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Isolation of $[CpCr(CO)_3]_2(\mu\text{-}SnCl_2)$ and $CpCrCl_2(THF)$ from the insertion-displacement of Se in $Cp_2Cr_2(CO)_4Se$ with $SnCl_2$. Crystal structure of $CpCrCl_2(CH_3CN)$ ($Cp = \eta^5\text{-}C_5H_5$)

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Abstract

The reaction of $Cp_2Cr_2(CO)_4Se$ with $SnCl_2$ in tetrahydrofuran results in the formation of $Cp_2Cr_2(CO)_6SnCl_2$ and $CpCrCl_2(THF)$ as the main stable products. The latter recrystallises from CH_3CN as $CpCrCl_2(CH_3CN)$ in the monoclinic, space group $P2_1/a$, a 12.868(6), b 5.863(2), c 12.875(5) Å, β 102.97(3)°, $Z = 4$, $R = 0.033$ (637 F).

Introduction

The insertion of divalent $M'X_2$ halides of group 4 into the metal–metal bonds of transition metal carbonyl complexes has been shown to provide a facile synthesis for complexes of the type $X_2M'(ML_n)_2$ [1]. In particular, $SnCl_2$ has inserted into the M–M bonds of numerous dimer species, e.g. $[CpFe(CO)_2]_2$ [2], $[Fe(\pi\text{-dienyl})(CO)_2]_2$ [3], $[Co(CO)_4]_2$ [4], $[Co(CO)_3P(C_6H_5)_3]_2$ [4], $[Co(CO)_3(PBu_3)]_2$ [5], $[CpNi(CO)]_2$ [4], $[CpM(CO)_3]_2$ (M = Cr, Mo, W [6,7]), $[Mn(CO)_5]_2$ [8], $[M(CO)_4P(C_6H_5)_3]_2$ (M = Mn, Re) [9] and lately the cluster $Os_3(\mu\text{-}CH_2)(CO)_{11}$ [10]. This study examines the reactivity of $SnCl_2$ towards $[CpCr(CO)_2]_2Se$ (1), the Cr≡Se bond of which has been found to undergo insertion reactions, as demonstrated in the insertion of a S atom [11], a Se atom [12], CR_2 groups from diazoalkanes [13] and a $Fe(CO)_3$ fragment from $Fe_2(CO)_9$ [14].

Experimental

All manipulations were performed using conventional Schlenk line techniques under nitrogen or in a Vacuum Atmospheres Dri-Box equipped with a Model

HE493 Dri-Train, under argon. IR spectra were measured on a Perkin Elmer 1330 spectrometer. NMR spectra were measured on a JEOL FX100 100 MHz spectrometer and referenced to residual C_6H_6 in C_6D_6. Mass spectra were measured on a Kratos AEI MS 3074. Chemical Analyses were performed by the Analytical Unit of the Research School of Chemistry, Australian National University.

$SnCl_2$ was obtained from Fluka Chemicals Ltd. $Cp_2Cr_2(CO)_6$ was synthesised from $Cr(CO)_6$ (Aldrich) as previously described [15]. All solvents were distilled from sodium/benzophenone prior to use.

Reaction with $SnCl_2$

(a) At 65 °C. To a filtered dark orange brown solution of $Cp_2Cr_2(CO)_4Se$ [16], prepared in situ from the reaction of $[CpCr(CO)_3]_2$ (400 mg, 1 mmol) and Se_8 (80 mg, 1 mmol) in THF (15 cm^3) was added a solution of $SnCl_2$ (379.2 mg, 2 mmol) in THF (10 cm^3) and the mixture was refluxed for 8 h. The resultant yellowish-brown suspension was filtered to remove 90 mg (12% yield based on Cr analysis) of a fine black pyrophoric CpCr carbonyl-containing solid, which analysed also for a high content of Se and $SnCl_2$. Highly insoluble in most solvents, it was not amenable to purification. Its mass spectrum shows only the fragmentation pattern of $Cp_4Cr_4Se_4$ [17].

