Supplementary Information

For

Divergent Reactivity of Nitric Oxide with Metal-Metal Quintuple Bonds

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Materials and Methods

General. Unless stated otherwise, all operations were performed using standard Schlenk techniques or in a Vacuum Atmospheres dry box under an atmosphere of nitrogen. Diethyl ether (Et_2O) and tetrahydrofuran (THF) were distilled under nitrogen from purple sodium benzophenone ketyl. *n*-Hexane and *n*-pentane were distilled from CaH_2. Distilled solvents were transferred under vacuum into vacuum-tight glass vessels before being transferred into a dry box. The quintuply bonded dichromium $Cr_2[\mu\text{-}\eta^2\text{-HC(N-2,6-R}_2C_6H_3)_2]_2$ (**1**: R = Et, **2**: R = *i*Pr)[1] and dimolybdenum complex $Mo_2[\mu\text{-}\eta^2\text{-PhC(N-2,6-}^i\text{Pr}_2C_6H_3)_2]_2$ (**3**).[2] The 4 Å sieves and Celite were dried in vacuo overnight at a temperature just above 200 °C. All other compounds were used as received. ^1H and ^{13}C NMR spectra were recorded on Bruker Avance 400 MHz spectrometers at room temperature. ^{13}C NMR spectra are proton decoupled. Chemical shifts for ^1H and ^{13}C spectra are reported with respect to internal solvent: 7.16 ppm and 128.00(t) ppm (C_6D_6). Elemental analysis was carried out with a Heraeus CHN-O rapid elementary analyzer.

Synthesis of $Cr(NO)_2[\kappa^2\text{-HC(N-2,6-Et}_2C_6H_3)_2]_2$ (4) and

$Cr_2(\mu\text{-}\kappa^1\text{-}ONO)_2(NO)_4[\mu\text{-}\kappa^2\text{-}HC(N\text{-}2,6\text{-}Et_2C_6H_3)_2]_2$ (5):

A portion of **1** (0.200 g, 0.278 mmol) was dissolved in 10 mL of THF in a 50 mL, thick-walled, round-bottom flask equipped with a screw-top Teflon stopcock and a sidearm for attachment onto a high-vacuum manifold. This flask was removed out of the drybox. This orange solution was subjected to 3 freeze-pump-thaw cycles before nitric oxide was transferred under vacuum to the solution. The flask was submerged in a bath of dry ice/acetone, and then nitric oxide was transferred into the flask. The color turned dark brown immediately upon exposure to NO. The reaction was allowed to stir at −78 °C for 30 min. The solvent was removed by vacuo at room temperature, and the flask was removed into the drybox. The dark residue was extracted with *n*-hexane to give a brown solution (compound **4**), and the residue was dissolved in toluene to give a green solution (compound **5**). The *n*-hexane solution of **4** was stripped to dryness under vacuum, and the residue was dissolved in *n*-pentane. Crystals of **4** for X-ray diffraction were grown in the drybox by storing the *n*-pentane solution at −35 °C (0.088 g, 43.2% yield). The X-ray quality crystals of **5** were grown by *n*-hexane diffusion into a toluene solution at −35 °C (0.076 g, 29.5% yield).

