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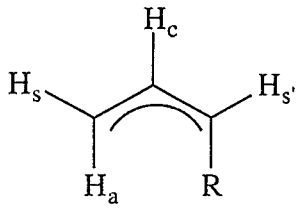
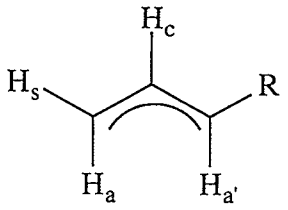
Characterization data for η^3-allyl complexes



anti-isomer (**a**)



syn-isomer (**s**)

Notation for mono-substituted allyl complexes

Tp'(CO)$_2$W(η^3-CH$_2$CHCH$_2$) (1). IR (KBr, cm^{-1}) ν_{BH}=2548; ν_{CO}=1919, 1817; ν_{CN}=1547. ^{1}H NMR (C_6D_6, δ): 5.48, 5.25 (2:1, Tp'C*H*), 3.36 (d, $^3J_{HcHs}$= 6.4 Hz, η^3-CH$_a$*H$_s$*CH$_c$CH$_a$*H$_s$*), 3.17 (tt, $^3J_{HsHc}$= 6.6 Hz, $^3J_{HaHc}$= 9.4 Hz, η^3-CH$_a$H$_s$C*H$_c$*CH$_a$H$_s$), 3.05, 2.34, 2.07, 1.77 (3:6:6:3, Tp'C*H$_3$*), 1.97 (d, $^3J_{HcHa}$= 8.8 Hz, η^3-C*H$_a$*H$_s$CH$_c$C*H$_a$*H$_s$). ^{13}C NMR (C_6D_6, δ): 221.1 ($^iJ_{WC}$= 160 Hz, *C*O), 155.2, 154.2, 145.5, 143.5 (1:2:1:2, Tp'*C*CH$_3$), 108.7, 107.1 (2:1, Tp'*C*H), 69.5 (d, $^1J_{CH}$= 169 Hz, η^3-CH$_2$*C*HCH$_2$), 56.1 (t, $^1J_{CH}$= 155 Hz, η^3-*C*H$_2$CH*C*H$_2$), 16.7, 16.3, 12.5 (2:1:3, Tp'C*C*H$_3$). Calculated for $WC_{20}H_{27}N_6BO_2$: C, 41.55; H, 4.71; N, 14.54. Found: C, 41.48; H, 4.69; N, 14.53.

Tp'(CO)$_2$W(η^3-CH$_2$CHCHMe) (2a, 2s). IR (KBr, cm^{-1}): **2a:** ν_{BH}=2548; ν_{CO}=1910, 1815; ν_{CN}=1545; **2s:** ν_{BH}=2540; ν_{CO}=1919, 1819; ν_{CN}=1549. ^{1}H NMR (C_6D_6, δ): **2a** 5.51, 5.49, 5.23 (Tp'C*H*), 4.14 (m., η^3-CH$_a$H$_s$CH$_c$C*H$_s$*'Me), 3.28 (m.obsc., η^3-CH$_a$H$_s$C*H$_c$*CH$_s$'Me), 3.28 (m.obsc., η^3-CH$_a$*H$_s$*CH$_c$CH$_s$'Me), 3.09, 2.47, 2.25, 2.08, 2.07, 1.76 (3:3:3:3:3:3, Tp'C*H$_3$*), 2.70 (m., η^3-C*H$_a$*H$_s$CH$_c$CH$_s$'Me), 1.61 (d, $^3J_{Ha'Me}$= 6.5 Hz, η^3-CH$_a$H$_s$CH$_c$CH$_s$'C*H*$_3$). **2s**: 5.52 5.46, 5.44 (Tp'C*H*), 4.97 (dt, $^3J_{HaHc}$= 8 Hz, $^3J_{HsHc}$=$^3J_{Ha'Hc}$= 6 Hz, η^3-CH$_a$H$_s$C*H$_c$*CH$_a$'Me), 2.69 (dq, $^3J_{MeHa'}$= 6 Hz, $^3J_{HcHa'}$= 6 Hz, η^3-CH$_a$H$_s$CH$_c$C*H$_a$*'Me), 2.54, 2.15, 2.08, 2.06, 1.95 (3:6:3:3:3, Tp'C*H$_3$*), 2.54 (d, $^3J_{Ha'Me}$= 6 Hz, η^3-CH$_a$H$_s$CH$_c$CH$_a$'C*H*$_3$), 1.96 (d, $^3J_{HcHs}$= 6 Hz, η^3-CH$_a$*H$_s$*CH$_c$CH$_a$'Me), 1.57 (d, $^3J_{HcHa}$= 8 Hz, η^3-C*H$_a$*H$_s$CH$_c$CH$_a$'Et). ^{13}C NMR (C_6D_6, δ): **2a**-*anti*-methyl: 224.0, 220.2 (*C*O), 155.6, 154.4, 154.3, 145.7, 145.6, 143.4 (Tp'*C*CH$_3$), 108.8, 108.6, 107.1 (Tp'*C*H), 70.9 (d, $^1J_{CH}$= 167 Hz, η^3-

$CH_aH_sCH_cCH_{s'}Me$), 65.1 (d, $^1J_{CH}$= 160 Hz, η^3-$CH_aH_sCH_cCH_{s'}Me$), 54.7 (t, $^1J_{CH}$= 160 Hz, η^3-$CH_aH_sCH_cCH_{s'}Me$). **2s**: 30.1, 228.6 (J_{WC}=160, 170 Hz, *C*O), 153.2, 151.5, 150.4, 144.5, 143.9, 143.7 (Tp'*C*CH_3), 107.9, 107.5, 107.4 (Tp'*C*H), 81.6 (d, $^1J_{CH}$= 175 Hz, η^3-$CH_aH_sCH_cCH_{a'}Me$), 58.4 (d, $^1J_{CH}$= 160 Hz, η^3-$CH_aH_sCH_cCH_{a'}Me$), 54.2 (t, $^1J_{CH}$= 160 Hz, η^3-$CH_aH_sCH_cCH_{a'}Me$), 20.3 (t, $^1J_{CH}$= 127 Hz, CH_3).

Tp'(CO)$_2$W(η^3-CH$_2$CHCHEt) (3a, 3s). IR (KBr, cm^{-1}): ν_{BH}=2558; ν_{CO}=1914, 1815; ν_{CN}=1545. ^{1}H NMR (C_6D_6, δ): **3a**: 5.52, 5.23 (2:1, Tp'C*H*), 4.15 (dddd, $^3J_{Hs'H}$= 11 Hz, $^3J_{Hs'Hc}$= 7.3 Hz, $^3J_{Hs'H}$= 3 Hz, $^4J_{Hs'Hs}$= 2 Hz, η^3-$CH_aH_sCH_cCH_{s'}Et$), 3.28 (ddd, $^3J_{HsHc}$= 7.3, $^4J_{HsHs'}$= 2 Hz, $^2J_{HsHa}$= 2 Hz, η^3-$CH_aH_sCH_cCH_{s'}Et$), 3.21 (dt, $^3J_{HaHc}$= 9.5 Hz, $^3J_{HsHc}$=$^3J_{Hs'Hc}$= 7.3 Hz, η^3-$CH_aH_sCH_cCH_{s'}Et$), 3.09, 2.47, 2.32, 2.09, 2.07, 1.76 (Tp'CH_3), 2.61 (br.d $^3J_{HaHc}$= 9.5 Hz, η^3-$CH_aH_sCH_cCH_{s'}Et$), 2.43-2.32 (m.obsc., $CHHCH_3$), 0.98 (t, $^3J_{HH}$= 7.3, Hz, CH_2CH_3), 0.72 (m, $CHHCH_3$): **3s**: 5.52, 5.47, 5.45 (Tp'C*H*), 5.02 (dt, $^3J_{HaHc}$= 8 Hz, $^3J_{HsHc}$=$^3J_{Ha'Hc}$= 6 Hz, η^3-$CH_aH_sCH_cCH_{a'}Et$),2.79-2.72 (m, η^3-$CH_aH_sCH_cCH_{a'}Et$), 2.7-2.6 (m.obsc., $CHHCH_3$), 2.58-2.51 (m.obsc., $CHHCH_3$), 2.56, 2.14, 2.13, 2.10, 2.07, 1.99 (Tp'CH_3), 1.99 ($^3J_{HcHs}$= 6 Hz, η^3-$CH_aH_sCH_cCH_{a'}Et$), 1.60 (d, $^3J_{HaHc}$=8 Hz, η^3-$CH_aH_sCH_cCH_{a'}Et$), 1.34 (t, $^3J_{HH}$=7.4 Hz, CH_2CH_3). ^{13}C NMR (C_6D_6, δ): **3a**: 223.6, 220.3 ($^1J_{WC}$=160, 170 Hz, *C*O), 155.5, 154.4, 154.3, 145.8, 145.6, 143.5 (Tp'*C*CH_3), 108.8, 108.7, 107.1 (Tp'*C*H), 72.3 (d, $^1J_{CH}$= 153 Hz, η^3-$CH_aH_sCH_cCH_{s'}Et$), 69.1 (d, $^1J_{CH}$= 166 Hz, η^3-$CH_aH_sCH_cCH_{s'}Et$), 54.6 (t, $^1J_{CH}$= 157 Hz, η^3-$CH_aH_sCH_cCH_{s'}Et$), 23.8 (t, $^1J_{CH}$= 129 Hz, CH_2CH_3). **3s**; 230.1 ($^1J_{WC}$= 160 Hz *C*O) ,228.8 (*C*O), 153.2, 151.5, 150.5, 144.6, 143.9, 143.8 (Tp'*C*CH_3), 107.9, 107.5, (1:2, Tp'*C*H), 80.7 (d, $^1J_{CH}$= 172 Hz, η^3-$CH_aH_sCH_cCH_{a'}Et$), 65.9 (d, $^1J_{CH}$= 160 Hz, η^3-$CH_aH_sCH_cCH_{a'}Et$), 54.6 (t, $^1J_{CH}$=157 Hz, η^3-$CH_aH_sCH_cCH_{a'}Et$), 29.4 ($^1J_{CH}$=125 Hz, CH_2CH_3). Calculated for $WC_{22}H_{31}N_6BO_2$: C, 43.59; H, 5.15; N, 13.86. Found: C, 43.70; H, 5.13; N, 13.93.

Tp'(CO)$_2$W(η^3-CH$_2$CHCHPr^n) (4a, 4s). IR (KBr, cm^{-1}): ν_{BH}=2556; ν_{CO}=1917, 1819; ν_{CN}=1545. ^{1}H NMR (C_6D_6, δ): **4a**: 5.52, 5.23 (2:1, Tp'C*H*), 4.15

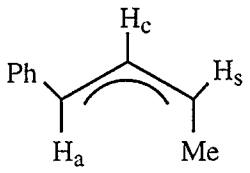
(dddd, $^3J_{Hs'H}$= 11 Hz, $^3J_{Hs'Hc}$= 7.3 Hz, $^3J_{Hs'H}$= 3 Hz, $^4J_{Hs'Hs}$= 2 Hz, η^3-$CH_aH_sCH_cCH_{s'}Pr^n$), 3.30 (ddd, $^3J_{HsHc}$= 7.3, $^4J_{HsHs'}$= 2 Hz, $^2J_{HsHa}$= 2 Hz, η^3-$CH_aH_sCH_cCH_{s'}Pr^n$), 3.21 (dt, $^3J_{HaHc}$= 9.5 Hz, $^3J_{HsHc}$=$^3J_{Hs'Hc}$= 7.3 Hz, η^3-$CH_aH_sCH_cCH_{s'}Pr^n$), 3.09, 2.47, 2.35, 2.10, 2.08, 1.77 (Tp'CH_3), 2.60 (br.d, $^3J_{HaHc}$= 10 Hz, η^3-$CH_aH_sCH_cCH_{s'}Pr)^n$, 2.42-2.36 (m, CHHCH$_2$CH$_3$), 1.5-1.2 (m, CH$_2$CH_2CH$_3$), 0.86 (t, $^3J_{HH}$= 7.5 Hz, CH$_2$CH$_2$CH_3), 0.71 (dddd, $^2J_{HHgem}$= 14 Hz, $^3J_{HHs'}$= 11 Hz, $^3J_{HHvic}$= 8.8 Hz, $^3J_{HHvic}$= 6.2 Hz, CHHCH$_2$CH$_3$): **4s**: 5.52, 5.48, 5.45 (Tp'CH), 5.06 (dt, $^3J_{HaHc}$= 8 Hz, $^3J_{HsHc}$=$^3J_{Ha'Hc}$= 6 Hz, η^3-$CH_aH_sCH_cCH_{a'}Pr^n$), 2.8-2.72 (m.obsc., η^3-$CH_aH_sCH_cCH_{a'}Pr^n$), 2.72-2.6 (m.obsc., CHHCH$_2$CH$_3$), 2.56, 2.15, 2.13, 2.10, 2.07, 2.00 (Tp'CH_3), 1.98 (d, $^3J_{HsHc}$= 6 Hz, η^3-$CH_aH_sCH_cCH_{a'}Pr^n$), 1.61 (d, $^3J_{HaHc}$= 8 Hz, η^3-$CH_aH_sCH_cCH_{a'}Pr^n$), 1.05 (t, $^3J_{HH}$= 7.5 Hz, CH$_2$CH$_2$CH_3); the remaining methylene proton for **4s** was not located ^{13}C NMR (C_6D_6, δ): **4a**: 223.5, 220.4 ($^1J_{WC}$=159, 164 Hz, CO), 155.5, 154.3, 145.8, 143.5 (1:2:2:1, Tp'CCH$_3$), 108.9, 108.7, 107.1 (Tp'CCH), 70.6 (d, $^1J_{CH}$=150 Hz, η^3-CH$_a$HsCH$_c$$CH_{s'}$Pr^n), 69.5 (d, $^1J_{CH}$=166 Hz, η^3-CH$_a$HsCH$_c$CH$_{s'}$ Pr^n), 55.5 (t, $^1J_{CH}$=156 Hz, η^3-CH$_a$HsCH$_c$CH$_{s'}$ Pr^n), 32.3 (t, $^1J_{CH}$=129 Hz, CH$_2$CH$_2$CH$_3$), 28.4 (t, $^1J_{CH}$=126 Hz, CH$_2$$CH_2CH_3$). **4s**: 230.3, 228.7 ($^1J_{WC}$=156, 174 Hz, CO), 153.2, 151.5, 150.4, 144.6, 143.9, 143.8 (Tp'CCH$_3$), 108.0, 107.6, 107.5 (Tp'CH), 81.2 (d, $^1J_{CH}$=173 Hz, η^3-CH$_a$HsCH$_c$CH$_{a'}$ Pr^n), 64.1 (d, $^1J_{CH}$=157 Hz, η^3-CH$_a$HsCH$_c$$CH_{a'}$ Pr^n), 54.5 (t, $^1J_{CH}$=156 Hz, η^3-CH$_a$HsCH$_c$CH$_{a'}$ Pr^n), 32.4 (t, $^1J_{CH}$=128 Hz, CH$_2$CH$_2$CH$_3$), 28.0 (t, $^1J_{CH}$=128 Hz, CH$_2$$CH_2CH_3$). Calculated for $WC_{23}H_{33}N_6BO_2$: C, 44.54; H, 5.36; N, 13.55. Found: C, 44.66; H, 5.38; N, 13.64.