The filtrate was concentrated to ca. 2 cm^3 and cooled at -30 °C for 1.5 h. A royal blue fluffy crystalline solid of $CpCrCl_2(THF)$ (**2**) was thrown down (87 mg, 0.32 mmol, 16% yield). Recrystallisation in THF–ether gave fine feather-like blue needles (60 mg). Analysis. Found: C, 38.30; H, 5.02; Cl, 25.59; Cr, 18.63%. $[(C_5H_5)CrCl_2(C_4H_8O)H_2O]$ calc.: C, 38.87; H, 5.44; Cl, 25.49; Cr, 18.70%. IR: ν 3520m, 3401m, 3300wbr, 3080m, 1600wbr, 1430s, 1013s, 866s, 845msh, 825s, 725w cm^{-1} (Nujol). ^1H NMR ($CDCl_3$): δ (Cp) 11.2 ($\nu_{1/2}$ ca. 200 Hz) and δ(THF) 3.77 and 1.86.

The mother liquor and washings were concentrated to ca. 4 cm^3 in THF and the concentrate loaded on a column (2.2 × 10 cm) of Merck Kieselgel. Three fractions were obtained: I, a dark orange brown eluate in n-hexane (55 cm^3); II, a muddy green eluate in 1 : 9 toluene–ether (30 cm^3); and III, a blue green eluate in CH_3CN (30 cm^3).

Fraction I gave brown solids of impure $Cp_2Cr_2(CO)_6SnCl_2$ (**3**) (232 mg, 0.39 mmole, 39%) which on dissolution in toluene and re-elution through a silica gel column (1.4 × 7 cm) with toluene–ether gave a clear golden orange solution which yielded orange solids (174 mg). A subsequent recrystallisation in toluene–ether or THF–ether gave lustrous polyhedral orange crystals of **3** (100 mg, 0.17 mmol, 17% yield), m.p. 193–194 °C. IR: ν(CO) 2010vs, 1983vs, 1940vs, 1900ssh cm^{-1} (THF) or 2010vs, 1987vs, 1940vs, 1920vs, 1895vs cm^{-1} (Nujol) (reported ν(CO) 2018vs, 1994vs, 1956vs, 1939s, 1911m cm^{-1} (CS_2) [6] and other bands at 3098w, 1420m, 1115vw, 1068w, 1020wsh, 1012w, 915vw, 880w, 860m, 720wbr, 646s, 620s, 605s, 598s, 550s, 508m, 472w, 432vw cm^{-1} (Nujol). NMR (C_6D_6): ^1H, δ(Cp) 4.42; ^{13}C, δ(Cp) 89.43 and δ(CO) 233.89, 239.25. Analysis. Found: C, 33.46; H, 1.58; Cr, 16.87; Cl, 11.19. $(C_5H_5)_2Cr_2(CO)_6SnCl_2$ calc.: C, 32.47; H, 1.70; Cr, 17.57; Cl, 11.98%. MS. *m/e* (for ^{120}Sn and ^{35}Cl): 592 $Cp_2Cr_2(CO)_6SnCl_2$, 557 $Cp_2Cr_2(CO)_6SnCl$, 508 $Cp_2Cr_2(CO)_3SnCl_2$, 473 $Cp_2Cr_2(CO)_3SnCl$, 424 $Cp_2Cr_2SnCl_2$, 389 Cp_2Cr_2SnCl, 318 $Cp_2Cr_2(CO)_3$, 307 $CpCrSnCl_2$, 290 $Cp_2Cr_2(CO)_2$, 262 $Cp_2Cr_2(CO)$, 234 Cp_2Cr_2, 220 CpSnCl, 201 $CpCr(CO)_3$, 190 $SnCl_2$, 188 $CpCrCl_2$, 185 CpSn, 182

Cp_2Cr, 173 $CpCr(CO)_2$, 155 SnCl, 152 CpCrCl, 145 CpCr(CO), 120 Sn and 117 CpCr.

Fraction II gave a mixture of green and yellow solids (220 mg). An exhaustive extraction with toluene gave a greenish yellow solution, which after rechromatography as described above gave more orange crystals of **3** (60 mg, 0.10 mmol, 10% yield). The grey-black residue (ca. 100 mg) recrystallised in THF–hexane to give greenish white solids of unreacted $SnCl_2$ contaminated with an unidentified unstable dark green compound, which showed no proton NMR signals.

