2D HetCOR NMR Spectrum and Structure of

Dicarbonyl(η^5-N-methylcarbamoylcyclopentadienyl)cobalt

$(CO)_2Co(\eta^5\text{-}C_5H_4CONHCH_3)$

Yu-Pin Wang[*], Chwan-Tzong Lin, Hsiu-Yao Cheng, Tso-Shen Lin,

Abstract

Dicarbonyl(η^5-N-methylcarbamoylcyclopentadienyl)cobalt (**5**) was prepared by the reaction of the corresponding acid chloride with methylamine. The structure of **5** has been determined by X-ray diffraction studies: space group, P2$_1$/c; monoclinic; a = 10.767(3), b = 9.869(2), c = 9.555(3) Å, β = 105.58(2)° ; Z = 4. The exocyclic carbon is bent away from the cobalt atom with an angle θ of –0.54°. The chemical shifts of C(2,5) and C(3,4) on the Cp ring were assigned using two-dimensional HetCOR NMR spectroscopy. The electron density distribution in the cyclopentadienyl ring of the Cp(Co) was discussed on the basis of ^{13}C NMR data and compared with calculations via the density functional B3LYP exchange-correlation method.

1. Introduction

Functionally substituted η^5-cyclopentadienyl metal compounds have been the subject of continuing interest in our laboratory [1]. From our previous studies [2], two facts emerge quite clearly. The first is the opposite correlation of the assignments of C(2,5) and C(3,4) on the Cp ring, in the ^{13}C NMR spectra, between cynichrodene (**1**) and ferrocene (**2**) derivatives bearing electron-withdrawing substituents. The second is the qualitative relationship of non-planarity of Cp–exocyclic carbon to substituent π-donor and π-acceptor interactions. The π-donor substituents and the ipso-carbon atoms to which they are attached are bent away from the ML_n fragments whereas the π-acceptor substituents and the ipso-carbon atoms to which they are attached are approximately in the Cp plane or are bent slightly toward the ML_n fragments. The magnitudes and directions of these distortions of the Cp planarity appear to be due primarily to electronic effects.
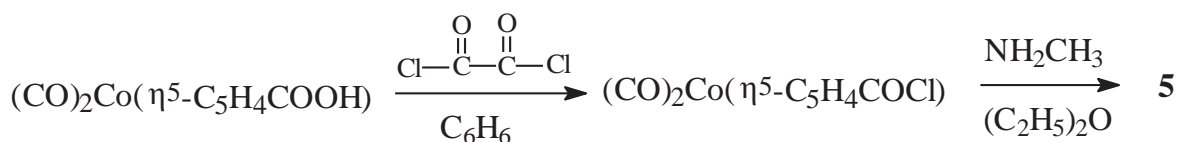
In hope of confirming those hypotheses and extending those hypotheses to the $Co(CO)_2$ analog have prompted us to synthesize complex $(CO)_2Co(\eta^5\text{-}C_5H_4CONHCH_3)$ (5).

1   **2**

3 R = COOH
4 R = COCl
5 R = CONHCH$_3$

6
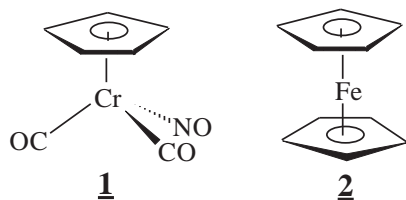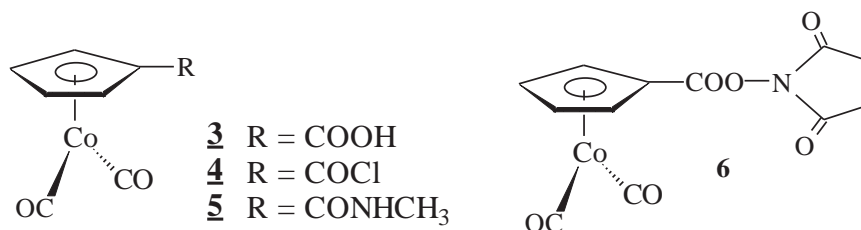
2. Results and discussion

By reacting with oxalyl chloride in benzene solution, dicarbonyl(η^5-carboxycyclopentadienyl)cobalt, $(CO)_2Co(\eta^5$-C$_5$H$_4$COOH) **3**, [3] was transformed into dicarbonyl(η^5-chloroformylcyclopentadienyl)cobalt, $(CO)_2Co(\eta^5$-C$_5$H$_4$COCl) **4**. Without further purification, **4** was treated with methylamine in diethyl ether leading to carboxamide **5** in a yield of 63%.

