



Supporting Information

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Homolytic bond strengths and formation rates in half-sandwich chromium-alkyl complexes: relevance for controlled radical polymerization

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1. Synthesis and characterization of Organochromium Complexes

General Considerations

All compounds were synthesized and stored under N₂ using standard Schlenk and glovebox techniques. Samples for X-ray diffraction, melting point determination, elemental analysis, and UV-visible spectroscopy were prepared in a glovebox. Melting point determinations were performed in flame-sealed tubes and are uncorrected. All UV-visible measurements were conducted in pentane solution in a specially-constructed cell for air-sensitive samples: a Kontes Hi-Vac® Valve with PTFE Plug was attached by a professional glassblower to a Hellma 10 mm path length quartz absorption cell with a quartz-to-glass graded seal. Elemental analyses were performed by Guelph Chemical Laboratories, Guelph, ON, Canada.

The symmetric β -diketiminato ligand, XylNHC(Me)CHC(Me)NXyl (Xyl = 2,6-Me₂C₆H₃) was prepared according to the literature procedure.¹ The mixed N-aryl β -diketiminato ligands, DppNHC(Me)CHC(Me)Ar (Ar = C₆H₅, *p*-C₆H₄OMe, or *p*-C₆H₄CF₃), were prepared by reacting the appropriate aniline (Aldrich) with DppNHC(Me)CHC(Me)O,² according to the literature procedure previously used to synthesize the corresponding Ar = *o*-C₆H₄OMe derivative.² CrCl₂(tmada) (tmada = N, N, N', N'-tetramethylethylenediamine) was prepared according to the literature procedure.³ THF, Et₂O, toluene and pentane were dried using Grubbs/Dow columns.⁴ Anhydrous reagents (2.0 M BuLi in pentane, 2.0 M NaCp in THF, 1.0 PhCH₂MgCl in Et₂O, 1,4-dioxane) were purchased from Aldrich, stored in a glovebox and used as received. Iodine was purified by sublimation and stored in a glovebox. Celite (Aldrich) was dried overnight in a 110 °C oven before being evacuated and stored in a glovebox. Filtrations were performed through Celite supported on a sintered glass frit, or through Celite supported on a Kimwipe in a glass pipette.

Synthesis of CpCr[(XylNCMe)₂CH] (2)

In a glovebox, XylNHC(Me)CHC(Me)NXyl (2.1834 g, 7.124 mmol) was dissolved in 10 mL THF in a 20 mL scintillation vial, and chilled in a -30 °C freezer for 30 min. To the cold solution was added BuLi (3.6 mL of 2.0 M solution in pentane, 7.2 mmol) by syringe. In a separate 100 mL Schlenk reaction flask, NaCp (3.6 mL of 2.0 M solution in THF, 7.2 mmol) was added by syringe to a stirred suspension of CrCl₂(tmada) (1.7034 g, 7.124 mmol) in 25 mL of THF at 25 °C. After both solutions had reacted for 30 min, the yellow solution of the deprotonated ligand was added dropwise to the reaction mixture in the Schlenk flask, which then turned green to incident light and magenta to transmitted light. After the reaction mixture had stirred overnight at 25 °C, the solvent was removed *in vacuo*, the residue was extracted with pentane and filtered. The solvent was again removed in vacuo, and the residue was extracted with pentane and filtered into four 20 mL scintillation vials which were placed in a -30 °C freezer overnight to yield 1.2185 g of product as black crystals (41.7% yield). Anal. Calcd.

¹ Budzelaar, P. H. M.; de Gelder, R.; Gal, A. W. *Organometallics* **1998**, *17*, 4121-4123.

² Dove, A. P.; Gibson, V. C.; Marshall, E. L.; White, A. J. P.; Williams, D. J. *Dalton Trans.* **2004**, 570-578.

³ Hao, S.; Song, J.-I.; Berno, P.; Gambarotta, S. *Organometallics* **1994**, *13*, 1326-1335.

⁴ Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996**, *15*, 1518-1520.

for C₂₆H₃₀CrN₂: C, 74.64; H, 7.61; N, 6.22. Found: C, 74.27; H, 7.49; N, 6.78. Melting point: 172–174 °C (dec). UV-vis (pentane): λ_{\max} (ϵ) 307 nm (11400 M⁻¹ cm⁻¹), 427 nm (6300 M⁻¹ cm⁻¹), 558 nm (1200 M⁻¹ cm⁻¹), 748 nm (850 M⁻¹ cm⁻¹).

Synthesis of CpCr[DppNC(Me)CHC(Me)NC₆H₅] (3)

This complex was prepared on a 1.558 mmol scale using the procedure described for **2**, above, using the DppNHC(Me)CHC(Me)NC₆H₅ ligand (yield: 0.4860g, 69.2%). UV-vis (pentane): λ_{\max} (ϵ) 300 nm (11000 M⁻¹ cm⁻¹), 419 nm (7400 M⁻¹ cm⁻¹), 559 nm (1100 M⁻¹ cm⁻¹), 738 nm (660 M⁻¹ cm⁻¹).

Synthesis of CpCr[DppNC(Me)CHC(Me)N(p-C₆H₄OMe)] (4)

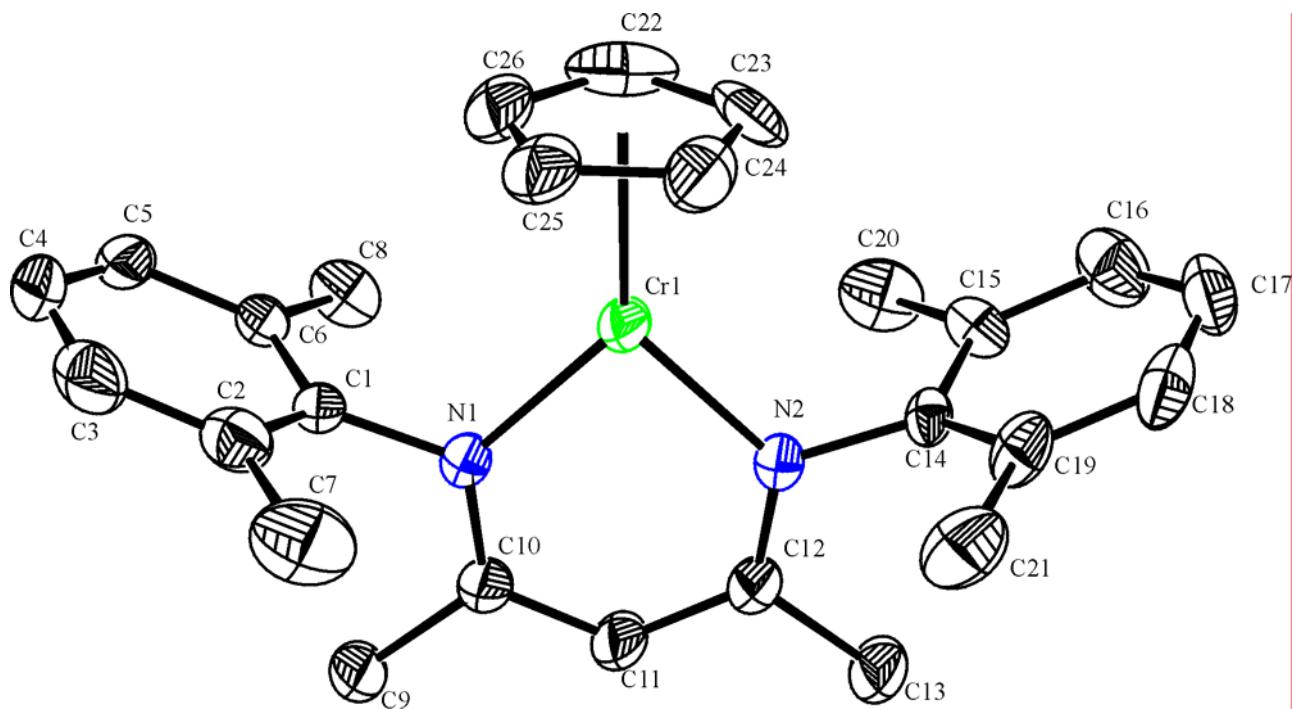
This complex was prepared on a 1.2042 mmol scale using the procedure described for **2**, above, using the DppNHC(Me)CHC(Me)N(p-C₆H₄OMe)ligand (yield: 0.0997g, 17.2%). UV-vis (pentane): λ_{\max} (ϵ) 309 nm (13900 M⁻¹ cm⁻¹), 429 nm (8600 M⁻¹ cm⁻¹), 564 nm (1100 M⁻¹ cm⁻¹), 761 nm (600 M⁻¹ cm⁻¹).

Synthesis of CpCr[DppNC(Me)CHC(Me)N(p-C₆H₄CF₃)] (5)

This complex was prepared on a 0.6581 mmol scale using the procedure described for **2**, above, using the DppNHC(Me)CHC(Me)NC₆H₅ ligand (yield: 0.1297 g, 38.0%). UV-vis (pentane): λ_{\max} (ϵ) 310 nm (12000 M⁻¹ cm⁻¹), 429 nm (6900 M⁻¹ cm⁻¹), 543 nm (1200 M⁻¹ cm⁻¹), 748 nm (750 M⁻¹ cm⁻¹).

2. X-ray analyses

2.1 Compound 2



Data Collection

A black prism crystal of $C_{26}H_{30}N_2Cr$ having approximate dimensions of $0.20 \times 0.30 \times 0.50$ mm was mounted on a glass fiber. All measurements were made on a Bruker X8 APEX diffractometer with graphite monochromated Mo-K α radiation. The data were collected at a temperature of $-100.0 \pm 0.1^\circ\text{C}$ to a maximum 2θ value of 55.7° . Data were collected in a series of ϕ and ω scans in 0.50° oscillations with 6.0 second exposures. The crystal-to-detector distance was 38.94 mm.

Data Reduction

Of the 31251 reflections that were collected, 5558 were unique ($R_{\text{int}} = 0.031$); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT¹ software package. The linear absorption coefficient, μ , for Mo-K α radiation is 12.01 cm^{-1} . Data were corrected for absorption effects using the multi-scan technique (SADABS²), with minimum and maximum transmission coefficients of 0.693 and 0.786, respectively. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods³. The material is crystallizes with disorder in the Cp ring as well as with one 2,6-dimethylphenyl group. Each disordered group was modeled in two orientations, with a roughly 60:40 ratio between the major and minor fragments. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included in calculated positions but were not refined. The final cycle of full-matrix least-squares refinement⁴ on F^2 was based on 5558 reflections and 355 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \sum |F_O| - |F_C| / \sum |F_O| = 0.057$$

$$wR2 = [\sum (w(F_O^2 - F_C^2)^2) / \sum w(F_O^2)^2]^{1/2} = 0.098$$

The standard deviation of an observation of unit weight⁵ was 1.01. The weighting scheme was based on counting statistics. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.23 and $-0.48 \text{ e}^-/\text{\AA}^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber⁶. Anomalous dispersion effects were included in F_{calc} ⁷; the values for Δf and $\Delta f''$ were those of Creagh and McAuley⁸. The values for the mass attenuation coefficients are those of Creagh and Hubbell⁹. All refinements were performed using the SHELXTL¹⁰ crystallographic software package of Bruker-AXS.

References

- (1) SAINT. Version 7.03A. Bruker AXS Inc., Madison, Wisconsin, USA. (1997-2003).
- (2) SADABS. Bruker Nonius area detector scaling and absorption correction - V2.10, Bruker AXS Inc., Madison, Wisconsin, USA (2003).
- (3) SIR97 - Altomare A., Burla M.C., Camalli M., Cascarano G.L., Giacovazzo C., Guagliardi A., Moliterni A.G.G., Polidori G., Spagna R. (1999) J. Appl. Cryst. 32, 115-119.
- (4) Least Squares function minimized:

$$\sum w(F_O^2 - F_C^2)^2$$
- (5) Standard deviation of an observation of unit weight:

$$[\sum w(F_O^2 - F_C^2)^2 / (N_O - N_V)]^{1/2}$$

where: N_O = number of observations
 N_V = number of variables
- (6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).
- (7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).
- (8) Creagh, D. C. & McAuley, W.J.; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).
- (9) Creagh, D. C. & Hubbell, J.H.; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).
- (10) SHELXTL Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA. (1997).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	C ₂₆ H ₃₀ N ₂ Cr
Formula Weight	422.52
Crystal Color, Habit	black, prism
Crystal Dimensions	0.20 X 0.35 X 0.50 mm
Crystal System	monoclinic
Lattice Type	primitive
Lattice Parameters	a = 8.2172(3) Å b = 16.2567(5) Å c = 17.5299(5) Å α = 90.0 ° β = 94.007(2) ° γ = 90.0 ° V = 2336.0(1) Å ³
Space Group	P 2 ₁ /c (#14)
Z value	4
D _{calc}	1.201 g/cm ³
F ₀₀₀	896.00
μ (MoK α)	12.01 cm ⁻¹

B. Intensity Measurements

Diffractometer	Bruker X8 APEX
Radiation	MoK α ($\lambda = 0.71073 \text{ \AA}$) graphite monochromated
Data Images	1560 exposures @ 6.0 seconds
Detector Position	38.94 mm
$2\theta_{\max}$	55.7°
No. of Reflections Measured	Total: 31251 Unique: 5558($R_{\text{int}} = 0.031$) Absorption ($T_{\min} = 0.693$, $T_{\max} = 0.786$) Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR97)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma w (F_o^2 - F_c^2)^2$
Least Squares Weights	$w=1/(\sigma^2(F_o^2)+(0.0424P)^2+0.9833P)$
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ($I > 0.00\sigma(I)$)	5558
No. Variables	355
Reflection/Parameter Ratio	15.66
Residuals (refined on F^2 , all data): R1; wR2	0.057; 0.098
Goodness of Fit Indicator	1.01
No. Observations ($I > 2.00\sigma(I)$)	4060
Residuals (refined on F): R1; wR2	0.035; 0.085
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.23 e $^-/\text{\AA}^3$
Minimum peak in Final Diff. Map	-0.48 e $^-/\text{\AA}^3$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ks043.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$	occ
C(1)	6119(2)	2448(1)	5228(1)	27(1)	
C(2)	4437(2)	2572(1)	5226(1)	39(1)	
C(3)	3794(2)	3318(1)	4955(1)	49(1)	
C(4)	4782(3)	3921(1)	4708(1)	50(1)	
C(5)	6442(2)	3798(1)	4711(1)	40(1)	
C(6)	7145(2)	3061(1)	4965(1)	29(1)	
C(7)	3349(3)	1914(2)	5521(2)	65(1)	
C(8)	8942(2)	2923(1)	4967(1)	42(1)	
C(9)	6403(3)	1116(1)	4260(1)	45(1)	
C(10)	7012(2)	1068(1)	5094(1)	36(1)	
C(11)	7749(3)	329(1)	5343(1)	44(1)	
C(12)	8370(2)	115(1)	6080(1)	37(1)	
C(13)	9087(3)	-741(1)	6181(1)	48(1)	
C(14)	9071(7)	298(5)	7393(3)	24(1) 0.60(2)	
C(15)	10694(7)	491(4)	7591(3)	30(1) 0.60(2)	
C(16)	11389(7)	289(4)	8313(3)	51(1) 0.60(2)	
C(17)	10460(9)	-106(4)	8836(2)	48(2) 0.60(2)	
C(18)	8837(9)	-298(4)	8638(3)	42(2) 0.60(2)	
C(19)	8143(7)	-96(5)	7917(4)	37(1) 0.60(2)	
C(20)	11648(13)	946(6)	7033(5)	53(2) 0.60(2)	
C(21)	6323(14)	-251(7)	7737(6)	54(2) 0.60(2)	
C(22)	8364(12)	2897(7)	7383(6)	58(2) 0.60(2)	
C(23)	8083(13)	2260(6)	7878(4)	54(3) 0.60(2)	
C(24)	6382(15)	2159(7)	7839(7)	48(2) 0.60(2)	
C(25)	5701(11)	2693(5)	7312(5)	44(1) 0.60(2)	
C(26)	6949(9)	3120(5)	7012(5)	48(3) 0.60(2)	
N(1)	6835(2)	1709(1)	5548(1)	31(1)	
N(2)	8342(2)	610(1)	6682(1)	32(1)	
Cr(1)	7467(1)	1770(1)	6678(1)	36(1)	
C(14B)	8817(11)	344(8)	7439(4)	27(2) 0.40(2)	
C(15B)	10405(11)	444(7)	7754(6)	48(2) 0.40(2)	
C(16B)	10861(16)	114(7)	8469(6)	56(3) 0.40(2)	
C(17B)	9730(20)	-315(6)	8869(4)	63(4) 0.40(2)	
C(18B)	8140(20)	-415(5)	8554(4)	56(3) 0.40(2)	
C(19B)	7686(13)	-85(7)	7839(5)	27(2) 0.40(2)	
C(20B)	11730(20)	864(13)	7309(11)	84(5) 0.40(2)	
C(21B)	6000(20)	-218(11)	7474(10)	61(3) 0.40(2)	
C(22B)	8746(13)	2977(8)	7268(7)	40(2) 0.40(2)	
C(23B)	8695(18)	2356(8)	7836(7)	54(3) 0.40(2)	
C(24B)	7040(20)	2136(7)	7899(7)	50(4) 0.40(2)	
C(25B)	6064(14)	2620(8)	7370(8)	74(5) 0.40(2)	
C(26B)	7119(14)	3140(7)	6980(7)	66(6) 0.40(2)	

Table 3. Bond lengths [Å] and angles [deg] for ks043.

C(1)-C(2)	1.396(2)
C(1)-C(6)	1.403(2)
C(1)-N(1)	1.4346(18)
C(2)-C(3)	1.393(3)
C(2)-C(7)	1.508(3)
C(3)-C(4)	1.364(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.378(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.390(2)
C(5)-H(5)	0.9500
C(6)-C(8)	1.493(2)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-C(10)	1.513(2)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-N(1)	1.325(2)
C(10)-C(11)	1.402(2)
C(11)-C(12)	1.400(2)
C(11)-H(11)	0.9500
C(12)-N(2)	1.329(2)
C(12)-C(13)	1.516(2)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(15)	1.3900
C(14)-C(19)	1.3900
C(14)-N(2)	1.437(4)
C(15)-C(16)	1.3900
C(15)-C(20)	1.493(9)
C(16)-C(17)	1.3900
C(16)-H(16)	0.9500
C(17)-C(18)	1.3900
C(17)-H(17)	0.9500
C(18)-C(19)	1.3900
C(18)-H(18)	0.9500
C(19)-C(21)	1.528(10)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(26)	1.342(8)
C(22)-C(23)	1.379(10)
C(22)-Cr(1)	2.301(10)
C(22)-H(22)	0.9500
C(23)-C(24)	1.404(9)
C(23)-Cr(1)	2.273(7)
C(23)-H(23)	0.9500
C(24)-C(25)	1.359(9)
C(24)-Cr(1)	2.365(13)
C(24)-H(24)	0.9500

C(25)-C(26)	1.373(8)
C(25)-Cr(1)	2.412(9)
C(25)-H(25)	0.9500
C(26)-Cr(1)	2.318(8)
C(26)-H(26)	0.9500
N(1)-Cr(1)	2.0147(13)
N(2)-C(14B)	1.424(6)
N(2)-Cr(1)	2.0185(13)
Cr(1)-C(25B)	2.216(13)
Cr(1)-C(24B)	2.273(13)
Cr(1)-C(26B)	2.311(13)
Cr(1)-C(23B)	2.400(13)
Cr(1)-C(22B)	2.422(13)
C(14B)-C(15B)	1.3900
C(14B)-C(19B)	1.3900
C(15B)-C(16B)	1.3900
C(15B)-C(20B)	1.546(17)
C(16B)-C(17B)	1.3900
C(16B)-H(16B)	0.9500
C(17B)-C(18B)	1.3900
C(17B)-H(17B)	0.9500
C(18B)-C(19B)	1.3900
C(18B)-H(18B)	0.9500
C(19B)-C(21B)	1.498(15)
C(20B)-H(20D)	0.9800
C(20B)-H(20E)	0.9800
C(20B)-H(20F)	0.9800
C(21B)-H(21D)	0.9800
C(21B)-H(21E)	0.9800
C(21B)-H(21F)	0.9800
C(22B)-C(26B)	1.4200
C(22B)-C(23B)	1.4200
C(22B)-H(22B)	0.9500
C(23B)-C(24B)	1.4200
C(23B)-H(23B)	0.9500
C(24B)-C(25B)	1.4200
C(24B)-H(24B)	0.9500
C(25B)-C(26B)	1.4200
C(25B)-H(25B)	0.9500
C(26B)-H(26B)	0.9500
C(2)-C(1)-C(6)	120.98(15)
C(2)-C(1)-N(1)	119.98(15)
C(6)-C(1)-N(1)	118.92(14)
C(3)-C(2)-C(1)	118.54(17)
C(3)-C(2)-C(7)	120.95(18)
C(1)-C(2)-C(7)	120.50(17)
C(4)-C(3)-C(2)	120.97(17)
C(4)-C(3)-H(3)	119.5
C(2)-C(3)-H(3)	119.5
C(3)-C(4)-C(5)	120.30(16)
C(3)-C(4)-H(4)	119.9
C(5)-C(4)-H(4)	119.9
C(4)-C(5)-C(6)	121.12(17)
C(4)-C(5)-H(5)	119.4
C(6)-C(5)-H(5)	119.4
C(5)-C(6)-C(1)	118.08(16)
C(5)-C(6)-C(8)	121.27(16)
C(1)-C(6)-C(8)	120.65(14)
C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5