Tp'(CO)$_2$W(η^3-CH$_2$CHCHCH$_2$Ph) (5a, 5s). IR (KBr, cm^{-1}) ν_{BH}=2548; ν_{CO}=1910, 1815; ν_{CN}=1545: ^{1}H NMR (C_6D_6, δ): 7.45-7.03 (*Ph*, both isomers), **5a**: 5.48, 5.47, 5.24 (Tp'CH), 4.31 (m., η^3-CH$_a$H$_s$CH$_c$C$H_{s'}$CH$_2$Ph), 3.65 (dd, $^2J_{HH}$= 14.4, $^3J_{HHs'}$= 3.2 Hz,η^3-CH$_a$H$_s$CH$_c$CH$_{s'}$CHHPh), 3.36 (ddd, $^3J_{HsHc}$= 6.8, $^4J_{HsHs'}$= 1.6 Hz, $^2J_{HsHa}$= 1.6 Hz η^3-CH$_a$$H_sCH_cCH_{s'}CH_2$Ph), 3.13 (dt, $^3J_{HaHc}$= 10 Hz, $^3J_{HsHc}$=$^3J_{Hs'Hc}$= 7.6 Hz, η^3-CH$_a$H$_s$CH_cCH$_{s'}$CH$_2$Ph), 3.10, 2.46, 2.31, 2.08, 2.07, 1.76 (3:3:3:3:3:3,

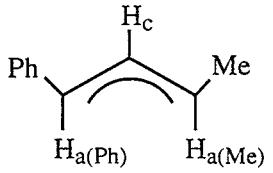
Tp'C*H*$_3$), 2.72 (m., η^3-C*H*$_a$H$_S$CH$_c$CH$_{s'}$CH$_2$Ph), 2.0-1.9 (m.,obsc., η^3-CH$_a$H$_S$CH$_c$CH$_{s'}$CH*H*Ph). **5s**: 5.52 5.48, (1:2, Tp'C*H*), 5.23 (dt, $^3J_{HaHc}$= 8 Hz, $^3J_{HsHc}$=$^3J_{Ha'Hc}$= 6 Hz, η^3-CH$_a$H$_s$C*H*$_c$CH$_{a'}$CH$_2$Ph), 3.96 (dd, $^2J_{HH}$= 14.4, $^3J_{HHa'}$= 3.2 Hz, η^3-CH$_a$H$_S$CH$_c$CH$_{a'}$C*H*HPh), 3.84 (dd, $^2J_{HH}$= 14.2, $^3J_{HHa'}$= 10.2 Hz,η^3-CH$_a$H$_S$CH$_c$CH$_{a'}$CH*H*Ph), 3.00 (dq, $^3J_{HHa'}$= 10 Hz, $^3J_{HcHs}$= 6 Hz, $^3J_{HHa'}$= 3.2 Hz, η^3-CH$_a$H$_S$CH$_c$C*H*$_{a'}$CHHPh), 2.58, 2.14, 2.12, 2.10, 1.89 (3:6:3:3:3, Tp'C*H*$_3$), 1.93 (d, $^3J_{HcHs}$= 6 Hz, η^3-CH$_a$*H*$_s$CH$_c$CH$_{a'}$CH$_2$Ph) 1.58 (d, $^3J_{HcHa}$= 8 Hz, η^3-C*H*$_a$H$_S$CH$_c$CH$_{a'}$CH$_2$Ph). ^{13}C NMR (C_6D_6, δ): **5a**: 223.4, 220.2 ($^1J_{WC}$= 160, 150 Hz, *C*O), 155.4, 154.4, 154.2, 145.8, 145.7, 143.5 (Tp'*C*CH$_3$), 108.8, 108.6, 107.1 (Tp'*C*H), 70.7 (d, $^1J_{CH}$= 160 Hz, η^3-CH$_a$H$_s$CH$_c$*C*H$_{s'}$CH$_2$Ph), 68.7 (d, $^1J_{CH}$= 167Hz, η^3-CH$_a$H$_s$*C*H$_c$CH$_{s'}$CH$_2$Ph), 54.8 (t, $^1J_{CH}$= 158 Hz, η^3-*C*H$_a$H$_s$CH$_c$CH$_{s'}$CH$_2$Ph), 36.3 (t, $^1J_{CH}$= 128 Hz, *C*H$_2$Ph); **5s**: 229.7, 228.4 (J_{WC}=150, 170 Hz, *C*O), 153.3, 151.5, 150.5, 144.7, 143.9, 143.8 (Tp'*C*CH$_3$), 107.9, 107.5, 107.4 (Tp'*C*H), 81.1 (d, $^1J_{CH}$= 173 Hz, η^3-CH$_a$H$_s$*C*H$_c$CH$_{a'}$CH$_2$Ph), 63.2 (d, $^1J_{CH}$= 159 Hz, η^3-CH$_a$H$_s$CH$_c$*C*H$_{a'}$CH$_2$Ph) 55.0 (t, $^1J_{CH}$= 157 Hz, η^3-*C*H$_a$H$_s$CH$_c$CH$_{a'}$CH$_2$Ph), 42.8 (t, $^1J_{CH}$= 129 Hz, *C*H$_2$Ph). Calculated for $WC_{27}H_{33}N_6BO_2$: C, 48.53; H, 4.98; N, 12.58. Found: C, 48.41; H, 4.92; N, 12.48.

Tp'(CO)$_2$W(η^3-CH$_2$CHCHPh) (6). ^{13}C NMR (-85°C, CD_2Cl_2:$CDCl_3$:CCl_4, 60:27:13, δ): 229.6, 227.8 (*C*O), 152.4, 150.7, 149.4, 145.3, 144.3, 144.2 (Tp'*C*CH$_3$), 139.2, 127.4, 126.8, 126.2 (*Ph*), 107.4, 107.0, 106.5 (Tp'*C*H), 77.2, 76.1 (η^3-CH$_2$*C*H*C*HPh), 59.8 ($^1J_{WC}$= 22 Hz, η^3-*C*H$_2$CHCHPh).15.3, 15.1, 14.1, 12.8, 12.7, 12.6 (Tp'C*C*H$_3$).

Tp'(CO)$_2$W(η^3-C(H)PhCHC(H)Me) (7a, 7s).



1-*syn*-phenyl-3-*anti*-methyl, **7a**



1-*syn*-phenyl-3-*syn*-methyl, **7s**

Notation for complex **7**

IR (KBr, cm^{-1}); ν_{CO}= 1902, 1808; ν_{CN}= 1545; ^1H NMR ($CDCl_3$, δ): **7a**: 6.6-6.2 (v.br., *Ph*), 5.84, 5.72, 5.11 (Tp'C*H*), 4.92 (d,$^1J_{HcHa}$= 10.4 Hz, η^3-CH_aPhCH$_c$CH$_s$CH$_3$), 4.84 (qd, $^3J_{HcHs}$= 8 Hz, $^3J_{MeHs}$= 6.4Hz, η^3-CH$_a$PhCH$_c$CH_sCH$_3$), 4.49 (dd, $^3J_{HaHc}$= 10.4, $^3J_{HsHc}$= 8, η^3-CH$_a$PhCH_cCH$_s$CH$_3$), 2.76, 2.41, 2.36, 2.17, 2.13, 1.56 (3:3:3:3:3:3, Tp'CH_3), 1.78 (d, $^3J_{HcHa}$= 6.4 η^3-CH$_a$PhCH$_c$CH$_s$CH_3); **7s**: 6.88-6.79 (m, *Ph*), 5.91, 5.79, 5.11 (Tp'C*H*), 5.42 (dd, $^3J_{Ha(Ph)Hc}$= 9.2, $^3J_{Ha(Me)Hc}$= 6, η^3-CH$_{a(Ph)}$PhCH_cCH$_{a(Me)}$CH$_3$), 3.24 (d,$^1J_{HcHa(Ph)}$= 9.2 Hz, η^3-C$H_{a(Ph)}$PhCH$_c$CH$_{a(Me)}$CH$_3$), 2.81 (qd, $^3J_{HcHs}$= 6 Hz, $^3J_{MeHa(Ph)}$= 6 Hz, η^3-CH$_{a(Ph)}$PhCH$_c$C$H_{a(Me)}$CH$_3$), 2.49, 2.33, 2.31, 2.20, 1.98 (3:3:3:6:3, Tp'CH_3), 2.46 (br., η^3-CH$_{a(Ph)}$PhCH$_c$CH$_{s(Me)}$CH_3). ^{13}C NMR (C_6D_6, δ); **7a**: 231.7, 220.9 ($^1J_{WC}$ = 140, --- Hz, *C*O), 154.7, 153.5, 153.0, 144.7, 144.6, 143.8 (Tp'*C*CH$_3$), 139.9 (C_{ipso}), 127.5 (br,), 127.0, 124.7 (2:2:1, *Ph*), 108.6, 107.1, 106.8 (Tp'*C*H), 92.0 (d, $^1J_{CH}$ = 164 Hz, η^3-CH$_a$Ph*C*H$_c$CH$_s$CH$_3$), 74.7 (d, $^1J_{CH}$ = 163, η^3-*C*H$_a$PhCH$_c$CH$_s$CH$_3$), 58.6 (d, $^1J_{CH}$ = 153 Hz, η^3-CH$_a$PhCH$_c$*C*H$_s$CH$_3$), 17.7 (q, $^1J_{CH}$ = 125 Hz, η^3-CH$_a$PhCH$_c$CH$_s$*C*H$_3$), 17.7, 16.1, 15.3, 12.9, 12.6, 12.3 (Tp'C*C*H$_3$). **7s**: 228.2, 227.5 ($^1J_{WC}$ = 180, 160 Hz, *C*O), 153.2, 151.9, 149.9, 144.9, 144.2, 143.8 (Tp'*C*CH$_3$), 139.4 (C_{ipso}), 127.3, 126.7, 125.4, (2:2:1, *Ph*), 107.8, 106.7, 106.6 (Tp'*C*H), 79.9 (d, $^1J_{CH}$ = 169 Hz, η^3-CH$_a$Ph*C*H$_c$CH$_s$CH$_3$), 72.8 (d, $^1J_{CH}$ = 157, η^3-*C*H$_{a(Ph)}$PhCH$_c$CH$_{a(Me)}$CH$_3$), 58.6 (d, $^1J_{CH}$ = 153 Hz, η^3-CH$_{a(Ph)}$PhCH$_c$*C*H$_{a(Me)}$CH$_3$), 19.9 (q, $^1J_{CH}$ = 124Hz, η^3-CH$_{(Ph)}$PhCH$_c$CH$_{a(Me)}$*C*H$_3$), 16.4, 15.7, 15.1, 13.0, 12.7, 12.4 (Tp'C*C*H$_3$).

Calculated for $WC_{27}H_{33}N_6BO_2$: C, 48.53; H, 4.98; N, 12.58. Found: C, 48.62; H, 4.95; N, 12.65.