4: ^{1}H NMR (C_6D_6, 400 MHz, 21 °C) δ 7.56 (*s*, 2 H, $NC(\mathit{H})N$), 7.06 (*br*, 12 H, $Et_2C_6\mathit{H}_3$), 2.99 (*q*, 2 H, $C\mathit{H}_2CH_3$), 2.75 (*q*, 4 H, $C\mathit{H}_2CH_3$), 2.24 (*q*, 4 H, $C\mathit{H}_2CH_3$), 2.61 (*q*, 4 H, $C\mathit{H}_2CH_3$), 2.35 (*q*, 2 H, $C\mathit{H}_2CH_3$), 2.13 (*q*, 2 H, $C\mathit{H}_2CH_3$), 1.24 (*t*, 6 H, $CH_2C\mathit{H}_3$), 1.17 (*t*, 6 H, $CH_2C\mathit{H}_3$), 1.11 (*t*, 6 H, $CH_2C\mathit{H}_3$), 0.84 (*t*, 6 H, $CH_2C\mathit{H}_3$). ^{13}C NMR (C_6D_6, 100.6 MHz, 21 °C) δ 167.62 (2 C, $N\mathit{C}(H)N$), 144.90 (2 C, *ipso*-2,6-$Et_2C_6H_3$), 143.83 (2 C, *ipso*-2,6-$Et_2C_6H_3$), 140.19 (4 C, *ortho*-2,6-$Et_2C_6H_3$), 139.68 (4 C, *ortho*-2,6-$Et_2C_6H_3$), 126.84 (4 C, *meta*-2,6-$Et_2C_6H_3$), 126.57 (4 C, *meta*-2,6-$Et_2C_6H_3$), 125.78 (2 C, *para*-2,6-$Et_2C_6H_3$), 124.49 (2 C, *para*-2,6-$Et_2C_6H_3$), 26.39 (1 C, $\mathit{C}H_2CH_3$), 25.66 (1 C, $\mathit{C}H_2CH_3$), 25.02 (1 C, $\mathit{C}H_2CH_3$), 24.04 (1 C, $\mathit{C}H_2CH_3$), 17.07 (1 C, $CH_2\mathit{C}H_3$), 15.63 (1 C, $CH_2\mathit{C}H_3$), 15.12 (1 C, $CH_2\mathit{C}H_3$), 14.84 (1 C, $CH_2\mathit{C}H_3$). Anal. Calcd for $C_{42}H_{54}N_6CrO_2$: C, 69.40; H, 7.49; N, 11.56. Found: C, 69.55; H, 7.22; N, 11.80. IR(THF): ν_{NO} = 1816(s), 1677(s) cm^{-1}.

5: ^{1}H NMR (C_6D_6, 400 MHz, 21 °C) δ 7.24 (*s*, 2 H, $NC(\mathit{H})N$), 6.96 (*t*, 4 H, *para*-2,6-$Et_2C_6H_3$), 6.88 (*d*, 8 H, *meta*-2,6-$Et_2C_6H_3$), 2.90 (*q*, 2 H, $C\mathit{H}_2CH_3$), 2.83 (*q*, 4 H, $C\mathit{H}_2CH_3$), 2.65 (*m*, 6 H, $C\mathit{H}_2CH_3$), 2.22 (*m*, 2 H, $C\mathit{H}_2CH_3$), 1.95 (*m*, 2 H, $C\mathit{H}_2CH_3$), 1.16 (*t*, 12 H, $CH_2C\mathit{H}_3$), 1.08 (*t*, 12 H, $CH_2C\mathit{H}_3$). ^{13}C NMR (C_6D_6, 100.6 MHz, 21 °C) δ 165.95 (2 C, $N\mathit{C}(H)N$), 149.90 (4 C, *ipso*-2,6-$Et_2C_6H_3$), 139.24 (8 C, *ortho*-2,6-$Et_2C_6H_3$), 125.99 (8 C, *meta*-2,6-$Et_2C_6H_3$), 125.52 (4 C, *para*-2,6-$Et_2C_6H_3$), 24.92 (1 C, $\mathit{C}H_2CH_3$), 25.66 (1 C, $\mathit{C}H_2CH_3$), 25.02 (1 C, $\mathit{C}H_2CH_3$), 24.04 (1 C, $\mathit{C}H_2CH_3$), 17.07 (1 C, $CH_2\mathit{C}H_3$), 15.63 (1 C, $CH_2\mathit{C}H_3$), 15.12 (1 C, $CH_2\mathit{C}H_3$), 14.84 (1 C, $CH_2\mathit{C}H_3$). Anal. Calcd for $C_{42}H_{54}N_{10}Cr_2O_8$: C, 54.19; H, 5.85; N, 15.05. Found: C, 54.42; H, 6.01; N, 14.83. IR(THF): ν_{NO} = 1814(s), 1705(s) cm^{-1}.

Synthesis of (κ^2-NO_2)Cr(μ-NO)$_2$[μ-κ^2-HC(N-2,6-*i*Pr$_2$C$_6$H$_3$)$_2$]$_2$CrNO (6):
A portion of **2** (0.114 g, 0.137 mmol) was dissolved in 10 mL of THF in a 50 mL, thick-walled, round-bottom flask equipped with a screw-top Teflon stopcock and a sidearm for attachment onto a high-vacuum manifold. This flask was removed out of the drybox. This orange solution was subjected to 3 freeze-pump-thaw cycles before nitric oxide was transferred under vacuum to the solution. The flask was submerged in a bath of dry ice/acetone, and then nitric oxide was transferred into the flask. The color turned purple immediately upon exposure to NO. The reaction was allowed to stir at –78 °C for 1 h, and the solvent was then removed by vacuo at room temperature, and the flask was removed into the drybox. The dark residue was extracted with *n*-hexane to give a dark brown solution. Crystals of **6** for X-ray diffraction were grown in the drybox by *n*-hexane diffusion into a THF solution at –35 °C (0.061 g, 46.1% yield).