H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-H(9A)	109.5
C(10)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(10)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
N(1)-C(10)-C(11)	123.38(15)
N(1)-C(10)-C(9)	119.78(14)
C(11)-C(10)-C(9)	116.84(14)
C(12)-C(11)-C(10)	128.50(16)
C(12)-C(11)-H(11)	115.7
C(10)-C(11)-H(11)	115.7
N(2)-C(12)-C(11)	123.84(15)
N(2)-C(12)-C(13)	119.47(15)
C(11)-C(12)-C(13)	116.69(15)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(19)	120.0
C(15)-C(14)-N(2)	118.2(3)
C(19)-C(14)-N(2)	121.4(3)
C(14)-C(15)-C(16)	120.0
C(14)-C(15)-C(20)	119.1(4)
C(16)-C(15)-C(20)	120.9(4)
C(17)-C(16)-C(15)	120.0
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(18)	120.0
C(16)-C(17)-H(17)	120.0
C(18)-C(17)-H(17)	120.0
C(17)-C(18)-C(19)	120.0
C(17)-C(18)-H(18)	120.0
C(19)-C(18)-H(18)	120.0
C(18)-C(19)-C(14)	120.0
C(18)-C(19)-C(21)	118.8(5)
C(14)-C(19)-C(21)	121.0(5)
C(26)-C(22)-C(23)	109.3(6)
C(26)-C(22)-Cr(1)	73.8(5)
C(23)-C(22)-Cr(1)	71.3(4)
C(26)-C(22)-H(22)	125.4
C(23)-C(22)-H(22)	125.4
Cr(1)-C(22)-H(22)	121.2
C(22)-C(23)-C(24)	105.5(6)
C(22)-C(23)-Cr(1)	73.6(4)
C(24)-C(23)-Cr(1)	76.0(6)
C(22)-C(23)-H(23)	127.3
C(24)-C(23)-H(23)	127.3
Cr(1)-C(23)-H(23)	115.7
C(25)-C(24)-C(23)	108.7(7)
C(25)-C(24)-Cr(1)	75.4(5)
C(23)-C(24)-Cr(1)	68.8(5)
C(25)-C(24)-H(24)	125.7

C(23)-C(24)-H(24)	125.7
Cr(1)-C(24)-H(24)	121.7
C(24)-C(25)-C(26)	107.4(7)
C(24)-C(25)-Cr(1)	71.6(6)
C(26)-C(25)-Cr(1)	69.4(4)
C(24)-C(25)-H(25)	126.3
C(26)-C(25)-H(25)	126.3
Cr(1)-C(25)-H(25)	124.4
C(22)-C(26)-C(25)	108.8(6)
C(22)-C(26)-Cr(1)	72.4(4)
C(25)-C(26)-Cr(1)	76.9(4)
C(22)-C(26)-H(26)	125.6
C(25)-C(26)-H(26)	125.6
Cr(1)-C(26)-H(26)	117.0
C(10)-N(1)-C(1)	118.88(13)
C(10)-N(1)-Cr(1)	126.70(11)
C(1)-N(1)-Cr(1)	114.41(9)
C(12)-N(2)-C(14B)	122.5(5)
C(12)-N(2)-C(14)	116.5(4)
C(14B)-N(2)-C(14)	9.6(7)
C(12)-N(2)-Cr(1)	126.10(11)
C(14B)-N(2)-Cr(1)	111.2(5)
C(14)-N(2)-Cr(1)	117.4(4)
N(1)-Cr(1)-N(2)	91.43(5)
N(1)-Cr(1)-C(25B)	117.5(4)
N(2)-Cr(1)-C(25B)	141.2(4)
N(1)-Cr(1)-C(23)	162.3(2)
N(2)-Cr(1)-C(23)	105.5(2)
N(1)-Cr(1)-C(24B)	153.2(4)
N(2)-Cr(1)-C(24B)	108.6(3)
C(25B)-Cr(1)-C(24B)	36.9(2)
N(1)-Cr(1)-C(22)	128.2(3)
N(2)-Cr(1)-C(22)	129.8(3)
C(23)-Cr(1)-C(22)	35.1(3)
N(1)-Cr(1)-C(26B)	104.2(3)
N(2)-Cr(1)-C(26B)	161.7(3)
C(25B)-Cr(1)-C(26B)	36.49(19)
C(24B)-Cr(1)-C(26B)	60.1(2)
C(22)-Cr(1)-C(26B)	31.8(4)
N(1)-Cr(1)-C(26)	104.8(2)
N(2)-Cr(1)-C(26)	162.8(2)
C(23)-Cr(1)-C(26)	57.8(2)
C(22)-Cr(1)-C(26)	33.8(2)
N(1)-Cr(1)-C(24)	140.6(3)
N(2)-Cr(1)-C(24)	113.7(3)
C(23)-Cr(1)-C(24)	35.2(2)
C(22)-Cr(1)-C(24)	56.7(3)
C(26)-Cr(1)-C(24)	56.1(3)
N(1)-Cr(1)-C(23B)	156.3(3)
N(2)-Cr(1)-C(23B)	103.8(3)
C(25B)-Cr(1)-C(23B)	59.5(2)
C(24B)-Cr(1)-C(23B)	35.24(18)
C(26B)-Cr(1)-C(23B)	58.3(2)
N(1)-Cr(1)-C(25)	111.2(2)
N(2)-Cr(1)-C(25)	143.58(17)
C(23)-Cr(1)-C(25)	57.2(3)
C(22)-Cr(1)-C(25)	55.8(3)
C(26)-Cr(1)-C(25)	33.7(2)
C(24)-Cr(1)-C(25)	33.0(2)
N(1)-Cr(1)-C(22B)	122.3(3)
N(2)-Cr(1)-C(22B)	127.7(3)
C(25B)-Cr(1)-C(22B)	59.2(2)
C(24B)-Cr(1)-C(22B)	58.5(2)

C(26B)-Cr(1)-C(22B)	34.82(17)
C(23B)-Cr(1)-C(22B)	34.25(17)
C(15B)-C(14B)-C(19B)	120.0
C(15B)-C(14B)-N(2)	121.5(5)
C(19B)-C(14B)-N(2)	118.2(5)
C(14B)-C(15B)-C(16B)	120.0
C(14B)-C(15B)-C(20B)	121.8(7)
C(16B)-C(15B)-C(20B)	118.0(7)
C(17B)-C(16B)-C(15B)	120.0
C(17B)-C(16B)-H(16B)	120.0
C(15B)-C(16B)-H(16B)	120.0
C(16B)-C(17B)-C(18B)	120.0
C(16B)-C(17B)-H(17B)	120.0
C(18B)-C(17B)-H(17B)	120.0
C(19B)-C(18B)-C(17B)	120.0
C(19B)-C(18B)-H(18B)	120.0
C(17B)-C(18B)-H(18B)	120.0
C(18B)-C(19B)-C(14B)	120.0
C(18B)-C(19B)-C(21B)	120.8(8)
C(14B)-C(19B)-C(21B)	119.1(8)
C(15B)-C(20B)-H(20D)	109.5
C(15B)-C(20B)-H(20E)	109.4
H(20D)-C(20B)-H(20E)	109.5
C(15B)-C(20B)-H(20F)	109.5
H(20D)-C(20B)-H(20F)	109.5
H(20E)-C(20B)-H(20F)	109.5
C(19B)-C(21B)-H(21D)	109.5
C(19B)-C(21B)-H(21E)	109.5
H(21D)-C(21B)-H(21E)	109.5
C(19B)-C(21B)-H(21F)	109.4
H(21D)-C(21B)-H(21F)	109.5
H(21E)-C(21B)-H(21F)	109.5
C(26B)-C(22B)-C(23B)	108.0
C(26B)-C(22B)-Cr(1)	68.3(5)
C(23B)-C(22B)-Cr(1)	72.0(5)
C(26B)-C(22B)-H(22B)	126.0
C(23B)-C(22B)-H(22B)	126.0
Cr(1)-C(22B)-H(22B)	125.2
C(24B)-C(23B)-C(22B)	108.0
C(24B)-C(23B)-Cr(1)	67.5(5)
C(22B)-C(23B)-Cr(1)	73.7(5)
C(24B)-C(23B)-H(23B)	126.0
C(22B)-C(23B)-H(23B)	126.0
Cr(1)-C(23B)-H(23B)	124.3
C(25B)-C(24B)-C(23B)	108.0
C(25B)-C(24B)-Cr(1)	69.4(5)
C(23B)-C(24B)-Cr(1)	77.3(5)
C(25B)-C(24B)-H(24B)	126.0
C(23B)-C(24B)-H(24B)	126.0
Cr(1)-C(24B)-H(24B)	119.2
C(26B)-C(25B)-C(24B)	108.0
C(26B)-C(25B)-Cr(1)	75.4(5)
C(24B)-C(25B)-Cr(1)	73.8(5)
C(26B)-C(25B)-H(25B)	126.0
C(24B)-C(25B)-H(25B)	126.0
Cr(1)-C(25B)-H(25B)	116.9
C(25B)-C(26B)-C(22B)	108.0
C(25B)-C(26B)-Cr(1)	68.1(5)
C(22B)-C(26B)-Cr(1)	76.9(5)
C(25B)-C(26B)-H(26B)	126.0
C(22B)-C(26B)-H(26B)	126.0
Cr(1)-C(26B)-H(26B)	120.7

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for ks043.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	35(1)	22(1)	23(1)	-3(1)	-3(1)	2(1)
C(2)	33(1)	43(1)	40(1)	-6(1)	-2(1)	-2(1)
C(3)	36(1)	55(1)	54(1)	-16(1)	-12(1)	18(1)
C(4)	64(1)	33(1)	48(1)	-6(1)	-21(1)	19(1)
C(5)	63(1)	25(1)	31(1)	2(1)	-7(1)	-5(1)
C(6)	37(1)	28(1)	21(1)	-2(1)	-1(1)	1(1)
C(7)	45(1)	77(2)	74(2)	-5(1)	7(1)	-23(1)
C(8)	36(1)	54(1)	37(1)	-2(1)	4(1)	-5(1)
C(9)	71(1)	33(1)	29(1)	-4(1)	-11(1)	8(1)
C(10)	55(1)	26(1)	27(1)	-2(1)	-5(1)	2(1)
C(11)	76(1)	24(1)	31(1)	-5(1)	-7(1)	11(1)
C(12)	51(1)	24(1)	33(1)	0(1)	-4(1)	4(1)
C(13)	73(1)	29(1)	40(1)	-1(1)	-5(1)	14(1)
C(14)	27(2)	23(2)	22(2)	2(2)	4(2)	10(2)
C(15)	20(2)	43(2)	27(2)	-7(2)	3(2)	5(2)
C(16)	38(3)	66(3)	47(3)	-4(2)	-9(2)	12(2)
C(17)	67(4)	50(3)	25(2)	4(2)	-3(2)	22(3)
C(18)	60(4)	32(2)	37(2)	14(2)	19(2)	15(2)
C(19)	29(3)	29(2)	54(3)	8(2)	4(2)	11(2)
C(20)	34(3)	64(3)	61(4)	-5(3)	8(3)	-13(2)
C(21)	52(5)	41(2)	70(5)	6(3)	12(3)	-9(3)
C(22)	60(4)	57(4)	59(4)	-34(3)	25(3)	-26(3)
C(23)	59(6)	64(5)	33(3)	-23(3)	-24(4)	21(5)
C(24)	78(6)	36(3)	32(3)	1(2)	12(4)	7(3)
C(25)	56(3)	34(2)	42(3)	-9(2)	9(2)	10(2)
C(26)	70(5)	31(5)	44(5)	-8(3)	1(3)	21(3)
N(1)	43(1)	22(1)	26(1)	1(1)	-4(1)	2(1)
N(2)	43(1)	24(1)	26(1)	3(1)	-4(1)	2(1)
Cr(1)	62(1)	22(1)	23(1)	-1(1)	-4(1)	6(1)
C(14B)	25(3)	27(4)	29(4)	-4(3)	3(3)	8(3)
C(15B)	43(5)	63(5)	41(4)	-14(3)	21(3)	11(3)
C(16B)	49(5)	69(5)	45(5)	-26(4)	-30(5)	30(4)
C(17B)	108(11)	41(4)	38(4)	-1(3)	-16(5)	29(6)
C(18B)	97(8)	34(3)	41(3)	9(3)	22(5)	12(5)
C(19B)	28(4)	23(2)	32(3)	10(2)	13(2)	13(3)
C(20B)	45(5)	118(11)	88(11)	-41(9)	-4(7)	-1(6)
C(21B)	44(6)	54(5)	85(9)	2(7)	16(6)	-16(4)
C(22B)	53(5)	37(3)	33(4)	-9(3)	10(4)	-15(4)
C(23B)	69(8)	37(3)	52(4)	-17(3)	-24(5)	7(5)
C(24B)	97(14)	33(3)	21(3)	-3(2)	6(9)	9(9)
C(25B)	59(7)	77(9)	85(10)	-48(7)	4(6)	23(6)
C(26B)	155(15)	21(6)	22(6)	0(4)	11(7)	-23(6)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ks043.

	x	y	z	U(eq)
H(3)	2650	3407	4943	59
H(4)	4324	4430	4532	60
H(5)	7116	4223	4537	48
H(7A)	2224	2116	5506	97
H(7B)	3721	1776	6049	97
H(7C)	3397	1422	5200	97
H(8A)	9453	3399	4737	63
H(8B)	9152	2428	4670	63
H(8C)	9399	2852	5494	63
H(9A)	5238	1252	4222	67
H(9B)	6569	585	4014	67
H(9C)	7007	1544	4005	67
H(11)	7838	-81	4962	53
H(13A)	10139	-708	6479	72
H(13B)	9245	-980	5678	72
H(13C)	8340	-1089	6451	72
H(16)	12498	420	8448	61
H(17)	10935	-244	9329	57
H(18)	8203	-567	8996	51
H(20A)	11581	653	6543	79
H(20B)	12791	984	7230	79
H(20C)	11198	1501	6958	79
H(21A)	5842	-459	8196	81
H(21B)	6173	-658	7326	81
H(21C)	5785	264	7575	81
H(22)	9396	3139	7315	69
H(23)	8874	1955	8181	64
H(24)	5804	1781	8132	58
H(25)	4568	2758	7176	52
H(26)	6830	3509	6608	58
H(16B)	11946	182	8684	67
H(17B)	10043	-540	9357	76
H(18B)	7370	-708	8827	68
H(20D)	12100	485	6921	126
H(20E)	12661	1013	7664	126
H(20F)	11284	1362	7058	126
H(21D)	5328	-488	7840	91
H(21E)	6062	-567	7021	91
H(21F)	5519	313	7323	91
H(22B)	9700	3237	7108	49
H(23B)	9610	2129	8123	64
H(24B)	6649	1735	8236	60
H(25B)	4909	2600	7291	89
H(26B)	6794	3529	6594	79

Table 6. Torsion angles [deg] for ks043.

C(6)-C(1)-C(2)-C(3)	0.1(2)
N(1)-C(1)-C(2)-C(3)	176.02(15)
C(6)-C(1)-C(2)-C(7)	-179.06(16)
N(1)-C(1)-C(2)-C(7)	-3.2(2)
C(1)-C(2)-C(3)-C(4)	-1.0(3)
C(7)-C(2)-C(3)-C(4)	178.20(19)
C(2)-C(3)-C(4)-C(5)	1.0(3)
C(3)-C(4)-C(5)-C(6)	0.0(3)
C(4)-C(5)-C(6)-C(1)	-0.8(2)
C(4)-C(5)-C(6)-C(8)	179.74(16)
C(2)-C(1)-C(6)-C(5)	0.7(2)
N(1)-C(1)-C(6)-C(5)	-175.19(13)
C(2)-C(1)-C(6)-C(8)	-179.80(15)
N(1)-C(1)-C(6)-C(8)	4.3(2)
N(1)-C(10)-C(11)-C(12)	2.0(4)
C(9)-C(10)-C(11)-C(12)	-178.1(2)
C(10)-C(11)-C(12)-N(2)	0.2(4)
C(10)-C(11)-C(12)-C(13)	179.4(2)
C(19)-C(14)-C(15)-C(16)	0.0
N(2)-C(14)-C(15)-C(16)	172.1(7)
C(19)-C(14)-C(15)-C(20)	-177.4(7)
N(2)-C(14)-C(15)-C(20)	-5.3(7)
C(14)-C(15)-C(16)-C(17)	0.0
C(20)-C(15)-C(16)-C(17)	177.3(7)
C(15)-C(16)-C(17)-C(18)	0.0
C(16)-C(17)-C(18)-C(19)	0.0
C(17)-C(18)-C(19)-C(14)	0.0
C(17)-C(18)-C(19)-C(21)	-175.1(8)
C(15)-C(14)-C(19)-C(18)	0.0
N(2)-C(14)-C(19)-C(18)	-171.9(7)
C(15)-C(14)-C(19)-C(21)	175.0(8)
N(2)-C(14)-C(19)-C(21)	3.1(7)
C(26)-C(22)-C(23)-C(24)	-5.4(8)
Cr(1)-C(22)-C(23)-C(24)	-69.9(6)
C(26)-C(22)-C(23)-Cr(1)	64.5(5)
C(22)-C(23)-C(24)-C(25)	2.8(9)
Cr(1)-C(23)-C(24)-C(25)	-65.4(7)
C(22)-C(23)-C(24)-Cr(1)	68.2(5)
C(23)-C(24)-C(25)-C(26)	0.8(8)
Cr(1)-C(24)-C(25)-C(26)	-60.4(4)
C(23)-C(24)-C(25)-Cr(1)	61.2(7)
C(23)-C(22)-C(26)-C(25)	6.0(6)
Cr(1)-C(22)-C(26)-C(25)	69.0(4)
C(23)-C(22)-C(26)-Cr(1)	-63.0(5)
C(24)-C(25)-C(26)-C(22)	-4.2(6)
Cr(1)-C(25)-C(26)-C(22)	-66.0(5)
C(24)-C(25)-C(26)-Cr(1)	61.8(6)
C(11)-C(10)-N(1)-C(1)	177.62(18)
C(9)-C(10)-N(1)-C(1)	-2.3(3)
C(11)-C(10)-N(1)-Cr(1)	-2.6(3)
C(9)-C(10)-N(1)-Cr(1)	177.46(13)
C(2)-C(1)-N(1)-C(10)	91.5(2)
C(6)-C(1)-N(1)-C(10)	-92.51(18)
C(2)-C(1)-N(1)-Cr(1)	-88.28(15)
C(6)-C(1)-N(1)-Cr(1)	87.68(15)
C(11)-C(12)-N(2)-C(14B)	172.9(5)
C(13)-C(12)-N(2)-C(14B)	-6.3(5)
C(11)-C(12)-N(2)-C(14)	-178.5(3)
C(13)-C(12)-N(2)-C(14)	2.4(4)