Tp'(CO)$_2$W(η^3-C(H)CH$_3$CHC(H)CH$_2$CH$_3$) (8x, 8y). IR (KBr, cm^{-1}): ν_{BH}=2554; ν_{CO}=1912, 1818; ν_{CN}=1546. ^1H NMR (-70 °C, CD_2Cl_2:$CDCl_3$:CCl_4, 60:27:13, δ): 5.86, 5.85, 5.83, 5.81, 5.80 (1:2:1:1:1, Tp'C*H* [both isomers]), 4.92 (dd, $^3J_{HH}$ = 9.2 Hz, $^3J_{HH}$ = 5. 2 Hz, H_c [1 isomer]), 4.86 (d (broad), $^3J_{HH}$ = 9.2 Hz, H_c [1 isomer]), 2.39, 2.35, 2.32, 2.30, 2.28, 2.03, 2.01 (9:6:3:12:3:3:3, Tp'CH_3 [both isomers],

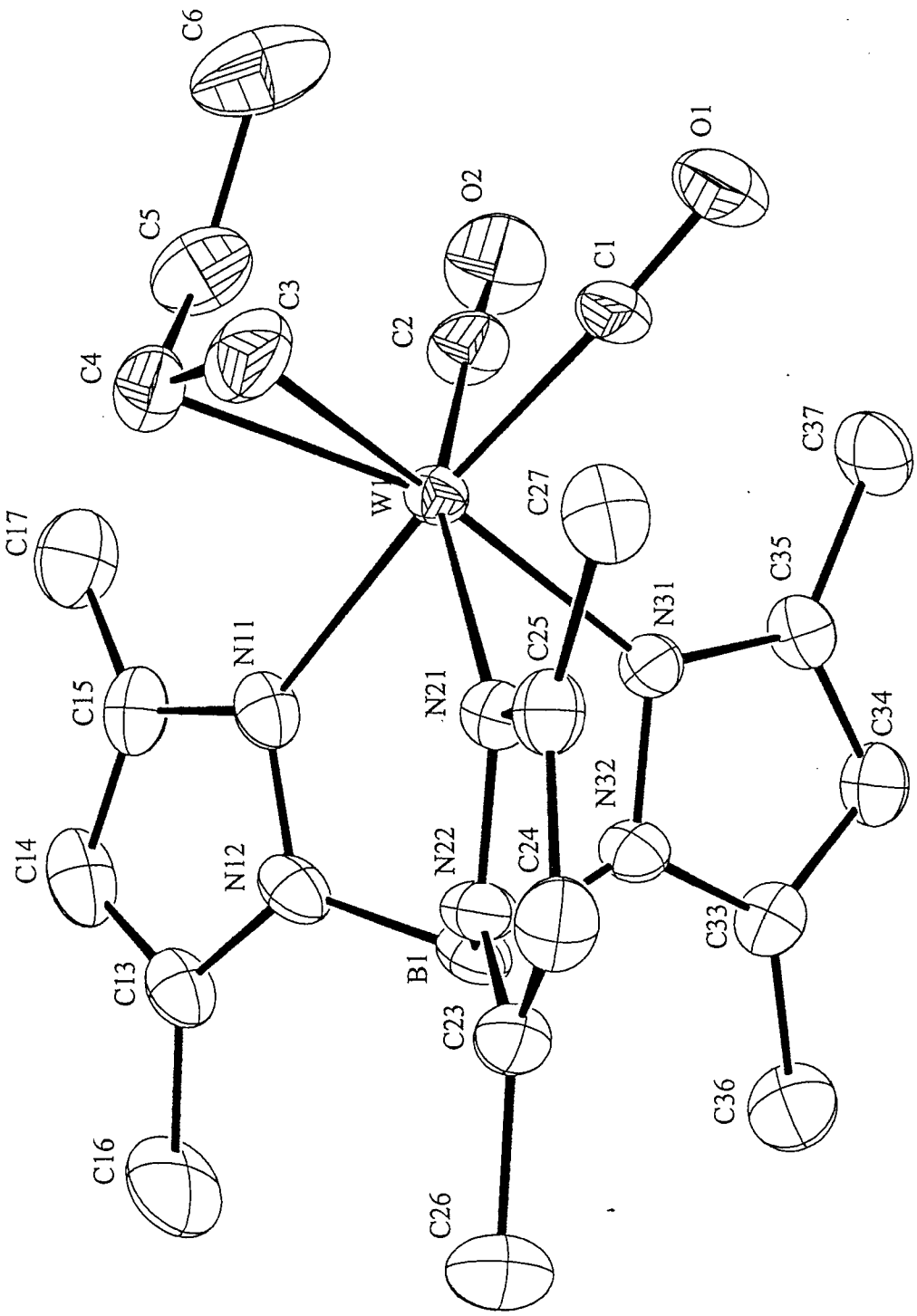
η^3-C(H)CH_3CHC(H)CH_2CH_3) [1 isomer]), 1.96 (dt, d-$^3J_{HH}$ = 5 Hz, t-$^3J_{HH}$ = 9 Hz, η^3-C(H)CH_3CHC(*H*)CH_2CH_3) [1 isomer]), 1.43 (m, η^3-C(H)CH_3CHC(H)CH_2CH_3 [1 isomer]), 1.32 (t, $^3J_{HH}$ = 7 Hz, η^3-C(H)CH_3CHC(H)CH_2CH_3 [1 isomer]), 0.80 (d, $^3J_{HH}$ = 6.1 Hz, η^3-C(H)CH_3CHC(H)CH_2CH_3 [1 isomer]), 0.61 (m, η^3-C(H)CH_3CHC(H)CH_2CH_3 [1 isomer]), 0.37 (t, $^3J_{HH}$ = 7.2 Hz, η^3-C(H)CH_3CHC(H)CH_2CH_3 [1 isomer]); the protons on the methyl substituted terminus for both isomers and the proton on the ethyl substituted terminus for one isomer could not be located unambiguously. ^{13}C NMR (-70 °C, CD_2Cl_2:$CDCl_3$:CCl_4, 60:27:13, δ) 228.0, 227.9, 227.5, 227.0 (*C*O [both isomers]), 152.6, 151.8,151.9, 149.8, 149.7 145.3, 145.1, 144.1 (2:1:1:1:1:3:1:2, Tp'*C*CH_3 [both isomers]), 107.4, 107.1, 106.6 (2:2:2, Tp'*C*H, [both isomers]), 85.0 (t, $^1J_{CH}$ = 173 Hz, η^3-C(H)CH_3*C*HC(H)CH_2CH_3 [1 isomer]), 83.6 (d, $^1J_{CH}$ = 171 Hz, η^3-C(H)CH_3*C*HC(H)CH_2CH_3 [1 isomer]), 80.1, 74.2, 64.2, 57.3(d each, $^1J_{CH}$ = 150, 156, 150, 161 Hz, resp.,η^3-*C*(H)CH_3CH*C*(H)CH_2CH_3 [both isomers]), 28.9, 22.5 (t each, $^1J_{CH}$ = 124, 125 Hz, resp., η^3-C(H)CH_3CHC(H)*C*H_2CH_3 [both isomers]), 20.1, 20.0 (q each, $^1J_{CH}$ = 126, 126 Hz, resp., η^3-C(H)CH_3CHC(H)CH_2*C*H_3 [both isomers]), 16.4, 16.1, 15.6, 14.9, 14.8, 13.2, 13.1, 13.0 (2:1:2:2:1:2:1:1:2, Tp'*C*H_3, η^3-C(H)*C*H_3CHC(H)CH_2CH_3 [both isomers])

Tp'(CO)$_2$Mo(η^3-CH$_2$CHCH$_2$) (9). IR (KBr, cm^{-1}) ν_{BH}=2544; ν_{CO}=1925, 1832; ν_{CN}=1545. ^{1}H NMR (C_6D_6, δ): 5.50, 5.35 (2:1, Tp'C*H*), 4.03 (tt, $^3J_{sc}$= 6.4 Hz, $^3J_{ac}$= 10.0 Hz, η^3-$CH_aH_sCH_cCH_aH_s$), 3.57 (d, $^3J_{cs}$= 6.4 Hz, η^3-$CH_aH_sCH_cCH_aH_s$), 3.03, 2.62, 2.09, 1.87 (3:6:6:3, Tp'C*H*$_3$), 1.88 (d, $^3J_{ca}$= obsc., η^3-$CH_aH_sCH_cCH_aH_s$). ^{13}C{^{1}H} NMR (C_6D_6, δ): 229.5 (*C*O), 154.0, 152.9, 147.4, 144.9 (1:2:1:2, Tp'*C*CH_3), 108.3, 107.2 (Tp'*C*H), 80.2 (η^3-CH_2*C*HCH_2), 63.5 (η^3-*C*H_2CHCH_2).

Tp'(CO)$_2$Mo(η^3-CH$_2$CHCHMe) (10a, 10s). IR (KBr, cm^{-1}): **10a:** ν_{BH}=2548; ν_{CO}=1919, 1827; ν_{CN}=1545; **10s:** ν_{BH}=2546; ν_{CO}=1921, 1825; ν_{CN}=1545. ^{1}H NMR (C_6D_6, δ): **10a**: 5.55, 5.51, 5.34 (Tp'C*H*), 4.59 (dqd, $^3J_{HcHs'}$= 7.6 Hz, $^3J_{MeHs'}$= 6.8 Hz, $^4J_{HsHs'}$= 1.9 Hz, η^3-$CH_aH_sCH_cCH_{s'}$Me), 4.12 (dt, $^3J_{HaHc}$= 10.8 Hz, $^3J_{HsHc}$=$^3J_{Hs'Hc}$= 7.6

Hz, η^3-$CH_aH_SCH_cCH_{s'}Me$), 3.50 (dd $^3J_{HcHs}$= 7.2 Hz, $^4J_{Hs'Hs}$= 1.2 Hz, η^3-$CH_aH_SCH_cCH_{s'}Me$), 2.97 (d, $^3J_{HaHc}$= 11.2 Hz, η^3-$CH_aH_SCH_cCH_{s'}Me$), 3.08, 2.47, 2.15, 2.10, 1.85 (3:3:3:6:3, Tp'CH_3), 1.28 (d, $^3J_{Hs'Me}$= 6.8 Hz, η^3-$CH_aH_SCH_cCH_{s'}CH_3$). **10s**: 5.53, 5.48 (2:1, Tp'C*H*), 5.06 (dt, $^3J_{HaHc}$= 10 Hz, $^3J_{HsHc}$=$^3J_{Ha'Hc}$= 6.8 Hz, η^3-$CH_aH_SCH_cCH_{a'}Me$), 2.68 (m.obsc., η^3-$CH_aH_SCH_cCH_{a'}Me$), 2.68 (d, $^3J_{HcHs}$= 6.0 Hz, η^3-$CH_aH_SCH_cCH_{a'}Me$), 2.54, 2.17, 2.14, 2.12, 2.10, 1.85 (3:3:3:3:3:3, Tp'CH_3), 2.20 (d, $^3J_{Ha'Me}$= 6.4 Hz, η^3-$CH_aH_SCH_cCH_{a'}CH_3$), 1.98 (d, $^3J_{HcHs}$= 10 Hz, η^3-$CH_aH_SCH_cCH_{a'}Me$). ^{13}C NMR (C_6D_6, δ): **10a**: 232.7, 228.6 ($^3J_{CH}$= 3.7 Hz, *C*O), 154.4, 153.0, 152.8, 145.0, 144.2 (1:1:1:2:1, Tp'*C*CH_3), 108.4, 108.2, 107.2 (Tp'*C*H), 82.0 (d, $^1J_{CH}$= 161 Hz, η^3-$CH_aH_SCH_cCH_{s'}CH_3$), 73.7, (d, $^1J_{CH}$= 153Hz, η^3-$CH_aH_SCH_cCH_{s'}CH_3$), 63.5 (t, $^1J_{CH}$= 160Hz, η^3-$CH_aH_SCH_cCH_{s'}CH_3$); **10s**; 235.0, 234.4 ($^3J_{CH}$= 3.7 Hz, *C*O), 152.4, 151.4, 150.7, 145.0, 144.9, 144.1 (Tp'*C*CH_3), 107.7, 107.4, 107.3 (Tp'*C*H), 89.1 (d, $^1J_{CH}$= 165 Hz, η^3-$CH_aH_SCH_cCH_{a'}CH_3$), 68.2 (d, $^1J_{CH}$= 162 Hz, η^3-$CH_aH_SCH_cCH_{a'}CH_3$), 65.1 (d, $^1J_{CH}$= 159 Hz, η^3-$CH_aH_SCH_cCH_{a'}CH_3$), 20.3 (q, $^1J_{CH}$= 128 Hz, η^3-$CH_aH_SCH_cCH_{a'}CH_3$)

Tp'(CO)$_2$W(η^3-*anti*-1-methylallyl) (2a)



Bond Lengths and Bond Angles for Tp'(CO)$_2$W(η^3-*anti*-1-methylallyl) (2a)

W(1)-C(1)	1.916(8)	C(13)-C(14)	1.345(14)
W(1)-C(2)	1.950(8)	C(13)-C(16)	1.492(14)
W(1)-C(3)	2.348(9)	C(14)-C(15)	1.391(14)
W(1)-C(4)	2.229(9)	C(15)-C(17)	1.477(14)
W(1)-C(5)	2.416(10)	N(21)-N(22)	1.387(8)
W(1)-N(11)	2.327(6)	N(21)-C(25)	1.355(9)
W(1)-N(21)	2.270(5)	N(22)-C(23)	1.342(9)
W(1)-N(31)	2.196(5)	C(23)-C(24)	1.355(12)
C(1)-O(1)	1.172(10)	C(23)-C(26)	1.504(11)
C(2)-O(2)	1.160(10)	C(24)-C(25)	1.396(11)
C(3)-C(4)	1.354(16)	C(25)-C(27)	1.483(11)
C(4)-C(5)	1.423(16)	N(31)-N(32)	1.384(8)
C(5)-C(6)	1.521(18)	N(31)-C(35)	1.353(9)
B(1)-N(12)	1.530(11)	N(32)-C(33)	1.341(9)
B(1)-N(22)	1.526(10)	C(33)-C(34)	1.370(12)
B(1)-N(32)	1.557(10)	C(33)-C(36)	1.481(12)
N(11)-N(12)	1.375(9)	C(34)-C(35)	1.374(11)
N(11)-C(15)	1.353(10)	C(35)-C(37)	1.508(11)
N(12)-C(13)	1.354(10)		