$$(CO)_2Co(\eta^5\text{-}C_5H_4COOH) \xrightarrow[C_6H_6]{Cl-\overset{O}{\underset{}{C}}-\overset{O}{\underset{}{C}}-Cl} (CO)_2Co(\eta^5\text{-}C_5H_4COCl) \xrightarrow[(C_2H_5)_2O]{NH_2CH_3} \textbf{5}$$

The IR spectrum of **5** contains two carbonyl stretching bands, the symmetric mode occurring at 2036 cm^{-1} and the asymmetric mode at 1971cm^{-1}, a characteristic carbamoyl stretching band at 1631 cm^{-1}, and a N–H bending band at 1558 cm^{-1}. The ^{1}H NMR spectrum of **5** exhibits a broad singlet owing to the NH proton at δ 5.80 and an A$_2$B$_2$ pattern related to the observed triplet. The downfield triplet can be assigned to the H(2,5) protons of the Cp ring. This assignment is made on the basis of the fact that the carbonyl group would exert a strong diamagnetic anisotropic effect and exhibit an electron-withdrawing property. As expected, H(2,5) would be deshielded to a greater extent than the protons on the more remote 3- and

4-positions. Accordingly, the following assignments for complex **5** were made: H(2,5) and H(3,4) of Cp(Co) resonate at δ 5.38 and δ 5.18, respectively.

The assignments of ^{13}C NMR spectra for **5** were based on standard ^{13}C NMR [4], 2D HetCOR, and DEPT correlation techniques. They were compared with other metallo-aromatic systems [5]. Three relatively less intense signals were observed at δ 202.38, δ 164.43, and δ 96.60 corresponding to the terminal carbonyl carbon, carbamoyl carbon, and C(1) of Cp(Co), respectively. The line assignments for C(2–5) of Cp(Co) were more difficult to make. Based on the 2D HetCOR results (Fig. 1), in which the magnetic fields of ^{1}H and ^{13}C NMR spectra increase toward the right and upper side, respectively, the upfield chemical shifts of C(2,5) correlate with the downfield chemical shifts of H(2,5) (δ 5.38) and the downfield chemical shifts of C(3,4) correlate with the upfield chemical shifts of H(3,4) (δ 5.18). Accordingly, chemical shifts at δ 83.10 and δ 86.10 were assigned to C(2,5) and C(3,4), respectively, of Cp(Co). The downfield and upfield chemical shifts are assigned to C(3,4) and C(2,5) owing to an electron-withdrawing carbonyl substituent on the Cp(Co) ring. These assignments reveal that positions 3 and 4 on the substituted Cp ring in (CO)$_2$CoCp, are more sensitive to electron-withdrawing substituents, as are ferrocene analogs [6]. After obtaining the X-ray structures of **5** and **6** [7], the average charges of C(2,5) and C(3,4) for complex **5** (–0.3709 and –0.2297) and complex **6** (–0.3953 and –0.3252) were determined by ab-initio calculations (Table 1). These values correlated well with the unequivocal assignments of the ^{13}C chemicals shifts for both **5** and **6** (Table 2) [8].

The molecular structure of **5** is shown in Fig. 2. Selected bond distances and angles are given in Table 3. The atomic coordinates of the atoms are listed in Table 4. For the purpose of comparison, selected structural data of **6** are also listed in Table 5. The structure of **6** [7]**,** bearing twist angles of 84.84 and 95.48°, shows that the –Co(CO)$_2$ unit is bonded almost symmetrically to the functionalized cyclopentadienyl ligand. In the case of **5**, the twist angles are 64.84 and 118.7°. The twist angle is defined as the torsional angle between the terminal carbonyl carbon atom, the Co atom, the Cp ring center and the ring carbon atom bearing the exocyclic carbon. The steric crowdedness may account for the difference. The plane containing the N-succinimidyl fragment is almost orthogonal to that of the Cp ring with dihedral angle of 93°, leading two carbonyl ligands away from the exocyclic carbon.