Fraction III gave dark blue-green solids (120 mg), consisting mainly of **2** and some unidentifiable insoluble compound.

(b) At ambient temperature. The reaction of $Cp_2Cr_2(CO)_4Se$ from $Cp_2Cr_2(CO)_6$ (800 mg, 2 mmol) and Se_8 (158 mg, 2 mmol) with $SnCl_2$ (758 mg, 4 mmol) in THF (ca. 35 cm^3) was allowed to proceed for 20 days at ambient temperature. No colour change was observed. A similar workup procedure, as described above, led to the isolation of (i) a brown black insoluble uncharacterisable mixture (300 mg, 12% yield based on Cr) consisting probably of $Cp_4Cr_4Se_4$, Se and CO-containing and $SnCl_2$-containing chromium complexes on the basis of its elemental analysis, and spectral and physical characteristics; (ii) dark blue fluffy crystals of $CpCrCl_2(THF)$ (**2**) (173 mg, 16% yield); (iii) orange yellow crystals of $Cp_2Cr_2(CO)_6SnCl_2$ (**3**) (310 mg, 26% yield); (iv) dark green solids (ca. 150 mg) which on fractional crystallisation in THF–ether gave partial separation into **3** (ca. 80 mg), grey-brown solids (10 mg) of $Cp_4Cr_4Se_4$ and dark green solids (yellow when pulverised) of **4** (ca. 50 mg); (v) dark green solids (ca. 300 mg), consisting mainly of **2** and $SnCl_2$, contaminated with a gummy dark green unidentified compound.

The species **4** possesses δ(Cp) at 3.85 in the ^1H NMR spectrum in C_6D_6, ν(CO) 2030vs, 2018vs, 1975m, 1940s cm^{-1} (Nujol) in the IR and a mass spectrum showing the fragmentation pattern of **3**. The solid decomposes during brief drying in vacuo to a partially soluble dirty greenish yellow residue. A solution of **4** in C_6D_6 undergoes a slow decomposition in 2 days at ambient temperature, resulting in a bluish solution and precipitation of royal blue solids of **2** and a metallic coating on the tube walls (presumably of Se or Sn since it gave a negative test for Cr). The solution still possesses some original complex (δ 3.85), as well as the complex **3** (δ 4.42).

In an attempt to maximise the yield of the species **4**, the progress of a similar reaction was monitored by ^1H NMR spectroscopy at regular intervals. This showed two new Cp-containing species after 1 h of reaction viz. **4** (δ 3.85) and **5** (δ 4.23). The intensity of the peak δ 3.85 remained constant for up to 4 h, at ca. 1/4 of the combined intensity of the peaks due to $Cp_2Cr_2(CO)_4Se$ (δ 4.36), **5** (δ 4.23) and the product **3** (δ 4.42) which had started to form. However, the relative intensity had fallen to 1/7 by 22 h and thereafter remained at that low level. Attempts to isolate the product **4**, after reaction times of 3.5 h, 6 h, and 5 days respectively, all gave low yields which defied further purification owing to decomposition.

X-Ray diffraction study

Diffraction-quality crystals of $CpCrCl_2(CH_3CN)$ (**2A**) were obtained as thick needles from recyrstallisation of **2** in a CH_3CN–ether mixture.

For diffractometry a crystal was mounted on a glass fibre with cyanoacrylate resin. Lattice parameters at 21° C were determined by a least-squares fit to the

