

Synthesis and oxidation of (benzimidazolylidene)Cr(CO)₅ complexes

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Abstract

A series of (benzimidazolylidene)pentacarbonylchromium(0) complexes were synthesized by the addition of lithium 1,2-phenylenediamides to Cr(CO)₆ in the presence of 12-crown-4, followed by the treatment of chlorotrimethylsilane. X-ray crystal structural analysis revealed a rather single-bond-like character between Cr and the carbene carbon. One reversible oxidation process was observed in the cyclic voltammograms of these complexes. Chemical oxidation using (4-BrC₆H₄)₃NSbCl₆ was studied by ESR to afford a hyperfine structure derived not from Cr but from N and H, indicating that the spin is delocalized on the benzimidazolidene moiety.

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Keywords: Cr(0) complex; Benzimidazolylidene; Carbene complex; Oxidation

1. Introduction

N-Heterocyclic carbenes such as imidazolylidenes possess advantageous characters as organometallic ligands, to broaden the scope of applications accessible to phosphanes [1]. *N,N'*-Heterocyclic carbenes exist in a singlet (σ^2) electronic ground state. Inductive effect of the nitrogen atoms induces a large σ - p_π gap by stabilizing the non-bonding σ orbital while leaving the p_π orbital energetically unchanged. Additional mesomeric stabilization of the heterocyclic carbene by the lone pairs at the nitrogen substituents results formally in a three-center, four-electron π -system [2]. The heteroatom-stabilized group 6 metal carbene complexes have received considerable attention due to the higher stability than the corresponding free carbenes. The carbene complexes have been employed as far beyond as a sim-

ple carbene-transferring reagent [3]. Use of the more stable carbene ligands, which may coordinate to chromium with the σ donor character, is expected to provide the more stable complexes with chromium pentacarbonyl. On the other hand, these type of carbenes show a very little π -acceptor character because it is rather difficult to induce back donation from d-orbital to p_π -orbital. The ratio of the back donation can be increased if the mesomeric stabilization of the heterocyclic moiety is reduced. Thus, the oxidized form of the imidazolylidene ligand is considered to increase the contribution of the back donation from metal center. Although some reactions of group 6 metal carbene complexes induced by oxidation and/or reduction have been reported [4], there are few reports concerning with the study of oxidized/reduced intermediates [5,6]. To clarify the oxidized state, the benzimidazolylidene ligand was chosen partly because the radical cation species might be stabilized by delocalization through the enlarged π -conjugation. In this paper, we describe a general route to a series of (benzimidazolylidene)Cr(CO)₅ complexes, and their structural and electronic characterization.

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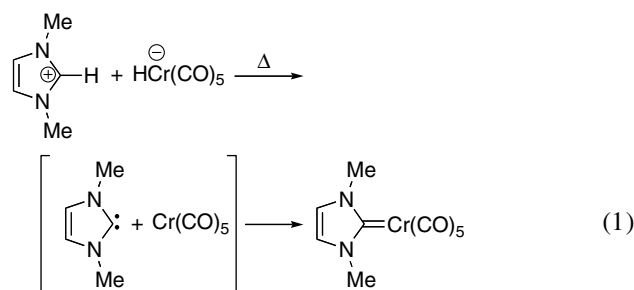
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2. Results and discussion