From Table 5, two interesting features are revealed: the exocyclic C–C bond of Cp(Co) in **6** is 1.438(7) Å (C(2)–C(1)), considerably shorter than 1.487(17) Å (C(1)–C(6)) in **5,** and **6** bears a large value of positive θ (2.61°), while **5** bears a negative θ value (–0.54°). The ability of the exocyclic double bond to donate electron density to the cobalt atom, reestablishing the favored 18-electron count, leads to the exocyclic carbon slightly bending towards the cobalt atom with an angle θ of 2.61° in the case of **6**. The θ angle is defined as the angle between the exocyclic C–C bond (C(1)–C(6) in **5** and C(2)–C(1) in **6**) and the corresponding Cp ring with a positive angle toward metal and a negative angle away from the metal.
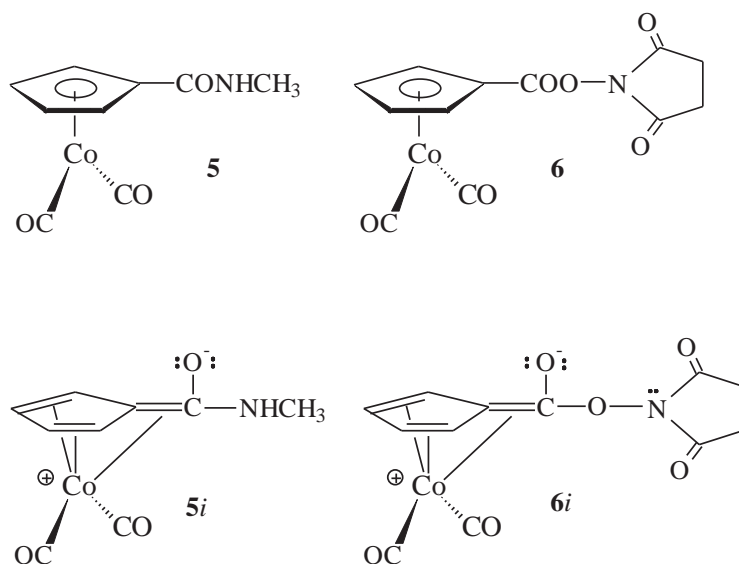
The smaller contribution of canonical form **5i** than **6i** to each of the corresponding structures **5** and **6** may explain a smaller θ (–0.54°) and a longer exocyclic C–C bond length (1.487(17) Å) of Cp(Co) in **5**. This phenomenon is plausible, since an amido nitrogen is stronger electron donating, compared to that of an ester oxygen. The more effective resonance, as shown in **5ii**, between the amido nitrogen and carbonyl group diminishes the extent of resonance between the carbonyl and Cp(Co) in **5**. The smaller contribution of **5i** to **5** leads to a longer exocyclic bond length of C(1)–C(6) and a smaller θ.
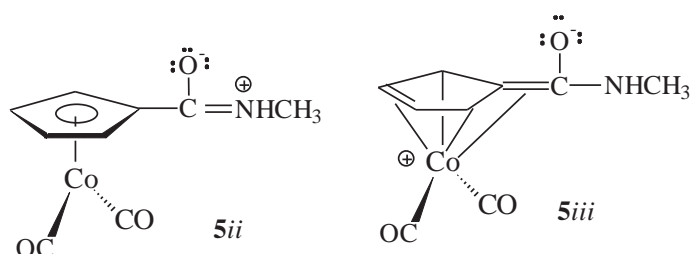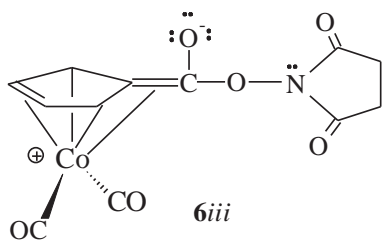
It is worth pointing out that a long-short-long pattern in η^4-1,3-diene canonical form was observed in both **5** and **6**. It reveals that in both complexes, the coordinated cobalt metal is fairly electron-rich. Given that the shortest bonds of C(3)–C(4) 1.378(18) Å in **5** and C(4)–C(5) 1.384(8) Å in **6** (Table 5) among each corresponding C–C bond lengths of Cp(Co) ring, a predominant weight was assigned to canonical form **5***iii* and **6***iii*, and an insignificant weight to **5***i* and **6***i,* respectively.

