fe-C bond distances (of carbonyl ligands) of 1.785(3) and 1.769(3) Å are in normal range for CpFe(CO)<sub>2</sub>X complexes. The Fe-Se bond length of 2.3958(5) Å is close to the range of Fe-Se bond lengths found in related iron complexes such as CpFe(CO)<sub>2</sub>SeSO<sub>2</sub>C<sub>6</sub>H<sub>5</sub> [29] and CpFe(CO)<sub>2</sub>-SeCO<sub>2</sub>C<sub>2</sub>H<sub>5</sub> [30]. The C=S bond distance of 1.633(3) Å is similar to that observed for  $(PPh_3)_2Pt(CS_3)$  and (dppe)PtCS<sub>3</sub> [36].

Table 2 Selected bond length  $(\mathring{A})$  and angles (°) of

Selected bond length (Å) and angles (°) of  $CpFe(CO)_2SeC(S)O-4-C_6H_4Cl$  (1b)

Fe–Se	2.3985(2)	C8–Se–Fe	107.80(7)
Fe-C1	1.785(3)	C1–Fe–Se	88.51(9)
Fe–C2	1.769(3)	C2–Fe–Se	90.10(9)
Fe-C3	2.081(3)	C2-Fe-C1	95.12(13)
Fe–C4	2.098(3)	C8–O3–C9	119.71(19)
Fe-C5	2.112(3)	O3–C8–S	124.98(19)
Fe–C6	2.100(3)	O3–C8–Se	112.99(17)
Fe–C7	2.083(3)	S1–C8–Se	122.03(14)
Se–C8	1.881(2)		
S1–C8	1.633(3)		
C101	1.131(3)		
C2–O2	1.145(3)		
C8–O3	1.351(3)		



Fig. 1. ORTEP drawing of CpFe(CO)<sub>2</sub>SeC(S)O-4-C<sub>6</sub>H<sub>4</sub>Cl (1b).

#### 4. Supplementary materials

Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC No. 277847 for compound **1b**. Copies of this information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK (fax: +44 1233 336 033; e-mail: deposit@ccdc. cam.ac.uk or www:http://www.ccdc.cam.ac.uk).

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