C(1)-W(1)-C(2)	80.5(4)	W(1)-N(11)-N(12)	117.3(4)
C(1)-W(1)-C(3)	77.9(3)	W(1)-N(11)-C(15)	137.8(6)
C(1)-W(1)-C(4)	103.6(3)	N(12)-N(11)-C(15)	104.5(6)
C(1)-W(1)-C(5)	93.2(4)	B(1)-N(12)-N(11)	119.8(5)
C(1)-W(1)-N(11)	172.5(3)	B(1)-N(12)-C(13)	127.2(7)
C(1)-W(1)-N(21)	92.9(3)	N(11)-N(12)-C(13)	111.2(7)
C(1)-W(1)-N(31)	94.2(3)	N(12)-C(13)-C(14)	107.1(7)
C(2)-W(1)-C(3)	115.9(3)	N(12)-C(13)-C(16)	123.0(8)
C(2)-W(1)-C(4)	98.4(4)	C(14)-C(13)-C(16)	129.8(8)
C(2)-W(1)-C(5)	63.2(4)	C(13)-C(14)-C(15)	107.4(7)
C(2)-W(1)-N(11)	95.7(3)	N(11)-C(15)-C(14)	109.8(8)
C(2)-W(1)-N(21)	162.0(3)	N(11)-C(15)-C(17)	123.5(8)
C(2)-W(1)-N(31)	87.0(3)	C(14)-C(15)-C(17)	126.6(8)
C(3)-W(1)-C(4)	34.3(4)	W(1)-N(21)-N(22)	119.4(4)
C(3)-W(1)-C(5)	58.7(3)	W(1)-N(21)-C(25)	134.9(5)
C(3)-W(1)-N(11)	109.7(3)	N(22)-N(21)-C(25)	105.7(5)
C(3)-W(1)-N(21)	78.6(3)	B(1)-N(22)-N(21)	119.1(5)
C(3)-W(1)-N(31)	153.6(3)	B(1)-N(22)-C(23)	129.2(6)
C(4)-W(1)-C(5)	35.4(4)	N(21)-N(22)-C(23)	110.2(6)
C(4)-W(1)-N(11)	83.3(3)	N(22)-C(23)-C(24)	108.0(6)
C(4)-W(1)-N(21)	99.5(3)	N(22)-C(23)-C(26)	123.6(8)
C(4)-W(1)-N(31)	162.0(3)	C(24)-C(23)-C(26)	128.5(7)
C(5)-W(1)-N(11)	90.8(3)	C(23)-C(24)-C(25)	107.3(6)
C(5)-W(1)-N(21)	134.3(3)	N(21)-C(25)-C(24)	108.8(6)
C(5)-W(1)-N(31)	147.6(3)	N(21)-C(25)-C(27)	125.3(6)
N(11)-W(1)-N(21)	88.76(22)	C(24)-C(25)-C(27)	125.9(7)
N(11)-W(1)-N(31)	79.01(22)	W(1)-N(31)-N(32)	120.0(4)
N(21)-W(1)-N(31)	76.70(19)	W(1)-N(31)-C(35)	134.5(5)
W(1)-C(1)-O(1)	176.5(7)	N(32)-N(31)-C(35)	105.4(5)
W(1)-C(2)-O(2)	175.3(9)	B(1)-N(32)-N(31)	121.1(5)
W(1)-C(3)-C(4)	68.0(5)	B(1)-N(32)-C(33)	128.4(6)
W(1)-C(4)-C(3)	77.7(5)	N(31)-N(32)-C(33)	110.4(6)
W(1)-C(4)-C(5)	79.5(6)	N(32)-C(33)-C(34)	107.1(7)
C(3)-C(4)-C(5)	114.7(9)	N(32)-C(33)-C(36)	124.0(7)
W(1)-C(5)-C(4)	65.1(5)	C(34)-C(33)-C(36)	128.8(7)
W(1)-C(5)-C(6)	115.4(8)	C(33)-C(34)-C(35)	107.5(6)
C(4)-C(5)-C(6)	125.3(10)	N(31)-C(35)-C(34)	109.6(6)
N(12)-B(1)-N(22)	111.0(6)	N(31)-C(35)-C(37)	123.6(7)
N(12)-B(1)-N(32)	109.0(6)	C(34)-C(35)-C(37)	126.8(7)
N(22)-B(1)-N(32)	108.0(6)		

Atomic Coordinates for Tp'(CO)$_2$W(η^3-*anti*-1-methylallyl) (2a)

Name	x	y	z
W(1)	0.22331(2)	0.55358(2)	0.23715(2)
C(1)	0.30449(78)	0.41726(78)	0.22853(74)
O(1)	0.34849(69)	0.33108(65)	0.22551(63)
C(2)	0.22296(89)	0.57153(94)	0.41336(78)
O(2)	0.22861(84)	0.57682(92)	0.51664(67)
C(3)	0.06360(92)	0.35389(103)	0.06574(97)
C(4)	0.00001(88)	0.43461(96)	0.14660(113)
C(5)	0.00830(110)	0.43738(104)	0.27188(99)
C(6)	0.00954(156)	0.31791(133)	0.29905(139)
B(1)	0.34443(90)	0.81599(78)	0.17180(82)
N(11)	0.14952(64)	0.73954(62)	0.27019(60)
N(12)	0.20682(66)	0.81946(57)	0.21306(59)
C(13)	0.14533(86)	0.91529(76)	0.22903(81)
C(14)	0.04616(95)	0.89728(85)	0.29540(92)
C(15)	0.05099(79)	0.79030(85)	0.32262(76)
C(16)	0.18306(128)	1.01344(109)	0.17334(146)
C(17)	-0.03143(108)	0.74125(120)	0.40248(111)
N(21)	0.29627(55)	0.56196(54)	0.05887(50)
N(22)	0.32514(59)	0.68307(56)	0.04935(55)
C(23)	0.35906(74)	0.66477(81)	-0.06580(73)
C(24)	0.35363(77)	0.53284(86)	-0.13257(67)
C(25)	0.31738(69)	0.47006(73)	-0.05310(66)
C(26)	0.39293(106)	0.77546(110)	-0.10814(101)
C(27)	0.30980(81)	0.32834(77)	-0.08267(74)
N(31)	0.42133(56)	0.72158(58)	0.32271(53)
N(32)	0.44746(60)	0.82410(55)	0.28449(56)
C(33)	0.57156(76)	0.91848(73)	0.35142(71)
C(34)	0.62830(77)	0.87685(83)	0.43337(72)
C(35)	0.53456(76)	0.75635(77)	0.41479(64)
C(36)	0.63122(99)	1.04100(90)	0.33297(103)
C(37)	0.55298(93)	0.66966(101)	0.48027(83)
H(3a)	0.05437(0)	0.35691(0)	-0.01663(0)
H(3b)	0.10176(0)	0.31123(0)	0.11004(0)
H(4)	-0.04470(0)	0.48731(0)	0.12135(0)
H(5)	0.01386(0)	0.52099(0)	0.34601(0)
H(6a)	0.01550(0)	0.34255(0)	0.39048(0)
H(6b)	-0.07445(0)	0.24363(0)	0.24843(0)
H(6c)	0.08758(0)	0.29039(0)	0.27259(0)
H(1)	0.38158(0)	0.89279(0)	0.15548(0)
H(14)	-0.01617(0)	0.94895(0)	0.32019(0)
H(16a)	0.12756(0)	1.07249(0)	0.19665(0)
H(16b)	0.27921(0)	1.06721(0)	0.20811(0)
H(16c)	0.16659(0)	0.96391(0)	0.07953(0)
H(17a)	-0.09536(0)	0.79092(0)	0.42805(0)
H(17b)	-0.08188(0)	0.64569(0)	0.35035(0)
H(17c)	0.02746(0)	0.75455(0)	0.47942(0)
H(24)	0.37489(0)	0.49102(0)	-0.21713(0)
H(26a)	0.41472(0)	0.74223(0)	-0.19326(0)
H(26b)	0.31511(0)	0.80713(0)	-0.11062(0)
H(26c)	0.47134(0)	0.84948(0)	-0.04510(0)
H(27a)	0.32525(0)	0.28331(0)	-0.16930(0)
H(27b)	0.38033(0)	0.33150(0)	-0.01998(0)
H(27c)	0.22060(0)	0.27883(0)	-0.07803(0)
H(34)	0.71757(0)	0.92249(0)	0.49232(0)
H(36a)	0.72085(0)	1.09297(0)	0.39066(0)
H(36b)	0.64019(0)	1.01324(0)	0.24369(0)
H(36c)	0.57180(0)	1.09625(0)	0.35276(0)
H(37a)	0.64015(0)	0.71252(0)	0.54235(0)
H(37b)	0.47907(0)	0.65789(0)	0.52471(0)
H(37c)	0.55032(0)	0.58208(0)	0.41423(0)

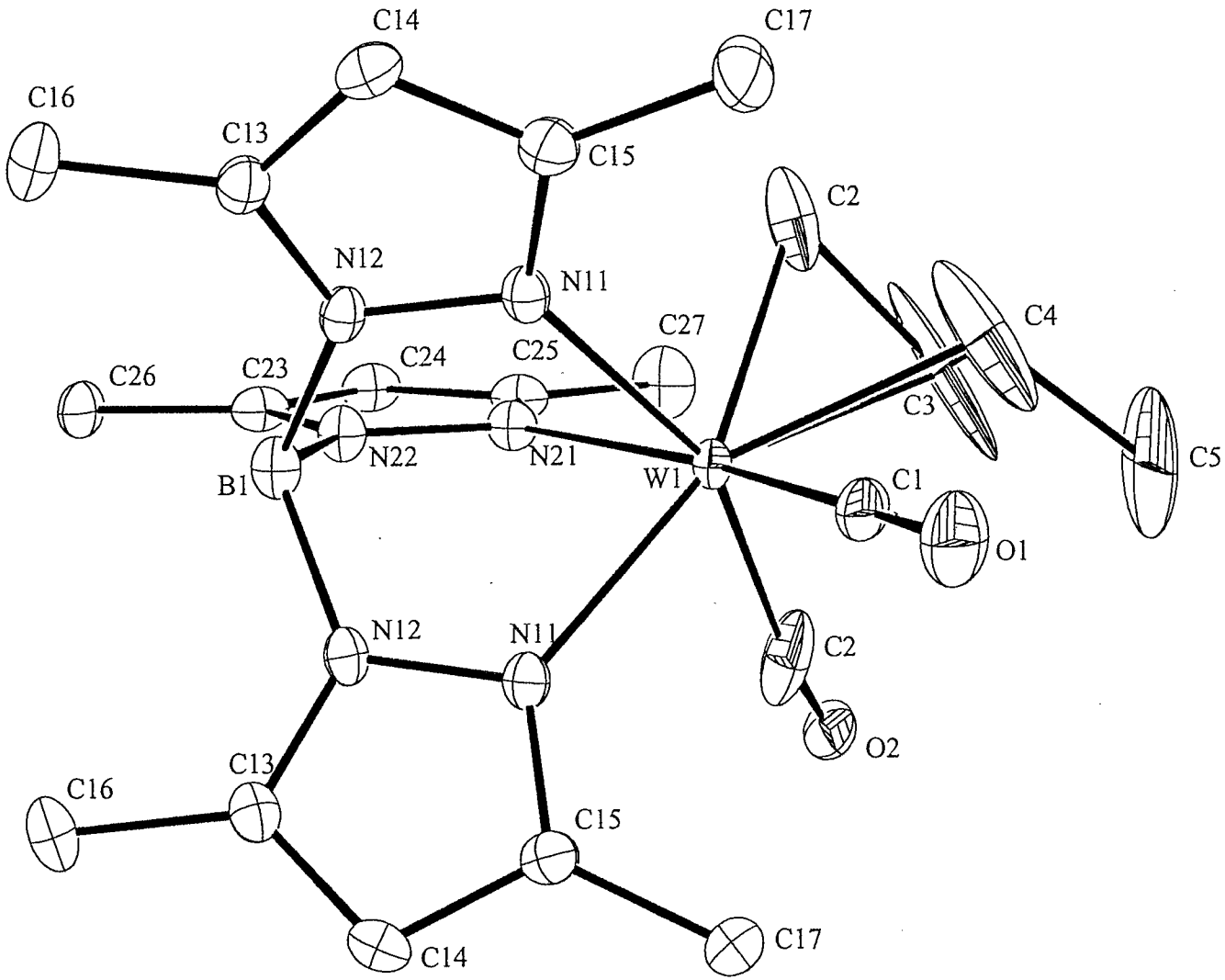
Table of u(i,j) values for $Tp'(CO)_2W(\eta^3$-*anti*-1-methylallyl) (2a)