^{1}H NMR (C_6D_6, 400 MHz, 21 °C) δ 7.82 (s, 2 H, NC(*H*)N), 7.09 (d, 8 H, *meta*-2,6-^{i}Pr$_2$C$_6$H$_3$), 7.02 (t, 4 H, *para*-2,6-^{i}Pr$_2$C$_6$H$_3$), 3.74 (septet, 2 H, C*H*Me$_2$), 3.00 (septet, 2 H, C*H*Me$_2$), 2.41 (septet, 2 H, C*H*Me$_2$), 2.21 (septet, 2 H, C*H*Me$_2$), 1.64 (d, 6 H, CH*Me*$_2$), 1.53 (d, 6 H, CH*Me*$_2$), 1.31 (d, 6 H, CH*Me*$_2$), 1.18 (d, 6 H, CH*Me*$_2$), 1.14 (d, 6 H, CH*Me*$_2$), 1.10 (d, 6 H, CH*Me*$_2$), 0.98 (d, 6 H, CH*Me*$_2$), 0.89 (d, 6 H, CH(C*H*$_3$)$_2$). ^{13}C NMR (100.6 MHz, C_6D_6, 23 °C): δ 165.22, 145.21, 143.48, 125.58, 125.56, 124.89, 124.30, 123.71, 123.12, 27.00, 25.11, 23.23, 15.23.

Anal. Calcd for $C_{50}H_{70}N_8Cr_2O_5$: C, 62.09; H, 7.30; N, 11.59; Found: C, 62.36; H, 7.02; N, 11.97. IR(THF): ν_{NO} = 1805(s), 1523(m) cm^{-1}.

Synthesis of *cis*-[Mo$_2$(μ-κ^1:κ^1-NO_2)$_2${μ-κ^2-PhC(N-2,6-^{i}Pr$_2$C$_6$H$_3$)$_2$}$_2$] (7)
A portion of **3** (0.102 g, 0.095 mmol) was dissolved in 8 mL of THF in a 50 mL, thick-walled, round-bottom flask equipped with a screw-top Teflon stopcock and a sidearm for attachment onto a high-vacuum manifold. This flask was removed out of the drybox. This burgundy solution was subjected to 3 freeze-pump-thaw cycles before nitric oxide was transferred under vacuum to the solution. The flask was submerged in a bath of dry ice/acetone, and then nitric oxide was transferred into the flask. The color turned dark brown immediately upon exposure to NO. The reaction was allowed to stir at –78 °C for 30 min, and the solvent was then removed by vacuo at room temperature, and the flask was removed into the drybox. The dark residue was extracted with *n*-hexane to give a dark brown solution. Crystals of **7** for X-ray diffraction were grown in the drybox by storing the *n*-hexane solution at –35 °C (0.066 g, 59.6% yield).

^{1}H NMR (C_6D_6, 400 MHz, 21 °C) δ 7.68 (*d*, 4 H, *ortho*-Ph), 7.41-6.51 (*m*, 18 H, Ph +