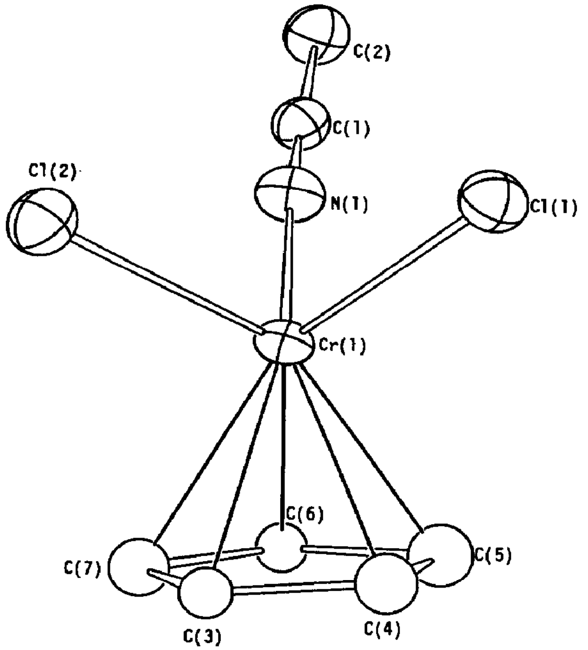

Fig. 1. An ORTEP plot of $CpCrCl_2(CH_3CN)$ giving atom numbering. Hydrogen atoms have arbitrary size and for all other atoms 30% thermal ellipsoids are shown.

setting parameters of 25 independent reflections, measured and refined on an Enraf–Nonius CAD4F four-circle diffractometer employing graphite monochromated Mo-K_α radiation.

Crystal data. Formula $C_7H_8Cl_2CrN$; *M* 229.05, monoclinic, space group $P2_1/a$, *a* 12.868(6), *b* 5.863(2), *c* 12.875(5) Å, *β* 102.97(3)°, *Z* = 4, *V* 946.6 $Å^3$, D_c 1.607 g cm^{-3}, μ(Mo-K_α) 16.54 cm^{-1}, λ(Mo-K_α) 0.7107 Å, *F*(000) 460 electrons.

Table 1

Positional parameters ($\times 10^4$) for $CpCrCl_2(CH_3CN)$

	x	*y*	*z*
Cr(1)	4393(1)	−894(1)	2360(1)
Cl(1)	3929(2)	1241(30	3665(1)
Cl(2)	5733(2)	1391(3)	2050(1)
N(1)	5388(6)	−3004(9)	3409(3)
C(1)	5870(7)	−4323(10)	3963(4)
C(2)	6469(11)	−5939(16)	4681(7)
C(3)	3455(20)	−587(29)	686(10)
C(4)	2742(18)	−715(3)	1353(13)
C(5)	2908(22)	−2937(45)	1867(9)
C(6)	3768(17)	−3998(21)	1455(13)
C(7)	4104(16)	−2549(38)	751(11)
C(3′)	3051(23)	−396(27)	1018(17)
C(4′)	2653(20)	−1850(46)	1727(13)
C(5′)	3370(24)	−3874(30)	1791(12)
C(6′)	3985(17)	−3464(33)	1062(15)
C(7′)	3782(25)	−1478(51)	624(10)

Primes indicate minor sites of disordered atoms, occupancy 0.47(2).

Table 2

Bond lengths (Å) and angles (°) for $CpCrCl_2(CH_3CN)$

Cl(1)–Cr(1)	2.280(1)	Cl(2)–Cr(1)	2.288(2)
N(1)–Cr(1)	2.053(6)	C(3)–Cr(1)	2.229(14)
C(4)–Cr(1)	2.230(21)	C(5)–Cr(1)	2.224(18)
C(6)–Cr(1)	2.213(12)	C(7)–Cr(1)	2.242(11)
C(3′)–Cr(1)	2.172(22)	C(4′)–Cr(1)	2.275(24)
C(5′)–Cr(1)	2.211(17)	C(6′)–Cr(1)	2.225(12)
C(7′)–Cr(1)	2.223(13)	C(1)–N(1)	1.137(8)
C(1)–C(2)	1.424(12)	C(4)–C(3)	1.392(23)
C(7)–C(3)	1.413(24)	C(5)–C(4)	1.456(22)
C(6)–C(5)	1.469(27)	C(7)–C(6)	1.381(19)
Cl(2)–Cr(1)–Cl(1)	98.0(1)	N(1)–Cr(1)–Cl(1)	94.2(1)
N(1)–Cr(1)–Cl(2)	94.9(2)	C(1)–N(1)–Cr(1)	173.7(6)
C(2)–C(1)–N(1)	178.4(6)	C(7)–C(3)–C(4)	112(1)
C(5)–C(4)–C(3)	106(2)	C(6)–C(5)–C(4)	105(1)
C(7)–C(6)–C(5)	110(1)	C(6)–C(7)–C(3)	105(2)
C(7′)–C(3′)–C(4′)	110(2)	C(5′)–C(4′)–C(3′)	101(2)
C(6′)–C(5′)–C(4′)	105(1)	C(7′)–C(6′)–C(5′)	111(2)
C(6′)–C(7′)–C(3′)	110(2)		