2.1. Synthesis and characterization of chromium complexes

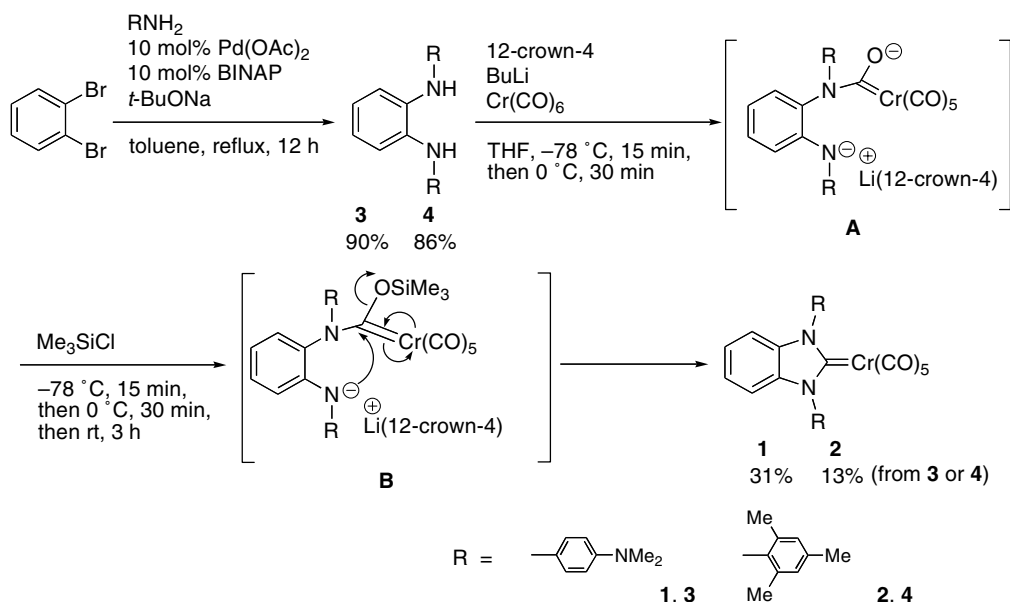
Since the first report by Öfele in 1968 [7], chromium complexes bearing the imidazolylidene ligand have been synthesized usually from the free imidazolylidene and coordinatively unsaturated “Cr(CO)₅” species (Eq. (1)). However, not a few imidazolylidenes have been isolated so far. Although several synthetic methods without isolation of imidazolylidenes have been developed [8,9], a more convenient route for the direct preparation from the corresponding 1,2-phenylenediamine derivatives was investigated. A new synthetic pathway to the benzimidazolylidene complexes is shown in Scheme 1. 4-Dimethylaminophenyl and mesityl (2,4,6-trimethylphenyl) groups are selected as a substituent on the nitrogen. 1,2-Dibromobenzene was treated with *N,N'*-dimethyl-1,4-phenylenediamine in the presence of *t*-BuONa, 10 mol% of Pd(OAc)₂, and 2,2'-bis(diphenylphosphino)-1,1'-binaphthyl (BINAP) in toluene [10,11], to give **3** in 90% yield. The mesityl derivatives **4** was also obtained in the similar manner in 86% yield. Thus-obtained diamine **3** or **4** was deprotonated with BuLi in the presence of 12-crown-4, followed by the addition of Cr(CO)₆, to generate the carbamoyl chromate intermediate **A** [12]. Chlorotrimethylsilane promoted the second intramolecular nucleophilic attack [13] of the lithium amide **B**. After the silica-gel column chromatography and recrystallization from MeCN or hexane, (1,3-diaryl-2-benzimidazolylidene)Cr(CO)₅ **1** or **2** was obtained as

a slightly pale yellow crystal. As expected, these complexes are stable enough to be handled under air.



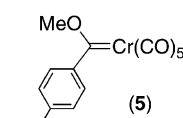
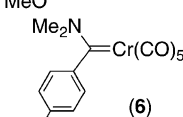
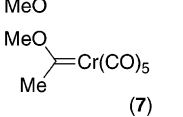
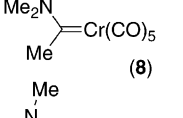
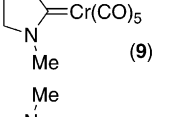
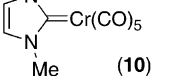
Chemical shifts of the carbene carbons in the ¹³C NMR spectra and IR stretching bands of the *trans*-carbonyl groups for representative Fischer-type chromium carbene complexes, together with **1** and **2** are listed in Table 1 [7,14,15]. As for ¹³C NMR, the more π-donating substituent such as the dialkylamino group tends to cause the higher-field shift of the carbene carbon, as exemplified by complexes **5** and **6**, **7** and **8**. The chemical shifts of the carbene carbons of **1** and **2** are 209.8 and 210.0 ppm, respectively, indicating that the *N,N'*-diaryl-1,2-phenylenediamine units possess very strong π-donating character. This inclination is in good agreement with the chemical shifts of the related imidazolylidene complexes **9** and **10**.

The frequency assignable to the *trans*-carbonyl group reflects on the π-back donation character of the ligands. The wavelength of ν_{CO*trans*} of Fischer-type chromium carbene complexes ranges from 1930 to 1960 cm⁻¹. The imidazolylidene complexes **9** and **10** showed the



Scheme 1. Preparation of the (benzimidazolylidene)Cr(CO)₅ complexes **1** and **2** via double nucleophilic attack route.