C(11)-C(12)-N(2)-Cr(1)	-1.4(3)
C(13)-C(12)-N(2)-Cr(1)	179.47(14)
C(15)-C(14)-N(2)-C(12)	94.0(4)
C(19)-C(14)-N(2)-C(12)	-94.0(5)
C(15)-C(14)-N(2)-C(14B)	-135(5)
C(19)-C(14)-N(2)-C(14B)	37(4)
C(15)-C(14)-N(2)-Cr(1)	-83.3(5)
C(19)-C(14)-N(2)-Cr(1)	88.7(4)
C(10)-N(1)-Cr(1)-N(2)	1.29(16)
C(1)-N(1)-Cr(1)-N(2)	-178.92(11)
C(10)-N(1)-Cr(1)-C(25B)	-151.8(4)
C(1)-N(1)-Cr(1)-C(25B)	28.0(4)
C(10)-N(1)-Cr(1)-C(23)	164.7(9)
C(1)-N(1)-Cr(1)-C(23)	-15.6(10)
C(10)-N(1)-Cr(1)-C(24B)	-138.0(6)
C(1)-N(1)-Cr(1)-C(24B)	41.8(6)
C(10)-N(1)-Cr(1)-C(22)	148.0(3)
C(1)-N(1)-Cr(1)-C(22)	-32.3(3)
C(10)-N(1)-Cr(1)-C(26B)	171.6(3)
C(1)-N(1)-Cr(1)-C(26B)	-8.6(3)
C(10)-N(1)-Cr(1)-C(26)	175.6(3)
C(1)-N(1)-Cr(1)-C(26)	-4.6(3)
C(10)-N(1)-Cr(1)-C(24)	-130.3(5)
C(1)-N(1)-Cr(1)-C(24)	49.5(5)
C(10)-N(1)-Cr(1)-C(23B)	131.9(9)
C(1)-N(1)-Cr(1)-C(23B)	-48.3(9)
C(10)-N(1)-Cr(1)-C(25)	-149.5(2)
C(1)-N(1)-Cr(1)-C(25)	30.3(2)
C(10)-N(1)-Cr(1)-C(22B)	139.0(4)
C(1)-N(1)-Cr(1)-C(22B)	-41.3(4)
C(12)-N(2)-Cr(1)-N(1)	0.65(16)
C(14B)-N(2)-Cr(1)-N(1)	-174.1(4)
C(14)-N(2)-Cr(1)-N(1)	177.7(3)
C(12)-N(2)-Cr(1)-C(25B)	140.8(5)
C(14B)-N(2)-Cr(1)-C(25B)	-34.0(8)
C(14)-N(2)-Cr(1)-C(25B)	-42.1(6)
C(12)-N(2)-Cr(1)-C(23)	-174.2(3)
C(14B)-N(2)-Cr(1)-C(23)	11.1(6)
C(14)-N(2)-Cr(1)-C(23)	2.9(5)
C(12)-N(2)-Cr(1)-C(24B)	162.5(4)
C(14B)-N(2)-Cr(1)-C(24B)	-12.2(7)
C(14)-N(2)-Cr(1)-C(24B)	-20.4(6)
C(12)-N(2)-Cr(1)-C(22)	-145.1(4)
C(14B)-N(2)-Cr(1)-C(22)	40.1(6)
C(14)-N(2)-Cr(1)-C(22)	32.0(5)
C(12)-N(2)-Cr(1)-C(26B)	-148.2(10)
C(14B)-N(2)-Cr(1)-C(26B)	37.0(11)
C(14)-N(2)-Cr(1)-C(26B)	28.9(11)
C(12)-N(2)-Cr(1)-C(26)	-160.5(8)
C(14B)-N(2)-Cr(1)-C(26)	24.8(9)
C(14)-N(2)-Cr(1)-C(26)	16.6(9)
C(12)-N(2)-Cr(1)-C(24)	149.4(4)
C(14B)-N(2)-Cr(1)-C(24)	-25.4(6)
C(14)-N(2)-Cr(1)-C(24)	-33.5(5)
C(12)-N(2)-Cr(1)-C(23B)	-161.0(4)
C(14B)-N(2)-Cr(1)-C(23B)	24.2(7)
C(14)-N(2)-Cr(1)-C(23B)	16.0(5)
C(12)-N(2)-Cr(1)-C(25)	130.7(4)
C(14B)-N(2)-Cr(1)-C(25)	-44.1(6)
C(14)-N(2)-Cr(1)-C(25)	-52.2(5)
C(12)-N(2)-Cr(1)-C(22B)	-133.3(4)
C(14B)-N(2)-Cr(1)-C(22B)	51.9(6)
C(14)-N(2)-Cr(1)-C(22B)	43.7(5)

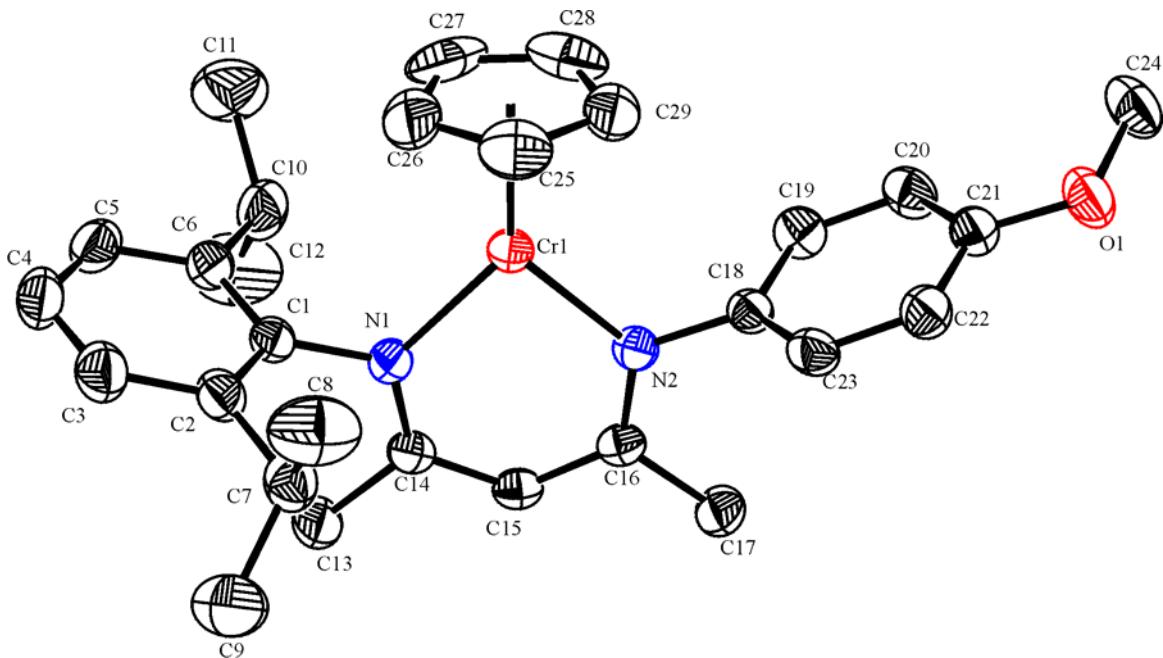
C(22)-C(23)-Cr(1)-N(1)	-23.1(12)
C(24)-C(23)-Cr(1)-N(1)	88.0(12)
C(22)-C(23)-Cr(1)-N(2)	139.6(4)
C(24)-C(23)-Cr(1)-N(2)	-109.3(5)
C(22)-C(23)-Cr(1)-C(25B)	-75.4(6)
C(24)-C(23)-Cr(1)-C(25B)	35.7(8)
C(22)-C(23)-Cr(1)-C(24B)	-119.1(11)
C(24)-C(23)-Cr(1)-C(24B)	-8.0(12)
C(24)-C(23)-Cr(1)-C(22)	111.1(7)
C(22)-C(23)-Cr(1)-C(26B)	-31.1(6)
C(24)-C(23)-Cr(1)-C(26B)	80.0(7)
C(22)-C(23)-Cr(1)-C(26)	-35.6(4)
C(24)-C(23)-Cr(1)-C(26)	75.5(5)
C(22)-C(23)-Cr(1)-C(24)	-111.1(7)
C(22)-C(23)-Cr(1)-C(23B)	55(2)
C(24)-C(23)-Cr(1)-C(23B)	167(2)
C(22)-C(23)-Cr(1)-C(25)	-75.8(4)
C(24)-C(23)-Cr(1)-C(25)	35.3(4)
C(22)-C(23)-Cr(1)-C(22B)	9.9(7)
C(24)-C(23)-Cr(1)-C(22B)	121.1(8)
C(26)-C(22)-Cr(1)-N(1)	53.8(6)
C(23)-C(22)-Cr(1)-N(1)	171.3(4)
C(26)-C(22)-Cr(1)-N(2)	-171.9(4)
C(23)-C(22)-Cr(1)-N(2)	-54.4(5)
C(26)-C(22)-Cr(1)-C(25B)	-42.9(8)
C(23)-C(22)-Cr(1)-C(25B)	74.6(6)
C(26)-C(22)-Cr(1)-C(23)	-117.5(6)
C(26)-C(22)-Cr(1)-C(24B)	-91.4(7)
C(23)-C(22)-Cr(1)-C(24B)	26.0(6)
C(26)-C(22)-Cr(1)-C(26B)	6.3(9)
C(23)-C(22)-Cr(1)-C(26B)	123.7(9)
C(23)-C(22)-Cr(1)-C(26)	117.5(6)
C(26)-C(22)-Cr(1)-C(24)	-77.4(5)
C(23)-C(22)-Cr(1)-C(24)	40.0(4)
C(26)-C(22)-Cr(1)-C(23B)	-139.2(9)
C(23)-C(22)-Cr(1)-C(23B)	-21.8(7)
C(26)-C(22)-Cr(1)-C(25)	-37.5(4)
C(23)-C(22)-Cr(1)-C(25)	80.0(4)
C(26)-C(22)-Cr(1)-C(22B)	108(3)
C(23)-C(22)-Cr(1)-C(22B)	-135(3)
C(22)-C(26)-Cr(1)-N(1)	-139.0(5)
C(25)-C(26)-Cr(1)-N(1)	106.1(4)
C(22)-C(26)-Cr(1)-N(2)	21.4(11)
C(25)-C(26)-Cr(1)-N(2)	-93.5(9)
C(22)-C(26)-Cr(1)-C(25B)	103.0(9)
C(25)-C(26)-Cr(1)-C(25B)	-11.9(9)
C(22)-C(26)-Cr(1)-C(23)	37.1(4)
C(25)-C(26)-Cr(1)-C(23)	-77.8(4)
C(22)-C(26)-Cr(1)-C(24B)	63.7(6)
C(25)-C(26)-Cr(1)-C(24B)	-51.2(6)
C(25)-C(26)-Cr(1)-C(22)	-114.9(5)
C(22)-C(26)-Cr(1)-C(26B)	-58(6)
C(25)-C(26)-Cr(1)-C(26B)	-173(6)
C(22)-C(26)-Cr(1)-C(24)	79.3(5)
C(25)-C(26)-Cr(1)-C(24)	-35.6(4)
C(22)-C(26)-Cr(1)-C(23B)	22.1(5)
C(25)-C(26)-Cr(1)-C(23B)	-92.8(5)
C(22)-C(26)-Cr(1)-C(25)	114.9(5)
C(22)-C(26)-Cr(1)-C(22B)	-14.8(7)
C(25)-C(26)-Cr(1)-C(22B)	-129.7(8)
C(25)-C(24)-Cr(1)-N(1)	-34.3(8)
C(23)-C(24)-Cr(1)-N(1)	-151.4(5)
C(25)-C(24)-Cr(1)-N(2)	-159.6(4)

C(23)-C(24)-Cr(1)-N(2)	83.3(5)
C(25)-C(24)-Cr(1)-C(25B)	9.0(8)
C(23)-C(24)-Cr(1)-C(25B)	-108.1(11)
C(25)-C(24)-Cr(1)-C(23)	117.1(7)
C(25)-C(24)-Cr(1)-C(24B)	130(2)
C(23)-C(24)-Cr(1)-C(24B)	13(2)
C(25)-C(24)-Cr(1)-C(22)	77.2(5)
C(23)-C(24)-Cr(1)-C(22)	-39.9(4)
C(25)-C(24)-Cr(1)-C(26B)	39.4(6)
C(23)-C(24)-Cr(1)-C(26B)	-77.7(7)
C(25)-C(24)-Cr(1)-C(26)	36.3(4)
C(23)-C(24)-Cr(1)-C(26)	-80.8(5)
C(25)-C(24)-Cr(1)-C(23B)	113.1(9)
C(23)-C(24)-Cr(1)-C(23B)	-4.0(6)
C(23)-C(24)-Cr(1)-C(25)	-117.1(7)
C(25)-C(24)-Cr(1)-C(22B)	78.1(6)
C(23)-C(24)-Cr(1)-C(22B)	-39.0(6)
C(24)-C(25)-Cr(1)-N(1)	157.4(5)
C(26)-C(25)-Cr(1)-N(1)	-85.0(4)
C(24)-C(25)-Cr(1)-N(2)	32.6(7)
C(26)-C(25)-Cr(1)-N(2)	150.1(4)
C(24)-C(25)-Cr(1)-C(25B)	-40(4)
C(26)-C(25)-Cr(1)-C(25B)	77(4)
C(24)-C(25)-Cr(1)-C(23)	-37.6(5)
C(26)-C(25)-Cr(1)-C(23)	79.9(4)
C(24)-C(25)-Cr(1)-C(24B)	-14.9(7)
C(26)-C(25)-Cr(1)-C(24B)	102.7(7)
C(24)-C(25)-Cr(1)-C(22)	-80.0(5)
C(26)-C(25)-Cr(1)-C(22)	37.6(3)
C(24)-C(25)-Cr(1)-C(26B)	-116.7(9)
C(26)-C(25)-Cr(1)-C(26B)	0.8(7)
C(24)-C(25)-Cr(1)-C(26)	-117.6(6)
C(26)-C(25)-Cr(1)-C(24)	117.6(6)
C(24)-C(25)-Cr(1)-C(23B)	-48.1(7)
C(26)-C(25)-Cr(1)-C(23B)	69.4(5)
C(24)-C(25)-Cr(1)-C(22B)	-86.0(7)
C(26)-C(25)-Cr(1)-C(22B)	31.6(5)
C(12)-N(2)-C(14B)-C(15B)	93.0(7)
C(14)-N(2)-C(14B)-C(15B)	39(4)
Cr(1)-N(2)-C(14B)-C(15B)	-92.0(6)
C(12)-N(2)-C(14B)-C(19B)	-81.6(7)
C(14)-N(2)-C(14B)-C(19B)	-135(5)
Cr(1)-N(2)-C(14B)-C(19B)	93.5(6)
C(19B)-C(14B)-C(15B)-C(16B)	0.0
N(2)-C(14B)-C(15B)-C(16B)	-174.5(10)
C(19B)-C(14B)-C(15B)-C(20B)	175.8(12)
N(2)-C(14B)-C(15B)-C(20B)	1.3(12)
C(14B)-C(15B)-C(16B)-C(17B)	0.0
C(20B)-C(15B)-C(16B)-C(17B)	-175.9(12)
C(15B)-C(16B)-C(17B)-C(18B)	0.0
C(16B)-C(17B)-C(18B)-C(19B)	0.0
C(17B)-C(18B)-C(19B)-C(14B)	0.0
C(17B)-C(18B)-C(19B)-C(21B)	177.2(12)
C(15B)-C(14B)-C(19B)-C(18B)	0.0
N(2)-C(14B)-C(19B)-C(18B)	174.6(10)
C(15B)-C(14B)-C(19B)-C(21B)	-177.2(12)
N(2)-C(14B)-C(19B)-C(21B)	-2.6(11)
N(1)-Cr(1)-C(22B)-C(26B)	66.4(5)
N(2)-Cr(1)-C(22B)-C(26B)	-171.9(5)
C(25B)-Cr(1)-C(22B)-C(26B)	-38.5(2)
C(23)-Cr(1)-C(22B)-C(26B)	-102.3(6)
C(24B)-Cr(1)-C(22B)-C(26B)	-81.9(3)
C(22)-Cr(1)-C(22B)-C(26B)	-65(3)

C(26)-Cr(1)-C(22B)-C(26B)	-4.7(8)
C(24)-Cr(1)-C(22B)-C(26B)	-69.6(6)
C(23B)-Cr(1)-C(22B)-C(26B)	-118.6(3)
C(25)-Cr(1)-C(22B)-C(26B)	-33.1(6)
N(1)-Cr(1)-C(22B)-C(23B)	-175.0(5)
N(2)-Cr(1)-C(22B)-C(23B)	-53.3(5)
C(25B)-Cr(1)-C(22B)-C(23B)	80.1(3)
C(23)-Cr(1)-C(22B)-C(23B)	16.3(6)
C(24B)-Cr(1)-C(22B)-C(23B)	36.7(2)
C(22)-Cr(1)-C(22B)-C(23B)	54(3)
C(26B)-Cr(1)-C(22B)-C(23B)	118.6(3)
C(26)-Cr(1)-C(22B)-C(23B)	113.9(8)
C(24)-Cr(1)-C(22B)-C(23B)	49.0(5)
C(25)-Cr(1)-C(22B)-C(23B)	85.5(5)
C(26B)-C(22B)-C(23B)-C(24B)	0.0
Cr(1)-C(22B)-C(23B)-C(24B)	-59.1(5)
C(26B)-C(22B)-C(23B)-Cr(1)	59.1(5)
N(1)-Cr(1)-C(23B)-C(24B)	128.6(11)
N(2)-Cr(1)-C(23B)-C(24B)	-102.8(4)
C(25B)-Cr(1)-C(23B)-C(24B)	39.1(2)
C(23)-Cr(1)-C(23B)-C(24B)	-3.6(18)
C(22)-Cr(1)-C(23B)-C(24B)	102.5(8)
C(26B)-Cr(1)-C(23B)-C(24B)	81.9(3)
C(26)-Cr(1)-C(23B)-C(24B)	77.4(6)
C(24)-Cr(1)-C(23B)-C(24B)	6.8(7)
C(25)-Cr(1)-C(23B)-C(24B)	40.1(5)
C(22B)-Cr(1)-C(23B)-C(24B)	118.0(3)
N(1)-Cr(1)-C(23B)-C(22B)	10.6(10)
N(2)-Cr(1)-C(23B)-C(22B)	139.2(4)
C(25B)-Cr(1)-C(23B)-C(22B)	-78.9(3)
C(23)-Cr(1)-C(23B)-C(22B)	-121.6(19)
C(24B)-Cr(1)-C(23B)-C(22B)	-118.0(3)
C(22)-Cr(1)-C(23B)-C(22B)	-15.5(8)
C(26B)-Cr(1)-C(23B)-C(22B)	-36.1(2)
C(26)-Cr(1)-C(23B)-C(22B)	-40.6(5)
C(24)-Cr(1)-C(23B)-C(22B)	-111.2(7)
C(25)-Cr(1)-C(23B)-C(22B)	-77.9(5)
C(22B)-C(23B)-C(24B)-C(25B)	0.0
Cr(1)-C(23B)-C(24B)-C(25B)	-63.0(5)
C(22B)-C(23B)-C(24B)-Cr(1)	63.0(5)
N(1)-Cr(1)-C(24B)-C(25B)	-20.7(7)
N(2)-Cr(1)-C(24B)-C(25B)	-157.2(4)
C(23)-Cr(1)-C(24B)-C(25B)	117.2(11)
C(22)-Cr(1)-C(24B)-C(25B)	75.8(6)
C(26B)-Cr(1)-C(24B)-C(25B)	38.75(18)
C(26)-Cr(1)-C(24B)-C(25B)	34.9(5)
C(24)-Cr(1)-C(24B)-C(25B)	-42(2)
C(23B)-Cr(1)-C(24B)-C(25B)	115.1(2)
C(25)-Cr(1)-C(24B)-C(25B)	-4.7(6)
C(22B)-Cr(1)-C(24B)-C(25B)	79.4(3)
N(1)-Cr(1)-C(24B)-C(23B)	-135.8(7)
N(2)-Cr(1)-C(24B)-C(23B)	87.7(4)
C(25B)-Cr(1)-C(24B)-C(23B)	-115.1(2)
C(23)-Cr(1)-C(24B)-C(23B)	2.1(11)
C(22)-Cr(1)-C(24B)-C(23B)	-39.3(6)
C(26B)-Cr(1)-C(24B)-C(23B)	-76.3(3)
C(26)-Cr(1)-C(24B)-C(23B)	-80.2(5)
C(24)-Cr(1)-C(24B)-C(23B)	-157(2)
C(25)-Cr(1)-C(24B)-C(23B)	-119.8(6)
C(22B)-Cr(1)-C(24B)-C(23B)	-35.66(17)
C(23B)-C(24B)-C(25B)-C(26B)	0.0
Cr(1)-C(24B)-C(25B)-C(26B)	-68.3(5)
C(23B)-C(24B)-C(25B)-Cr(1)	68.3(5)

N(1)-Cr(1)-C(25B)-C(26B)	-76.3(4)
N(2)-Cr(1)-C(25B)-C(26B)	150.0(5)
C(23)-Cr(1)-C(25B)-C(26B)	88.0(5)
C(24B)-Cr(1)-C(25B)-C(26B)	114.1(2)
C(22)-Cr(1)-C(25B)-C(26B)	42.1(6)
C(26)-Cr(1)-C(25B)-C(26B)	-2.2(8)
C(24)-Cr(1)-C(25B)-C(26B)	133.1(9)
C(23B)-Cr(1)-C(25B)-C(26B)	76.8(2)
C(25)-Cr(1)-C(25B)-C(26B)	-95(4)
C(22B)-Cr(1)-C(25B)-C(26B)	36.75(16)
N(1)-Cr(1)-C(25B)-C(24B)	169.6(4)
N(2)-Cr(1)-C(25B)-C(24B)	35.9(5)
C(23)-Cr(1)-C(25B)-C(24B)	-26.1(5)
C(22)-Cr(1)-C(25B)-C(24B)	-72.0(5)
C(26B)-Cr(1)-C(25B)-C(24B)	-114.1(2)
C(26)-Cr(1)-C(25B)-C(24B)	-116.3(8)
C(24)-Cr(1)-C(25B)-C(24B)	19.0(9)
C(23B)-Cr(1)-C(25B)-C(24B)	-37.33(16)
C(25)-Cr(1)-C(25B)-C(24B)	151(4)
C(22B)-Cr(1)-C(25B)-C(24B)	-77.3(2)
C(24B)-C(25B)-C(26B)-C(22B)	0.0
Cr(1)-C(25B)-C(26B)-C(22B)	-67.2(5)
C(24B)-C(25B)-C(26B)-Cr(1)	67.2(5)
C(23B)-C(22B)-C(26B)-C(25B)	0.0
Cr(1)-C(22B)-C(26B)-C(25B)	61.4(5)
C(23B)-C(22B)-C(26B)-Cr(1)	-61.4(5)
N(1)-Cr(1)-C(26B)-C(25B)	117.2(5)
N(2)-Cr(1)-C(26B)-C(25B)	-95.0(12)
C(23)-Cr(1)-C(26B)-C(25B)	-65.3(4)
C(24B)-Cr(1)-C(26B)-C(25B)	-39.14(19)
C(22)-Cr(1)-C(26B)-C(25B)	-99.5(7)
C(26)-Cr(1)-C(26B)-C(25B)	17(6)
C(24)-Cr(1)-C(26B)-C(25B)	-23.8(5)
C(23B)-Cr(1)-C(26B)-C(25B)	-80.3(3)
C(25)-Cr(1)-C(26B)-C(25B)	10.8(8)
C(22B)-Cr(1)-C(26B)-C(25B)	-115.8(2)
N(1)-Cr(1)-C(26B)-C(22B)	-127.0(5)
N(2)-Cr(1)-C(26B)-C(22B)	20.8(12)
C(25B)-Cr(1)-C(26B)-C(22B)	115.8(2)
C(23)-Cr(1)-C(26B)-C(22B)	50.6(4)
C(24B)-Cr(1)-C(26B)-C(22B)	76.7(3)
C(22)-Cr(1)-C(26B)-C(22B)	16.3(7)
C(26)-Cr(1)-C(26B)-C(22B)	133(6)
C(24)-Cr(1)-C(26B)-C(22B)	92.0(5)
C(23B)-Cr(1)-C(26B)-C(22B)	35.49(18)
C(25)-Cr(1)-C(26B)-C(22B)	126.6(8)

2.2 Compound 4



Data Collection

A purple rod crystal of $C_{29}H_{36}N_2OCr$ having approximate dimensions of $0.10 \times 0.12 \times 0.35$ mm was mounted on a glass fiber. All measurements were made on a Bruker X8 APEX diffractometer with graphite monochromated Mo-K α radiation.