3. Experimental

3.1   Preparation of dicarbonyl[η^5-N-methylcarbamoylcyclopentadienyl)cobalt (**5**)

To a solution of dicarbonyl (η^5-carboxycyclopentadienyl)cobalt **3** (0.72 g, 3.2 mmol) in 70 ml of benzene, oxalyl chloride (0.70 ml, 8.0 mmol) was added, The reaction mixture was stirred at room temperature for 18 h with the outlet interfaced to a mercury overpressure valve. The dark solution was filtered, the solvent was removed in vacuum, and the red residue was extracted with pentane. Removal of the solvent in vacuum afforded dicarbonyl(η^5-chloroformylcyclopentadienyl)cobalt **4**. Without further purification, the dark red liquid was dissolved in 60 ml of diethyl ether and dry methylamine was passed through the solution for 1 h, resulting in an

immediate precipitation of yellow crystals. After removal of the solvent, 60 ml of methylene chloride was added and the solution was washed with deoxygenated water until the washings were neutral. After the solution was dried over anhydrous magnesium sulfate for 1h, it was filtered through an alumina plug (2 x 2.5 cm) and was chromatographed on an alumina column using THF as the eluent. Removal of the solvent in vacuum produced 0.48 g (63%) of dicarbonyl(η^5-N-methylcarbamoylcyclopentadienyl)cobalt **5**.

An analytical sample, m.p. 107–109°C, was obtained as an orange solid by recrystallization from Hexane/Ether/CH_2Cl_2 (5/1/1). Anal. Found: C, 45.64; H, 3.37; N, 5.99. $C_9H_8NO_3Co$ Calc.: C, 45.59; H, 3.40; N, 5.91 %. Proton NMR ($CDCl_3$): δ (relative intensity, multiplicity, assignment): 2.93 (3H, d, $J = 4.5$ Hz, $-CH_3$); 5.18 (2H, s, Cp(Co) H(3,4)); 5.38 (2H, s, Cp(Co) H(2,5)); 5.80 (1H, bs, $-NH-$). Carbon-13 NMR ($CDCl_3$): δ (assignment): 26.50(CH_3); 83.10 (Cp(Co), C(2,5)); 86.10 (Cp(Co), C(3,4)); 96.60 (Cp(Co), C(1)); 164.43 ($-C(O)-$); 202.38(Co-C≡O). IR(KBr): ν (cm^{-1}) (intensity): 3323(m), 3092(w), 2036(s), 1971(s), 1631(m), 1558(m), 1309(w), 622(w). Mass spectrum: *m/z 237*(M)$^+$.

3.2. X-ray Diffraction analysis of *5*

The intensity data were collected on a Siemens R3m/V diffractometer with a graphite monochromator (Mo-K$_\alpha$ radiation). θ $-$2θ scan data were collected at room temperature (23°C). The data were corrected for absorption, Lorentz and polarization effects. The absorption correction is according to the empirical psi rotation. The details of crystal data and intensity collection are summarized in Table 6.

The structures were solved by direct methods and were refined by full matrix least squares refinement based on F values. All of the non-hydrogen atoms were refined with anisotropic thermal parameters. All of the hydrogen atoms were positioned at calculated coordinate with a fixed isotropic thermal parameter (U = U(attached atom) + 0.01 Å^2). Atomic scattering factors and corrections for anomalous dispersion were from *International Tables for X-ray Crystallography* [9]. All calculations were performed on a PC computer using Shelex software package [10].

Computational Method

Calculations based on DFT are carried out using B3LYP hybrid method involving three-parameter Becke exchange functional [11] and a Lee-Yang-Parr correlation functional [12]. All calculations are performed using the Gaussian 09 program [13]. The geometry for **5** is taken from the crystallographic data. The atomic charges have been analyzed using the Mulliken population analysis.