Table 1
Selected data for the representative chromium carbene complexes including **1** and **2** [7,14,15]

	$^{13}\text{C-NMR}$ (CDCl_3) C_{carbene} (ppm)	IR CO_{trans} ν_{CO} (cm^{-1})
1	209.8 (CD_2Cl_2)	1912
2	210.0 (CD_2Cl_2)	1916
 (5)	342.6	1941
 (6)	275.8	1931
 (7)	361.0	1948
 (8)	274.3	1930
 (9)	220.7	1926
 (10)	188.3 (CD_3CN)	1925

wavelength around 1925 cm^{-1} due to the lack of their π -back donation character. On the other hand, $\nu_{\text{CO}_{\text{trans}}}$ of **1** and **2** was further shifted to 1912 and 1916 cm^{-1} , respectively. These results indicate that the benzimidazolylidene complexes **1** and **2** exhibit very strong π -donating and very weak π -back donating characters. It should be noted that the values of $\nu_{\text{CO}_{\text{trans}}}$ are not attributed only to π -back donation abilities [16].

2.2. X-ray crystallography

The structures of **1** and **2** were furthermore determined by X-ray crystallography (Fig. 1). The bond lengths of Cr–C1(carbene) in **1** and **2** are 2.125 and 2.131 \AA , respectively, representing medium bond characters between a single bond and a double bond one (cf. **8**, 2.116 \AA ; **10**, 2.139 \AA). Little d– p_{π} electronic back donation is present in both complexes. The plane angles between the *N*-attached benzene ring and center imidazolidene ring were 79.1° and 99.8° for **1**, and 96.2° and 91.6° for **2**, respectively. Due to the steric effect of the methyl group of **2**, the mesitylene ring of **2** was more perpendicular to the central imidazolidene ring than the

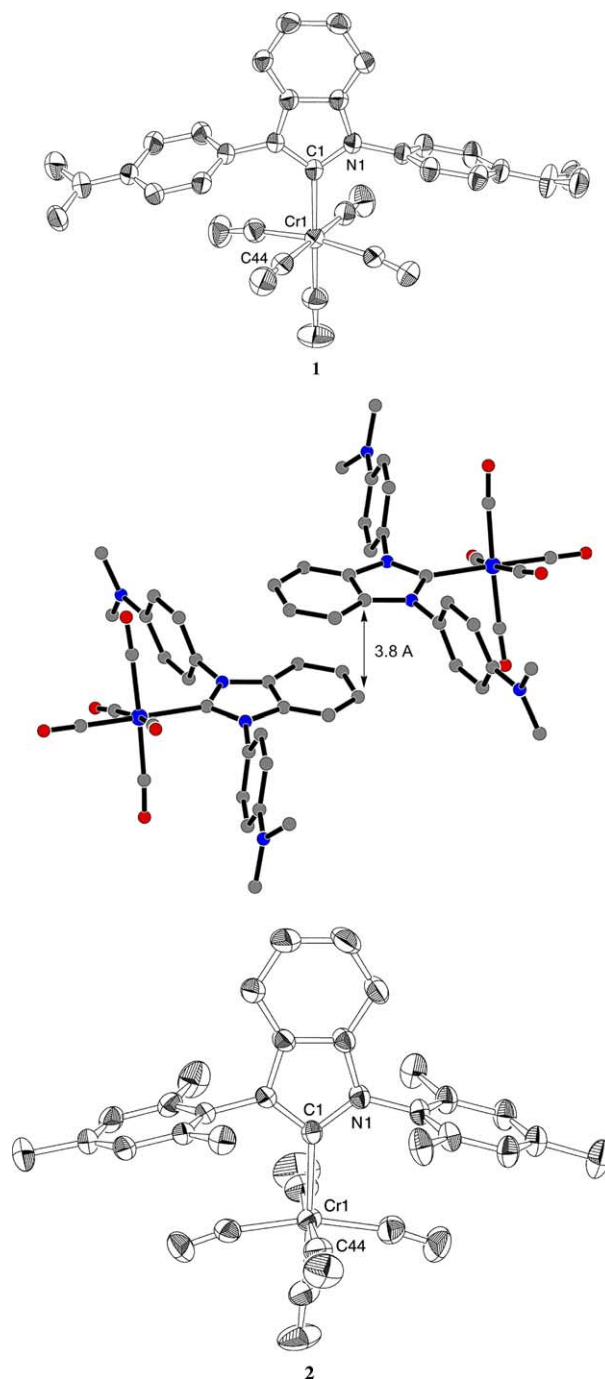


Fig. 1. ORTEP diagram of **1** and **2** and the crystal packing of **1**. Hydrogen atoms are omitted for clarity.