2,6-^{i}Pr$_2$C$_6$*H*$_3$), 5.07 (*sept*, 1 H, C*H*Me$_2$), 4.53 (*sept*, 1 H, C*H*Me$_2$), 4.36 (*sept*, 1 H, C*H*Me$_2$), 4.11 (*sept*, 1 H, C*H*Me$_2$), 3.83 (*sept*, 1 H, C*H*Me$_2$), 3.25 (*sept*, 1 H, C*H*Me$_2$), 2.91 (*sept*, 1 H, C*H*Me$_2$), 2.41 (*sept*, 1 H, C*H*Me$_2$), 1.83 (*d* , 3 H, CH*Me*$_2$), 1.72 (*d*, 3 H, CH*Me*$_2$), 1.62 (d, 3 H, CH*Me*$_2$), 1.58 (*d*, 3 H, CH*Me*$_2$), 1.52 (*d*, 3 H, CH*Me*$_2$), 1.29 (*d*, 3 H, CH*Me*$_2$), 0.97 (*d*, 3 H, CH*Me*$_2$), 0.74 (*d*, 3 H, CH*Me*$_2$), 0.70 (*d*, 3 H, CH*Me*$_2$), 0.64 (*d*, 3 H, CH*Me*$_2$), 0.57 (*d*, 3 H, CH*Me*$_2$), 0.53 (*d*, 3 H, CH*Me*$_2$), 0.47 (*d*, 3 H, CH*Me*$_2$), 0.28 (*d*, 3 H, CH*Me*$_2$), –0.02 (*d*, 3 H, CH*Me*$_2$), –0.28 (*d*, 3 H, CH*Me*$_2$). ^{13}C NMR (C$_6$D$_6$, 100.6 MHz, 21 °C) δ 171.50 (N*C*(Ph)N), 152.88 (N*C*(Ph)N), 146.42, 145.00, 144.71, 144.59, 144.25, 144.11, 143.89, 142.85, 140.85, 139.52, 135.05, 134.28, 132.57, 132.21, 130.51, 130.10, 129.57, 129.44, 129.28, 129.27, 127.25, 127.20, 127.08, 126.41, 125.64, 125.25, 124.72, 124.52, 124.30, 124.21, 124.11, 124.03, 123.97, 123.74, 123.40, 123.21, 31.89, 29.29, 29.14, 28.74, 28.61, 28.40, 28.24, 28.08, 27.12, 25.60, 25.26, 25.21, 24.92, 24.66, 24.55, 24.51, 24.26, 24.24, 23.77, 23.26, 23.00, 22.40, 15.49, 14.31. Anal. Calcd for C$_{62}$H$_{72}$N$_6$Mo$_2$O$_4$: C, 64.02; H, 6.76; N, 7.22. Found: C, 63.65; H, 6.88; N, 6.88.

X-ray Crystallography

The chosen crystals were mounted on a glass fiber. Data collection were carried out on a NONIUS Kappa CCD diffractometer[3] with Mo radiation (λ = 0.71073 Å) at 150(2) K. Cell parameters were retrieved and refined using *DENZO-SMN*[4] software on all observed reflections. Data reduction was performed with the *DENZO-SMN*[4] software. An empirical absorption was based on the symmetry-equivalent reflections and applied the data using the *SORTAV*[5] program. Using *SHELXTL*[6] program on PC computer made the structure analysis. The structure was solved using the *SHELXS-97*[7] program and refined using *SHELXL-97*[8] program by full-matrix least squares on F^2 values. All of non-hydrogen atoms are refined anisotropically. Hydrogen atoms attached to the carbons were fixed at calculated positions and refined using a riding mode.

X-ray Crystal structure of Cr(NO)$_2$[κ^2-HC(N-2,6-Et$_2$C$_6$H$_3$)$_2$]$_2$·1.3*n*-C$_5$H$_{12}$ (4·1.3*n*-C$_5$H$_{12}$), CCDC 903290

Dark brown crystals of **4·1.3*n*-C$_5$H$_{12}$** were coated with Paratone N oil and placed on a microscope slide. A crystal of approximate dimensions 0.38 × 0.12 × 0.04 mm^3 was selected and mounted with wax on the end of a glass fiber. A total of 14996 reflections ($-14 \leqq h \leqq 15$, $-12 \leqq k \leqq 12$, $-19 \leqq l \leqq 18$) were collected at 200(2) K in the θ range 1.66 to 25.04°, of which 3962 (R_{int} = 0.0403) were unique. The structure was solved using direct methods in conjunction with standard difference Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were generated using HFIX 23 (for methylene groups), HFIX 33 (for methyl groups), HFIX 43 (for phenyl rings), and their orientation may not be totally reliable. The unit cell volume comprises a large region of disordered solvent (2.6 *n*-pentane molecules) which could not be modeled as discrete atomic sites, so they were squeezed by using PLATON SQUEEZE option. The residual peak and hole electron density were 0.463 and –0.344 e·Å^{-3}, respectively. An empirical absorption correction (multi-scan) was applied with maximum and minimum transmissions equal to 0.9884 and 0.8971, respectively. The least squares refinement converged normally with residuals R_1 = 0.0801, wR_2 = 0.2343 based upon I > 2σ(I) and GOF = 1.032 based upon F^2. No extinction coefficient was applied to the refinement. Crystal and refinement data: formula $C_{48.50}H_{69.60}CrN_6O_2$, formula weight = 820.70, space group P2/c, a = 12.6712(12) Å, b = 11.3892(11) Å, c = 16.3973(15) Å, β = 104.700(5)°, V = 2288.9(4) Å^3, Z = 2, μ = 0.292 mm^{-1}, ρ(calc) = 1.159 g/cm^{-3}, F(000) = 860, R_1 (based on F) = 0.1235, wR_2 (based on F^2) = 0.2553.