Acknowledgements

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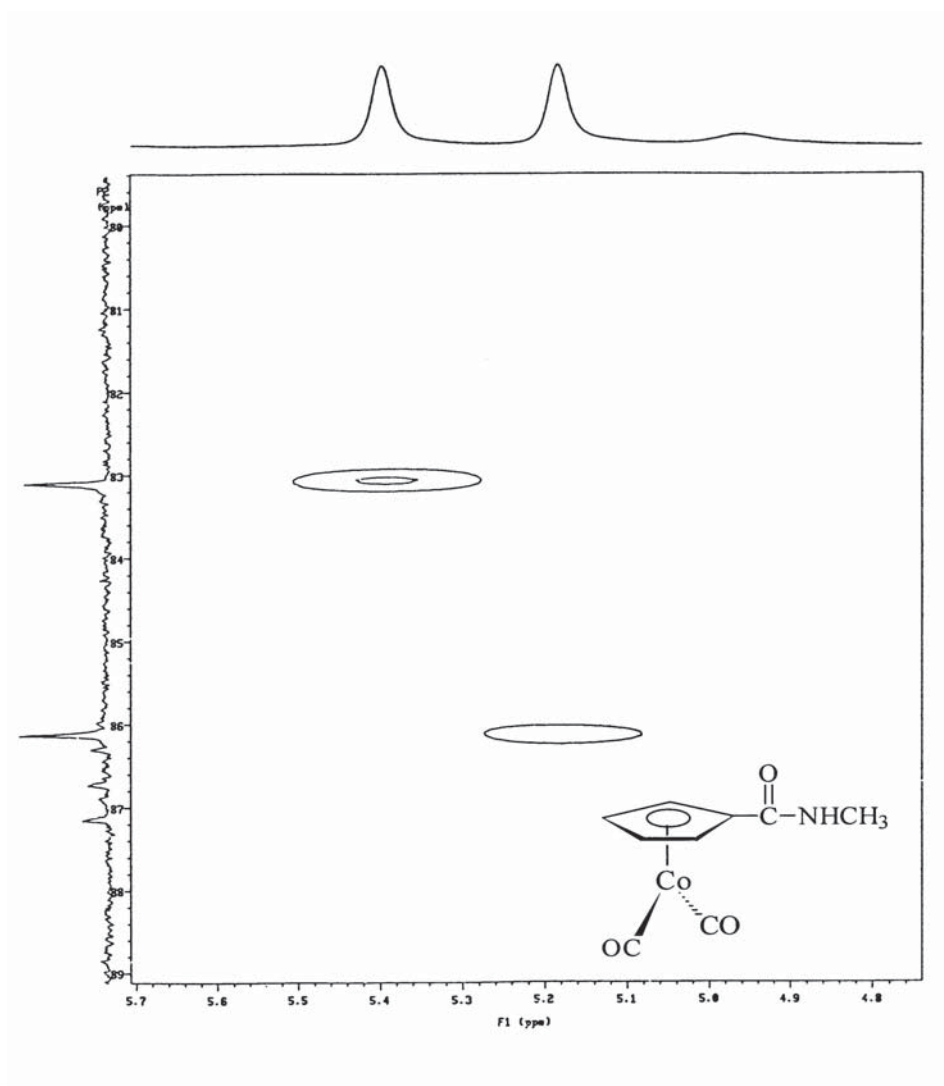
Fig. 1. Two-dimensional ^{1}H-^{13}C HetCOR