Structure determination

Intensity data were collected in the range $1.0 < \theta < 25.0$° by use of an $\omega - 1.33\theta$ scan. The scan widths and horizontal counter apertures employed were $(1.00 + 0.34 \tan \theta)$° and $(2.70 + 1.05 \tan \theta)$mm. Data reduction and application of Lorentz, polarization and absorption (max. trans. 0.847, min. trans. 0.808) corrections were carried out by use of the Enraf–Nonius Structure Determination Package. Of the 788 independent non-zero reflections collected 637 with $I > 2.5\sigma(I)$ were considered observed and used in the calculations.

The structure was solved by direct methods using SHELX-76 [18] which enabled the location of the heavier atoms and the solution was extended by difference Fourier methods. The cyclopentadienyl ligand was found to be rotationally disordered; two sites with occupancies 0.53 : 0.47 successfully modelled the observed electron density. Hydrogen atoms of the CH_3CN ligand were refined with isotropic thermal parameters and those of the cyclopentadienyl ligand were included at calculated sites with a group isotropic thermal parameter. The contributors to the cyclopentadienyl ligand atoms were refined isotropically and all other atoms were refined anisotropically.

Blocked-matrix least-square refinement of an overall scale factor, positional and thermal parameters converged (all shifts $< 0.1\sigma$ for full occupancy atoms) with R * $= 0.033$, $R_w = 0.029$ and $w = 1.21/(\sigma^2(F_o) + 0.000617F_o^2)$. Maximum excursions in a final difference map were $+0.25$ eÅ^{-3} and -0.25 eÅ^{-3}. Scattering factors and anomalous dispersion terms used for Cr were taken from ref. [19] and for all other atoms the values supplied with SHELX-76 were used [18]. All calculations were carried out by use of SHELX-76 [18] and plots were drawn with ORTEP [20].

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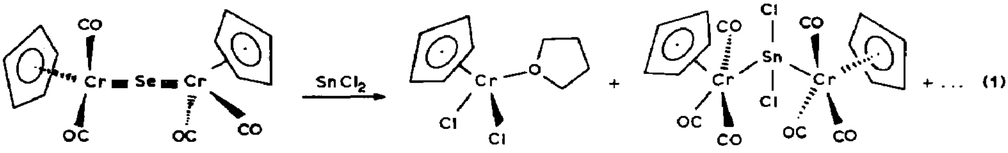
* $R = \Sigma(||F_o| - |F_c||)/\Sigma|F_o|$, $R_w = (\Sigma w(|F_o| - |F_c|)^2/\Sigma w F_o^2)^{1/2}$.

The atom numbering scheme is given in Fig. 1. Final atomic coordinates are listed in Table 1 and bond lengths and bond angles in Table 2. Listings of observed and calculated structure factors, hydrogen atom coordinates and thermal parameters and details of least-squares planes calculations (Tables S1–S4) are available from the authors.

Results and discussion

Reaction of $Cp_2Cr_2(CO)_4Se$ with $SnCl_2$

Products. The reaction of $Cp_2Cr_2(CO)_4Se$ with two mole equivalents of $SnCl_2$ in THF for 8 h at 65° or for an extended period of 20 days at ambient temperature led to the isolation of the stable products $CpCrCl_2(THF)$ (**2**) and $Cp_2Cr_2(CO)_6SnCl_2$ (**3**) in 16 and 26% yields respectively (eq. 1), in addition to the other unstable products discussed below. Whereas the insertion of $SnCl_2$ into the $Cr{\equiv}Se{\equiv}Cr$ bond of (**1**) was expected on account of previously demonstrated facile insertions of S [11], Se [12], CR_2 groups [13] and $Fe(CO)_3$ fragments [14], the accompanying extrusion of Se to form **3** as well as **2** was not.