X-ray Crystal structure of $Cr_2(\mu\text{-}\kappa^1\text{-}ONO)_2(NO)_4[\mu\text{-}\kappa^2\text{-}HC(N\text{-}2,6\text{-}Et_2C_6H_3)_2]_2$·*n*-toluene ($5\cdot0.7C_7H_8$), CCDC 903291

Dark green crystals of **5·toluene** were coated with Paratone N oil and placed on a microscope slide. A crystal of approximate dimensions 0.31 × 0.21 × 0.09 mm^3 was selected and mounted with wax on the end of a glass fiber. A total of 22628 reflections (–23 ≦ h ≦ 23, –21 ≦ k ≦ 21, –17 ≦ l ≦ 13) were collected at 200 (2) K in the θ range 2.10 to 25.07°, of which 4532 (R_{int} = 0.0756) were unique. The structure was solved using direct methods in conjunction with standard difference Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were generated using HFIX 13 (for methine groups), HFIX 33 (for methyl groups), HFIX 43 (for phenyl rings), and their orientation may not be totally reliable. The unit cell volume comprises a large region of disordered solvent (2.8 toluene molecules) which could not be modeled as discrete atomic sites, so they were squeezed by using PLATON SQUEEZE option. The residual peak and hole electron density were 0.607 and –1.056 e·Å^{-3}, respectively. An empirical absorption correction (multi-scan) was applied with maximum and minimum transmissions equal to 0.9639 and 0.8232, respectively. The least squares refinement converged normally with residuals R_1 = 0.0837, wR_2 = 0.2297 based upon I > 2σ(I) and GOF = 1.140 based upon F^2. No extinction coefficient was applied to the refinement. Crystal and refinement data: formula $C_{46.9}H_{59.6}Cr_2N_{10}O_8$, formula weight = 996.55, space group C2/c, a = 19.5267(5) Å, b = 17.9584(5) Å, c = 14.7203(5) Å, β = 97.6360(10)°, V = 5116.2(3) Å^3, Z = 4, μ = 0.479 mm^{-1}, ρ(calc) = 1.209 g/cm^{-3}, F(000) = 1952, R_1

(based on F) = 0.1173, wR_2 (based on F^2) = 0.2471.

X-ray Crystal structure of (κ^2-NO_2)Cr(μ-NO)$_2$[μ-κ^2-HC(N-2,6-*i*$Pr_2C_6H_3$)$_2$]$_2$CrNO (6·THF), CCDC 903292

Purple crystals of **6·THF** were coated with Paratone N oil and placed on a microscope slide. A crystal of approximate dimensions 0.40 × 0.15 x 0.12 mm^3 was selected and mounted with wax on the end of a glass fiber. A total of 15876 reflections ($-28 \leqq h \leqq 28$, $-12 \leqq k \leqq 12$, $-26 \leqq l \leqq 26$) were collected at 150 (2) K in the θ range 1.77 to 25.00°, of which 4727 (R_{int} = 0.0346) were unique. The structure was solved using direct methods in conjunction with standard difference Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were generated using HFIX 13 (for methine groups), HFIX 23 (for methylene groups), HFIX 33 (for methyl groups), HFIX 43 (for phenyl rings), and their orientation may not be totally reliable. The residual peak and hole electron density were 1.435 and –0.484 e·$Å^{-3}$, respectively. An empirical absorption correction (multi-scan) was applied with maximum and minimum transmissions equal to 0.9467 and 0.8370, respectively. The least squares refinement converged normally with residuals R_1 = 0.0732, wR_2 = 0.1710 based upon $I > 2\sigma(I)$ and GOF = 1.100 based upon F^2. No extinction coefficient was applied to the refinement. Crystal and refinement data: formula $C_{54}H_{78}Cr_2N_8O_6$, formula weight = 1039.24, space group C2/c, a = 24.1046(14) Å, b = 10.2903(6) Å, c = 22.6641(13) Å, β = 107.516(1)°, V = 5361.0(5) $Å^3$, Z = 4, μ = 0.461 mm^{-1}, ρ(calc) = 1.288 g/cm^{-3}, F(000) = 2216, R_1 (based on F) = 0.0795, wR_2 (based on F^2) = 0.1751. It should be noted that we also tried to solve this structure in space group Cc, but it was not possible to obtain and refine a satisfactory non-disordered model. The current model was obtained and refined in space group C2/c with the metal complex disordered about an inversion centre.