NMR spectrum of **5** in CDCl$_3$.
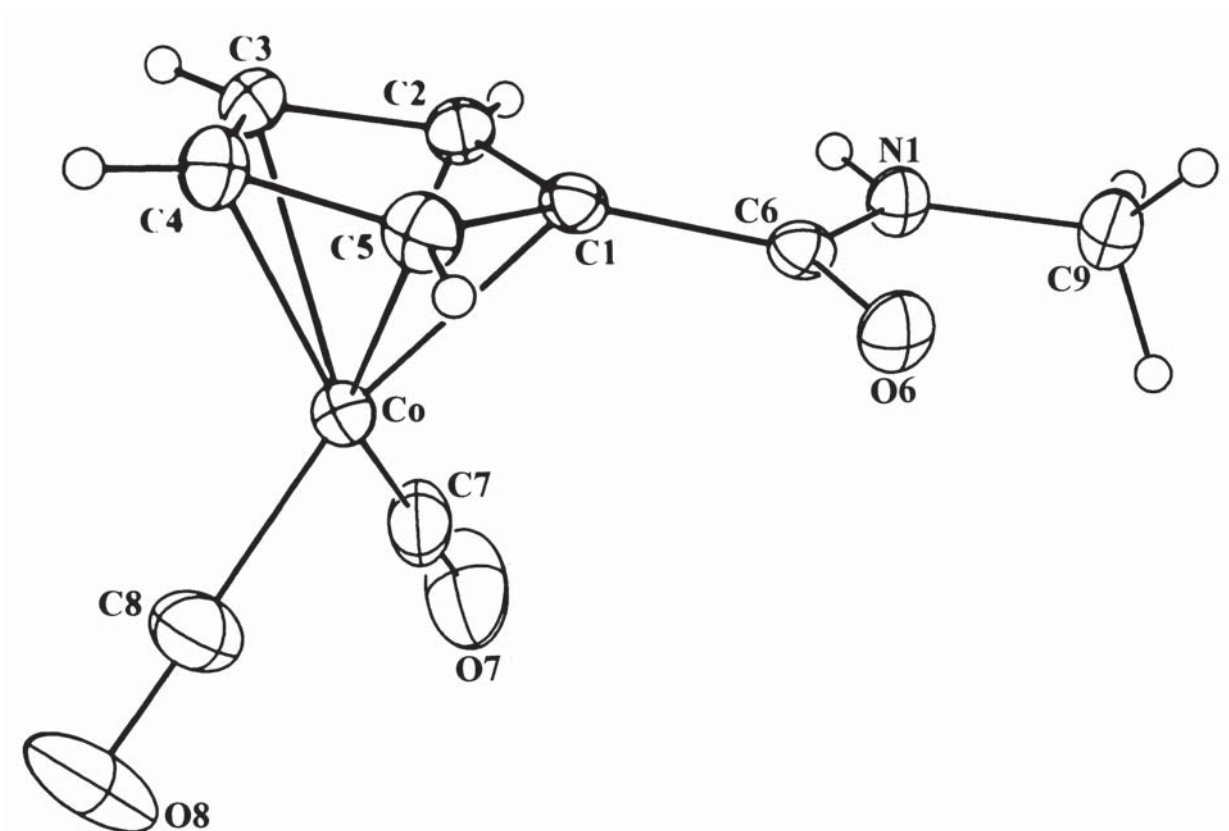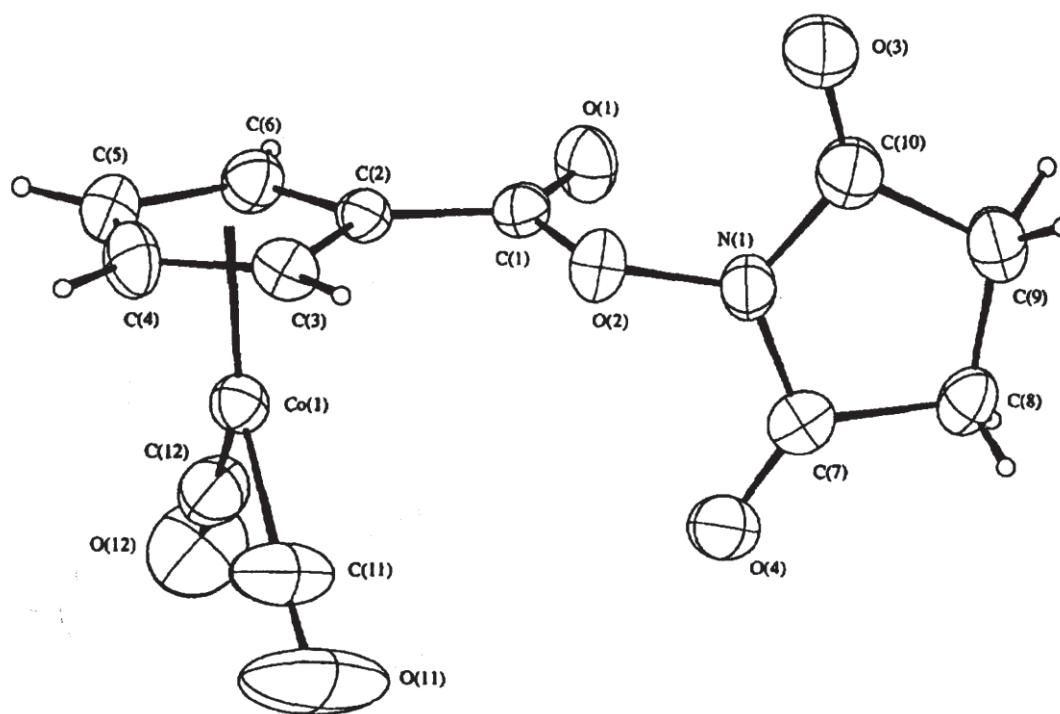
Fig. 2. Molecular structure of **5**

