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Figure 1. Labeled ORTEP Diagram of $Tp(CO)_2Re(\mu\text{-}N_2)Re(CO)_2Tp$ (**9**)

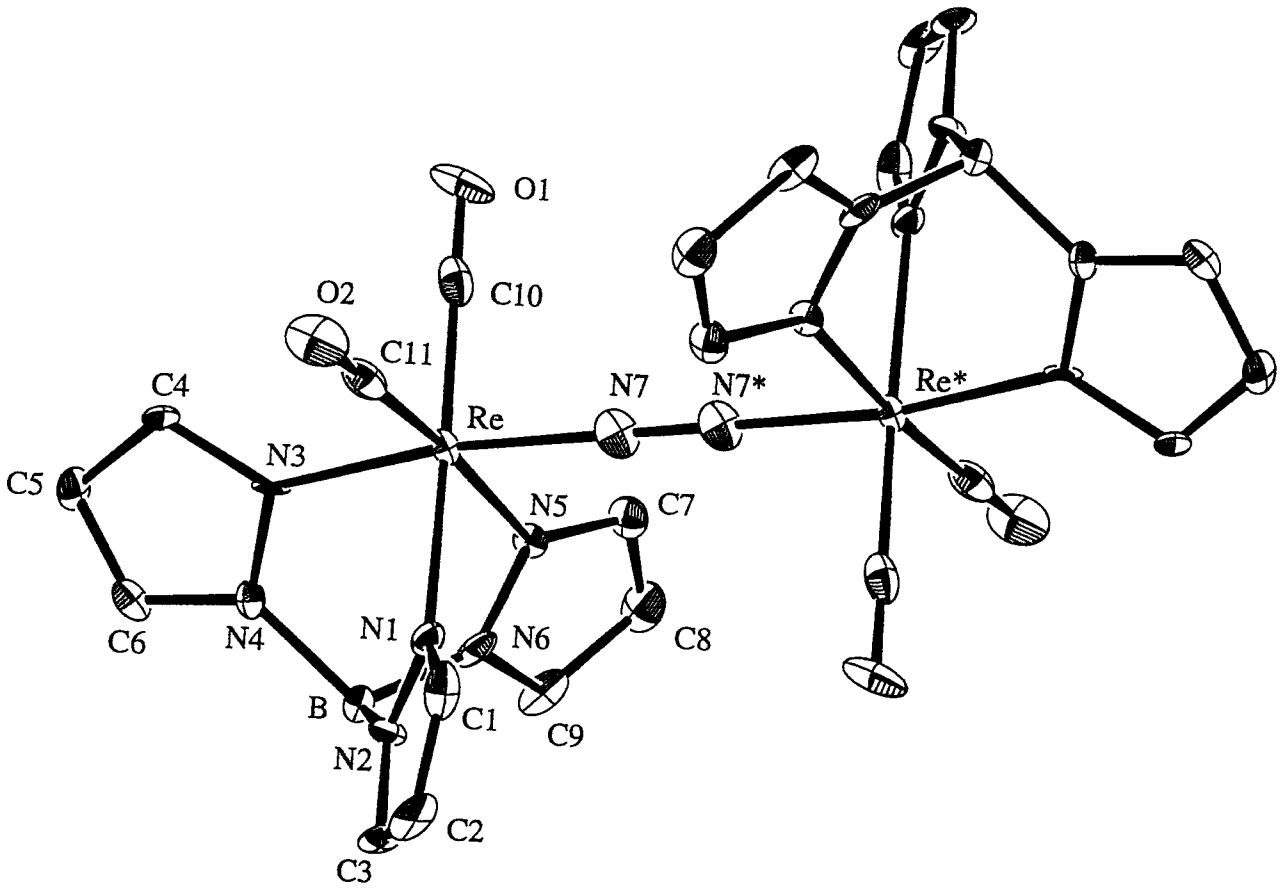


Table I. Crystallographic Data

Empirical Formula	$C_{23}H_{20}N_{14}O_4B_2Cl_2Re_2$
Formula Weight	1021.44
Crystal Color and Habit	brown prism
Crystal Dimensions	0.28 x 0.31 x 0.43 mm
Crystal System	monoclinic
Lattice Parameters	a = 7.675(2) Å
	b = 13.090(4) Å
	c = 16.567(6) Å
	$\beta = 96.80(3)^o$
	$V = 1653(1)$ Å^3
Space Group	$P2_1/c$ (No.14)
Z	2
D_{calc}	2.05 gcm^{-3}
Radiation	MoKa (λ = 0.71069 Å)
μ(MoKα)	75.36 cm^{-1}
Absorption Corrections	ψ scans (transmission factors 0.53 - 1.00)
Temperature	-100^{o}C
$2\theta_{max}$	46^o
No.of Reflections Measured	Total: 2683 Unique: 2427 (R_{int}=0.038)
No.of Reflections (I>3σ(I)	1746
No.of Variables	208