dimethylaminobenzene ring of **1**. The torsion angles of N1, C1, Cr1, C44 in **1** and **2** were 116.5° and 92° , respectively, suggesting that the degree of d– p_{π} orbital overlap is sterically affected by the steric effect of the *N*-substituent attached to the benzimidazolidene ring.

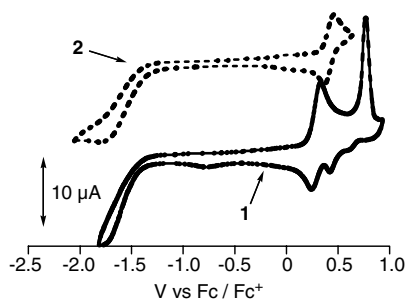
The electronic repulsion between the π -electrons of the *N*-attached benzene ring and the carbonyl group is considered to cause the distortion of coordination geometry of Cr center, resulting in the angles C41–Cr1–C43

of $169.56(10)^\circ$ for **1** and $164.7(1)^\circ$ for **2**. Furthermore, the benzimidazolide rings of **1** are intermolecularly overlapped in a face-to-face manner to form the π -stack dimer in the crystal packing.

2.3. Oxidation of the chromium complexes

Electrochemical behavior of **1** and **2** was next investigated. In the cyclic voltammogram of **1** in CH_2Cl_2 , one reversible oxidation wave and one irreversible oxidation wave were observed at the potentials of 330 and 770 mV vs. Fc/Fc^+ , respectively, being in contrast to one reversible oxidation wave at 450 mV with **2** (Fig. 2). These reversible oxidation waves might correspond to the one-electron process attributable to the oxidation of the benzimidazolide ring, suggesting that the radical cation species is stable.

To confirm the radical cation species, chemical oxidation of **2** was conducted. As an oxidant, tris-(4-bromophenyl)aminium hexachloroantimonate [17] ($E_{1/2} = 0.70$ V vs. Fc/Fc^+) was chosen. Chemical oxidation of **2** with one equivalent of $(4\text{-BrC}_6\text{H}_4)_3\text{NSbCl}_6$ in CH_2Cl_2 at 233 K yielded a reddish purple solution, which might correspond to a radical species of the imidazolide ring, and the color did not change when the solution was warmed up to 297 K. The ESR spectrum at 297 K showed no peak derived from the coupling of ^{53}Cr , but a hyperfine structure resulting from ^{14}N and ^1H nuclei at the benzimidazolide ring ($g = 2.005$, $A_{\text{N}} = 5.0$ G, $A_{\text{H}} = 1.3$ G) (Fig. 3). These coupling constant suggests that the radical cation is delocalized at the benzimidazolide ring. The very similar ESR spectrum was also observed in the oxidation of **1** ($g = 2.005$, $A_{\text{N}} = 5.0$ G, $A_{\text{H}} = 1.3$ G) with $(4\text{-BrC}_6\text{H}_4)_3\text{NSbCl}_6$. In contrast, in Lappert's imidazolylidene chromium radical cation complexes [5], these radicals are not coupled with nitrogen but coupled with only Cr and coordinated phosphines (Fig. 4). These differ-



Complex	E_1^{ox} (V)	E_2^{ox} (V)
1	0.33	0.77
2	0.45	-

Fig. 2. Cyclic voltammograms of **1** and **2**. 5.0×10^{-4} M in CH_2Cl_2 (0.1 M Bu_4NPF_6) with a platinum working electrode at 100 mV/s scan rate.