Fig. 3. Molecular structure of **6**

Table 1

Selected net atomic charges for **5** and **6** using the LANL2DZ basis set

	C(1)	C(2)	C(3)	C(4)	C(5)
5	0.24002	–0.37101	–0.21087	–0.24852	–0.37084
6	0.19836	–0.38213	–0.29913	–0.35122	–0.40843

Table 2
^{13}C{1H} NMR data and Δ ^{a}

Compound	Cp(Co) δ (ppm)				-C(O)-	Co(CO)	Others
	C(1)	C(2,5)	C(3,4)	Δ (ppm)			
(CO)$_2$CoCp		84.51(C(1–5))		0			
(CO)$_2$Co(C$_5$H$_4$–CHO)	100.55	83.44	**89.47**	–6.03	184.73	201.84	
(CO)$_2$Co(C$_5$H$_4$–COCH$_3$)	100.22	83.58	**88.33**	–4.75	193.66	201.75	26.57(–CH$_3$)
(CO)$_2$Co(C$_5$H$_4$–COOCH$_3$)	92.85	86.06	**88.80**	–2.74	165.17	203.64	52.07(–OCH$_3$)
(CO)$_2$Co(C$_5$H$_4$–CONHCH$_3$) **5**	96.60	83.10	**86.10**	–3.00	164.43	202.38	26.50(–CH$_3$)
(CO)$_2$Co(C$_5$H$_4$–COONS)^b **6**	106.50	85.18	**90.49**	–5.31	169.74	201.48	159.69(C(O)), 24.91(–CH$_2$–CH$_2$–)

^{a} $\Delta = \delta[C(2,5)] - \delta[C(3,4)]$

(+: C(2.5)downfield, C(3,4) upfield; – : C(2,5) upfield, C(3,4) downfield). The lower-field chemical shift of each pair is underlined.

^{b} NS = N-succinimidyl

Table 3
Selected bond length (Å) and selected bond angles (°) for **5**

Co–C(1)	2.098(11)	C(7)–Co–C(8)	93.7(6)
Co–C(2)	2.054(12)	C(6)–C(1)–C(2)	128.4(6)
Co–C(3)	2.099(15)	C(6)–C(1)–C(5)	124.9(6)
Co–C(4)	2.073(14)	C(6)–N(1)–C(9)	121.8(5)
Co–C(5)	2.088(13)	C(1)–C(6)–N(1)	116.2(7)
C(1)–C(2)	1.433(12)	C(1)–C(6)–O(6)	121.1(6)
C(1)–C(5)	1.398(17)	N(1)–C(6)–O(6)	122.71(18)
C(1)–C(6)	1.487(17)	Co–C(7)–O(7)	179.49(12)
C(2)–C(3)	1.408(19)	Co–C(8)–O(8)	178.51(13)
C(3)–C(4)	1.378(18)	Cp(cen.)–Co–C(7)	132.45
C(4)–C(5)	1.436(19)	Cp(cen.)–Co–C(8)	133.81
Co–C(7)	1.717(13)		
Co–C(8)	1.729(13)		
C(7)–O(7)	1.138(20)		
C(8)–O(8)	1.143(18)		
C(6)–O(6)	1.231(18)		
C(6)–N(1)	1.329(14)		
C(9)–N(1)	1.462(14)		
Co..Cp(cen.)	1.702		

Dihedral angles between planes

Cp(cen.), Co, C(7) and Cp(cen.), Co, C(1)	64.84
Cp(cen.), Co, C(8) and Cp(cen.), Co, C(1)	118.70
Cp(Co) and carbonyl plane (C1, C6, O6, N1)	3.52

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

	x	y	z	U(eq)
Co	1824(1)	998(1)	364(1)	49(1)
O(7)	1151(3)	61(5)	2891(3)	134(2)
O(8)	-271(3)	2897(4)	-384(5)	138(2)
O(6)	5198(2)	2571(2)	2021(2)	52(1)
N(1)	5319((2)	462(2)	2935(2)	44(1)
C(7)	1415(3)	431(5)	1880(4)	77(2)
C(8)	574(3)	2155(4)	-82(5)	81(2)
C(1)	3821(3)	900(2)	633(3)	41(1)
C(5)	3243(3)	169(3)	-582(3)	52(1)
C(4)	2319(3)	861(4)	-1583(4)	64(1)
C(3)	2354(3)	-423(3)	-1006(3)	57(1)
C(2)	3232(3)	-412(3)	384(3)	48(1)
C(6)	4832(2)	1384(3)	1923(3)	38(1)
C(9)	6357(3)	789(3)	4227(4)	56(1)

Table 5
Selected structural data of **5** and **6**

Compound	Bond length (Å)	$\omega_W(°)$[a]	$\theta_M(°)$[b] M–C(exocyclic)	C(Cp(Co))–C(exocyclic) Cp				
				C1–C2	C2–C3	C3–C4	C4–C5	C1–C5
5 $(CO)_2Co(C_5H_4–CONHCH_3)$	1.487(17)(C1–C6)	64.84, 118.70	–0.54 3.203	1.433(12)	1.408(19)	1.378(18)	1.436(19)	1.398(17)
				C2–C3	C3–C4	C4–C5	C5–C6	C6–C2
6[c] $(CO)_2Co(C_5H_4–COONS)$	1.438(7)(C2–C1)	84.84, 95.48	2.61 3.090	1.435(7)	1.395(8)	1.384(8)	1.423(8)	1.413(7)

[a] $\omega_M(°)$: the twist angle is defined as the torsional angle between terminal carbonyl atom, the cobalt atom, the Cp center and the ring carbon atom bearing the exocyclic carbon atom.