The data were collected at a temperature of $-100.0 \pm 0.1^\circ\text{C}$ to a maximum 2θ value of 50.1° . Data were collected in a series of ϕ and ω scans in 0.50° oscillations with 10.0 second exposures. The crystal-to-detector distance was 38.94 mm.

Data Reduction

Of the 22097 reflections that were collected, 4609 were unique ($R_{\text{int}} = 0.038$); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT¹ software package. The linear absorption coefficient, μ , for Mo-K α radiation is 4.63 cm^{-1} . Data were corrected for absorption effects using the multi-scan technique (SADABS²), with minimum and maximum transmission coefficients of 0.821 and 0.955, respectively. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods³. All non-hydrogen atoms were refined anisotropically. All C-H hydrogen atoms were included in calculated positions but were not refined. The final cycle of full-matrix least-squares refinement⁴ on

F^2 was based on 4609 reflections and 305 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \sum |Fo| - |Fc| / \sum |Fo| = 0.052$$

$$wR2 = [\sum (w(Fo^2 - Fc^2)^2) / \sum w(Fo^2)^2]^{1/2} = 0.100$$

The standard deviation of an observation of unit weight⁵ was 1.04. The weighting scheme was based on counting statistics. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.22 and $-0.20 \text{ e}^-/\text{\AA}^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber⁶. Anomalous dispersion effects were included in F_{calc} ⁷; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley⁸. The values for the mass attenuation coefficients are those of Creagh and Hubbell⁹. All refinements were performed using the SHELXTL¹⁰ crystallographic software package of Bruker-AXS.

References

- (1) SAINT. Version 7.03A. Bruker AXS Inc., Madison, Wisconsin, USA. (1997-2003).
- (2) SADABS. Bruker Nonius area detector scaling and absorption correction - V2.10, Bruker AXS Inc., Madison, Wisconsin, USA (2003).
- (3) SIR97 - Altomare A., Burla M.C., Camalli M., Cascarano G.L., Giacovazzo C., Guagliardi A., Moliterni A.G.G., Polidori G., Spagna R. (1999) *J. Appl. Cryst.* 32, 115-119.
- (4) Least Squares function minimized:

$$\sum w(F_o^2 - F_c^2)^2$$
- (5) Standard deviation of an observation of unit weight:

$$[\sum w(F_o^2 - F_c^2)^2 / (N_o - N_v)]^{1/2}$$

where: N_o = number of observations
 N_v = number of variables
- (6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).
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EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	C ₂₉ H ₃₆ N ₂ OCr
Formula Weight	480.60
Crystal Color, Habit	purple, rod
Crystal Dimensions	0.10 X 0.12 X 0.35 mm
Crystal System	monoclinic
Lattice Type	primitive
Lattice Parameters	a = 9.4111(4) Å b = 19.3774(9) Å c = 14.2505(7) Å α = 90.0 ° β = 90.981(2) ° γ = 90.0 ° V = 2598.4(2) Å ³
Space Group	P 2 ₁ /n (#14)
Z value	4
D _{calc}	1.229 g/cm ³
F ₀₀₀	1024.00
μ(MoKα)	4.63 cm ⁻¹

B. Intensity Measurements

Diffractometer	Bruker X8 APEX
Radiation	MoK α ($\lambda = 0.71073 \text{ \AA}$) graphite monochromated
Data Images	1013 exposures @ 10.0 seconds
Detector Position	38.94 mm
$2\theta_{\max}$	50.1°
No. of Reflections Measured	Total: 22097 Unique: 4609 ($R_{\text{int}} = 0.038$) Absorption ($T_{\min} = 0.821$, $T_{\max} = 0.955$) Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR97)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma w (F_o^2 - F_c^2)^2$
Least Squares Weights	$w=1/(\sigma^2(F_o^2)+(0.0496P)^2+0.7264P)$
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ($I > 0.00\sigma(I)$)	4609
No. Variables	305
Reflection/Parameter Ratio	15.11
Residuals (refined on F^2 , all data): R1; wR2	0.052; 0.100
Goodness of Fit Indicator	1.04
No. Observations ($I > 2.00\sigma(I)$)	3536
Residuals (refined on F): R1; wR2	0.036; 0.092
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.22 e $^-/\text{\AA}^3$
Minimum peak in Final Diff. Map	-0.20 e $^-/\text{\AA}^3$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ks049.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	7170(2)	206(1)	3409(1)	32(1)
C(2)	7439(2)	-507(1)	3420(1)	38(1)
C(3)	8017(2)	-794(1)	4238(2)	46(1)
C(4)	8305(2)	-398(2)	5011(2)	50(1)
C(5)	8053(2)	300(1)	4991(2)	47(1)
C(6)	7486(2)	617(1)	4192(1)	38(1)
C(7)	7129(3)	-966(1)	2575(2)	43(1)
C(8)	8481(3)	-1224(2)	2129(2)	73(1)
C(9)	6182(3)	-1582(2)	2805(2)	71(1)
C(10)	7215(3)	1390(1)	4188(2)	52(1)
C(11)	8425(4)	1804(2)	4644(2)	78(1)
C(12)	5842(4)	1568(2)	4667(3)	97(1)
C(13)	4261(2)	178(1)	3203(2)	47(1)
C(14)	5175(2)	483(1)	2448(1)	31(1)
C(15)	4455(2)	699(1)	1633(1)	31(1)
C(16)	5009(2)	964(1)	809(1)	29(1)
C(17)	3974(2)	1071(1)	4(2)	40(1)
C(18)	6833(2)	1366(1)	-188(1)	29(1)
C(19)	7053(2)	2063(1)	-337(2)	37(1)
C(20)	7549(2)	2306(1)	-1194(2)	39(1)
C(21)	7827(2)	1843(1)	-1901(2)	36(1)
C(22)	7616(2)	1145(1)	-1753(2)	39(1)
C(23)	7119(2)	912(1)	-909(2)	35(1)
C(24)	8713(3)	2713(1)	-2918(2)	52(1)
C(25)	10208(2)	481(1)	1277(2)	51(1)
C(26)	10191(2)	640(2)	2226(2)	60(1)
C(27)	10058(3)	1347(2)	2311(2)	69(1)
C(28)	9937(3)	1626(2)	1411(2)	61(1)
C(29)	10010(2)	1090(1)	779(2)	48(1)
N(1)	6576(2)	516(1)	2569(1)	30(1)
N(2)	6380(2)	1112(1)	707(1)	30(1)
O(1)	8311(2)	2016(1)	-2773(1)	49(1)
Cr(1)	7957(1)	922(1)	1644(1)	31(1)

Table 3. Bond lengths [Å] and angles [deg] for ks049.

C(1)-C(6)	1.400(3)
C(1)-C(2)	1.405(3)
C(1)-N(1)	1.443(2)
C(2)-C(3)	1.393(3)
C(2)-C(7)	1.522(3)
C(3)-C(4)	1.365(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.375(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.392(3)
C(5)-H(5)	0.9500
C(6)-C(10)	1.519(3)
C(7)-C(8)	1.516(4)
C(7)-C(9)	1.528(3)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(12)	1.512(4)
C(10)-C(11)	1.528(4)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.510(3)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-N(1)	1.328(2)
C(14)-C(15)	1.398(3)
C(15)-C(16)	1.391(3)
C(15)-H(15)	0.9500
C(16)-N(2)	1.332(2)
C(16)-C(17)	1.506(3)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.382(3)
C(18)-C(23)	1.384(3)
C(18)-N(2)	1.438(2)
C(19)-C(20)	1.397(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.378(3)
C(20)-H(20)	0.9500
C(21)-O(1)	1.371(2)
C(21)-C(22)	1.384(3)
C(22)-C(23)	1.373(3)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(24)-O(1)	1.420(3)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800

C(25)-C(26)	1.386(4)
C(25)-C(29)	1.389(4)
C(25)-Cr(1)	2.351(2)
C(25)-H(25)	0.9500
C(26)-C(27)	1.382(4)
C(26)-Cr(1)	2.312(2)
C(26)-H(26)	0.9500
C(27)-C(28)	1.395(4)
C(27)-Cr(1)	2.329(2)
C(27)-H(27)	0.9500
C(28)-C(29)	1.376(4)
C(28)-Cr(1)	2.338(2)
C(28)-H(28)	0.9500
C(29)-Cr(1)	2.333(2)
C(29)-H(29)	0.9500
N(1)-Cr(1)	2.0251(16)
N(2)-Cr(1)	2.0139(16)
C(6)-C(1)-C(2)	121.00(19)
C(6)-C(1)-N(1)	119.89(19)
C(2)-C(1)-N(1)	119.10(18)
C(3)-C(2)-C(1)	118.0(2)
C(3)-C(2)-C(7)	119.7(2)
C(1)-C(2)-C(7)	122.22(18)
C(4)-C(3)-C(2)	121.4(2)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	120.3(2)
C(3)-C(4)-H(4)	119.8
C(5)-C(4)-H(4)	119.8
C(4)-C(5)-C(6)	121.0(2)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
C(5)-C(6)-C(1)	118.3(2)
C(5)-C(6)-C(10)	120.0(2)
C(1)-C(6)-C(10)	121.66(19)
C(8)-C(7)-C(2)	111.9(2)
C(8)-C(7)-C(9)	109.2(2)
C(2)-C(7)-C(9)	113.0(2)
C(8)-C(7)-H(7)	107.5
C(2)-C(7)-H(7)	107.5
C(9)-C(7)-H(7)	107.5
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(12)-C(10)-C(6)	111.6(2)
C(12)-C(10)-C(11)	109.0(2)
C(6)-C(10)-C(11)	113.0(2)
C(12)-C(10)-H(10)	107.7
C(6)-C(10)-H(10)	107.7
C(11)-C(10)-H(10)	107.7
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5

C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(1)-C(14)-C(15)	124.03(18)
N(1)-C(14)-C(13)	120.19(18)
C(15)-C(14)-C(13)	115.75(18)
C(16)-C(15)-C(14)	128.88(18)
C(16)-C(15)-H(15)	115.6
C(14)-C(15)-H(15)	115.6
N(2)-C(16)-C(15)	123.35(18)
N(2)-C(16)-C(17)	120.11(18)
C(15)-C(16)-C(17)	116.53(18)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(19)-C(18)-C(23)	118.43(19)
C(19)-C(18)-N(2)	121.19(18)
C(23)-C(18)-N(2)	120.32(18)
C(18)-C(19)-C(20)	121.1(2)
C(18)-C(19)-H(19)	119.4
C(20)-C(19)-H(19)	119.4
C(21)-C(20)-C(19)	119.4(2)
C(21)-C(20)-H(20)	120.3
C(19)-C(20)-H(20)	120.3
O(1)-C(21)-C(20)	124.99(19)
O(1)-C(21)-C(22)	115.36(19)
C(20)-C(21)-C(22)	119.7(2)
C(23)-C(22)-C(21)	120.5(2)
C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(22)-C(23)-C(18)	120.92(19)
C(22)-C(23)-H(23)	119.5
C(18)-C(23)-H(23)	119.5
O(1)-C(24)-H(24A)	109.5
O(1)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
O(1)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-C(29)	107.8(3)
C(26)-C(25)-Cr(1)	71.17(14)
C(29)-C(25)-Cr(1)	72.05(13)
C(26)-C(25)-H(25)	126.1
C(29)-C(25)-H(25)	126.1
Cr(1)-C(25)-H(25)	122.4
C(27)-C(26)-C(25)	108.0(3)
C(27)-C(26)-Cr(1)	73.38(15)
C(25)-C(26)-Cr(1)	74.25(14)

C(27)-C(26)-H(26)	126.0
C(25)-C(26)-H(26)	126.0
Cr(1)-C(26)-H(26)	118.3
C(26)-C(27)-C(28)	108.0(2)
C(26)-C(27)-Cr(1)	71.99(14)
C(28)-C(27)-Cr(1)	72.95(14)
C(26)-C(27)-H(27)	126.0
C(28)-C(27)-H(27)	126.0
Cr(1)-C(27)-H(27)	120.8
C(29)-C(28)-C(27)	107.8(3)
C(29)-C(28)-Cr(1)	72.67(14)
C(27)-C(28)-Cr(1)	72.28(14)
C(29)-C(28)-H(28)	126.1
C(27)-C(28)-H(28)	126.1
Cr(1)-C(28)-H(28)	120.7
C(28)-C(29)-C(25)	108.3(2)
C(28)-C(29)-Cr(1)	73.06(14)
C(25)-C(29)-Cr(1)	73.45(13)
C(28)-C(29)-H(29)	125.8
C(25)-C(29)-H(29)	125.8
Cr(1)-C(29)-H(29)	119.5
C(14)-N(1)-C(1)	117.22(16)
C(14)-N(1)-Cr(1)	125.50(13)
C(1)-N(1)-Cr(1)	117.21(12)
C(16)-N(2)-C(18)	118.24(16)
C(16)-N(2)-Cr(1)	126.30(13)
C(18)-N(2)-Cr(1)	115.12(12)
C(21)-O(1)-C(24)	117.28(18)
N(2)-Cr(1)-N(1)	91.66(7)
N(2)-Cr(1)-C(26)	159.43(9)
N(1)-Cr(1)-C(26)	105.36(8)
N(2)-Cr(1)-C(27)	144.72(11)
N(1)-Cr(1)-C(27)	114.94(9)
C(26)-Cr(1)-C(27)	34.63(11)
N(2)-Cr(1)-C(29)	103.37(8)
N(1)-Cr(1)-C(29)	160.88(8)
C(26)-Cr(1)-C(29)	57.74(9)
C(27)-Cr(1)-C(29)	57.39(9)
N(2)-Cr(1)-C(28)	112.25(9)
N(1)-Cr(1)-C(28)	147.25(9)
C(26)-Cr(1)-C(28)	57.78(10)
C(27)-Cr(1)-C(28)	34.78(10)
C(29)-Cr(1)-C(28)	34.27(9)
N(2)-Cr(1)-C(25)	125.13(8)
N(1)-Cr(1)-C(25)	126.48(8)
C(26)-Cr(1)-C(25)	34.58(9)
C(27)-Cr(1)-C(25)	57.15(10)
C(29)-Cr(1)-C(25)	34.49(9)
C(28)-Cr(1)-C(25)	57.11(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{A}^2 \times 10^3$) for ks049.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	25(1)	43(1)	30(1)	6(1)	3(1)	-4(1)
C(2)	33(1)	42(1)	38(1)	10(1)	3(1)	-2(1)
C(3)	41(1)	52(2)	45(1)	13(1)	-1(1)	2(1)
C(4)	38(1)	73(2)	39(1)	20(1)	-4(1)	-1(1)
C(5)	39(1)	71(2)	31(1)	1(1)	-2(1)	-9(1)
C(6)	34(1)	49(1)	31(1)	3(1)	2(1)	-6(1)
C(7)	51(1)	38(1)	41(1)	6(1)	-2(1)	2(1)
C(8)	64(2)	70(2)	87(2)	-27(2)	14(2)	-6(2)
C(9)	71(2)	72(2)	70(2)	-2(2)	2(2)	-23(2)
C(10)	71(2)	53(2)	34(1)	-5(1)	-6(1)	-5(1)
C(11)	90(2)	65(2)	77(2)	-20(2)	-2(2)	-21(2)
C(12)	72(2)	71(2)	149(4)	-16(2)	9(2)	14(2)
C(13)	32(1)	67(2)	41(1)	11(1)	3(1)	-8(1)
C(14)	30(1)	30(1)	33(1)	-2(1)	3(1)	-3(1)
C(15)	24(1)	32(1)	36(1)	-3(1)	1(1)	-2(1)
C(16)	28(1)	23(1)	35(1)	-3(1)	-2(1)	2(1)
C(17)	32(1)	50(1)	39(1)	5(1)	-4(1)	1(1)
C(18)	26(1)	30(1)	32(1)	3(1)	-1(1)	0(1)
C(19)	41(1)	31(1)	41(1)	-2(1)	2(1)	2(1)
C(20)	45(1)	26(1)	47(1)	7(1)	2(1)	-1(1)
C(21)	34(1)	40(1)	35(1)	6(1)	-1(1)	-4(1)
C(22)	47(1)	37(1)	32(1)	-5(1)	4(1)	-5(1)
C(23)	41(1)	27(1)	38(1)	0(1)	2(1)	-6(1)
C(24)	59(2)	47(2)	52(2)	19(1)	10(1)	-7(1)
C(25)	29(1)	57(2)	67(2)	-5(1)	7(1)	7(1)
C(26)	26(1)	100(2)	55(2)	23(2)	-6(1)	-4(1)
C(27)	33(1)	114(3)	60(2)	-37(2)	2(1)	-26(2)
C(28)	35(1)	51(2)	98(2)	1(2)	12(1)	-13(1)
C(29)	26(1)	77(2)	42(1)	9(1)	6(1)	-2(1)
N(1)	28(1)	33(1)	28(1)	1(1)	-1(1)	-1(1)
N(2)	29(1)	29(1)	31(1)	1(1)	1(1)	-1(1)
O(1)	62(1)	44(1)	40(1)	9(1)	10(1)	-10(1)
Cr(1)	24(1)	37(1)	31(1)	2(1)	1(1)	-3(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ks049.

	x	y	z	U(eq)
H(3)	8215	-1274	4258	55
H(4)	8682	-607	5564	60
H(5)	8267	571	5531	56
H(7)	6610	-680	2096	52
H(8A)	9058	-829	1938	110
H(8B)	8238	-1505	1578	110
H(8C)	9019	-1504	2584	110
H(9A)	6708	-1903	3212	107
H(9B)	5897	-1817	2223	107
H(9C)	5334	-1420	3128	107
H(10)	7123	1541	3519	63
H(11A)	8438	1724	5323	116
H(11B)	8280	2296	4518	116
H(11C)	9332	1656	4382	116
H(12A)	5042	1362	4318	146
H(12B)	5728	2070	4686	146
H(12C)	5866	1386	5309	146
H(13A)	4316	-327	3178	70
H(13B)	3273	324	3101	70
H(13C)	4599	339	3819	70
H(15)	3449	658	1643	37
H(17A)	4168	1515	-298	60
H(17B)	3002	1071	240	60
H(17C)	4080	698	-453	60
H(19)	6865	2381	152	45
H(20)	7692	2786	-1289	47
H(22)	7816	825	-2237	47
H(23)	6970	431	-820	42
H(24A)	7880	3012	-2858	79
H(24B)	9102	2763	-3548	79
H(24C)	9436	2845	-2449	79
H(25)	10332	35	1015	61
H(26)	10259	318	2728	72
H(27)	10050	1599	2883	83
H(28)	9825	2100	1261	73
H(29)	9938	1131	115	58

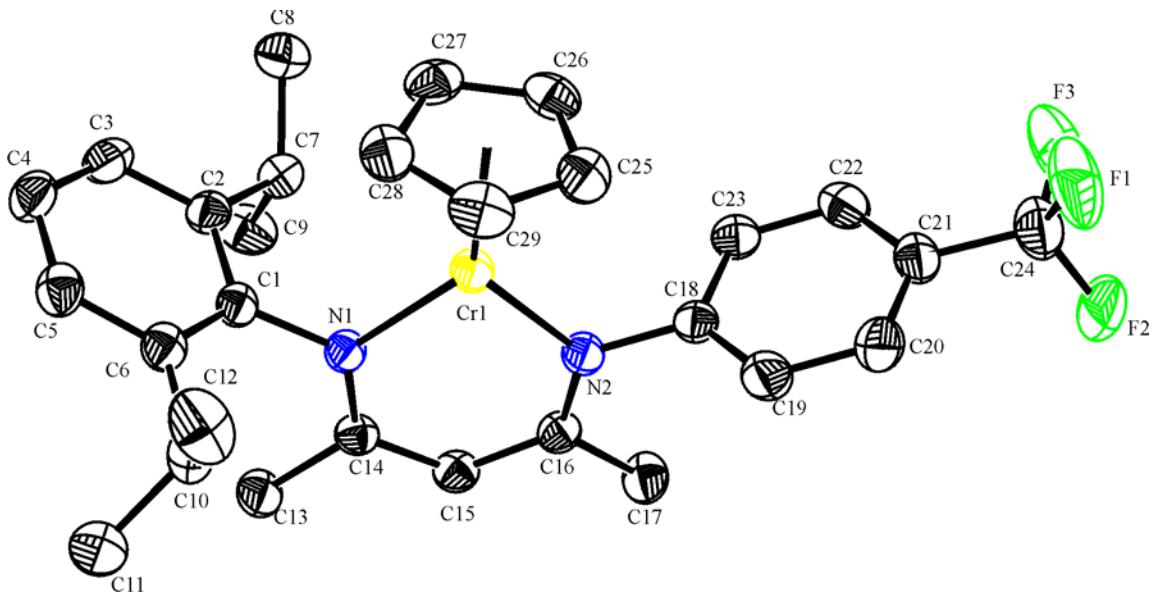
Table 6. Torsion angles [deg] for ks049.