X-ray Crystal structure of [Mo_2(μ-κ^1:κ^1-NO_2)$_2${μ-κ^2-PhC(N-2,6-$^iPr_2C_6H_3$)$_2$}$_2$]·0.7*n*-hexane (7·0.7*n*-hexane), CCDC 903293

Brown crystals of **7·0.7*n*-hexane** were coated with Paratone N oil and placed on a microscope slide. A crystal of approximate dimensions 0.50 × 0.45 × 0.14 mm^3 was selected and mounted with wax on the end of a glass fiber. A total of 40388 reflections ($-15 \leqq h \leqq 15$, $-16 \leqq k \leqq 13$, $-40 \leqq l \leqq 40$) were collected at 200 (2) K in the θ range 1.20 to 25.05°, of which 10894 (R_{int} = 0.0366) were unique. The structure was solved using direct methods in conjunction with standard difference Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were generated using HFIX 13 (for methine groups), HFIX 33 (for methyl groups), HFIX 43 (for phenyl rings), and their orientation may not be totally reliable. The unit cell volume comprises a large region of disordered solvent (2.8 *n*-hexane molecules) which could not be modeled as discrete atomic sites, so they were squeezed by using PLATON SQUEEZE option. The residual peak and hole electron density were 0.959 and –0.520 e·$Å^{-3}$, respectively. An empirical absorption correction (multi-scan) was applied with maximum and minimum transmissions equal to 0.9391 and 0.8047, respectively. The least squares refinement converged normally with residuals R_1 = 0.0378, wR_2 = 0.1033 based upon I > 2σ(I) and GOF = 1.053 based upon F^2. No extinction coefficient was applied to the refinement. Crystal and refinement data: formula $C_{66.20}H_{87.80}Mo_2N_6O_4$, formula weight = 1223.50, space group $P2_1/c$, a = 13.5514(13) Å, b = 13.6186(13) Å, c = 34.248(3) Å, β = 99.118(2)°, V = 6240.6(10) $Å^3$, Z = 4, μ = 0.454 mm^{-1}, ρ(calc) = 1.330 g/cm^{-3}, F(000) = 2632, R_1 (based on F) = 0.0490, wR_2 (based on F^2) = 0.1078.

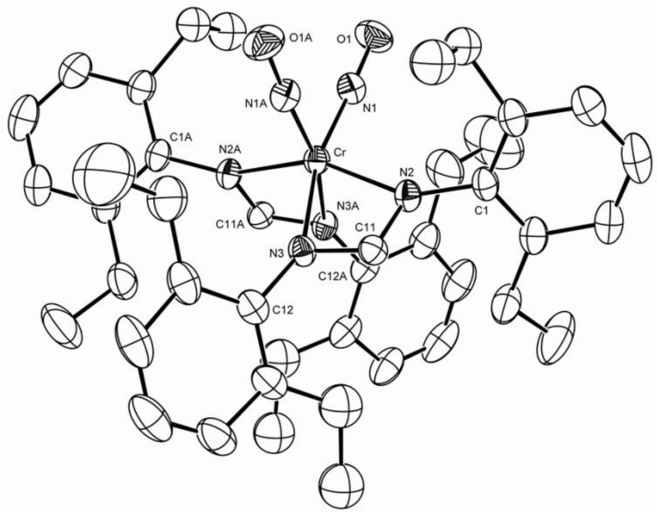

Fig. *S*1 The solid-state molecular structure of Cr(NO)$_2$[κ^2-HC(N-2,6-Et$_2$C$_6$H$_3$)$_2$]$_2$ (**4**) (without solvent and H atoms) with thermal ellipsoids shown at the 35% probability level. Those atoms with an additional “A” letter are at equivalent position (1–x, y, 1/2–z). Selected bond distances(Å) and angles (°): Cr–N1, 1.725(4); N1–O1, 1.169(4); Cr–N2, 2.049(3); Cr–N3, 2.128(3); N1–Cr–N1A, 83.8(2); N1–Cr–N2, 99.65(15); N1A–Cr–N2, 99.74(15); N2–Cr–N2A, 153.8(2); N1–Cr–N3, 94.55(15); N1A–Cr–N3, 162.51(15); N2–Cr–N3, 63.27(13); N2A–Cr–N3, 97.80(13); N3–Cr–N3A, 92.10(18); O1–N1–Cr, 170.5(3).

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