	u11(U)	u22	u33	u12	u13	u23
W1	3.727(17)	3.427(17)	3.193(16)	1.135(11)	0.579(10)	1.675(12)
C1	5.1 (4)	4.7 (4)	4.8 (4)	1.8 (4)	0.8 (3)	3.1 (4)
O1	8.4 (4)	6.9 (4)	7.4 (4)	4.0 (4)	2.4 (3)	4.8 (3)
C2	6.3 (5)	7.5 (6)	4.3 (4)	1.7 (4)	1.7 (4)	3.4 (4)
O2	10.7 (6)	13.9 (7)	5.7 (4)	3.6 (5)	2.6 (4)	5.5 (5)
C3	5.0 (5)	7.2 (6)	7.0 (6)	-0.7 (5)	-0.8 (4)	3.2 (5)
C4	4.2 (5)	5.8 (5)	10.3 (8)	1.0 (4)	0.2 (5)	3.7 (5)
C5	8.3 (7)	6.6 (6)	6.6 (6)	1.0 (5)	2.2 (5)	2.3 (5)
C6	14.6 (12)	8.5 (8)	11.5 (10)	1.5 (8)	6.8 (10)	5.1 (8)
B1	5.2 (5)	2.9 (4)	4.5 (4)	1.1 (3)	-0.1 (4)	1.7 (3)
N11	4.7 (3)	4.2 (3)	4.6 (3)	1.8 (3)	0.2 (3)	1.2 (3)
N12	5.7 (4)	3.2 (3)	4.6 (3)	1.8 (3)	-0.1 (3)	1.4 (3)
C13	5.7 (5)	3.7 (4)	5.6 (5)	2.0 (4)	-0.3 (4)	1.2 (4)
C14	6.2 (5)	4.5 (5)	6.8 (6)	3.0 (4)	-0.9 (4)	-0.2 (4)
C15	4.3 (4)	5.6 (5)	4.4 (4)	1.7 (4)	0.4 (3)	0.4 (4)
C16	10.3 (8)	5.8 (6)	14.2 (11)	4.5 (6)	0.8 (8)	4.8 (7)
C17	7.0 (6)	9.3 (8)	8.5 (7)	4.1 (6)	3.3 (6)	2.8 (6)
N21	3.9 (3)	3.4 (3)	3.0 (3)	0.88 (24)	0.17 (23)	1.21 (24)
N22	4.6 (3)	3.5 (3)	4.1 (3)	0.9 (3)	0.5 (3)	2.2 (3)
C23	4.2 (4)	5.7 (5)	4.8 (4)	1.2 (3)	0.8 (3)	3.3 (4)
C24	4.7 (4)	6.9 (5)	3.2 (4)	2.0 (4)	1.2 (3)	2.1 (4)
C25	3.6 (4)	4.3 (4)	3.6 (4)	1.0 (3)	0.1 (3)	1.1 (3)
C26	8.1 (6)	8.8 (7)	7.6 (6)	2.4 (5)	2.3 (5)	6.1 (6)
C27	5.3 (5)	4.4 (4)	4.5 (4)	1.9 (4)	0.5 (3)	0.7 (3)
N31	3.8 (3)	4.1 (3)	3.4 (3)	1.0 (3)	0.50 (24)	1.7 (3)
N32	4.6 (3)	3.0 (3)	4.1 (3)	0.8 (3)	0.3 (3)	1.4 (3)
C33	4.7 (4)	3.7 (4)	4.3 (4)	0.9 (3)	0.8 (3)	0.7 (3)
C34	4.3 (4)	5.6 (5)	3.9 (4)	1.0 (4)	-0.3 (3)	0.9 (4)
C35	4.8 (4)	5.0 (4)	2.9 (3)	1.7 (3)	0.3 (3)	1.2 (3)
C36	6.6 (6)	4.4 (5)	8.5 (7)	0.1 (4)	0.0 (5)	1.8 (5)
C37	6.3 (5)	8.2 (6)	5.1 (5)	2.6 (5)	-0.2 (4)	3.4 (5)
H3a	7.4					
H3b	7.4					
H4	7.7					
H5	8.2					
H6a	12.5					
H6b	12.5					
H6c	12.5					
H1	5.2					
H14	6.8					
H16a	11.1					
H16b	11.1					
H16c	11.1					
H17a	9.3					
H17b	9.3					
H17c	9.3					
H24	5.9					
H26a	9.2					
H26b	9.2					
H26c	9.2					
H27a	5.7					
H27b	5.7					
H27c	5.7					
H34	5.6					
H36a	7.5					
H36b	7.5					
H36c	7.5					
H37a	7.5					
H37b	7.5					
H37c	7.5					

u(i,j) values listed as u(i,j) x 100

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)

$Tp'(CO)_2W(\eta^3\text{-}syn\text{-}1\text{-methylallyl})$ (2s)



Bond Lengths and Bond Angles for

$Tp'(CO)_2W(\eta^3\text{-}syn\text{-}1\text{-methylallyl})$ (2s)

W(1)-C(1)	1.969(12)	B(1)-N(12)	1.562(9)
W(1)-C(2)	2.122(14)	B(1)-N(12)a	1.562(9)
W(1)-C(2)a	2.122(14)	B(1)-N(22)	1.481(15)
W(1)-C(3)	2.273(22)	N(11)-N(12)	1.366(8)
W(1)-C(3)a	2.273(22)	N(11)-C(15)	1.348(10)
W(1)-C(4)	2.314(24)	N(12)-C(13)	1.346(10)
W(1)-C(4)a	2.314(24)	C(13)-C(14)	1.359(11)
W(1)-N(11)	2.241(6)	C(13)-C(16)	1.487(11)
W(1)-N(11)a	2.241(6)	C(14)-C(15)	1.390(12)
W(1)-N(21)	2.258(9)	C(15)-C(17)	1.506(12)
C(1)-O(1)	1.136(15)	N(21)-N(22)	1.408(13)
C(2)-O(2)	0.939(18)	N(21)-C(25)	1.356(13)
C(2)-C(3)	1.73(5)	N(22)-C(23)	1.375(13)
C(3)-C(3)a	1.08(10)	C(23)-C(24)	1.373(17)
C(3)-C(4)	1.14(4)	C(23)-C(26)	1.479(16)
C(4)-C(5)	1.64(5)	C(24)-C(25)	1.387(16)
C(5)-C(4)a	1.64(5)	C(25)-C(27)	1.467(18)

C(1)-W(1)-C(2)	104.1(3)	N(11)a-W(1)-N(21)	82.73(23)
C(1)-W(1)-C(2)a	104.1(3)	W(1)-C(1)-O(1)	178.4(12)
C(1)-W(1)-C(3)	90.1(10)	W(1)-C(2)-O(2)	172.7(13)
C(1)-W(1)-C(3)a	90.1(10)	W(1)-C(2)-C(3)	71.5(11)
C(1)-W(1)-C(4)	64.8(9)	O(2)-C(2)-C(3)	101.2(15)
C(1)-W(1)-C(4)a	64.8(9)	W(1)-C(3)-C(2)	62.3(10)
C(1)-W(1)-N(11)	87.4(3)	W(1)-C(3)-C(3)a	76.3(18)
C(1)-W(1)-N(11)a	87.4(3)	W(1)-C(3)-C(4)	77.6(17)
C(1)-W(1)-N(21)	167.2(5)	C(2)-C(3)-C(3)a	134(3)
C(2)-W(1)-C(2)a	111.0(4)	C(2)-C(3)-C(4)	77(3)
C(2)-W(1)-C(3)	46.2(14)	C(3)a-C(3)-C(4)	112(5)
C(2)-W(1)-C(3)a	72.4(12)	W(1)-C(4)-C(3)	73.7(16)
C(2)-W(1)-C(4)	49.2(11)	W(1)-C(4)-C(5)	118.3(19)
C(2)-W(1)-C(4)a	92.5(10)	C(3)-C(4)-C(5)	83(4)
C(2)-W(1)-N(11)	82.9(4)	C(4)-C(5)-C(4)a	73.3(15)
C(2)-W(1)-N(11)a	158.5(3)	N(12)-B(1)-N(12)a	108.8(8)
C(2)-W(1)-N(21)	82.9(3)	N(12)-B(1)-N(22)	109.7(6)
C(2)a-W(1)-C(3)	72.4(12)	N(12)a-B(1)-N(22)	109.7(6)
C(2)a-W(1)-C(3)a	46.2(14)	W(1)-N(11)-N(12)	120.9(4)
C(2)a-W(1)-C(4)	92.5(10)	W(1)-N(11)-C(15)	133.1(5)
C(2)a-W(1)-C(4)a	49.2(11)	N(12)-N(11)-C(15)	106.0(6)
C(2)a-W(1)-N(11)	158.5(3)	B(1)-N(12)-N(11)	119.7(7)
C(2)a-W(1)-N(11)a	82.9(4)	B(1)-N(12)-C(13)	129.7(7)
C(2)a-W(1)-N(21)	82.9(3)	N(11)-N(12)-C(13)	110.6(6)
C(3)-W(1)-C(3)a	27.4(18)	N(12)-C(13)-C(14)	107.3(7)
C(3)-W(1)-C(4)	28.8(9)	N(12)-C(13)-C(16)	124.2(7)
C(3)-W(1)-C(4)a	47.4(16)	C(14)-C(13)-C(16)	128.4(7)
C(3)-W(1)-N(11)	126.5(13)	C(13)-C(14)-C(15)	107.0(7)
C(3)-W(1)-N(11)a	153.8(13)	N(11)-C(15)-C(14)	109.1(7)
C(3)-W(1)-N(21)	102.4(10)	N(11)-C(15)-C(17)	123.6(7)
C(3)a-W(1)-C(4)	47.4(16)	C(14)-C(15)-C(17)	127.2(7)
C(3)a-W(1)-C(4)a	28.8(9)	W(1)-N(21)-N(22)	119.5(6)
C(3)a-W(1)-N(11)	153.8(13)	W(1)-N(21)-C(25)	134.4(8)
C(3)a-W(1)-N(11)a	126.5(13)	N(22)-N(21)-C(25)	106.0(8)
C(3)a-W(1)-N(21)	102.4(10)	B(1)-N(22)-N(21)	120.5(8)
C(4)-W(1)-C(4)a	50.1(16)	B(1)-N(22)-C(23)	130.3(10)
C(4)-W(1)-N(11)	108.9(10)	N(21)-N(22)-C(23)	109.2(8)
C(4)-W(1)-N(11)a	149.9(10)	N(22)-C(23)-C(24)	107.0(10)
C(4)-W(1)-N(21)	126.3(9)	N(22)-C(23)-C(26)	121.9(10)
C(4)a-W(1)-N(11)	149.9(10)	C(24)-C(23)-C(26)	131.0(10)
C(4)a-W(1)-N(11)a	108.9(10)	C(23)-C(24)-C(25)	108.2(9)
C(4)a-W(1)-N(21)	126.3(9)	N(21)-C(25)-C(24)	109.5(10)
N(11)-W(1)-N(11)a	79.49(22)	N(21)-C(25)-C(27)	122.8(10)
N(11)-W(1)-N(21)	82.73(23)	C(24)-C(25)-C(27)	127.6(10)

Atomic Coordinates for Tp'(CO)$_2$W(η^3-*syn*-1-methylallyl) (2s)

Name	x	y	z	
W(1)	0.55784(5)	0.75000(0)	0.31970(3)	
C(1)	0.78521(165)	0.75000(0)	0.43759(107)	
O(1)	0.91816(125)	0.75000(0)	0.50335(89)	
C(2)	0.43497(130)	0.61723(113)	0.36451(91)	*
O(2)	0.37921(174)	0.56298(91)	0.39340(114)	
C(3)	0.42875(391)	0.70919(373)	0.47381(321)	*
C(4)	0.56385(358)	0.67572(301)	0.50799(305)	*
C(5)	0.57145(424)	0.75000(0)	0.62662(184)	
B(1)	0.54410(152)	0.75000(0)	0.01879(115)	
N(11)	0.66962(73)	0.64127(46)	0.20556(54)	*
N(12)	0.64138(72)	0.65360(45)	0.08111(52)	*
C(13)	0.71517(93)	0.57770(55)	0.03137(67)	
C(14)	0.79238(112)	0.51481(56)	0.12462(79)	
C(15)	0.76324(108)	0.55549(57)	0.23247(75)	
C(16)	0.70149(112)	0.56574(69)	-0.10271(75)	
C(17)	0.82714(151)	0.51489(71)	0.36116(85)	
N(21)	0.33269(106)	0.75000(0)	0.15283(83)	
N(22)	0.36449(106)	0.75000(0)	0.03440(83)	
C(23)	0.20936(128)	0.75000(0)	-0.05207(104)	
C(24)	0.08093(130)	0.75000(0)	0.01080(109)	
C(25)	0.15827(130)	0.75000(0)	0.13581(109)	
C(26)	0.20048(160)	0.75000(0)	-0.18560(100)	
C(27)	0.07257(155)	0.75000(0)	0.23815(139)	
H(14)	0.85621(0)	0.45416(0)	0.11770(0)	
H(16a)	0.76474(0)	0.50685(0)	-0.11729(0)	
H(16b)	0.58180(0)	0.55807(0)	-0.14409(0)	
H(16c)	0.74765(0)	0.62486(0)	-0.13353(0)	
H(17a)	0.88977(0)	0.45296(0)	0.35875(0)	
H(17b)	0.90207(0)	0.56399(0)	0.41050(0)	
H(17c)	0.73040(0)	0.50194(0)	0.39628(0)	
H(24)	-0.04102(0)	0.75000(0)	-0.02616(0)	
H(26a)	0.08097(0)	0.75000(0)	-0.22923(0)	
H(26b)	0.25623(0)	0.80949(0)	-0.20727(0)	
H(27a)	-0.05054(0)	0.75000(0)	0.20596(0)	
H(27b)	0.10593(0)	0.69051(0)	0.28767(0)	

There are Symmetry Equivalent atoms.
The Bond and Angle Tables may need editting.

The following Atoms are the Symmetry Equivalents

Name	x	y	z			
C(2)a	0.43497	0.88277	0.36451	x	1.500-y	z
C(3)a	0.42875	0.79081	0.47381	x	1.500-y	z
C(4)a	0.56385	0.82428	0.50799	x	1.500-y	z
N(11)a	0.66962	0.85873	0.20556	x	1.500-y	z
N(12)a	0.64138	0.84640	0.08111	x	1.500-y	z