C(6)-C(1)-C(2)-C(3)	0.6(3)
N(1)-C(1)-C(2)-C(3)	179.79(18)
C(6)-C(1)-C(2)-C(7)	-179.03(19)
N(1)-C(1)-C(2)-C(7)	0.2(3)
C(1)-C(2)-C(3)-C(4)	0.6(3)
C(7)-C(2)-C(3)-C(4)	-179.8(2)
C(2)-C(3)-C(4)-C(5)	-1.2(4)
C(3)-C(4)-C(5)-C(6)	0.7(3)
C(4)-C(5)-C(6)-C(1)	0.4(3)
C(4)-C(5)-C(6)-C(10)	179.9(2)
C(2)-C(1)-C(6)-C(5)	-1.1(3)
N(1)-C(1)-C(6)-C(5)	179.73(18)
C(2)-C(1)-C(6)-C(10)	179.4(2)
N(1)-C(1)-C(6)-C(10)	0.2(3)
C(3)-C(2)-C(7)-C(8)	-69.3(3)
C(1)-C(2)-C(7)-C(8)	110.3(3)
C(3)-C(2)-C(7)-C(9)	54.5(3)
C(1)-C(2)-C(7)-C(9)	-125.9(2)
C(5)-C(6)-C(10)-C(12)	-80.3(3)
C(1)-C(6)-C(10)-C(12)	99.1(3)
C(5)-C(6)-C(10)-C(11)	42.9(3)
C(1)-C(6)-C(10)-C(11)	-137.6(2)
N(1)-C(14)-C(15)-C(16)	1.6(3)
C(13)-C(14)-C(15)-C(16)	-176.5(2)
C(14)-C(15)-C(16)-N(2)	-6.2(3)
C(14)-C(15)-C(16)-C(17)	172.8(2)
C(23)-C(18)-C(19)-C(20)	0.2(3)
N(2)-C(18)-C(19)-C(20)	177.39(18)
C(18)-C(19)-C(20)-C(21)	-0.3(3)
C(19)-C(20)-C(21)-O(1)	179.8(2)
C(19)-C(20)-C(21)-C(22)	-0.1(3)
O(1)-C(21)-C(22)-C(23)	-179.34(19)
C(20)-C(21)-C(22)-C(23)	0.6(3)
C(21)-C(22)-C(23)-C(18)	-0.7(3)
C(19)-C(18)-C(23)-C(22)	0.3(3)
N(2)-C(18)-C(23)-C(22)	-176.95(19)
C(29)-C(25)-C(26)-C(27)	-3.0(3)
Cr(1)-C(25)-C(26)-C(27)	-66.18(17)
C(29)-C(25)-C(26)-Cr(1)	63.15(16)
C(25)-C(26)-C(27)-C(28)	2.2(3)
Cr(1)-C(26)-C(27)-C(28)	-64.52(17)
C(25)-C(26)-C(27)-Cr(1)	66.76(17)
C(26)-C(27)-C(28)-C(29)	-0.6(3)
Cr(1)-C(27)-C(28)-C(29)	-64.47(17)
C(26)-C(27)-C(28)-Cr(1)	63.90(17)
C(27)-C(28)-C(29)-C(25)	-1.3(3)
Cr(1)-C(28)-C(29)-C(25)	-65.52(16)
C(27)-C(28)-C(29)-Cr(1)	64.21(17)
C(26)-C(25)-C(29)-C(28)	2.7(3)
Cr(1)-C(25)-C(29)-C(28)	65.26(16)
C(26)-C(25)-C(29)-Cr(1)	-62.58(16)
C(15)-C(14)-N(1)-C(1)	-173.63(19)
C(13)-C(14)-N(1)-C(1)	4.4(3)
C(15)-C(14)-N(1)-Cr(1)	3.1(3)
C(13)-C(14)-N(1)-Cr(1)	-178.85(15)
C(6)-C(1)-N(1)-C(14)	-97.5(2)
C(2)-C(1)-N(1)-C(14)	83.3(2)
C(6)-C(1)-N(1)-Cr(1)	85.54(19)
C(2)-C(1)-N(1)-Cr(1)	-93.67(19)

C(15)-C(16)-N(2)-C(18)	178.27(18)
C(17)-C(16)-N(2)-C(18)	-0.6(3)
C(15)-C(16)-N(2)-Cr(1)	5.3(3)
C(17)-C(16)-N(2)-Cr(1)	-173.64(14)
C(19)-C(18)-N(2)-C(16)	99.9(2)
C(23)-C(18)-N(2)-C(16)	-82.9(2)
C(19)-C(18)-N(2)-Cr(1)	-86.3(2)
C(23)-C(18)-N(2)-Cr(1)	90.83(19)
C(20)-C(21)-O(1)-C(24)	7.8(3)
C(22)-C(21)-O(1)-C(24)	-172.2(2)
C(16)-N(2)-Cr(1)-N(1)	-1.18(16)
C(18)-N(2)-Cr(1)-N(1)	-174.36(14)
C(16)-N(2)-Cr(1)-C(26)	145.1(3)
C(18)-N(2)-Cr(1)-C(26)	-28.1(3)
C(16)-N(2)-Cr(1)-C(27)	-141.65(18)
C(18)-N(2)-Cr(1)-C(27)	45.2(2)
C(16)-N(2)-Cr(1)-C(29)	166.90(16)
C(18)-N(2)-Cr(1)-C(29)	-6.28(15)
C(16)-N(2)-Cr(1)-C(28)	-158.24(16)
C(18)-N(2)-Cr(1)-C(28)	28.57(16)
C(16)-N(2)-Cr(1)-C(25)	137.20(16)
C(18)-N(2)-Cr(1)-C(25)	-35.99(17)
C(14)-N(1)-Cr(1)-N(2)	-2.89(17)
C(1)-N(1)-Cr(1)-N(2)	173.83(14)
C(14)-N(1)-Cr(1)-C(26)	-171.22(17)
C(1)-N(1)-Cr(1)-C(26)	5.50(18)
C(14)-N(1)-Cr(1)-C(27)	153.20(18)
C(1)-N(1)-Cr(1)-C(27)	-30.08(19)
C(14)-N(1)-Cr(1)-C(29)	-145.0(2)
C(1)-N(1)-Cr(1)-C(29)	31.7(3)
C(14)-N(1)-Cr(1)-C(28)	135.29(19)
C(1)-N(1)-Cr(1)-C(28)	-48.0(2)
C(14)-N(1)-Cr(1)-C(25)	-140.39(17)
C(1)-N(1)-Cr(1)-C(25)	36.33(18)
C(27)-C(26)-Cr(1)-N(2)	103.3(3)
C(25)-C(26)-Cr(1)-N(2)	-11.4(4)
C(27)-C(26)-Cr(1)-N(1)	-111.82(17)
C(25)-C(26)-Cr(1)-N(1)	133.44(16)
C(25)-C(26)-Cr(1)-C(27)	-114.7(2)
C(27)-C(26)-Cr(1)-C(29)	78.02(18)
C(25)-C(26)-Cr(1)-C(29)	-36.72(16)
C(27)-C(26)-Cr(1)-C(28)	37.25(16)
C(25)-C(26)-Cr(1)-C(28)	-77.48(18)
C(27)-C(26)-Cr(1)-C(25)	114.7(2)
C(26)-C(27)-Cr(1)-N(2)	-143.71(17)
C(28)-C(27)-Cr(1)-N(2)	-27.6(3)
C(26)-C(27)-Cr(1)-N(1)	80.84(17)
C(28)-C(27)-Cr(1)-N(1)	-163.04(16)
C(28)-C(27)-Cr(1)-C(26)	116.1(2)
C(26)-C(27)-Cr(1)-C(29)	-79.13(17)
C(28)-C(27)-Cr(1)-C(29)	36.99(16)
C(26)-C(27)-Cr(1)-C(28)	-116.1(2)
C(26)-C(27)-Cr(1)-C(25)	-37.85(15)
C(28)-C(27)-Cr(1)-C(25)	78.26(18)
C(28)-C(29)-Cr(1)-N(2)	110.02(17)
C(25)-C(29)-Cr(1)-N(2)	-134.31(15)
C(28)-C(29)-Cr(1)-N(1)	-109.1(3)
C(25)-C(29)-Cr(1)-N(1)	6.6(3)
C(28)-C(29)-Cr(1)-C(26)	-78.85(19)
C(25)-C(29)-Cr(1)-C(26)	36.81(16)
C(28)-C(29)-Cr(1)-C(27)	-37.55(18)
C(25)-C(29)-Cr(1)-C(27)	78.11(18)
C(25)-C(29)-Cr(1)-C(28)	115.7(2)

C(28)-C(29)-Cr(1)-C(25)	-115.7(2)
C(29)-C(28)-Cr(1)-N(2)	-80.98(17)
C(27)-C(28)-Cr(1)-N(2)	163.20(17)
C(29)-C(28)-Cr(1)-N(1)	145.09(16)
C(27)-C(28)-Cr(1)-N(1)	29.3(3)
C(29)-C(28)-Cr(1)-C(26)	78.73(18)
C(27)-C(28)-Cr(1)-C(26)	-37.10(17)
C(29)-C(28)-Cr(1)-C(27)	115.8(3)
C(27)-C(28)-Cr(1)-C(29)	-115.8(3)
C(29)-C(28)-Cr(1)-C(25)	37.44(15)
C(27)-C(28)-Cr(1)-C(25)	-78.39(19)
C(26)-C(25)-Cr(1)-N(2)	175.12(16)
C(29)-C(25)-Cr(1)-N(2)	58.35(18)
C(26)-C(25)-Cr(1)-N(1)	-60.5(2)
C(29)-C(25)-Cr(1)-N(1)	-177.31(14)
C(29)-C(25)-Cr(1)-C(26)	-116.8(2)
C(26)-C(25)-Cr(1)-C(27)	37.91(18)
C(29)-C(25)-Cr(1)-C(27)	-78.87(19)
C(26)-C(25)-Cr(1)-C(29)	116.8(2)
C(26)-C(25)-Cr(1)-C(28)	79.6(2)
C(29)-C(25)-Cr(1)-C(28)	-37.18(16)

2.3 Compound 5



Data Collection

A red tablet crystal of $C_{29}H_{33}N_2F_3Cr$ having approximate dimensions of $0.30 \times 0.40 \times 0.50$ mm was mounted on a glass fiber. All measurements were made on a Bruker X8 APEX diffractometer with graphite monochromated Mo-K α radiation.

The data were collected at a temperature of $-100.0 \pm 0.1^\circ\text{C}$ to a maximum 2θ value of 55.90° . Data were collected in a series of ϕ and ω scans in 0.50° oscillations with 5.0 second exposures. The crystal-to-detector distance was 38.94 mm.

Data Reduction

Of the 26408 reflections that were collected, 6359 were unique ($R_{\text{int}} = 0.028$); equivalent reflections were merged. Data were collected and integrated using the Bruker SAINT¹ software package. The linear absorption coefficient, μ , for Mo-K α radiation is 4.70 cm^{-1} . Data were corrected for absorption effects using the multi-scan technique (SADABS²), with minimum and maximum transmission coefficients of 0.706 and 0.868, respectively. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods³. All non-hydrogen atoms were refined anisotropically. All C-H hydrogen atoms were included in calculated positions but were not refined. The final cycle of full-matrix least-squares refinement⁴ on F^2 was based on 6359 reflections and 350 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \sum \|F_O - F_C\| / \sum |F_O| = 0.048$$

$$wR2 = [\sum (w(F_O^2 - F_C^2)^2) / \sum w(F_O^2)^2]^{1/2} = 0.100$$

The standard deviation of an observation of unit weight⁵ was 1.03. The weighting scheme was based on counting statistics. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.28 and $-0.25 \text{ e}^-/\text{\AA}^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber⁶. Anomalous dispersion effects were included in Fcalc⁷; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley⁸. The values for the mass attenuation coefficients are those of Creagh and Hubbell⁹. All refinements were performed using the SHELXTL¹⁰ crystallographic software package of Bruker-AXS.

References

- (1) [SAINT](#). Version 7.03A. Bruker AXS Inc., Madison, Wisconsin, USA. (1997-2003).
- (2) [SADABS](#). Bruker Nonius area detector scaling and absorption correction - V2.10, Bruker AXS Inc., Madison, Wisconsin, USA (2003).
- (3) [SIR97](#) - Altomare A., Burla M.C., Camalli M., Cascarano G.L., Giacovazzo C., Guagliardi A., Moliterni A.G.G., Polidori G., Spagna R. (1999) J. Appl. Cryst. 32, 115-119.
- (4) Least Squares function minimized:
$$\sum w(F_O^2 - F_C^2)^2$$
- (5) Standard deviation of an observation of unit weight:
$$[\sum w(F_O^2 - F_C^2)^2 / (N_O - N_V)]^{1/2}$$

where: N_O = number of observations
 N_V = number of variables

- (6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).
- (7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).
- (8) Creagh, D. C. & McAuley, W.J.; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).
- (9) Creagh, D. C. & Hubbell, J.H.; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).
- (10) [SHELXTL](#) Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA. (1997).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	C ₂₉ H ₃₃ N ₂ F ₃ Cr
Formula Weight	518.57
Crystal Color, Habit	red, tablet
Crystal Dimensions	0.30 X 0.40 X 0.50 mm
Crystal System	triclinic
Lattice Type	primitive
Lattice Parameters	a = 9.4535(3) Å b = 9.6773(4) Å c = 14.8723(6) Å α = 79.991(2) ° β = 83.696(2) ° γ = 86.467(2) ° V = 1330.52(9) Å ³
Space Group	P -1 (#2)
Z value	2
D _{calc}	1.294 g/cm ³
F ₀₀₀	544.00
μ(MoKα)	4.70 cm ⁻¹

B. Intensity Measurements

Diffractometer	Bruker X8 APEX
Radiation	MoK α ($\lambda = 0.71073 \text{ \AA}$) graphite monochromated
Data Images	2263 exposures @ 5.0 seconds
Detector Position	38.94 mm
$2\theta_{\max}$	55.9°
No. of Reflections Measured	Total: 26408 Unique: 6359 ($R_{\text{int}} = 0.028$) Absorption ($T_{\min} = 0.706$, $T_{\max} = 0.868$) Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR97)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma w (F_o^2 - F_c^2)^2$
Least Squares Weights	$w=1/(\sigma^2(F_o^2)+(0.0490P)^2+0.4393P)$
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ($I > 0.00\sigma(I)$)	6359
No. Variables	350
Reflection/Parameter Ratio	18.17
Residuals (refined on F^2 , all data): R1; wR2	0.048; 0.100
Goodness of Fit Indicator	1.03
No. Observations ($I > 2.00\sigma(I)$)	5202
Residuals (refined on F): R1; wR2	0.036; 0.093
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.28 e $^-/\text{\AA}^3$
Minimum peak in Final Diff. Map	-0.25 e $^-/\text{\AA}^3$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ks051.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	8035(2)	4602(2)	1841(1)	28(1)
C(2)	7480(2)	5993(2)	1843(1)	31(1)
C(3)	6739(2)	6637(2)	1112(1)	38(1)
C(4)	6531(2)	5936(2)	406(1)	39(1)
C(5)	7085(2)	4576(2)	413(1)	35(1)
C(6)	7850(2)	3883(2)	1122(1)	31(1)
C(7)	7746(2)	6798(2)	2597(1)	34(1)
C(8)	6492(2)	7773(2)	2865(1)	40(1)
C(9)	9083(2)	7642(2)	2312(1)	47(1)
C(10)	8452(2)	2398(2)	1087(1)	39(1)
C(11)	9472(2)	2338(2)	216(1)	47(1)
C(12)	7251(3)	1383(2)	1133(2)	57(1)
C(13)	11044(2)	4378(2)	1762(1)	37(1)
C(14)	10105(2)	3891(2)	2639(1)	28(1)
C(15)	10813(2)	3434(2)	3426(1)	30(1)
C(16)	10233(2)	2956(2)	4326(1)	28(1)
C(17)	11256(2)	2727(2)	5056(1)	39(1)
C(18)	8401(2)	2207(2)	5504(1)	28(1)
C(19)	8396(2)	769(2)	5809(1)	40(1)
C(20)	7951(2)	234(2)	6715(1)	45(1)
C(21)	7482(2)	1139(2)	7318(1)	38(1)
C(22)	7451(2)	2573(2)	7016(1)	37(1)
C(23)	7911(2)	3108(2)	6111(1)	33(1)
C(24)	7049(2)	540(3)	8302(1)	54(1)
C(25)	5392(2)	1864(2)	4524(1)	39(1)
C(26)	5121(2)	3298(2)	4564(1)	37(1)
C(27)	4961(2)	4001(2)	3676(1)	39(1)
C(28)	5152(2)	3003(2)	3079(1)	41(1)
C(29)	5374(2)	1671(2)	3612(1)	41(1)
N(1)	8699(1)	3912(1)	2637(1)	26(1)
N(2)	8851(1)	2739(1)	4561(1)	28(1)
F(1)	5946(5)	-155(12)	8412(4)	78(2)
F(2)	8068(11)	-140(16)	8721(8)	95(3)
F(3)	6642(9)	1586(8)	8794(4)	86(2)
F(1B)	6420(20)	-785(18)	8384(6)	125(5)
F(2B)	8150(14)	183(19)	8760(9)	78(3)
F(3B)	6234(16)	1304(18)	8768(6)	124(5)
Cr(1)	7304(1)	3075(1)	3700(1)	28(1)

Table 3. Bond lengths [Å] and angles [deg] for ks051.

