Supporting Information

A bimetallic N-heterocyclic carbene complex featuring a short Cr-Cr distance

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X-ray Experimental for 2 $[C_{35}H_{52}Cr_2N_4]\bullet(C_4H_{10}O)$. A suitable crystal of **2** was selected, mounted with viscous oil and cooled to 120 K. Data was collected on a Bruker APEX CCD diffractometer using graphite monochromated Mo-K_α radiation (λ = 0.71073). Unit cell parameters were obtained from three sets of 20 frames using 0.3E scans from different sections of the Ewald sphere. The data set was corrected for absorption using SADABS multiscan methods.[1] Details of the crystal data, data collection and structure refinement can be found in Table S1. Systematic absences in the diffraction data and unit cell parameters are consistent for $P2_1/n$. The centrosymmetric space group option yielded chemically reasonable and computationally stable results of refinement. Structures were solved using direct methods and refined with full-matrix least-squares methods based on F^2. Hydrogen atoms were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms). The hydrogen atoms on the bridging methyl ligands C32 and C33 were observed in a ΔF map and refined with isotropic displacement parameters. All structure factors are included in the SHELXTL program library.[1]

References:

1. G. M. Sheldrick, *SHELXTL*, version 6.01; University of Göttingen: Germany, and Bruker-AXS, Inc.: Madison WI, USA, 2001.

Table S1. Crystal data and structure refinement for **2**.

Empirical formula	C39 H62 Cr2 N4 O
Formula weight	706.93
Temperature	120(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 12.3754(17) A alpha = 90 deg. b = 17.081(2) A beta = 96.698(2) deg. c = 18.753(3) A gamma = 90 deg.
Volume	3937.0(9) A^3
Z, Calculated density	4, 1.193 Mg/m^3
Absorption coefficient	0.585 mm^-1
F(000)	1520
Crystal size	0.22 x 0.12 x 0.05 mm
Theta range for data collection	1.62 to 25.00 deg.
Limiting indices	-14<=h<=14, -20<=k<=20, -22<=l<=22
Reflections collected / unique	33353 / 6929 [R(int) = 0.0247]
Completeness to theta = 25.00	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9713 and 0.8821
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6929 / 0 / 445
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.1020

R indices (all data)	R1 = 0.0421, wR2 = 0.1043
Largest diff. peak and hole	0.551 and -0.232 e.A^-3