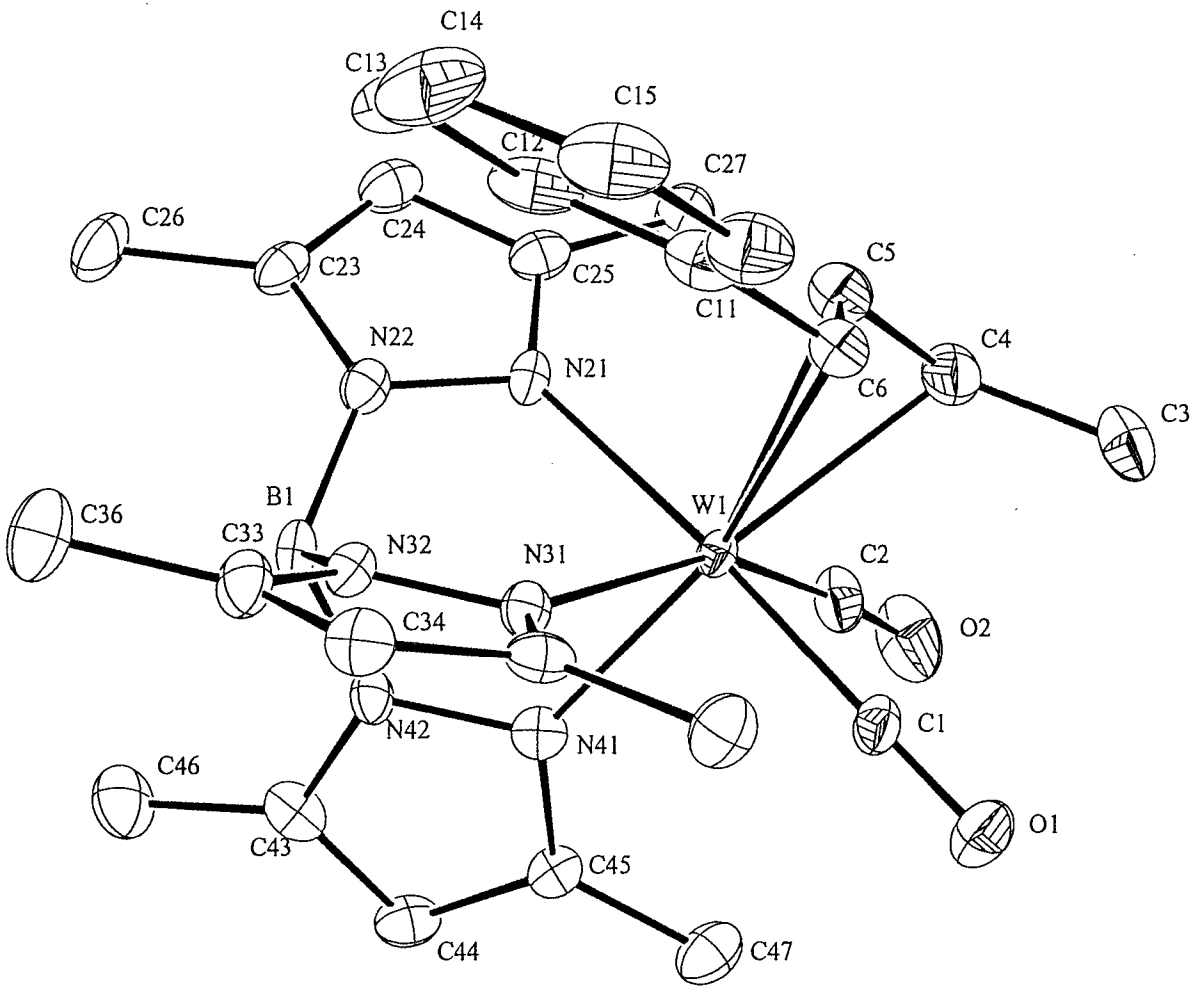
Table of u(i,j) values for Tp'(CO)$_2$W(η^3-*syn*-1-methylallyl) (2s)

	u11(U)	u22	u33	u12	u13	u23
W1	2.089(23)	2.525(22)	1.549(22)	0.0	0.339(15)	0.0
C1	4.1 (7)	3.4 (6)	2.4 (6)	0.0	-0.7 (5)	0.0
O1	4.4 (6)	7.6 (7)	3.7 (5)	0.0	-0.3 (5)	0.0
C2	3.6 (5)	11.1 (10)	3.3 (5)	1.2 (6)	1.4 (4)	2.5 (6)
O2	5.7 (8)	3.3 (6)	3.4 (7)	-1.1 (6)	1.8 (6)	0.6 (5)
C3	10.0 (21)	32. (8)	15. (3)	12. (3)	10.2 (23)	20. (5)
C4	7.1 (18)	21. (4)	12. (3)	7.4 (21)	6.8 (18)	13. (3)
C5	19. (3)	24. (3)	3.1 (10)	0.0	6.3 (15)	0.0
B1	1.9 (6)	3.9 (7)	2.5 (6)	0.0	0.6 (5)	0.0
N11	2.1 (3)	3.0 (3)	2.2 (3)	-0.16(24)	0.62 (24)	0.05(25)
N12	1.9 (3)	3.1 (3)	1.9 (3)	-0.34(24)	0.34 (23)	-0.31(24)
C13	2.5 (4)	3.0 (4)	2.6 (4)	-0.8 (3)	0.7 (3)	-0.4 (3)
C14	4.4 (5)	2.5 (4)	3.8 (5)	0.4 (3)	1.2 (4)	-0.6 (3)
C15	4.1 (5)	2.6 (4)	3.1 (4)	0.5 (3)	0.4 (4)	0.1 (3)
C16	3.9 (5)	5.1 (5)	2.6 (4)	-0.1 (4)	1.2 (3)	-1.0 (4)
C17	8.8 (8)	4.1 (5)	3.1 (5)	2.7 (5)	0.8 (5)	0.6 (4)
N21	1.7 (4)	2.9 (4)	2.9 (5)	0.0	0.8 (4)	0.0
N22	1.7 (4)	3.6 (5)	2.6 (5)	0.0	0.5 (4)	0.0
C23	1.8 (5)	2.5 (5)	3.5 (6)	0.0	-0.4 (5)	0.0
C24	1.6 (5)	3.0 (5)	3.9 (7)	0.0	-0.6 (5)	0.0
C25	1.6 (5)	2.6 (5)	4.1 (7)	0.0	0.9 (5)	0.0
C26	4.2 (7)	3.9 (6)	1.6 (5)	0.0	-0.6 (5)	0.0
C27	2.1 (6)	7.2 (9)	5.6 (9)	0.0	1.8 (6)	0.0
H14	4.6					
H16a	4.9					
H16b	4.9					
H16c	4.9					
H17a	6.3					
H17b	6.3					
H17c	6.3					
H24	3.8					
H26a	4.2					
H26b	4.2					
H27a	6.0					
H27b	6.0					

u(i,j) values listed as u(i,j) x 100

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)

Tp'(CO)$_2$W(η^3-*syn*-1-phenyl-*anti*-3-methylallyl) (7a)



Bond Lengths and Bond Angles for

$Tp'(CO)_2W(\eta^3$-*syn*-1-phenyl-*anti*-3-methylallyl) (7a)

W(1)-C(1)	1.931(6)	B(1)-N(42)	1.544(8)
W(1)-C(2)	1.979(6)	N(21)-N(22)	1.376(6)
W(1)-C(4)	2.422(6)	N(21)-C(25)	1.359(7)
W(1)-C(5)	2.267(6)	N(22)-C(23)	1.353(7)
W(1)-C(6)	2.454(6)	C(23)-C(24)	1.376(8)
W(1)-N(21)	2.309(5)	C(23)-C(26)	1.491(9)
W(1)-N(31)	2.250(5)	C(24)-C(25)	1.400(8)
W(1)-N(41)	2.201(5)	C(25)-C(27)	1.501(9)
C(1)-O(1)	1.169(7)	N(31)-N(32)	1.365(6)
C(2)-O(2)	1.165(8)	N(31)-C(35)	1.345(7)
C(3)-C(4)	1.515(9)	N(32)-C(33)	1.358(7)
C(4)-C(5)	1.432(9)	C(33)-C(34)	1.379(8)
C(5)-C(6)	1.369(9)	C(33)-C(36)	1.484(9)
C(6)-C(11)	1.525(9)	C(34)-C(35)	1.393(8)
C(11)-C(12)	1.388(9)	C(35)-C(37)	1.498(8)
C(11)-C(16)	1.393(9)	N(41)-N(42)	1.392(7)
C(12)-C(13)	1.388(10)	N(41)-C(45)	1.347(7)
C(13)-C(14)	1.409(10)	N(42)-C(43)	1.348(7)
C(14)-C(15)	1.371(11)	C(43)-C(44)	1.381(8)
C(15)-C(16)	1.395(9)	C(43)-C(46)	1.491(9)
B(1)-N(22)	1.547(7)	C(44)-C(45)	1.390(8)
B(1)-N(32)	1.540(8)	C(45)-C(47)	1.494(8)

C(1)-W(1)-C(2)	81.20(24)	C(14)-C(15)-C(16)	121.1(6)
C(1)-W(1)-C(4)	88.47(22)	C(11)-C(16)-C(15)	120.8(6)
C(1)-W(1)-C(5)	104.59(23)	N(22)-B(1)-N(32)	111.0(4)
C(1)-W(1)-C(6)	85.43(22)	N(22)-B(1)-N(42)	107.3(4)
C(1)-W(1)-N(21)	175.39(19)	N(32)-B(1)-N(42)	108.7(4)
C(1)-W(1)-N(31)	90.32(20)	W(1)-N(21)-N(22)	117.9(3)
C(1)-W(1)-N(41)	96.72(21)	W(1)-N(21)-C(25)	135.9(4)
C(2)-W(1)-C(4)	62.49(22)	N(22)-N(21)-C(25)	105.9(4)
C(2)-W(1)-C(5)	96.22(24)	B(1)-N(22)-N(21)	118.8(4)
C(2)-W(1)-C(6)	120.47(22)	B(1)-N(22)-C(23)	128.6(5)
C(2)-W(1)-N(21)	96.60(21)	N(21)-N(22)-C(23)	110.5(4)
C(2)-W(1)-N(31)	156.96(20)	N(22)-C(23)-C(24)	107.8(5)
C(2)-W(1)-N(41)	84.84(21)	N(22)-C(23)-C(26)	122.7(5)
C(4)-W(1)-C(5)	35.36(22)	C(24)-C(23)-C(26)	129.5(5)
C(4)-W(1)-C(6)	59.40(21)	C(23)-C(24)-C(25)	106.3(5)
C(4)-W(1)-N(21)	94.11(19)	N(21)-C(25)-C(24)	109.5(5)
C(4)-W(1)-N(31)	139.10(19)	N(21)-C(25)-C(27)	124.0(5)
C(4)-W(1)-N(41)	145.79(19)	C(24)-C(25)-C(27)	126.3(5)
C(5)-W(1)-C(6)	33.42(21)	W(1)-N(31)-N(32)	119.4(3)
C(5)-W(1)-N(21)	79.63(19)	W(1)-N(31)-C(35)	133.3(4)
C(5)-W(1)-N(31)	106.66(20)	N(32)-N(31)-C(35)	106.4(4)
C(5)-W(1)-N(41)	158.59(19)	B(1)-N(32)-N(31)	119.2(4)
C(6)-W(1)-N(21)	99.18(18)	B(1)-N(32)-C(33)	129.9(5)
C(6)-W(1)-N(31)	79.75(18)	N(31)-N(32)-C(33)	110.0(4)
C(6)-W(1)-N(41)	154.53(19)	N(32)-C(33)-C(34)	107.7(5)
N(21)-W(1)-N(31)	90.22(16)	N(32)-C(33)-C(36)	124.0(5)
N(21)-W(1)-N(41)	79.00(17)	C(34)-C(33)-C(36)	128.3(5)
N(31)-W(1)-N(41)	74.87(17)	C(33)-C(34)-C(35)	105.8(5)
W(1)-C(1)-O(1)	175.5(5)	N(31)-C(35)-C(34)	110.1(5)
W(1)-C(2)-O(2)	173.0(5)	N(31)-C(35)-C(37)	124.2(5)
W(1)-C(4)-C(3)	115.8(4)	C(34)-C(35)-C(37)	125.6(5)
W(1)-C(4)-C(5)	66.4(3)	W(1)-N(41)-N(42)	119.3(3)
C(3)-C(4)-C(5)	125.5(6)	W(1)-N(41)-C(45)	134.7(4)
W(1)-C(5)-C(4)	78.2(3)	N(42)-N(41)-C(45)	105.9(4)
W(1)-C(5)-C(6)	80.8(3)	B(1)-N(42)-N(41)	120.8(4)
C(4)-C(5)-C(6)	119.2(5)	B(1)-N(42)-C(43)	128.6(5)
W(1)-C(6)-C(5)	65.8(3)	N(41)-N(42)-C(43)	110.1(4)
W(1)-C(6)-C(11)	116.1(4)	N(42)-C(43)-C(44)	107.4(5)
C(5)-C(6)-C(11)	120.7(5)	N(42)-C(43)-C(46)	123.6(5)
C(6)-C(11)-C(12)	123.2(5)	C(44)-C(43)-C(46)	128.8(5)
C(6)-C(11)-C(16)	118.6(6)	C(43)-C(44)-C(45)	106.7(5)
C(12)-C(11)-C(16)	118.2(6)	N(41)-C(45)-C(44)	109.9(5)
C(11)-C(12)-C(13)	121.1(5)	N(41)-C(45)-C(47)	123.8(5)
C(12)-C(13)-C(14)	120.3(6)	C(44)-C(45)-C(47)	126.4(5)
C(13)-C(14)-C(15)	118.5(6)		

Atomic Coordinates for $Tp'(CO)_2W(\eta^3$-*syn*-1-phenyl-*anti*-3-methylallyl) (7a)