C(1)-C(6)	1.404(2)
C(1)-C(2)	1.415(2)
C(1)-N(1)	1.4413(18)
C(2)-C(3)	1.393(2)
C(2)-C(7)	1.522(2)
C(3)-C(4)	1.383(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.385(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.395(2)
C(5)-H(5)	0.9500
C(6)-C(10)	1.521(2)
C(7)-C(9)	1.527(2)
C(7)-C(8)	1.531(2)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(12)	1.535(3)
C(10)-C(11)	1.535(3)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.515(2)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-N(1)	1.3280(19)
C(14)-C(15)	1.404(2)
C(15)-C(16)	1.399(2)
C(15)-H(15)	0.9500
C(16)-N(2)	1.3355(19)
C(16)-C(17)	1.511(2)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(23)	1.386(2)
C(18)-C(19)	1.387(2)
C(18)-N(2)	1.4343(19)
C(19)-C(20)	1.386(2)
C(19)-H(19)	0.9500
C(20)-C(21)	1.380(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.382(3)
C(21)-C(24)	1.499(2)
C(22)-C(23)	1.388(2)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(24)-F(1)	1.256(6)
C(24)-F(3B)	1.269(10)
C(24)-F(2)	1.289(9)
C(24)-F(2B)	1.303(11)

C(24)-F(3)	1.363(7)
C(24)-F(1B)	1.429(9)
C(25)-C(29)	1.402(3)
C(25)-C(26)	1.407(2)
C(25)-Cr(1)	2.3282(16)
C(25)-H(25)	0.9500
C(26)-C(27)	1.395(3)
C(26)-Cr(1)	2.3275(16)
C(26)-H(26)	0.9500
C(27)-C(28)	1.412(3)
C(27)-Cr(1)	2.3392(16)
C(27)-H(27)	0.9500
C(28)-C(29)	1.407(3)
C(28)-Cr(1)	2.3347(16)
C(28)-H(28)	0.9500
C(29)-Cr(1)	2.3695(16)
C(29)-H(29)	0.9500
N(1)-Cr(1)	2.0303(12)
N(2)-Cr(1)	2.0224(12)
C(6)-C(1)-C(2)	121.14(14)
C(6)-C(1)-N(1)	121.14(13)
C(2)-C(1)-N(1)	117.55(13)
C(3)-C(2)-C(1)	118.30(14)
C(3)-C(2)-C(7)	120.51(14)
C(1)-C(2)-C(7)	121.12(13)
C(4)-C(3)-C(2)	121.19(15)
C(4)-C(3)-H(3)	119.4
C(2)-C(3)-H(3)	119.4
C(5)-C(4)-C(3)	119.77(15)
C(5)-C(4)-H(4)	120.1
C(3)-C(4)-H(4)	120.1
C(4)-C(5)-C(6)	121.56(15)
C(4)-C(5)-H(5)	119.2
C(6)-C(5)-H(5)	119.2
C(5)-C(6)-C(1)	118.02(14)
C(5)-C(6)-C(10)	119.25(14)
C(1)-C(6)-C(10)	122.72(14)
C(2)-C(7)-C(9)	110.06(14)
C(2)-C(7)-C(8)	113.93(14)
C(9)-C(7)-C(8)	109.64(14)
C(2)-C(7)-H(7)	107.7
C(9)-C(7)-H(7)	107.7
C(8)-C(7)-H(7)	107.7
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(6)-C(10)-C(12)	110.87(16)
C(6)-C(10)-C(11)	111.38(14)
C(12)-C(10)-C(11)	109.65(15)
C(6)-C(10)-H(10)	108.3
C(12)-C(10)-H(10)	108.3
C(11)-C(10)-H(10)	108.3
C(10)-C(11)-H(11A)	109.5

C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(1)-C(14)-C(15)	123.62(14)
N(1)-C(14)-C(13)	120.41(14)
C(15)-C(14)-C(13)	115.97(13)
C(16)-C(15)-C(14)	128.79(14)
C(16)-C(15)-H(15)	115.6
C(14)-C(15)-H(15)	115.6
N(2)-C(16)-C(15)	123.67(13)
N(2)-C(16)-C(17)	119.80(14)
C(15)-C(16)-C(17)	116.50(13)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(23)-C(18)-C(19)	119.11(15)
C(23)-C(18)-N(2)	121.03(13)
C(19)-C(18)-N(2)	119.81(14)
C(20)-C(19)-C(18)	120.67(16)
C(20)-C(19)-H(19)	119.7
C(18)-C(19)-H(19)	119.7
C(21)-C(20)-C(19)	119.84(16)
C(21)-C(20)-H(20)	120.1
C(19)-C(20)-H(20)	120.1
C(20)-C(21)-C(22)	119.97(15)
C(20)-C(21)-C(24)	118.95(18)
C(22)-C(21)-C(24)	121.06(17)
C(21)-C(22)-C(23)	120.14(15)
C(21)-C(22)-H(22)	119.9
C(23)-C(22)-H(22)	119.9
C(18)-C(23)-C(22)	120.26(15)
C(18)-C(23)-H(23)	119.9
C(22)-C(23)-H(23)	119.9
F(1)-C(24)-F(3B)	81.0(8)
F(1)-C(24)-F(2)	111.8(6)
F(3B)-C(24)-F(2)	115.4(7)
F(1)-C(24)-F(2B)	123.8(8)
F(3B)-C(24)-F(2B)	106.0(9)
F(2)-C(24)-F(2B)	15.2(12)
F(1)-C(24)-F(3)	102.0(5)
F(3B)-C(24)-F(3)	21.3(10)
F(2)-C(24)-F(3)	104.1(7)
F(2B)-C(24)-F(3)	91.6(8)
F(1)-C(24)-F(1B)	31.0(7)
F(3B)-C(24)-F(1B)	108.1(7)
F(2)-C(24)-F(1B)	86.5(8)

F(2B)-C(24)-F(1B)	101.0(10)
F(3)-C(24)-F(1B)	127.3(7)
F(1)-C(24)-C(21)	113.4(3)
F(3B)-C(24)-C(21)	117.3(5)
F(2)-C(24)-C(21)	113.8(6)
F(2B)-C(24)-C(21)	111.7(7)
F(3)-C(24)-C(21)	110.6(4)
F(1B)-C(24)-C(21)	111.3(4)
C(29)-C(25)-C(26)	108.44(16)
C(29)-C(25)-Cr(1)	74.26(10)
C(26)-C(25)-Cr(1)	72.39(9)
C(29)-C(25)-H(25)	125.8
C(26)-C(25)-H(25)	125.8
Cr(1)-C(25)-H(25)	119.4
C(27)-C(26)-C(25)	107.95(16)
C(27)-C(26)-Cr(1)	73.06(9)
C(25)-C(26)-Cr(1)	72.44(9)
C(27)-C(26)-H(26)	126.0
C(25)-C(26)-H(26)	126.0
Cr(1)-C(26)-H(26)	120.3
C(26)-C(27)-C(28)	108.03(15)
C(26)-C(27)-Cr(1)	72.15(9)
C(28)-C(27)-Cr(1)	72.24(9)
C(26)-C(27)-H(27)	126.0
C(28)-C(27)-H(27)	126.0
Cr(1)-C(27)-H(27)	121.4
C(29)-C(28)-C(27)	107.94(16)
C(29)-C(28)-Cr(1)	73.95(10)
C(27)-C(28)-Cr(1)	72.58(9)
C(29)-C(28)-H(28)	126.0
C(27)-C(28)-H(28)	126.0
Cr(1)-C(28)-H(28)	119.3
C(25)-C(29)-C(28)	107.55(15)
C(25)-C(29)-Cr(1)	71.04(9)
C(28)-C(29)-Cr(1)	71.25(9)
C(25)-C(29)-H(29)	126.2
C(28)-C(29)-H(29)	126.2
Cr(1)-C(29)-H(29)	123.2
C(14)-N(1)-C(1)	120.27(12)
C(14)-N(1)-Cr(1)	125.64(10)
C(1)-N(1)-Cr(1)	114.07(9)
C(16)-N(2)-C(18)	118.09(12)
C(16)-N(2)-Cr(1)	125.82(10)
C(18)-N(2)-Cr(1)	116.08(9)
N(2)-Cr(1)-N(1)	91.59(5)
N(2)-Cr(1)-C(26)	108.46(6)
N(1)-Cr(1)-C(26)	147.78(6)
N(2)-Cr(1)-C(25)	104.12(6)
N(1)-Cr(1)-C(25)	161.00(6)
C(26)-Cr(1)-C(25)	35.17(6)
N(2)-Cr(1)-C(28)	162.25(6)
N(1)-Cr(1)-C(28)	105.65(6)
C(26)-Cr(1)-C(28)	58.32(6)
C(25)-Cr(1)-C(28)	58.15(6)
N(2)-Cr(1)-C(27)	138.91(6)
N(1)-Cr(1)-C(27)	115.56(6)
C(26)-Cr(1)-C(27)	34.79(6)
C(25)-Cr(1)-C(27)	58.09(6)
C(28)-Cr(1)-C(27)	35.18(6)
N(2)-Cr(1)-C(29)	129.54(6)
N(1)-Cr(1)-C(29)	126.31(6)
C(26)-Cr(1)-C(29)	58.02(6)
C(25)-Cr(1)-C(29)	34.70(6)

C(28)-Cr(1)-C(29) 34.80(6)
C(27)-Cr(1)-C(29) 57.93(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{A}^2 \times 10^3$) for ks051.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	22(1)	32(1)	27(1)	1(1)	-1(1)	-5(1)
C(2)	23(1)	34(1)	33(1)	-2(1)	-2(1)	-2(1)
C(3)	32(1)	37(1)	43(1)	-2(1)	-8(1)	5(1)
C(4)	31(1)	48(1)	36(1)	0(1)	-10(1)	1(1)
C(5)	31(1)	43(1)	32(1)	-4(1)	-6(1)	-7(1)
C(6)	29(1)	32(1)	31(1)	-1(1)	0(1)	-6(1)
C(7)	33(1)	32(1)	35(1)	-4(1)	-5(1)	1(1)
C(8)	35(1)	36(1)	49(1)	-9(1)	2(1)	-2(1)
C(9)	32(1)	60(1)	55(1)	-22(1)	-3(1)	-10(1)
C(10)	51(1)	34(1)	32(1)	-4(1)	-8(1)	-2(1)
C(11)	50(1)	45(1)	45(1)	-12(1)	-4(1)	4(1)
C(12)	79(2)	40(1)	51(1)	-10(1)	9(1)	-21(1)
C(13)	26(1)	47(1)	34(1)	0(1)	1(1)	-5(1)
C(14)	24(1)	26(1)	32(1)	-4(1)	0(1)	-3(1)
C(15)	21(1)	33(1)	36(1)	-4(1)	-2(1)	-3(1)
C(16)	26(1)	28(1)	32(1)	-5(1)	-5(1)	-2(1)
C(17)	29(1)	52(1)	36(1)	-3(1)	-8(1)	-6(1)
C(18)	22(1)	32(1)	31(1)	-4(1)	-4(1)	-2(1)
C(19)	47(1)	32(1)	40(1)	-6(1)	3(1)	2(1)
C(20)	46(1)	36(1)	45(1)	6(1)	2(1)	-1(1)
C(21)	22(1)	56(1)	32(1)	1(1)	-4(1)	-5(1)
C(22)	29(1)	51(1)	33(1)	-14(1)	-4(1)	-1(1)
C(23)	30(1)	32(1)	37(1)	-8(1)	-4(1)	-2(1)
C(24)	37(1)	83(2)	37(1)	7(1)	-5(1)	-8(1)
C(25)	28(1)	41(1)	44(1)	4(1)	1(1)	-12(1)
C(26)	24(1)	47(1)	42(1)	-12(1)	5(1)	-7(1)
C(27)	22(1)	38(1)	54(1)	-2(1)	-2(1)	-2(1)
C(28)	25(1)	61(1)	37(1)	-5(1)	-5(1)	-10(1)
C(29)	32(1)	40(1)	55(1)	-15(1)	-1(1)	-12(1)
N(1)	24(1)	27(1)	27(1)	-1(1)	-2(1)	-3(1)
N(2)	25(1)	31(1)	28(1)	-2(1)	-2(1)	-3(1)
F(1)	64(3)	114(5)	49(2)	20(3)	-2(2)	-52(2)
F(2)	60(5)	138(6)	59(4)	43(3)	-2(3)	35(4)
F(3)	106(5)	119(3)	32(2)	-15(2)	13(2)	-12(4)
F(1B)	218(11)	105(7)	52(3)	6(4)	16(5)	-110(7)
F(2B)	53(4)	138(8)	36(3)	20(4)	-22(3)	-22(5)
F(3B)	86(6)	196(11)	49(4)	37(5)	30(3)	93(7)
Cr(1)	20(1)	33(1)	29(1)	0(1)	-1(1)	-5(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ks051.

	x	y	z	U(eq)
H(3)	6370	7576	1098	45
H(4)	6008	6385	-83	46
H(5)	6942	4104	-77	42
H(7)	7925	6094	3154	40
H(8A)	6356	8534	2350	60
H(8B)	6692	8170	3399	60
H(8C)	5626	7239	3019	60
H(9A)	9912	6998	2234	71
H(9B)	9220	8191	2788	71
H(9C)	8976	8276	1731	71
H(10)	8997	2086	1632	47
H(11A)	8943	2581	-324	70
H(11B)	9903	1387	238	70
H(11C)	10222	3006	180	70
H(12A)	6653	1357	1717	85
H(12B)	7663	440	1088	85
H(12C)	6670	1703	624	85
H(13A)	11291	3585	1437	55
H(13B)	11916	4747	1912	55
H(13C)	10532	5118	1371	55
H(15)	11823	3451	3336	36
H(17A)	11081	3464	5436	58
H(17B)	12237	2760	4764	58
H(17C)	11112	1807	5442	58
H(19)	8700	143	5392	48
H(20)	7968	-752	6920	53
H(22)	7115	3195	7429	44
H(23)	7891	4094	5907	39
H(25)	5559	1146	5029	47
H(26)	5057	3716	5100	45
H(27)	4760	4979	3503	46
H(28)	5134	3196	2432	49
H(29)	5489	801	3394	49

Table 6. Torsion angles [deg] for ks051.

C(6)-C(1)-C(2)-C(3)	0.1(2)
N(1)-C(1)-C(2)-C(3)	-175.20(13)
C(6)-C(1)-C(2)-C(7)	-176.80(14)
N(1)-C(1)-C(2)-C(7)	7.9(2)
C(1)-C(2)-C(3)-C(4)	0.8(2)
C(7)-C(2)-C(3)-C(4)	177.79(16)
C(2)-C(3)-C(4)-C(5)	-1.1(3)
C(3)-C(4)-C(5)-C(6)	0.4(3)
C(4)-C(5)-C(6)-C(1)	0.6(2)
C(4)-C(5)-C(6)-C(10)	-179.16(16)
C(2)-C(1)-C(6)-C(5)	-0.8(2)
N(1)-C(1)-C(6)-C(5)	174.36(13)
C(2)-C(1)-C(6)-C(10)	178.89(14)
N(1)-C(1)-C(6)-C(10)	-5.9(2)
C(3)-C(2)-C(7)-C(9)	-85.01(19)
C(1)-C(2)-C(7)-C(9)	91.86(18)
C(3)-C(2)-C(7)-C(8)	38.6(2)
C(1)-C(2)-C(7)-C(8)	-144.54(15)
C(5)-C(6)-C(10)-C(12)	-63.7(2)
C(1)-C(6)-C(10)-C(12)	116.58(17)
C(5)-C(6)-C(10)-C(11)	58.7(2)
C(1)-C(6)-C(10)-C(11)	-121.02(17)
N(1)-C(14)-C(15)-C(16)	-1.3(3)
C(13)-C(14)-C(15)-C(16)	178.69(15)
C(14)-C(15)-C(16)-N(2)	6.5(3)
C(14)-C(15)-C(16)-C(17)	-171.63(15)
C(23)-C(18)-C(19)-C(20)	-2.0(3)
N(2)-C(18)-C(19)-C(20)	-179.34(16)
C(18)-C(19)-C(20)-C(21)	1.2(3)
C(19)-C(20)-C(21)-C(22)	0.3(3)
C(19)-C(20)-C(21)-C(24)	-178.10(17)
C(20)-C(21)-C(22)-C(23)	-1.0(2)
C(24)-C(21)-C(22)-C(23)	177.38(15)
C(19)-C(18)-C(23)-C(22)	1.3(2)
N(2)-C(18)-C(23)-C(22)	178.60(14)
C(21)-C(22)-C(23)-C(18)	0.2(2)
C(20)-C(21)-C(24)-F(1)	-67.1(6)
C(22)-C(21)-C(24)-F(1)	114.6(6)
C(20)-C(21)-C(24)-F(3B)	-158.8(11)
C(22)-C(21)-C(24)-F(3B)	22.8(11)
C(20)-C(21)-C(24)-F(2)	62.2(8)
C(22)-C(21)-C(24)-F(2)	-116.2(8)
C(20)-C(21)-C(24)-F(2B)	78.5(8)
C(22)-C(21)-C(24)-F(2B)	-99.8(8)
C(20)-C(21)-C(24)-F(3)	179.0(4)
C(22)-C(21)-C(24)-F(3)	0.6(5)
C(20)-C(21)-C(24)-F(1B)	-33.6(12)
C(22)-C(21)-C(24)-F(1B)	148.1(12)
C(29)-C(25)-C(26)-C(27)	-1.12(19)
Cr(1)-C(25)-C(26)-C(27)	64.93(11)
C(29)-C(25)-C(26)-Cr(1)	-66.05(12)
C(25)-C(26)-C(27)-C(28)	-0.75(18)
Cr(1)-C(26)-C(27)-C(28)	63.78(11)
C(25)-C(26)-C(27)-Cr(1)	-64.52(11)
C(26)-C(27)-C(28)-C(29)	2.32(19)
Cr(1)-C(27)-C(28)-C(29)	66.04(12)
C(26)-C(27)-C(28)-Cr(1)	-63.72(11)
C(26)-C(25)-C(29)-C(28)	2.55(19)
Cr(1)-C(25)-C(29)-C(28)	-62.28(12)

C(26)-C(25)-C(29)-Cr(1)	64.82(11)
C(27)-C(28)-C(29)-C(25)	-2.99(19)
Cr(1)-C(28)-C(29)-C(25)	62.14(12)
C(27)-C(28)-C(29)-Cr(1)	-65.13(11)
C(15)-C(14)-N(1)-C(1)	170.01(14)
C(13)-C(14)-N(1)-C(1)	-10.0(2)
C(15)-C(14)-N(1)-Cr(1)	-8.3(2)
C(13)-C(14)-N(1)-Cr(1)	171.77(11)
C(6)-C(1)-N(1)-C(14)	87.74(18)
C(2)-C(1)-N(1)-C(14)	-96.92(17)
C(6)-C(1)-N(1)-Cr(1)	-93.80(14)
C(2)-C(1)-N(1)-Cr(1)	81.54(14)
C(15)-C(16)-N(2)-C(18)	178.19(14)
C(17)-C(16)-N(2)-C(18)	-3.8(2)
C(15)-C(16)-N(2)-Cr(1)	-1.2(2)
C(17)-C(16)-N(2)-Cr(1)	176.84(11)
C(23)-C(18)-N(2)-C(16)	93.97(17)
C(19)-C(18)-N(2)-C(16)	-88.76(18)
C(23)-C(18)-N(2)-Cr(1)	-86.60(15)
C(19)-C(18)-N(2)-Cr(1)	90.67(16)
C(16)-N(2)-Cr(1)-N(1)	-5.13(13)
C(18)-N(2)-Cr(1)-N(1)	175.49(10)
C(16)-N(2)-Cr(1)-C(26)	-159.48(12)
C(18)-N(2)-Cr(1)-C(26)	21.14(12)
C(16)-N(2)-Cr(1)-C(25)	164.09(12)
C(18)-N(2)-Cr(1)-C(25)	-15.29(11)
C(16)-N(2)-Cr(1)-C(28)	161.13(18)
C(18)-N(2)-Cr(1)-C(28)	-18.3(2)
C(16)-N(2)-Cr(1)-C(27)	-138.65(12)
C(18)-N(2)-Cr(1)-C(27)	41.97(14)
C(16)-N(2)-Cr(1)-C(29)	137.16(12)
C(18)-N(2)-Cr(1)-C(29)	-42.23(13)
C(14)-N(1)-Cr(1)-N(2)	9.73(12)
C(1)-N(1)-Cr(1)-N(2)	-168.63(10)
C(14)-N(1)-Cr(1)-C(26)	139.38(13)
C(1)-N(1)-Cr(1)-C(26)	-38.98(15)
C(14)-N(1)-Cr(1)-C(25)	-136.40(17)
C(1)-N(1)-Cr(1)-C(25)	45.2(2)
C(14)-N(1)-Cr(1)-C(28)	-165.95(12)
C(1)-N(1)-Cr(1)-C(28)	15.69(11)
C(14)-N(1)-Cr(1)-C(27)	157.84(12)
C(1)-N(1)-Cr(1)-C(27)	-20.51(12)
C(14)-N(1)-Cr(1)-C(29)	-134.43(12)
C(1)-N(1)-Cr(1)-C(29)	47.22(12)
C(27)-C(26)-Cr(1)-N(2)	155.81(10)
C(25)-C(26)-Cr(1)-N(2)	-88.44(11)
C(27)-C(26)-Cr(1)-N(1)	30.05(16)
C(25)-C(26)-Cr(1)-N(1)	145.79(11)
C(27)-C(26)-Cr(1)-C(25)	-115.74(15)
C(27)-C(26)-Cr(1)-C(28)	-37.33(10)
C(25)-C(26)-Cr(1)-C(28)	78.41(11)
C(25)-C(26)-Cr(1)-C(27)	115.74(15)
C(27)-C(26)-Cr(1)-C(29)	-78.54(11)
C(25)-C(26)-Cr(1)-C(29)	37.20(10)
C(29)-C(25)-Cr(1)-N(2)	-142.15(10)
C(26)-C(25)-Cr(1)-N(2)	102.11(10)
C(29)-C(25)-Cr(1)-N(1)	2.8(2)
C(26)-C(25)-Cr(1)-N(1)	-112.95(18)
C(29)-C(25)-Cr(1)-C(26)	115.74(15)
C(29)-C(25)-Cr(1)-C(28)	36.79(11)
C(26)-C(25)-Cr(1)-C(28)	-78.95(11)
C(29)-C(25)-Cr(1)-C(27)	78.49(12)
C(26)-C(25)-Cr(1)-C(27)	-37.26(10)