[b] $\theta_M(°)$: the θ angle is defined as the angle between the exocyclic C–C bond and the corresponding Cp ring with a positive angle toward metal and a negative angle away from the metal.

[c] NS= N-succinimidyl, from [7].

Table 6

Selected crystal data and refinement parameters for **5**

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Identification code	920163
Empirical formula	$C_9 H_8 CoNO_3$
Color; Habit	Red; Columnar
Crystal size	$0.64 \times 0.30 \times 0.20$ mm^3
Formula weight	237.1
Temperature	296 K
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 10.767(3)$ Å
	$b = 9.869(2)$ Å $\qquad \beta = 105.58(2)°.$
	$c = 9.555(3)$ Å
No. Reflns. For Indexing	17 ($13.36° <= 2\theta <= 26.45°$)
Volume	978.0(4) Å^3
Z	4
Density (calculated)	1.610 Mg/m^3
Absorption coefficient	1.732 mm^{-1}
F(000)	480
Diffractometer used	Siemens R3m/V
Radiation	MoKα ($\lambda = 0.71073$ Å^3)
Monochromator	Highly oriented graphite crystal
2θ Range	2.5 to 50.00°.
Scan Type	$\theta/2\theta$
Scan Speed	Variable; 2.93 to 14.65° /min. in ω
Scan Range (ω)	1.00° plus Kα-separation
Background Measurement	Stationary crystal and stationary
	Counter at beginning and end of
	scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 50 reflections
Index ranges	$-12<=h<=12$, $-11<=k<=0$, $0<=l<=11$
Reflections collected	1965 ($2513 >= 3.0\sigma(I)$)
Independent reflections	1737 ($1391 >= 3.0\sigma(I)$) ($R_{int} = 1.42\%$)
Max. and min. transmission	0.9645 and 0.6985
Extinction Correction	$\chi = 0.0002(3)$, where
	$F^* = F[1+ 0.002 \chi F^2/\sin(2\theta)]^{-1/4}$
Hydrogen Atoms	Located on difference map
Weithting Scheme	$w^{-1} = \sigma^2(F) + .00003F^2$
Number of Parameters refined	152

Largest and Mean Δ/σ	0.003, 0.000
Data-to-Parameter Ratio	9.2:1
Goodness-of-fit	1.60
Final R indices (obs. Data)]	R = 0.0299, Rw = 0.0336
Largest diff. peak and hole	0.26 and -0.33 e.$\mathring{A}^{-3}$

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化合物 (CO)$_2$Co(η^5-C$_5$H$_4$CONHCH$_3$)

二維異核 NMR 光譜及結構分析

王玉蘋*, 林傳宗, 鄭秀瑤, 林哲生

摘 要

化合物(CO)$_2$Co(C$_5$H$_4$-COCl)(**4**)與(CO)$_2$Cl$_2$反應得化合物(CO)$_2$Co[η^5-(C$_5$H$_4$CONHCH$_3$) (**5**). **5** 的結構已由 X-ray 繞射法解析出. 晶體參數如下: Space group, P2$_1$/c; monoclinic; a = 10.767(3), b = 9.869(2), c = 9.555(3) Å, β = 105.58 (2)°; Z = 4. 五環上羰取代基的碳位向與 Cr 原子的位向相反, θ 角為 –0.54°. 經由二維異核相對應 NMR 光譜儀, 化合物 (CO)$_2$Co(η^5 - C$_5$H$_4$CONHCH$_3$) C(2)-C(5)的 ^{13}C 化學位移得以確認. 文中論述以 B3LYP correlation- exchange 理論計算法得出的電子密度分佈, 呼應於由 C13 NMR 化學位移所得之 Cp(Co)的電子密度分佈.

關鍵字:鈷, [η^5- (環戊二烯)]二羰基鈷, 醯胺基, HetCOR NMR, B3LYP