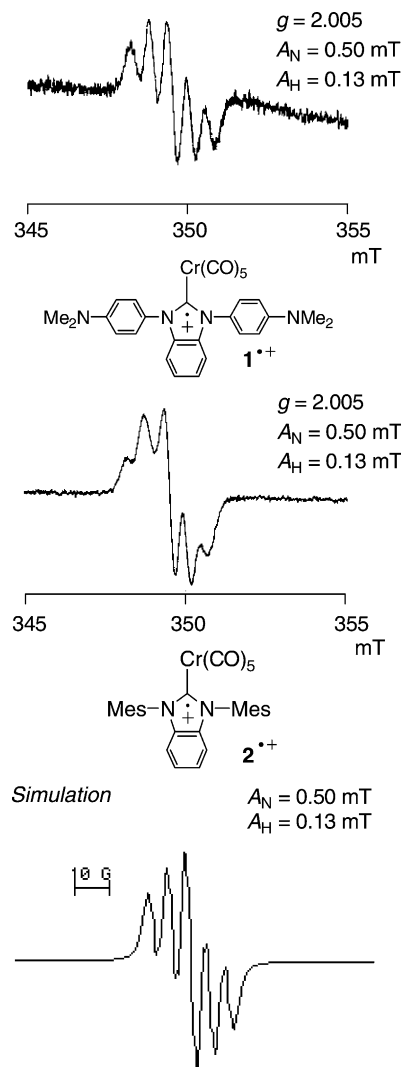


Fig. 3. ESR spectra of radical cation species of **1** and **2** and simulation.

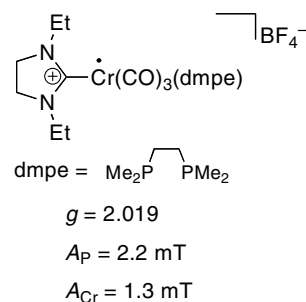


Fig. 4. Lappert's radical cation complex of (imidazolylidene)- $\text{Cr}(\text{CO})_3(\text{dmpe})$.

ences suggest that the electronic character of chromium carbene complexes is dependent on the ligands. The benzimidazolide ligand, which possesses larger π -conjugation, effectively stabilizes the radical cation species, diminishing the donation effect from d-orbital of Cr to p_{π} -orbital.

3. Summary

As described above, (benzimidazolylidene)pentacarbonylchromium(0) complexes were synthesized and characterized. Spectroscopic and X-ray crystal structural analysis of the neutral carbene complex revealed that the back-donation effect from d-orbital of Cr to p_{π} -orbital of carbene carbon is limited. Chemical oxidation of **1** and **2** afforded the radical cation complexes, which were detected by ESR spectra. Since the hyperfine structure resulting from the coupling of ^{53}Cr was not observed, the d- p_{π} back donation effect is also restricted even in the oxidized state. It is probably because the expansion of π -conjugation in the ligand affects the characters of the chromium complexes. These phenomena indicate that the ligand design of carbene complexes might be important to control the characteristics and reactivities of the metal center.

4. Experimental

4.1. General procedures

All melting points are uncorrected. ^1H (300 MHz) and ^{13}C (75 MHz) NMR spectra were measured on a Varian Mercury 300 spectrometer. CDCl_3 was used as a solvent and residual chloroform ($\delta = 7.24$ ppm; ^{13}C , 77.0 ppm) or Me_4Si was used as an internal standard. Infrared spectra were recorded on JASCO FT/IR-480plus. Mass spectra were measured on a JEOL JMS-DX-303 spectrometer using either electron impact (EI) or chemical ionization (CI) modes. ESR spectra were measured with Bruker ESP 300 electron spin resonance spectrophotometer. The cyclic voltammetry measurements were performed on a BAS CV-50W voltammetry analyzer in deaerated CH_2Cl_2 containing 0.1 M Bu_4NClO_4 as a supporting electrolyte at 298 K with a three-electrode system consisting of a stationary platinum working electrode (BAS), a platinum auxiliary electrode (BAS), and an Ag/AgCl (0.01 M) reference electrode (BAS) at 100 mV/s scan rate. Potentials are given vs. Fc/Fc^+ . Elemental analyses were carried out at the Analytical Center, Graduate School of Engineering, Osaka University. Column chromatography was conducted on silica gel (Wakogel C-200). Toluene was freshly distilled from CaH_2 . THF was purchased from Kanto Chemical Co., Inc. as dehydrated stabilizer free grade, and were collected with argon stream introduced directly into the apparatus. All reagents were purchased from commercial sources and were further purified prior to use with the standard methods. All of the operations were performed under argon atmosphere.