C(26)-C(25)-Cr(1)-C(29)	-115.74(15)
C(29)-C(28)-Cr(1)-N(2)	-33.3(3)
C(27)-C(28)-Cr(1)-N(2)	81.9(2)
C(29)-C(28)-Cr(1)-N(1)	132.42(10)
C(27)-C(28)-Cr(1)-N(1)	-112.36(10)
C(29)-C(28)-Cr(1)-C(26)	-78.32(11)
C(27)-C(28)-Cr(1)-C(26)	36.90(10)
C(29)-C(28)-Cr(1)-C(25)	-36.68(10)
C(27)-C(28)-Cr(1)-C(25)	78.54(11)
C(29)-C(28)-Cr(1)-C(27)	-115.22(15)
C(27)-C(28)-Cr(1)-C(29)	115.22(15)
C(26)-C(27)-Cr(1)-N(2)	-36.25(14)
C(28)-C(27)-Cr(1)-N(2)	-152.65(10)
C(26)-C(27)-Cr(1)-N(1)	-162.78(9)
C(28)-C(27)-Cr(1)-N(1)	80.81(11)
C(28)-C(27)-Cr(1)-C(26)	-116.40(15)
C(26)-C(27)-Cr(1)-C(25)	37.68(10)
C(28)-C(27)-Cr(1)-C(25)	-78.72(11)
C(26)-C(27)-Cr(1)-C(28)	116.40(15)
C(26)-C(27)-Cr(1)-C(29)	78.86(11)
C(28)-C(27)-Cr(1)-C(29)	-37.54(10)
C(25)-C(29)-Cr(1)-N(2)	50.50(13)
C(28)-C(29)-Cr(1)-N(2)	167.46(10)
C(25)-C(29)-Cr(1)-N(1)	-178.87(9)
C(28)-C(29)-Cr(1)-N(1)	-61.91(12)
C(25)-C(29)-Cr(1)-C(26)	-37.71(10)
C(28)-C(29)-Cr(1)-C(26)	79.25(11)
C(28)-C(29)-Cr(1)-C(25)	116.96(16)
C(25)-C(29)-Cr(1)-C(28)	-116.96(16)
C(25)-C(29)-Cr(1)-C(27)	-79.00(11)
C(28)-C(29)-Cr(1)-C(27)	37.96(11)

3. Polymerization results

Materials

Tetrahydrofuran (THF, synthesis grade, SDS) was filtered (pore size = 0.2 µm) before use. Toluene (synthesis grade, SDS) was dried over sodium and freshly distilled before use. Vinyl acetate (VAc, 99 %) and methyl metacrylate (MMA, 99 %, Acros Organics) were passed through a neutral alumina column to remove the stabilizer, dried over calcium hydride, distilled under reduced pressure, and degassed with argon. Styrene (99 %, Acros Organics) was dried over calcium hydride and distilled under reduced pressure before use. 2,2'-azobisisobutyronitrile (AIBN, 98 %, Acros Organics), 2,2'-Azobis(4-methoxy-2,4-dimethylvaleronitrile) (V-70, 96 %, Wako), and Bromoethylbenzene (BEB, 97 %, Aldrich) and Anisol (99 %, Fluka) were used as received.

The isolated polymer samples were dissolved for at least 12 h in THF and the polymer solutions were filtered (pore size = 0.2 µm) before analysis with size exclusion chromatography (SEC).

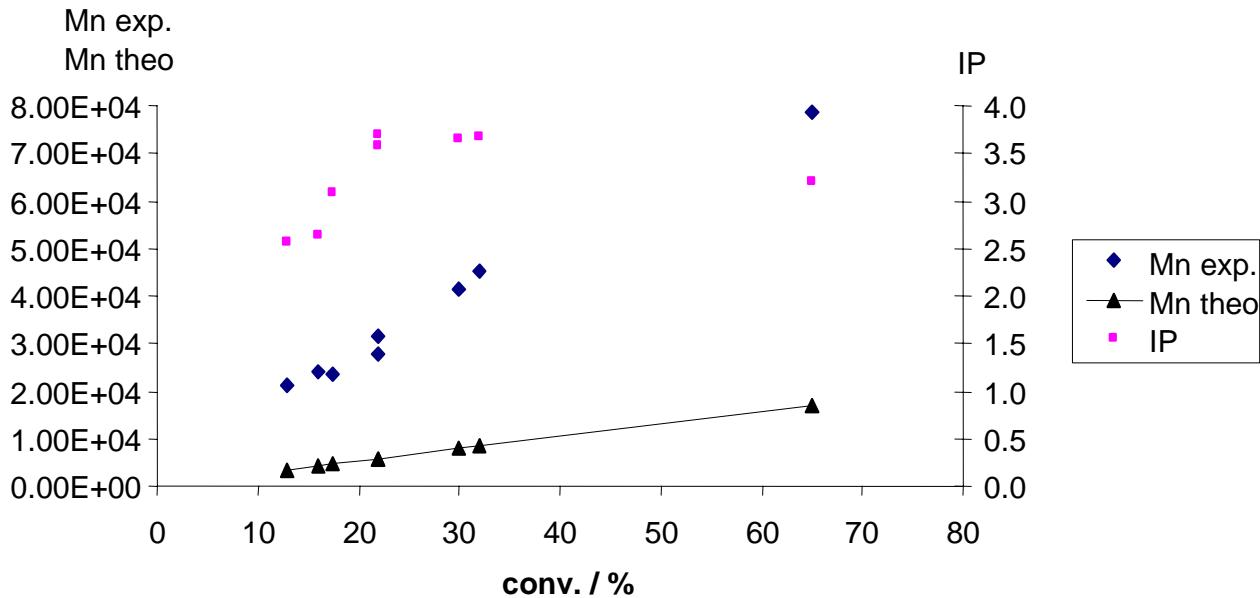
Techniques

The molecular weight distribution, \overline{M}_n and $\overline{M}_w / \overline{M}_n$ of the polymers were measured by size-exclusion chromatography (SEC) using THF as eluent (1mL/min) at room temperature on a 300x7,5 mm PLgel 5µm Mixed-D column (Polymer Laboratories), equipped with multiangle light scattering (miniDawn Tristar, Wyatt Technology Corp.) and refractive index (RI2000, Soparès) detector or with a Waters column pack (300x7,5 mm, Ultrastyragel 104, 103, 100 Å), equipped with multiangle light scattering (miniDawn Tristar, Wyatt Technology Corp.) and refractive index (Waters 410) detector.

3.1. OMRP of styrene in the presence of compound 2 (YC111)

Catalyst: [CpCr{(XylNCMe)₂CH}]
Monomer: Styrene
Initiator: V-70
Solvent: - (BULK)
Temperature: 50 °C for 44 h. Then 70 °C from 44 h until 68 h then 90 °C
Ratio: (Cat. : Monom. : Init.) = 1 : 250 : 0.8
Result:

Time/h	T/°C	conv/%	Mn PVAc	Mn theo	M _w /M _n
16.4	50	13	2.14 E+04	0.34 E+04	2.56
23	50	16	2.42 E+04	0.42 E+04	2.64
26.5	50	18	2.37 E+04	0.47 E+04	3.08
41.5	50	22	2.76 E+04	0.57 E+04	3.57
49	70	22	3.17 E+04	0.57 E+04	3.7
64.5	70	30	4.13 E+04	0.78 E+04	3.65
69.5	90	32	4.52 E+04	0.83 E+04	3.68
87.5	90	65	7.87 E+04	1.69 E+04	3.19



Note that polymer continues to form after the end of the radical generation (the half life of V-70 at 50°C is ca. 40 min), indicating that radical continue to be released in solution from a presumed dormant organochromium(III) species. This suggests that the Cr^{III}-PS bond has sufficient strength to be formed, but the trapping of the active PS radical is not efficient. Indeed, most radicals initially generated from V-70 are lost (low efficiency factor as shown by the high M_{n(exp)/M_{n(th)} ratio), and the PDI remains high at high conversion.}

3.2. OMRP of vinyl acetate in the presence of compound 2 (YC55)

Catalyst: [CpCr{(XylNCMe)₂CH}]

Monomer: Vinyl Acetate

Initiator: V-70

Solvent: - (BULK)

Temperature: 50 °C for 4 h then 90 °C for 62 h

Ratio: (Cat. : Monom. : Init.) = 1 : 500 : 08

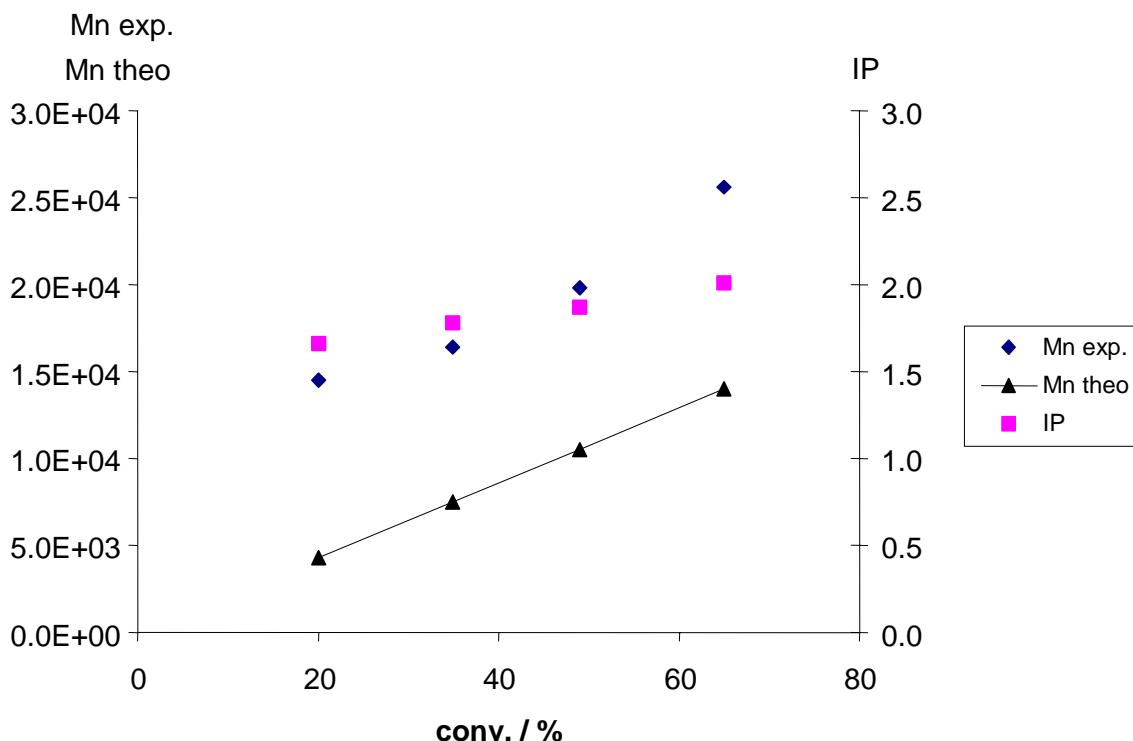
Result:

Time/min	T/°C	conv/%	Mn PVAc	Mn theo	M _w /M _n
210	50	2.0	-	-	-
480	90	11.0	1.05 E+04	0.47 E+04	1.81
1080	90	11.6	1.02 E+04	0.52 E+04	1.86
1350	90	11.4	1.07 E+04	0.47 E+04	1.74
2880	90	12.0	1.13 E+04	0.52 E+04	1.67
3960	90	12.2	1.13 E+04	0.52 E+04	1.68

3.3. OMRP of vinyl acetate in the presence of compound 1 at 50°C (YC79)

Catalyst: [CpCr{(DippNCMe)₂CH}]
Monomer: Vinyl Acetate
Initiator: V-70
Solvent: - (BULK)
Temperature: 50 °C
Ratio: (Cat. : Monom. : Init.) = 1 : 250 : 08
Result:

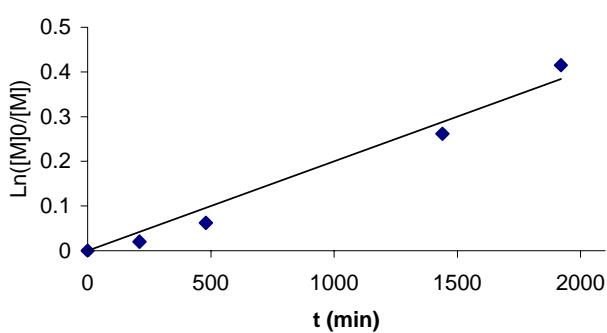
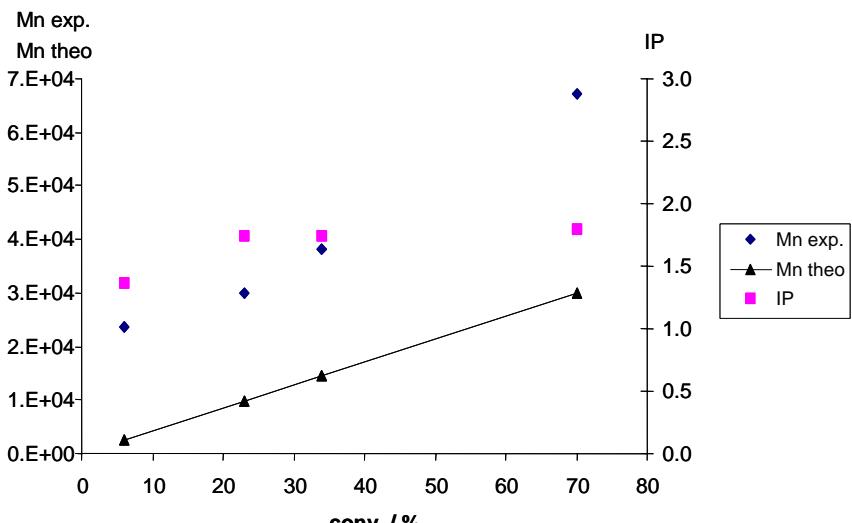
Time/min	T/°C	conv/%	Mn PVAc	Mn theo	M _w /M _n
210	50	20	1.45 E+04	0.43 E+04	1.66
255	50	35	1.64 E+04	0.75 E+04	1.78
390	50	49	1.98 E+04	1.05 E+04	1.87
480	50	65	2.56 E+04	1.40 E+04	2.01



3.4. OMRP of vinyl acetate in the presence of compound 1 at 30°C (YC96)

Catalyst: [CpCr{(DippNCMe)₂CH}]
Monomer: Vinyl Acetate
Initiator: V-70
Solvent: - (BULK)
Temperature: 30 °C
Ratio: (Cat. : Monom. : Init.) = 1 : 500 : 08
Result:

Time/min	T/°C	conv/%	Mn PVAc	Mn theo	M _w /M _n
210	30	2	-	-	-
480	30	6	2.38 E+04	0.25 E+04	1.36
1440	30	23	2.98 E+04	0.99 E+04	1.75
1920	30	34	3.80 E+04	1.46 E+04	1.74
2760	30	70	6.73 E+04	3.01 E+04	1.80



OMRP of vinyl acetate in the presence of compound 3 (UB053)

Catalyst: (LT94) [CpCr{($\text{C}_6\text{H}_3^i\text{Pr}_2$)NCMeCHCMeN(C_6H_5)}]

Monomer: Vinylacetate

Initiator: V-70

Solvent: - (BULK)

Temperature: 50 °C (115 min), 70 °C (225 min), 90 °C (24h 25min)

Ratio: (Cat. : Monom. : Init.) = 1 : 250 : 1.8

Result:

Time/min	T/°C	conv/%	Mn PVAc	Mn theo	M _w /M _n
255	70	2.9411	42210.000	765.579	1.891
534	90	3.2440	23790.000	844.421	1.715
1489	90	3.4447	6603.000	896.647	1.202
1895	90	4.0833	5601.000	1062.884	1.148

3.5. OMRP of vinyl acetate in the presence of compound 4 (UB050)

Catalyst: (LT100) [CpCr{($C_6H_5^iPr_2$)NCMeCHCMeN(C_6H_5OMe)}]

Monomer: Vinylacetate

Initiator: V-70

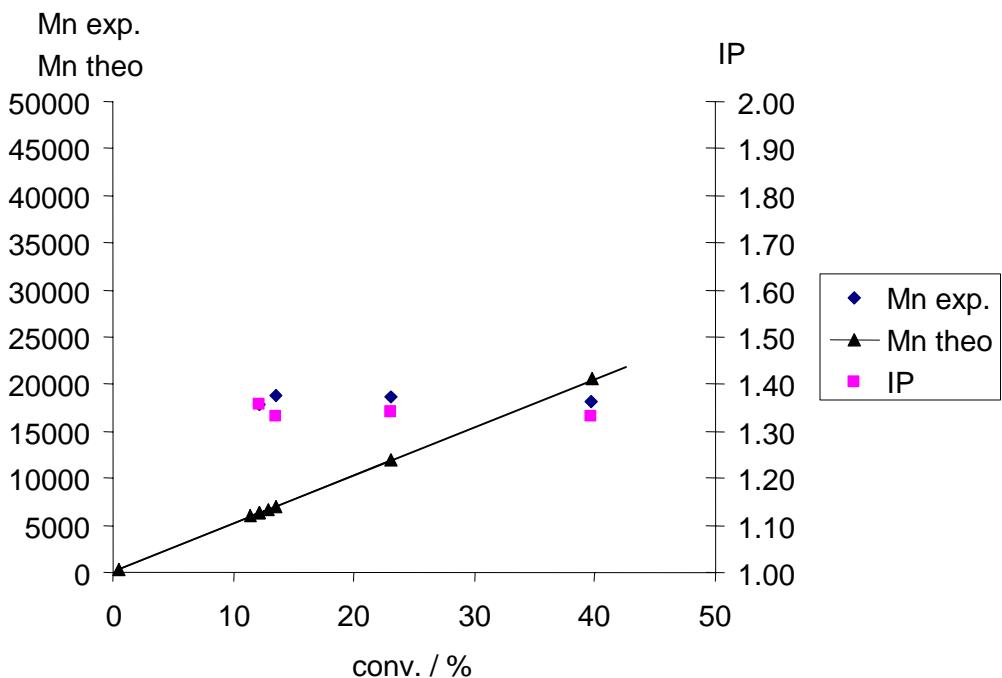
Solvent: - (BULK)

Temperature: 50 °C (115 min); 60 °C (5h 13min min); 80 °C (26h 3min);
100 °C (51h 32min)

Ratio: (Cat. : Monom. : Init.) = 1 : 500 : 1.8

Result:

Time/min	T/°C	conv	Mn PVAc	Mn theo	M _w /M _n
313	60	12.2	1.79E+04	6.33E+03	1.36
3283	100	13.5	1.88E+04	7.04E+03	1.33
5013	100	23.1	1.86E+04	1.20E+04	1.34
6375	100	39.6	1.82E+04	2.06E+04	1.33



Note that the M_n remains approximately constant while the conversion increases at 100°C ($1.8\text{-}1.9 \cdot 10^4$ with $M_w/M_n = 1.33\text{-}1.34$). This suggests the intervention of a catalyzed chain transfer.