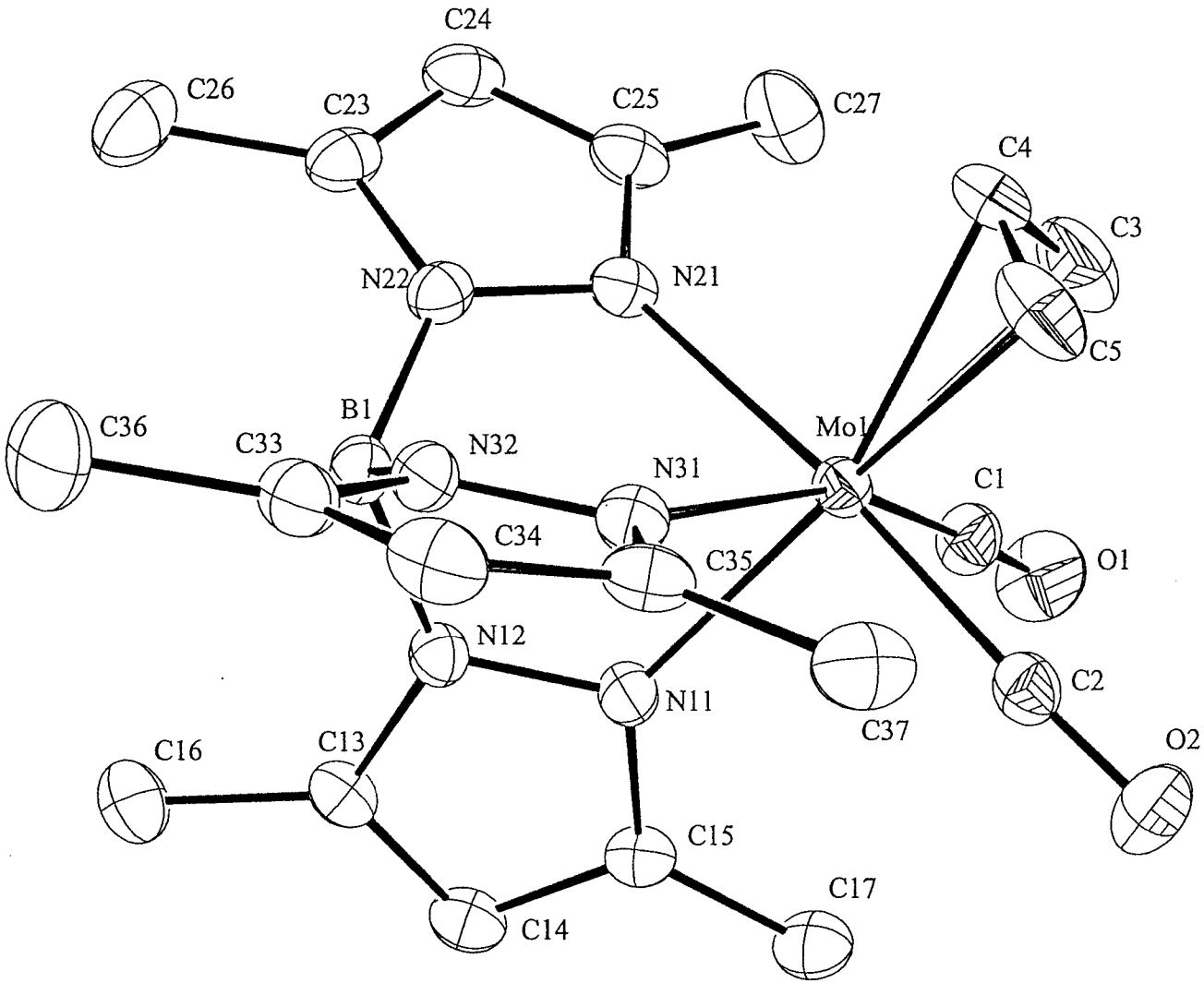
Name	x	y	z
W(1)	0.29208(2)	0.48181(2)	0.22364(1)
C(1)	0.35762(65)	0.68740(59)	0.27828(35)
O(1)	0.40590(53)	0.81461(44)	0.30885(28)
C(2)	0.49500(71)	0.58197(66)	0.18445(39)
O(2)	0.61908(54)	0.65343(58)	0.16859(32)
C(3)	0.32018(77)	0.70228(73)	0.07844(40)
C(4)	0.27471(71)	0.54102(68)	0.07737(40)
C(5)	0.12425(74)	0.42910(67)	0.08832(38)
C(6)	0.04563(72)	0.47079(64)	0.14373(36)
C(11)	-0.11221(69)	0.35399(67)	0.15938(36)
C(12)	-0.15181(67)	0.20549(73)	0.15381(37)
C(13)	-0.29601(78)	0.10376(72)	0.16999(44)
C(14)	-0.40536(73)	0.14996(79)	0.19265(47)
C(15)	-0.36828(73)	0.29550(79)	0.19533(41)
C(16)	-0.22368(73)	0.39729(73)	0.17861(40)
B(1)	0.19709(76)	0.19203(67)	0.31873(41)
N(21)	0.23254(52)	0.23887(47)	0.16558(29)
N(22)	0.16936(53)	0.13542(49)	0.21590(29)
C(23)	0.12576(65)	-0.00357(59)	0.16865(37)
C(24)	0.16231(69)	0.00851(62)	0.08611(38)
C(25)	0.22966(65)	0.16069(62)	0.08600(36)
C(26)	0.05526(78)	-0.13859(63)	0.20626(43)
C(27)	0.29909(81)	0.23141(70)	0.01302(39)
N(31)	0.13542(53)	0.40262(48)	0.32082(28)
N(32)	0.09420(52)	0.26559(47)	0.33827(28)
C(33)	-0.02236(66)	0.22780(62)	0.38495(36)
C(34)	-0.05462(66)	0.34473(63)	0.39966(36)
C(35)	0.04673(64)	0.45183(61)	0.35948(33)
C(36)	-0.10237(75)	0.08147(69)	0.40940(44)
C(37)	0.06256(70)	0.60340(63)	0.36241(37)
N(41)	0.43870(53)	0.44922(50)	0.33267(28)
N(42)	0.37693(53)	0.31109(48)	0.35527(28)
C(43)	0.48922(68)	0.31048(65)	0.41840(35)
C(44)	0.62517(66)	0.45015(64)	0.43869(37)
C(45)	0.58996(63)	0.53306(59)	0.38477(35)
C(46)	0.46593(79)	0.17561(73)	0.45211(42)
C(47)	0.70056(72)	0.69118(68)	0.38261(42)
H(1)	0.17100(0)	0.11032(0)	0.34764(0)
H(3a)	0.43545(0)	0.76339(0)	0.09447(0)
H(3b)	0.27580(0)	0.73752(0)	0.12185(0)
H(3c)	0.27810(0)	0.70810(0)	0.01960(0)
H(4)	0.35278(0)	0.51079(0)	0.06783(0)
H(5)	0.07905(0)	0.32595(0)	0.05744(0)
H(6)	0.09062(0)	0.57467(0)	0.17291(0)
H(12)	-0.07835(0)	0.17343(0)	0.13726(0)
H(13)	-0.32018(0)	0.00199(0)	0.16670(0)
H(14)	-0.50405(0)	0.08095(0)	0.20545(0)
H(15)	-0.44261(0)	0.32812(0)	0.20941(0)
H(16)	-0.20007(0)	0.49841(0)	0.17978(0)
H(24)	0.14488(0)	-0.07152(0)	0.03815(0)
H(26a)	0.01204(0)	-0.22735(0)	0.15865(0)
H(26b)	-0.02927(0)	-0.14005(0)	0.23298(0)
H(26c)	0.13761(0)	-0.13530(0)	0.25138(0)
H(27a)	0.32669(0)	0.16722(0)	-0.02300(0)
H(27b)	0.39401(0)	0.32676(0)	0.03981(0)
H(27c)	0.22081(0)	0.24545(0)	-0.02446(0)
H(34)	-0.13018(0)	0.35161(0)	0.43169(0)
H(36a)	-0.17001(0)	0.08427(0)	0.44875(0)
H(36b)	-0.02196(0)	0.06213(0)	0.43963(0)
H(36c)	-0.16678(0)	0.00333(0)	0.35564(0)
H(37a)	-0.02253(0)	0.60835(0)	0.38559(0)
H(37b)	0.05556(0)	0.62009(0)	0.30263(0)
H(37c)	0.16485(0)	0.67894(0)	0.40100(0)
H(44)	0.72442(0)	0.48335(0)	0.48190(0)
H(46a)	0.54570(0)	0.20568(0)	0.50718(0)
H(46b)	0.47679(0)	0.10806(0)	0.40764(0)
H(46c)	0.36033(0)	0.12624(0)	0.46320(0)
H(47a)	0.77886(0)	0.74251(0)	0.43937(0)
H(47b)	0.63926(0)	0.74121(0)	0.37205(0)
H(47c)	0.75461(0)	0.69140(0)	0.33498(0)

Table of u(i,j) values for $Tp'(CO)_2W(\eta^3$-*syn*-1-phenyl-*anti*-3-methylallyl) (7a)

	u11(U)	u22	u33	u12	u13	u23
W1	1.127(14)	1.067(14)	1.618(14)	0.423(10)	0.403(8)	0.412(8)
C1	1.6 (3)	1.5 (3)	2.3 (3)	0.59 (23)	0.48 (22)	0.72 (22)
O1	3.5 (3)	1.79 (22)	3.39 (23)	1.18 (20)	0.25 (19)	0.26 (18)
C2	2.2 (3)	2.6 (3)	3.0 (3)	1.3 (3)	0.76 (25)	1.4 (3)
O2	2.5 (3)	5.6 (3)	5.0 (3)	1.60 (24)	1.94 (22)	3.27 (25)
C3	3.2 (4)	3.6 (4)	2.9 (3)	1.9 (3)	1.1 (3)	2.0 (3)
C4	2.0 (3)	2.8 (3)	3.2 (3)	0.8 (3)	-0.01 (25)	1.1 (3)
C5	2.5 (3)	2.7 (3)	2.5 (3)	1.3 (3)	0.26 (24)	0.61 (24)
C6	2.7 (3)	2.2 (3)	2.0 (3)	1.1 (3)	0.07 (23)	0.51 (22)
C11	2.0 (3)	3.2 (3)	1.9 (3)	1.2 (3)	0.25 (22)	0.39 (24)
C12	1.6 (3)	4.4 (4)	2.0 (3)	1.7 (3)	0.03 (23)	-0.3 (3)
C13	2.6 (3)	2.9 (3)	3.7 (4)	0.9 (3)	-0.4 (3)	-0.8 (3)
C14	1.3 (3)	3.9 (4)	4.6 (4)	0.2 (3)	0.4 (3)	-0.1 (3)
C15	1.8 (3)	4.8 (4)	3.0 (3)	1.7 (3)	0.28 (25)	-0.1 (3)
C16	2.2 (3)	3.5 (3)	2.8 (3)	1.3 (3)	0.26 (25)	0.4 (3)
B1	2.1 (3)	1.4 (3)	2.3 (3)	0.9 (3)	0.8 (3)	0.99 (24)
N21	1.51 (23)	1.36 (22)	2.21 (23)	0.70 (19)	0.67 (18)	0.76 (18)
N22	1.67 (24)	1.57 (23)	2.31 (24)	0.92 (20)	0.47 (18)	0.54 (18)
C23	1.6 (3)	1.4 (3)	2.9 (3)	0.78 (23)	0.05 (22)	0.21 (22)
C24	2.2 (3)	2.0 (3)	2.8 (3)	1.1 (3)	0.21 (24)	-0.11 (23)
C25	1.5 (3)	2.2 (3)	2.5 (3)	0.83 (24)	0.20 (22)	0.09 (23)
C26	3.3 (4)	1.3 (3)	4.1 (4)	0.8 (3)	0.6 (3)	0.6 (3)
C27	4.1 (4)	2.7 (3)	2.3 (3)	1.5 (3)	1.4 (3)	0.54 (24)
N31	1.62 (23)	1.56 (22)	1.86 (22)	0.93 (19)	0.45 (18)	0.54 (17)
N32	1.52 (23)	1.35 (22)	1.94 (22)	0.57 (19)	0.39 (18)	0.37 (17)
C33	1.7 (3)	2.0 (3)	2.5 (3)	0.64 (24)	0.69 (22)	0.90 (22)
C34	1.6 (3)	2.5 (3)	2.3 (3)	0.98 (24)	0.76 (22)	0.52 (22)
C35	1.6 (3)	2.2 (3)	1.56 (25)	1.15 (24)	0.03 (21)	-0.05 (21)
C36	2.5 (3)	2.6 (3)	4.5 (4)	1.0 (3)	1.7 (3)	1.6 (3)
C37	2.5 (3)	2.0 (3)	2.7 (3)	1.3 (3)	0.98 (24)	0.43 (23)
N41	1.56 (23)	2.10 (24)	1.91 (22)	0.96 (20)	0.48 (18)	0.34 (18)
N42	1.83 (24)	1.68 (23)	1.97 (22)	1.07 (20)	0.43 (18)	0.79 (18)
C43	2.3 (3)	3.2 (3)	2.0 (3)	2.0 (3)	0.69 (23)	0.68 (23)
C44	1.5 (3)	2.6 (3)	2.5 (3)	1.05 (25)	-0.09 (22)	-0.03 (23)
C45	1.4 (3)	1.8 (3)	2.1 (3)	0.80 (23)	0.52 (21)	0.29 (21)
C46	3.2 (4)	3.6 (4)	3.6 (3)	2.1 (3)	0.6 (3)	1.6 (3)
C47	1.9 (3)	2.3 (3)	3.7 (3)	0.7 (3)	0.2 (3)	0.2 (3)
H1	3.0					
H3a	4.2					
H3b	4.2					
H3c	4.2					
H4	3.7					
H5	3.6					
H6	3.3					
H12	3.7					
H13	4.1					
H14	4.3					
H15	4.2					
H16	3.8					
H24	3.3					
H26a	3.9					
H26b	3.9					
H26c	3.9					
H27a	4.0					
H27b	4.0					
H27c	4.0					
H34	3.1					
H36a	4.2					
H36b	4.2					
H36c	4.2					
H37a	3.4					
H37b	3.4					
H37c	3.4					
H44	3.2					
H46a	4.4					
H46b	4.4					
H46c	4.4					
H47a	3.6					
H47b	3.6					
H47c	3.6					

u(i,j) values listed as u(i,j) x 100

$Tp'(CO)_2Mo(\eta^3\text{-}C_3H_5)$ (9)



Bond Lengths and Bond Angles for $Tp'(CO)_2Mo(\eta^3\text{-allyl})$ (9)

Mo(1)-C(1)	1.961(4)	C(13)-C(14)	1.376(6)
Mo(1)-C(2)	1.930(4)	C(13)-C(16)	1.491(6)
Mo(1)-C(3)	2.370(5)	C(14)-C(15)	1.390(6)
Mo(1)-C(4)	2.245(4)	C(15)-C(17)	1.493(6)
Mo(1)-C(5)	2.363(4)	N(21)-N(22)	1.372(5)
Mo(1)-N(11)	2.215(3)	N(21)-C(25)	1.354(5)
Mo(1)-N(21)	2.340(3)	N(22)-C(23)	1.350(5)
Mo(1)-N(31)	2.289(3)	C(23)-C(24)	1.360(7)
C(1)-O(1)	1.158(5)	C(23)-C(26)	1.493(7)
C(2)-O(2)	1.159(5)	C(24)-C(25)	1.388(7)
C(3)-C(4)	1.393(9)	C(25)-C(27)	1.487(7)
C(4)-C(5)	1.379(8)	N(31)-N(32)	1.384(4)
B(1)-N(12)	1.563(5)	N(31)-C(35)	1.348(5)
B(1)-N(22)	1.538(6)	N(32)-C(33)	1.346(5)
B(1)-N(32)	1.526(5)	C(33)-C(34)	1.383(6)
N(11)-N(12)	1.380(4)	C(33)-C(36)	1.489(7)
N(11)-C(15)	1.348(5)	C(34)-C(35)	1.372(6)
N(12)-C(13)	1.344(5)	C(35)-C(37)	1.493(6)