(1) (2) (3)

The monohydrate of **2** crystallised as hygroscopic fine royal blue needles from THF–ether and was characterised by its elemental analysis and IR spectrum. Its ^1H NMR spectrum in $CDCl_3$ shows a broad Cp resonance at δ 11.2 ($\nu_{1/2}$ ca. 200 Hz) and resonances for THF at δ 3.77 and 1.86. Though first reported in 1962 as the product of the reaction of Cp_2Cr with CCl_4 in THF [21], studies on such paramagnetic half-sandwich complexes have been scarce, owing to the unavailability of a rapid and efficient analytical method. Recently, the application of paramagnetic NMR spectroscopy [22,23], together with the emerging catalytic role of paramagnetic complexes [24,25], has led to a reawakening of interest in the structure and reactivity of these chromium complexes. This is illustrated by Köhler's studies on the antiferromagnetic dinuclear $[Cp'CrX_2]_2$ complexes ($Cp' = \eta^5\text{-}C_5H_5$ and $\eta^5\text{-}C_5Me_5$, X = Cl, Br, I) and the monomeric $CpCrX_2(L)$ complexes (L = THF, PMe_3, PEt_3) and related compounds where X is substituted by alkyl and aryl groups [22,23]. Recent work by Theopold [26–28] on paramagnetic cyclopentadienylchromium alkyls of the type $[Cp'Cr(R)Cl]_2$ ($Cp' = \eta^5\text{-}C_5H_5$ and $\eta^5\text{-}C_5Me_5$; R = Me, Et) demonstrated the tendency of these complexes to undergo facile insertion of nitriles and other unsaturated molecules into the metal–carbon bond and to catalyse the polymerisation of olefins.

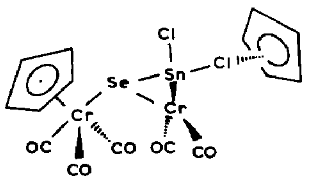
The compound **3** was isolated as orange polyhedral crystals and characterised by elemental analysis, from its mass spectrum, and a comparison of its IR data with those of $Cp_2Cr_2(CO)_6SnCl_2$, previously synthesised from the reaction of $Cp_2Cr_2(CO)_6$ with $SnCl_2$ [6] and structurally determined to possess a Cr–Sn–Cr bond with a bond angle of 130.2(1)° [29]. The solution in C_6D_6 shows resonances

δ(Cp) 4.42 in the ^{1}H NMR spectrum and δ(Cp) 89.43 with δ(CO) 233.89 and 239.25 in the ^{13}C spectrum.

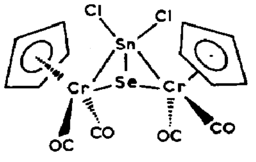
Whereas the less soluble complex **2** separates readily from the product mixture and readily recrystallises as pure beautiful feather-like blue crystals, the complex **3** was generally contaminated with dark brown or dark green impurities and required two chromatographic workups before pure lustrous golden yellow crystals could be obtained. The re-occurrence of **3** in later chromatographic fractions indicate disproportionation/decomposition of insertion complexes **4** and **5** (discussed below) on the column.

Intermediate species. ^{1}H NMR spectral monitoring of the reaction at ambient temperature indicated that the formation of one or two intermediate species **4** (δ 3.85) and **5** (δ 4.24), constitutes the slow rate-determining step, so that its concentration remained low ($<$ 20% of reactant and product mixture) throughout the reaction. Hence attempts at isolation produced only in very low yield, an impure sample of **4** which was not stable enough to endure purification procedures. A fairly pure sample of **4** obtained was found to possess CO stretching frequencies in the IR and a mass fragmentation pattern similar to that of **3**. In the solid state, the intermediate (**4**) decomposes within a few hours in vacuo into an insoluble greenish yellow solid. In solution in C_6D_6, it converts to **2**, **3** and a metallic coating on the tube walls presumably of elemental Se and/or Sn. This deposition of Se and Sn is consistent with the relatively high S and Sn content present in the insoluble uncharacterisable byproducts of the reaction. Furthermore, the finely divided nature of these metallic deposits is the likely cause of their pyrophoric character.