4.2. Synthesis of (benzimidazolylidene)pentacarbonylchromium(0) complexes

4.2.1. *N,N'*-Bis(4-dimethylaminophenyl)-1,2-phenylenediamine (**3**)

A well-dried three-necked round bottomed flask equipped with a condenser, a magnetic stirring bar, and a septum, was charged with (*rac*)-BINAP (250 mg, 0.4 mmol), $\text{Pd}(\text{OAc})_2$ (90 mg, 0.4 mmol), and toluene (20 mL). The mixture was heated to 60 °C with stirring, then 1,2-dibromobenzene (242 μL , 2.0 mmol) was added, followed by *N,N'*-dimethyl-1,4-phenylenediamine (637 mg, 4.7 mmol) and *t*-BuONa (480 mg, 5.0 mmol). The reaction mixture was heated to reflux until the 1,2-dibromobenzene was consumed (monitored by TLC). After cooling to room temperature, the reaction mixture was filtered through Celite and silica-gel pad and was washed with AcOEt, then the solvent was evaporated under vacuum. Column chromatography (hexane/AcOEt = 3/2, $R_f = 0.26$) of the residue afforded 624 mg (90%) of **3**; m.p. 108 °C (from hexane); IR (KBr) 3358, 2878, 2359, 1517, 1339, 1286 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) $\delta = 2.89$ (12H, s), 5.35 (2H, br), 6.74 (4H, d, $J = 9.0$ Hz), 6.82 (2H, dd, $J = 3.3$ and 5.7 Hz), 6.92 (4H, d, $J = 9.0$ Hz), 7.04 (2H, dd, $J = 3.3$ and 5.7 Hz); ^{13}C NMR (75 MHz, CDCl_3) 41.5, 114.4, 117.7, 120.8, 121.3, 134.1, 135.9, 146.3 ppm. Found: C, 76.19; H, 7.56; N, 16.03%. Calc. for $\text{C}_{22}\text{H}_{26}\text{N}_4$: C, 76.27; H, 7.56; N, 16.17%.

4.2.2. *N,N'*-Bis(mesityl)-1,2-phenylenediamine (**4**)

Compound **4** was prepared from 2,4,6-trimethylaniline according to the similar procedure as the preparation of **3**. Yield 86%; m.p. 180 °C (from hexane); IR (KBr) 3333, 3015, 2964, 2915, 2854, 1598, 1507, 1498, 1482, 1457, 1399 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) $\delta = 2.19$ (12H, s), 2.31 (6H, s), 5.11 (2H, br), 6.29 (2H, dd, $J = 3.3$ and 5.7 Hz), 6.66 (2H, dd, $J = 3.3$ and 5.7 Hz), 6.95 (4H, s); ^{13}C NMR (75 MHz, CDCl_3) 18.2, 20.9, 114.2, 119.9, 129.2, 133.3, 133.9, 135.1, 136.8 ppm. Found: C, 83.28; H, 8.06; N, 8.09%. Calc. for $\text{C}_{24}\text{H}_{28}\text{N}_2$: C, 83.68; H, 8.19; N, 8.13%.

4.2.3. (1,3-Bis(4'-dimethylaminophenyl)benzimidazol-2-ylidene)pentacarbonylchromium(0) (**1**)

A well-dried three-necked round bottomed flask equipped with a condenser, a magnetic stirring bar, and a septum, was charged with 12-crown-4 (867 μL , 5.36 mmol), which was azeotropically dehydrated with toluene. After the addition of THF (12 mL) solution of the 1,2-phenylenediamine **3** (928 mg, 2.68 mmol), the mixture was cooled to -78 °C and BuLi (4.53 mL, 5.36 mmol) was added dropwise via syringe. A THF (20 mL) solution of $\text{Cr}(\text{CO})_6$ (590 mg, 2.68 mmol) was added to the reaction mixture via can-