C(1)-Mo(1)-C(2)	80.73(17)	Mo(1)-N(11)-C(15)	133.9(3)
C(1)-Mo(1)-C(3)	64.36(21)	N(12)-N(11)-C(15)	106.5(3)
C(1)-Mo(1)-C(4)	99.35(19)	B(1)-N(12)-N(11)	120.9(3)
C(1)-Mo(1)-C(5)	115.32(18)	B(1)-N(12)-C(13)	129.1(3)
C(1)-Mo(1)-N(11)	87.08(15)	N(11)-N(12)-C(13)	109.8(3)
C(1)-Mo(1)-N(21)	94.89(15)	N(12)-C(13)-C(14)	107.8(3)
C(1)-Mo(1)-N(31)	162.25(15)	N(12)-C(13)-C(16)	123.7(4)
C(2)-Mo(1)-C(3)	94.80(18)	C(14)-C(13)-C(16)	128.5(4)
C(2)-Mo(1)-C(4)	102.65(17)	C(13)-C(14)-C(15)	106.6(3)
C(2)-Mo(1)-C(5)	75.45(18)	N(11)-C(15)-C(14)	109.2(3)
C(2)-Mo(1)-N(11)	95.36(14)	N(11)-C(15)-C(17)	123.8(4)
C(2)-Mo(1)-N(21)	172.81(14)	C(14)-C(15)-C(17)	127.0(3)
C(2)-Mo(1)-N(31)	92.89(14)	Mo(1)-N(21)-N(22)	116.76(22)
C(3)-Mo(1)-C(4)	35.01(22)	Mo(1)-N(21)-C(25)	137.4(3)
C(3)-Mo(1)-C(5)	59.09(19)	N(22)-N(21)-C(25)	105.6(3)
C(3)-Mo(1)-N(11)	147.57(16)	B(1)-N(22)-N(21)	120.0(3)
C(3)-Mo(1)-N(21)	88.36(16)	B(1)-N(22)-C(23)	128.3(3)
C(3)-Mo(1)-N(31)	133.06(18)	N(21)-N(22)-C(23)	110.4(3)
C(4)-Mo(1)-C(5)	34.70(20)	N(22)-C(23)-C(24)	107.5(4)
C(4)-Mo(1)-N(11)	161.62(15)	N(22)-C(23)-C(26)	123.5(4)
C(4)-Mo(1)-N(21)	83.63(15)	C(24)-C(23)-C(26)	129.0(4)
C(4)-Mo(1)-N(31)	98.21(17)	C(23)-C(24)-C(25)	106.9(4)
C(5)-Mo(1)-N(11)	153.30(15)	N(21)-C(25)-C(24)	109.5(4)
C(5)-Mo(1)-N(21)	111.67(16)	N(21)-C(25)-C(27)	124.5(4)
C(5)-Mo(1)-N(31)	78.49(15)	C(24)-C(25)-C(27)	126.0(4)
N(11)-Mo(1)-N(21)	78.64(11)	Mo(1)-N(31)-N(32)	118.47(21)
N(11)-Mo(1)-N(31)	76.98(11)	Mo(1)-N(31)-C(35)	135.9(3)
N(21)-Mo(1)-N(31)	89.64(11)	N(32)-N(31)-C(35)	105.6(3)
Mo(1)-C(1)-O(1)	175.4(4)	B(1)-N(32)-N(31)	119.5(3)
Mo(1)-C(2)-O(2)	175.3(3)	B(1)-N(32)-C(33)	128.5(3)
Mo(1)-C(3)-C(4)	67.6(3)	N(31)-N(32)-C(33)	110.1(3)
Mo(1)-C(4)-C(3)	77.4(3)	N(32)-C(33)-C(34)	107.3(4)
Mo(1)-C(4)-C(5)	77.3(3)	N(32)-C(33)-C(36)	123.8(4)
C(3)-C(4)-C(5)	114.7(5)	C(34)-C(33)-C(36)	128.9(4)
Mo(1)-C(5)-C(4)	67.97(25)	C(33)-C(34)-C(35)	106.7(3)
N(12)-B(1)-N(22)	108.6(3)	N(31)-C(35)-C(34)	110.3(4)
N(12)-B(1)-N(32)	108.1(3)	N(31)-C(35)-C(37)	124.8(4)
N(22)-B(1)-N(32)	112.4(3)	C(34)-C(35)-C(37)	124.9(4)
Mo(1)-N(11)-N(12)	119.58(21)		

Atomic Coordinates for Tp'(CO)$_2$Mo(η^3-allyl) (9)

	x	y	z	Biso
Mo1	0.72492(3)	0.54446(3)	0.24207(3)	2.431(16)
C1	0.7311 (4)	0.5572 (4)	0.4198 (4)	3.52 (21)
O1	0.7402 (4)	0.5589 (4)	0.5227 (3)	5.79 (24)
C2	0.8135 (4)	0.4042 (4)	0.2257 (4)	2.95 (18)
O2	0.8611 (4)	0.3179 (3)	0.2216 (3)	4.57 (18)
C3	0.5160 (5)	0.4272 (5)	0.2775 (6)	5.5 (3)
C4	0.5023 (4)	0.4186 (5)	0.1511 (6)	4.5 (3)
C5	0.5721 (5)	0.3372 (5)	0.0699 (5)	4.84 (24)
B1	0.8249 (5)	0.8165 (4)	0.1789 (4)	2.83 (20)
N11	0.9188 (3)	0.7206 (3)	0.3268 (3)	2.63 (14)
N12	0.9360 (3)	0.8253 (3)	0.2883 (3)	2.59 (14)
C13	1.0604 (4)	0.9205 (4)	0.3505 (4)	2.92 (17)
C14	1.1255 (4)	0.8784 (4)	0.4310 (4)	3.31 (19)
C15	1.0354 (4)	0.7536 (4)	0.4141 (3)	2.86 (19)
C16	1.1140 (5)	1.0448 (5)	0.3277 (5)	4.22 (23)
C17	1.0595 (4)	0.6665 (5)	0.4797 (4)	3.83 (23)
N21	0.6393 (3)	0.7331 (3)	0.2855 (3)	2.98 (16)
N22	0.6889 (3)	0.8177 (3)	0.2286 (3)	2.84 (15)
C23	0.6189 (4)	0.9113 (4)	0.2483 (4)	3.40 (19)
C24	0.5247 (4)	0.8899 (4)	0.3213 (5)	3.95 (21)
C25	0.5402 (4)	0.7808 (4)	0.3456 (4)	3.70 (21)
C26	0.6456 (6)	1.0155 (5)	0.1952 (5)	5.1 (3)
C27	0.4642 (6)	0.7260 (5)	0.4280 (6)	5.6 (3)
N31	0.7899 (3)	0.5596 (3)	0.0595 (3)	2.74 (15)
N32	0.8088 (3)	0.6844 (3)	0.0532 (3)	2.76 (15)
C33	0.8418 (4)	0.6725 (4)	-0.0624 (4)	3.27 (20)
C34	0.8442 (4)	0.5376 (5)	-0.1330 (4)	3.59 (22)
C35	0.8157 (4)	0.4727 (4)	-0.0541 (4)	3.07 (19)
C36	0.8658 (6)	0.7870 (6)	-0.1020 (5)	4.9 (3)
C37	0.8198 (5)	0.3289 (5)	-0.0864 (4)	3.92 (22)
H3a	0.457	0.465	0.335	6.0
H3b	0.559	0.373	0.306	6.0
H4	0.422	0.443	0.129	5.1
H5a	0.570	0.323	-0.020	4.9
H5b	0.583	0.273	0.103	4.9
H1	0.857	0.896	0.162	3.7
H14	1.215	0.927	0.488	3.7
H16a	1.193	1.109	0.397	4.8
H16b	1.043	1.089	0.328	4.8
H16c	1.141	1.017	0.244	4.8
H17a	1.158	0.686	0.506	4.6
H17b	1.019	0.570	0.420	4.6
H17c	1.019	0.689	0.557	4.6
H24	0.459	0.939	0.350	4.4
H26a	0.574	1.059	0.205	6.1
H26b	0.647	0.968	0.103	6.1
H26c	0.733	1.085	0.242	6.1
H27a	0.425	0.794	0.484	6.4
H27b	0.527	0.708	0.482	6.4
H27c	0.392	0.642	0.372	6.4
H34	0.863	0.497	-0.220	4.3
H36a	0.874	0.752	-0.193	6.2
H36b	0.950	0.858	-0.047	6.2
H36c	0.790	0.825	-0.091	6.2
H37a	0.886	0.307	-0.141	4.3
H37b	0.730	0.264	-0.133	4.3
H37c	0.846	0.322	-0.007	4.3

Biso is the Mean of the Principal Axes of the Thermal Ellipsoid

Table of u(i,j) values for Tp'$(CO)_2$Mo(η^3-allyl) (9)

	u11(U)	u22	u33	u12	u13	u23
Mo1	2.837(20)	3.240(21)	3.194(20)	0.707(13)	0.649(12)	1.585(14)
C1	5.0 (3)	5.05 (24)	4.57 (24)	2.03 (20)	1.97 (19)	2.85 (20)
O1	8.9 (3)	10.6 (3)	5.45 (21)	4.12 (23)	3.20 (19)	5.31 (21)
C2	3.74 (21)	4.11 (21)	3.49 (20)	0.90 (17)	0.94 (16)	1.94 (17)
O2	7.16 (22)	5.56 (19)	6.54 (21)	3.48 (17)	2.05 (17)	3.51 (17)
C3	5.4 (3)	5.4 (3)	9.2 (4)	0.75 (23)	3.8 (3)	2.5 (3)
C4	2.66 (21)	5.4 (3)	8.4 (4)	-0.23 (19)	-0.11 (22)	3.3 (3)
C5	4.9 (3)	5.5 (3)	5.4 (3)	-1.27 (22)	0.41 (22)	1.66 (23)
B1	3.71 (23)	3.59 (22)	3.62 (22)	0.85 (18)	0.56 (18)	1.95 (19)
N11	3.28 (16)	3.56 (16)	3.03 (15)	0.71 (13)	0.38 (13)	1.60 (13)
N12	3.36 (17)	3.30 (16)	3.13 (15)	0.77 (13)	0.60 (13)	1.53 (13)
C13	3.41 (20)	3.47 (19)	3.23 (19)	0.51 (16)	0.76 (16)	0.85 (16)
C14	3.34 (20)	4.76 (23)	3.13 (19)	0.68 (17)	0.12 (16)	0.89 (17)
C15	3.41 (20)	4.59 (22)	2.62 (18)	1.34 (17)	0.52 (15)	1.33 (16)
C16	5.1 (3)	4.17 (23)	5.9 (3)	0.11 (20)	0.90 (21)	2.20 (21)
C17	4.32 (24)	6.2 (3)	3.85 (22)	1.67 (20)	0.06 (18)	2.18 (20)
N21	3.02 (17)	4.00 (18)	4.07 (18)	1.05 (14)	0.71 (14)	1.59 (15)
N22	3.53 (17)	3.47 (16)	3.50 (17)	1.06 (14)	0.16 (13)	1.39 (13)
C23	4.12 (23)	3.54 (20)	4.33 (22)	1.34 (17)	-0.30 (18)	1.03 (17)
C24	3.71 (23)	4.16 (23)	5.9 (3)	1.76 (18)	0.47 (20)	0.86 (20)
C25	3.36 (21)	4.56 (23)	4.85 (24)	1.22 (18)	1.00 (18)	0.88 (19)
C26	7.5 (4)	5.4 (3)	7.2 (3)	3.0 (3)	0.5 (3)	3.16 (25)
C27	6.6 (3)	5.7 (3)	8.9 (4)	2.3 (3)	4.6 (3)	2.6 (3)
N31	3.33 (17)	3.61 (16)	3.02 (16)	0.88 (13)	0.35 (13)	1.24 (13)
N32	3.51 (17)	4.00 (17)	3.19 (16)	0.96 (14)	0.55 (13)	1.94 (14)
C33	3.53 (21)	5.55 (25)	3.62 (21)	0.91 (18)	0.71 (16)	2.56 (19)
C34	3.94 (22)	6.2 (3)	3.04 (20)	1.28 (19)	1.02 (17)	1.68 (19)
C35	2.74 (19)	4.72 (22)	3.18 (19)	1.03 (17)	0.22 (15)	0.96 (17)
C36	7.3 (3)	8.0 (3)	5.2 (3)	2.0 (3)	2.04 (24)	4.5 (3)
C37	4.47 (25)	4.78 (24)	4.24 (24)	1.55 (20)	0.32 (19)	0.73 (19)
H3a	7.7					
H3b	7.7					
H4	6.5					
H5a	6.3					
H5b	6.3					
H1	4.6					
H14	4.7					
H16a	6.1					
H16b	6.1					
H16c	6.1					
H17a	5.8					
H17b	5.8					
H17c	5.8					
H24	5.6					
H26a	7.7					
H26b	7.7					
H26c	7.7					
H27a	8.1					
H27b	8.1					
H27c	8.1					
H34	5.4					
H36a	7.8					
H36b	7.8					
H36c	7.8					
H37a	5.5					
H37b	5.5					
H37c	5.5					

u(i,j) values listed as u(i,j) x 100

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)