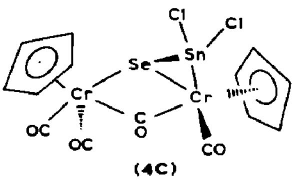
On the basis of insertion products arising from the reaction of $Cp_2Cr_2(CO)_4Se$ with S [11], Se [12], diazoalkanes [13] and $Fe_2(CO)_9$ [14], probable formulations for the species **4** and **5** could be represented by **4A**–**4C**. The observed singlet Cp resonance of **4** seems to favour the symmetrical structural form **4B**. An expulsion of Se to form **3** finds a precedent in the insertion of elemental sulphur to yield $Cp_2Cr_2(CO)_4S$ (eq. 2) [11]. Other mechanistic pathways that may be envisaged for the dissociation of these intermediate species to **2** and **3** are numerous, but are beyond the scope of this study to delineate.



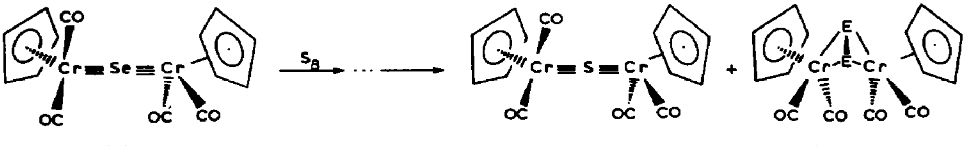
(4A)



(4B)



(4C)



(2)

(1)

(E = S, Se)

Structure of $CpCrCl_2(CH_3CN)$ (2A)

Structural studies on these Cr^{III} half-sandwich complexes are scarce. The only ones that we are aware of are the recent X-ray diffraction studies of $[CpCrMeCl]_2$ [26], $[Cp^{\star}CrEt(py)_2]^+$ [28], $[Cp^{\star}CrCl_2]_2$ and $[Cp^{\star}CrMe_2(PMe_3)]$ ($Cp^{\star} = \eta^5$-C_5Me_5) [22,23]. In view of this current interest, it would be desirable to do the structural analysis of **2** for comparative purposes, if diffraction-quality crystals were available. Attempts to crystallise **2** in THF or THF–ether produced only fine feather-like needles of the complex. quality crystals in the form of thick needles were obtained only in CH_3CN–ether mixtures, which gave the solvent-exchanged derivative $CpCrCl_2(CH_3CN)$ (**2A**). This ease of exchange of a coordinated solvent molecule is consistent with Theopold's observation of this facile coordination of acetonitrile in $[Cp^{\star}CrMeCl]_2$, prior to the formation of nitrile-insertion products [27].

The structure consists of neutral molecules with no unusually short contacts between the molecules. The Cr atom is coordinated to two Cl^- ligands, an anionic cyclopentadienyl ligand and a neutral CH_3CN ligand, giving a three-legged piano-stool geometry. Unknown until recently, this coordination geometry for Cr^{III} has now been observed for several complexes, viz. $[CpCrCl_2]_2$ [22], $Cp^{\star}CrMe_2(PMe_3)$ [23], $[CpCrMeCl]_2$ [26], and $Cp^{\star}CrEt(py)_2^+$ [28]. The bond lengths of $CpCrCl_2(CH_3CN)$ (**2A**) are very similar to their counterparts in $[CpCrCl_2]_2$ [22]. Thus the Cr–Cl (nonbridging) bond lengths in $[CpCrCl_2]_2$ are 2.287(1) and 2.294(2) Å [22], almost identical to the values of 2.280(1) and 2.288(1) Å in **2A**. The coordination of the Cp ring is also almost identical in the two structures, the Cr–Cp (centroid) distances being 1.88 [22] and 1.87 Å respectively. The Cr–N bond length is short [2.053(6) Å], comparable with Cr^{III}–N(amine) bond lengths and indicates a strong interaction.

Acknowledgements

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