3.6. OMRP of vinyl acetate in the presence of compound 5 (UB049)

Catalyst: (LT102) [CpCr{(C₆H₃ⁱPr₂)NCMeCHCMeN(C₆H₅CF₃)}]

Monomer: Vinylacetate

Initiator: V-70

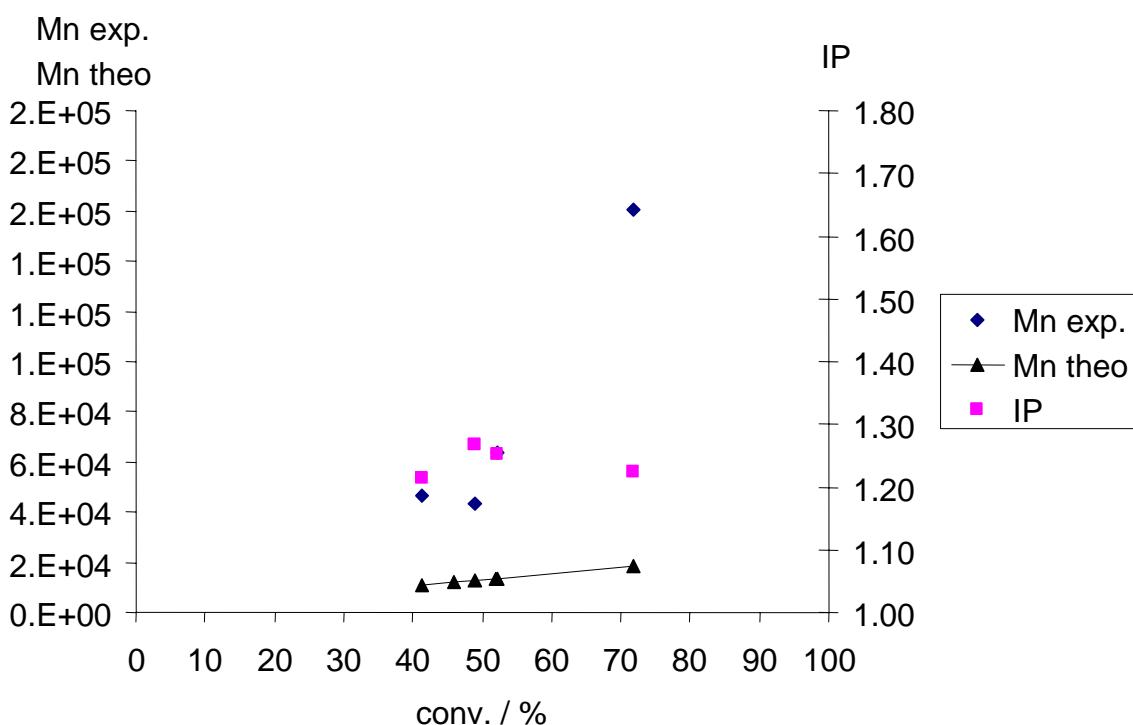
Solvent: - (BULK)

Temperature: 50 °C (2 d 6 h 40 min); 80 °C (14 h 50min)

Ratio: (Cat. : Monom. : Init.) = 1 : 250 : 1.8

Result:

Time/min	T/°C	conv	Mn PVAc	Mn theo	M _w /M _n
110	50	41.4	4.65E+04	1.08E+04	1.21
464	50	48.9	4.33E+04	1.27E+04	1.27
3280	50	52.2	6.36E+04	1.36E+04	1.25
4170	80	71.7	1.60E+05	1.87E+04	1.23



4. DFT calculations

4.1 Computational details

All geometry optimizations were performed using the B3LYP three-parameter hybrid density functional method of Becke,¹ as implemented in the Gaussian03 suite of programs.² The basis functions consisted of the standard 6-31G* for all atoms. All geometry optimizations were carried out without any symmetry constraint and all final geometries were characterized as local minima of the potential energy surface (PES) by verifying that all second derivatives of the energy were positive. The unrestricted formulation was used for open-shell molecules. The mean value of the spin of the first-order electron wave function, which is not an exact eigenstate of S^2 for unrestricted calculations on open-shell systems, was considered to identify unambiguously the spin state. The value of $\langle S^2 \rangle$ at convergence was very close to the expected value of 0.75 (maximum value 0.784 for the PhCH₂ radical) for the radical species, to 6.0 for the spin quintet Cr^{II} species (maximum value 6.023 for the Xyl system), and to 3.75 for the spin quartet Cr^{III} species (maximum value 3.842 for the Xyl-CH₂Ph system), indicating minor spin contamination. All energies were corrected for zero point vibrational energy and for thermal energy to obtain the bond dissociation enthalpies at 298 K. The standard approximations for estimating these corrections were used (ideal gas, rigid rotor and harmonic oscillator) as implemented into Gaussian03. As we are interested in qualitative trends and not in absolute values, these dissociation enthalpies have not been corrected for the basis set superposition error. The table below reports all optimized geometries in Cartesian coordinates.

References

- ¹ A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648–5652.
- ² G. W. T. M. J. Frisch, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. Montgomery, J. A., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, **2004**.

4.2 Cartesian coordinates for all DFT-optimized structures.

PhCH ₂	H 1.072801 6.431292 0.633230 H -0.142079 6.724512 -1.134194 H 5.967489 1.783725 3.415567 H 5.018154 1.435082 5.689574 H -1.436594 5.532237 -1.362116 H 2.646703 2.043179 6.137522 H -0.026703 5.492970 -2.408564 H 1.794262 -0.001900 2.802366 H 3.368895 -0.040442 0.623178 H -3.708600 2.044118 -2.516497 H -0.777248 -0.048930 1.990600 H -0.117529 1.784436 -4.870379 H 1.769855 -0.040270 -1.555193 H -0.781062 -0.001576 -0.705982 H -2.571474 1.436077 -4.645218	C 4.583097 -0.944746 0.327964 N 0.977924 -1.584214 -0.448096 C 0.562940 -2.437918 -1.391414 C 1.554071 -3.390069 -2.042635 C -0.759621 -2.524607 -1.855292 C -1.903797 -1.846318 -1.402755 C -3.219256 -2.260166 -2.041752 N -1.889028 -0.879911 -0.479174 C -3.149904 -0.328795 -0.073105 C -3.936756 -0.983673 0.887101 C -5.150616 -0.438676 1.304921 C -5.601507 0.769981 0.769649 C -4.831349 1.421153 -0.194942 C -3.616889 0.876302 -0.617014 Cr -0.181281 -0.103417 0.397559 C -1.128783 0.900623 2.256198 C 0.184782 1.412045 2.097271 C 1.097468 0.343526 2.277015 C 0.345593 -0.823354 2.602592 C -1.019171 -0.480757 2.592426 C 0.007570 1.462803 -1.097238 C 0.926797 2.624944 -0.866871 C 0.469786 3.786264 -0.206617 C 1.294347 4.888054 0.011472 C 2.618055 4.878950 -0.436041 C 3.087418 3.756560 -1.118430 C 2.255504 2.656696 -1.335293 H -3.586652 -1.925520 1.300379 H -3.029041 1.375670 -1.380189 H 1.855036 -3.579884 1.099905 H 3.058466 0.063016 -0.815505 H -3.888374 -2.723537 -1.308952 H -3.048541 -2.974923 -2.849062 H 1.130617 -3.813238 -2.956096 H -3.750791 -1.392955 -2.447256 H -0.928435 -3.244218 -2.646445 H 1.815617 -4.219029 -1.376664 H -5.744707 -0.960344 2.050850 H 2.487784 -2.876647 -2.291817 H 4.135671 -3.849725 2.033708 H -6.545193 1.196640 1.097752 H -5.176747 2.356113 -0.628490 H -1.016532 1.851931 -1.007724 H 5.893540 -2.154217 1.544898 C 0.169743 0.857743 -2.500527 H 0.755481 -1.808688 2.779402 H -1.845493 -1.156808 2.763120 H 5.339608 -0.195429 0.109911 H -0.565434 3.823455 0.129355 H 2.174331 0.407341 2.200934 H -2.049730 1.461896 2.167053 H 2.640789 1.817829 -1.907287 H 0.448798 2.428265 1.845444 H 0.897670 5.762929 0.521791 H 4.106972 3.738029 -1.497348 H 3.264167 5.736767 -0.270174 H -0.613529 0.127173 -2.716056 H 0.126501 1.635518 -3.278837 H 1.124676 0.335304 -2.626269	
PhCH(CH ₃)	scf done: -310.233367 C -0.483361 -1.714286 0.775013 C -1.336178 -1.758383 2.004430 H -0.870755 -1.231070 2.851065 H -2.316392 -1.283200 1.846368 H -1.519078 -2.789282 2.320935 H -0.156287 -2.659100 0.347121 C -0.067900 -0.528462 0.122194 C -0.430872 0.769671 0.584553 C -0.005730 1.911530 -0.080257 C 0.793778 1.815040 -1.226610 C 0.746009 -0.597209 -1.046225 C 1.165095 0.549219 -1.702514 H -1.050217 0.865490 1.471493 H -0.297321 2.889788 0.294142 H 1.123096 2.712748 -1.742224 H 1.785322 0.464925 -2.591389 H 1.037789 -1.575821 -1.420929	CpCr[PhNC(CH ₃ CHC(CH ₃)NPh)(CH ₂ Ph)] scf done: -2276.501846 C 0.497384 5.544177 -0.537841 C -0.774848 4.974073 -0.621602 C -0.922403 3.609495 -0.867337 C 0.189867 2.759470 -1.035331 C 1.462024 3.361740 -0.956923 C 1.615762 4.725616 -0.711128 C 0.025534 1.301524 -1.282700 Cr -0.032060 -0.111844 0.317591 C 0.749262 1.344473 9.136953 C 1.110146 0.052263 2.366165 C -0.077549 -0.680553 2.625475 C -1.176840 0.174205 2.351090 C -0.673963 1.420126 1.904234 N -1.544355 -1.200550 -0.560277 C -2.870438 -1.048867 -0.041379 C -3.433812 -2.049007 0.765220 C -4.707782 -1.885751 1.309904 C -5.437770 -0.721718 1.058164 C -4.883289 0.275950 0.254218 C -3.609294 0.115592 -0.293219 H -2.855618 -2.946053 0.970315 H -3.178022 0.890307 -0.919581 C -1.382505 -1.941674 -1.660538 C -0.131193 -2.279226 -2.202119 C 1.141961 -2.077764 -1.644523 N 1.368652 -1.352006 -0.545455 C 2.697126 -1.340286 -0.011426 C 3.139417 -2.386455 0.811830 C 4.418837 -2.357656 1.367341 C 5.274801 -1.283968 1.110215 C 4.840722 -0.241121 0.289652 C 3.561734 -0.267719 -0.268772 H 2.464079 -3.211892 1.020696 H 3.22960 0.540199 -0.909943 C -2.598275 -2.488346 -2.389555 C 2.301243 -2.755927 -2.354724 H -3.111537 -3.247372 -1.789027 H -2.306296 -2.944555 -3.337594 H 1.973482 -3.187794 -3.302449 H -3.328734 -1.697673 -2.589177 H -0.156582 -2.854344 -3.119104 H 2.724835 -3.558541 -1.741209 H -5.128878 -2.668644 1.935464 H 3.113121 -2.048354 -2.551602 H 4.745852 -3.174465 2.005569 H -6.428481 -0.593543 1.485135 H -5.443728 1.184464 0.049472 H -0.914412 1.110730 -1.814374 H 6.269608 -1.260245 1.546139 H 0.837649 0.922951 -1.914877 H -0.134670 -1.706894 2.965538 H -2.221342 -0.091572 2.434716 H 5.499279 0.597898 0.080525 H -1.922978 3.186837 -0.943553 H 2.119026 -0.323351 2.464533 H -1.256757 2.280096 1.603233 H 2.346691 2.744581 -1.102899 H 1.424409 2.135713 1.617206 H -1.658692 5.596955 -0.502590 H 2.614881 5.153117 -0.662403 H 0.615075 6.607766 -0.348835	
(CH ₃ COO)CH(CH ₃)	scf done: -307.042610 C -0.970339 0.001584 -2.466051 C -0.958808 -0.001033 -0.983320 O 0.277655 -0.000164 -0.379948 C 0.341252 -0.000877 0.988379 C 1.778564 0.000686 1.444738 O -0.637421 -0.002139 1.699633 H -1.819496 -0.000953 -0.329685 H -1.489158 -0.877904 -2.877874 H -1.483794 0.885510 -2.875280 H 0.053493 -0.000870 -2.852681 H 1.809634 -0.002730 2.534735 H 2.303150 -0.878914 1.056108 H 2.299066 0.885353 1.062058	CpCr[PhNC(CH ₃ CHC(CH ₃)NPh)] scf done: -2005.550393 C 0.094398 -0.006477 -0.068919 C 0.095998 -0.038514 1.349594 C 1.448832 -0.006649 1.776227 C 2.285819 -0.030746 0.618597 C 1.449645 -0.030658 -0.520523 Cr 0.089170 1.998728 0.620741 N 0.244414 3.422093 -0.580351 C -0.521885 2.925808 -1.682773 C -1.904881 2.725962 -1.563064 C -2.637477 2.194193 -2.625132 C -2.000445 1.852895 -3.820250 C -0.623445 2.047944 -3.945056 C 0.111695 2.579510 -2.884687 H -2.394977 2.983632 -0.627830 H 1.184357 2.729032 -2.974226 C 0.346463 4.744434 -0.409299 C -0.351532 5.681501 -1.379472 C 1.083104 5.348391 0.625549 C 1.849997 4.744128 1.638052 N 1.982543 3.421843 1.786434 C 2.805044 2.925341 2.847485 C 4.141475 2.579009 2.602638 C 4.933175 2.047254 3.621375 C 4.401938 1.852046 4.897866 C 3.070957 2.193501 5.148039 C 2.276875 2.725333 4.131223 H 4.547972 2.728660 1.605973 H 1.237840 2.983034 4.318972 C 2.566890 5.681085 2.594542 H 2.395620 6.724150 2.321441 H 3.646014 5.492469 2.592552 H 2.225589 5.531693 3.624658	CpCr[PhNC(CH ₃ CHC(CH ₃)NPh)][CHPh(CH ₃)] scf done: -2312.644207 Cr -0.127338 0.085287 0.378914 C -0.111101 1.926289 1.763009 C 1.046224 1.151800 2.044277 C 0.617609 -0.082526 2.614575 C -0.790932 -0.084167 2.652870 C -1.246130 1.153415 2.111216 H -0.132542 2.911736 1.317740 H 2.072327 1.448301 1.872727 H 1.266640 -0.892529 2.919412 H -1.420427 -0.894710 2.996520 H -2.277942 1.456153 1.995613 N 1.208131 -1.313558 -0.306266 C 0.899770 -2.328531 -1.119984 C -0.405948 -2.637988 -1.539412 C -1.620152 -2.040063 -1.166807 N -1.714453 -0.970964 -0.368853 C 2.569445 -1.183495 0.126202 C 3.383905 -0.162309 -0.382183 C 4.700944 -0.027780 0.062711 C 5.222157 -0.903064 1.017330 C 4.412384 -1.918481 1.530439 C 3.095985 -2.056822 1.090769 H 2.972519 0.528862 -1.109460 H 5.322625 0.766176 -0.343649

H 6.247099 -0.793602 1.360803
 H 4.803790 -2.603692 2.278036
 H 2.461537 -2.841196 1.495464
 C 1.999609 -3.226945 -1.662373
 H 2.838444 -2.636622 -2.044182
 H 1.616603 -3.856319 -2.468299
 H 2.402957 -3.881945 -0.882857
 H -0.488818 -3.473580 -2.222951
 C -2.880187 -2.664808 -1.741644
 H -2.629363 -3.425838 -2.483205
 H -3.485088 -3.135414 -0.959293
 H -3.513170 -1.906972 -2.214919
 C -3.020317 -0.494716 -0.019229
 C -3.549645 0.647157 -0.636766
 C -4.801439 1.137636 -0.261140
 C -5.542695 0.495961 0.732792
 C -5.022313 -0.644401 1.349060
 C -3.770809 -1.135781 0.977855
 H -2.973788 1.147988 -1.408363
 H -5.195947 2.025015 -0.749005
 H -6.515275 0.881313 1.025727
 H -5.589534 -1.151450 2.125396
 H -3.358049 -2.015376 1.464551
 C -0.015384 1.409610 -1.258429
 H -0.828895 2.134491 -1.149978
 C -0.057017 0.800244 -2.654591
 H -0.989584 0.247246 -2.803206
 H 0.769281 0.101336 -2.821019
 H 0.001035 1.578806 -3.429650
 O 1.236699 2.190744 -1.209685
 C 1.184902 3.518632 -1.014957
 C 2.571975 4.127043 -1.074677
 O 0.169182 4.154639 -0.803321
 H 2.504027 5.203963 -0.915242
 H 3.215099 3.679919 -0.309045
 H 3.032749 3.924199 -2.047222

CpCr[XylNC(CH₃CHC(CH₃)NXYl](CH₂Ph)
 scf done: -2433.760486
 H 3.359355 -1.918141 2.516846
 H 2.492485 -1.224093 3.895413
 C 2.775002 -1.054314 2.854274
 H -1.685520 -2.123770 3.868717
 H 3.441107 -0.187581 2.807899
 H 0.353951 -1.411350 3.648358
 H 2.297928 -3.169753 0.585296
 H -0.762956 -4.122622 0.800787
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 H -1.081344 -4.855087 -0.776394
 C -1.966864 -2.150292 2.813598
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 H -0.131706 -3.361918 -0.645988
 C -0.921277 -1.447511 1.963209
 C 4.794705 -1.649278 -0.973016
 C 3.519551 -1.655264 -0.396595
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 C 5.564809 -0.490052 -0.006809
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 C -2.262764 -3.093368 -0.393643
 C 5.059121 0.677728 -0.445334
 C -3.380210 -3.666430 -0.1011992
 C 3.787452 0.716616 0.142304
 H 5.659558 1.584343 -0.450094
 N -1.187117 -1.158519 0.685249
 C 3.308675 2.010599 0.754311
 C -2.348478 -1.766572 0.086673
 H 4.126790 2.735587 0.806238
 C -4.569518 -2.956690 -1.152601
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 H -5.428091 -3.414542 -1.636309
 H 2.501972 2.461206 0.167941
 H -0.958162 1.362226 1.774913
 Cr 0.009423 0.173599 -0.350722
 C -3.554956 -1.045087 -0.038232
 H -3.427568 0.420842 1.555144
 H -0.512286 -1.840175 -2.614865
 C -4.649868 -1.656636 -0.661417
 C -0.339871 1.811943 0.990702
 H 1.954077 -0.763528 -2.520884
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 C 1.017557 -0.226955 -2.449299
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 H -3.021942 1.055854 -0.027132
 H -2.294331 0.147931 -2.295504
 C -1.218767 0.261222 -2.310777
 C 0.889691 3.147940 0.614191
 C -0.119993 4.102229 -0.085163
 C 0.883728 1.173895 -2.226795
 C -0.504723 1.474859 -2.173819
 H 1.695564 1.885356 -2.151033
 H -2.810270 2.851764 1.547460
 C -2.196747 3.537481 0.969156
 H -0.934117 2.452981 -0.021119
 C -0.626663 3.535889 -0.421607
 H 0.003061 6.062875 -0.957263
 C -2.712029 4.789336 0.630288
 C -1.932704 5.709153 -0.071811
 H -3.725198 5.049775 0.928607
 H -2.330013 6.686095 -0.333790

CpCr[XylNC(CH₃CHC(CH₃)NXYl][CH(OOCC
 H₁)(CH₃)]
 scf done: -2469.899829
 C 3.289178 -1.824610 -0.573655
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 C 3.799277 0.458261 0.154323
 C 5.038960 0.354798 -0.492056
 C 5.406418 -0.796534 -1.180652
 C 4.532611 -1.880669 -1.211253
 N 1.597696 -0.573611 0.694206
 C 1.441588 -1.150526 1.892738
 C 2.666746 -1.544841 2.701279
 C 0.196410 -1.448960 2.469861
 C -1.073756 -1.436560 1.862865
 C -2.178578 -2.145324 2.629870

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 C -3.711291 -0.345180 0.184059
 C -4.908911 -0.683861 -0.460533
 C -5.031958 -1.858092 -1.196504
 C -3.945095 -2.723975 -1.285484
 C -2.728284 -2.423541 -0.662969
 Cr 0.028202 0.319459 -0.315734
 C -0.054633 2.040927 0.925907
 O -1.111087 2.978355 0.485288
 C -0.764626 4.201025 0.049894
 O 0.379128 4.595661 -0.086775
 C 0.317202 1.801679 -2.057646
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 C 0.497481 -0.441730 -2.531754
 C 1.235690 0.748882 -2.273773
 C -0.248622 1.892996 2.429681
 C -1.988396 5.022473 -0.302803
 H 0.575106 2.825969 -1.826094
 H -1.921935 1.803213 -2.016714
 H -1.700384 -0.808300 -2.591594
 H 0.919923 -1.415323 -2.740552
 H 2.313604 0.830715 -2.245787
 C -3.651473 0.914201 1.013341
 H -5.758787 -0.011807 -0.368097
 H -5.969977 -2.102476 -1.687634
 H -4.034503 -3.651623 -1.845956
 C -1.570780 -3.384044 -0.802251
 H -3.090297 -1.542805 2.674212
 H -1.856241 -2.370260 3.648807
 H -2.448409 -3.090333 2.144684
 H 0.230902 -1.860022 3.471261
 H 2.381007 -1.857444 3.707944
 H 3.207381 -2.372160 2.228985
 H 3.372618 -0.711754 2.778969
 C 3.472271 1.737751 0.887569
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