nula. The solution was stirred for 15 min at $-78\text{ }^{\circ}\text{C}$ and for 30 min at $0\text{ }^{\circ}\text{C}$, then was cooled to $-78\text{ }^{\circ}\text{C}$ again. Chlorotrimethylsilane ($400\text{ }\mu\text{L}$, 3.15 mmol) was added dropwise. The thus-obtained reaction mixture was stirred for 15 min at $-78\text{ }^{\circ}\text{C}$, for 30 min at $0\text{ }^{\circ}\text{C}$, and then for 1 h at room temperature. The solvent was removed under vacuum. The crude product was purified by silica-gel column chromatography (CH_2Cl_2) to afford 451 mg (31%) of **1**; m.p. $172\text{ }^{\circ}\text{C}$ (dec.) (from MeCN); IR (KBr) 2051 , 1972 , 1912 , 1895 cm^{-1} ; ^1H NMR (300 MHz , CD_2Cl_2) $\delta = 3.07$ (12H , s), 6.88 (4H , d, $J = 8.4\text{ Hz}$), 6.89 (2H , dd, $J = 3.0$ and 6.0 Hz), 7.17 (2H , dd, $J = 3.0$ and 6.0 Hz), 7.31 (4H , d, $J = 8.4\text{ Hz}$); ^{13}C NMR (75 MHz , CDCl_3) 40.0 , 110.3 , 112.1 , 122.5 , 127.2 , 129.5 , 137.2 , 151.0 , 209.8 (*Ccarbene*), 217.0 (*COcis*), 222.1 (*COtrans*) ppm. Found: C, 61.05% ; H, 4.42% ; N, 10.20% . Calc. for $\text{C}_{28}\text{H}_{24}\text{CrN}_4\text{O}_5$: C, 61.31% ; H, 4.41% ; N, 10.21% .

4.2.4. (1,3-Bis(2',4',6'-trimethylphenyl)benzimidazol-2-ylidene)pentacarbonyl chromium(0) (**2**)

Compound **2** was prepared from **4** according to the similar procedure as the preparation of **1** except hexane/EtOAc = $95/5$ was used as an eluent for chromatography. Yield 13% ; m.p. $161\text{ }^{\circ}\text{C}$ (dec.) (from hexane); IR (KBr) 2052 , 1950 , 1916 , 1883 cm^{-1} ; ^1H NMR (300 MHz , CD_2Cl_2) $\delta = 2.00$ (12H , s), 2.42 (6H , s), 6.77 (2H , dd, $J = 3.3$ and 6.3 Hz), 7.13 (4H , s), 7.21 (2H , dd, $J = 3.3$ and 6.3 Hz); ^{13}C NMR (75 MHz , CD_2Cl_2) 17.1 , 20.7 , 110.1 , 123.3 , 129.4 , 134.0 , 135.4 , 136.2 , 139.7 , 210.0 (*Ccarbene*), 215.7 (*COcis*), 220.9 (*COtrans*) ppm. Found: C, 65.97% ; H, 4.83% ; N, 5.11% . Calc. for $\text{C}_{30}\text{H}_{26}\text{CrN}_2\text{O}_5$: C, 65.93% ; H, 4.80% ; N, 5.13% .

4.3. X-ray structure analysis

All measurements for **1** and **2** were made on a Rigaku RAXIS-RAPID Imaging Plate diffractometer with

graphite monochromated Mo $\text{K}\alpha$ radiation. The structures of **1** and **2** were solved by direct methods and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. The H atoms were placed in idealized positions and allowed to ride with the C atoms to which each was bonded. Crystallographic details are given in Table 2. Crystallographic data (excluding structure factors) for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-256806 for **1** and no. CCDC-256807 for **2**. Copies of this information may be obtained free of charge from: The Director, CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK (fax: +44 1223 336 033; email: deposit@ccdc.cam.ac.uk or www: <http://www.ccdc.cam.ac.uk>).

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Table 2
Crystallographic data for **1** and **2**

	1	2
Formula	$\text{C}_{28}\text{H}_{24}\text{CrN}_4\text{O}_5$	$\text{C}_{30}\text{H}_{26}\text{CrN}_2\text{O}_5$
Formula weight	548.12	546.12
Crystal system	Triclinic	Monoclinic
Space Group	$P\bar{1}$ (#2)	$P2_1/c$ (#14)
a (Å)	10.886(1)	9.8901(3)
b (Å)	13.728(1)	17.6812(6)
c (Å)	10.2393(8)	16.6486(7)
α (°)	101.392(3)	
β (°)	109.249(4)	101.949(1)
γ (°)	67.020(4)	
Volume (Å ³)	1325.8(2)	2848.2(2)
Z	2	4
R_1	0.046	0.051
wR_2	0.157	0.181