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Residuals R; R_w	0.040; 0.054
Goodness of Fit	1.75
Maximum Peak in Final Diff. Map	1.65 e/A^3

Table II. Positional Parameters

atom	x	y	z
Re	0.41493(7)	0.12971(4)	0.60348(3)
Cl(1)	0.1613(8)	0.4512(5)	0.4890(4)
O(1)	0.058(1)	0.1642(9)	0.5047(6)
O(2)	0.567(1)	0.3118(8)	0.5197(7)
N(1)	0.660(1)	0.1048(7)	0.6812(7)
N(2)	0.660(1)	0.0868(8)	0.7610(6)
N(3)	0.348(1)	0.2162(7)	0.7033(6)
N(4)	0.391(1)	0.1838(7)	0.7801(6)
N(5)	0.333(1)	0.0013(7)	0.6708(6)
N(6)	0.376(1)	-0.0042(8)	0.7544(7)
N(7)	0.484(2)	0.0308(9)	0.5228(7)
C(1)	0.829(2)	0.110(1)	0.6670(10)
C(2)	0.937(2)	0.093(1)	0.738(1)
C(3)	0.829(2)	0.0789(10)	0.7944(9)
C(4)	0.263(2)	0.3078(9)	0.7078(8)
C(5)	0.253(2)	0.3299(10)	0.7890(8)
C(6)	0.333(2)	0.2527(10)	0.8320(8)
C(7)	0.235(2)	-0.081(1)	0.6520(9)
C(8)	0.222(2)	-0.140(1)	0.717(1)
C(9)	0.313(2)	-0.0895(10)	0.7836(9)
C(10)	0.193(2)	0.1522(10)	0.5409(9)
C(11)	0.506(2)	0.244(1)	0.5516(8)
C(12)	0.061(4)	0.587(2)	0.478(2)
B	0.489(2)	0.079(1)	0.7973(9)

Table III. Anisotropic Thermal Displacement Parameters

atom	U11	U22	U33	U12	U13	U23
Re	0.0217(4)	0.0222(3)	0.0211(4)	-0.0039(3)	0.0031(2)	-0.0059(2)
O(1)	0.044(8)	0.084(8)	0.033(6)	-0.015(7)	-0.020(6)	0.004(6)
O(2)	0.059(8)	0.058(7)	0.047(7)	-0.028(6)	0.003(6)	0.019(6)
N(1)	0.019(6)	0.020(6)	0.036(7)	0.004(5)	-0.002(5)	-0.002(5)
N(2)	0.023(6)	0.028(6)	0.017(6)	0.000(5)	-0.006(5)	0.000(5)
N(3)	0.025(6)	0.025(6)	0.008(6)	0.003(5)	-0.007(4)	0.008(4)
N(4)	0.019(6)	0.018(5)	0.024(6)	-0.004(5)	0.008(5)	-0.005(5)
N(5)	0.005(5)	0.023(6)	0.032(7)	-0.007(4)	0.000(5)	-0.002(5)
N(6)	0.016(6)	0.022(6)	0.046(8)	0.010(5)	0.002(5)	0.006(5)
N(7)	0.038(7)	0.044(8)	0.031(8)	-0.009(7)	0.014(6)	-0.003(5)
C(1)	0.026(8)	0.030(8)	0.06(1)	-0.006(7)	0.025(8)	-0.014(7)
C(2)	0.006(7)	0.037(8)	0.08(1)	0.011(6)	0.002(8)	-0.003(8)
C(3)	0.014(7)	0.028(7)	0.047(10)	0.002(6)	-0.014(7)	0.006(6)
C(4)	0.020(8)	0.026(7)	0.030(9)	0.008(6)	-0.013(6)	-0.001(6)
C(5)	0.016(8)	0.031(7)	0.043(9)	0.007(6)	0.005(7)	-0.015(7)
C(6)	0.025(8)	0.035(8)	0.023(8)	-0.008(6)	0.003(6)	-0.007(6)
C(7)	0.021(8)	0.032(8)	0.043(9)	-0.005(6)	0.000(6)	-0.007(7)
C(8)	0.028(9)	0.030(8)	0.07(1)	-0.007(7)	0.001(8)	-0.003(8)
C(9)	0.009(7)	0.028(8)	0.06(1)	0.000(6)	0.019(7)	0.017(7)
C(10)	0.05(1)	0.026(8)	0.029(8)	-0.012(7)	0.012(8)	-0.005(6)
C(11)	0.022(8)	0.048(9)	0.031(9)	-0.008(7)	-0.002(6)	-0.008(7)
B	0.031(9)	0.019(8)	0.028(9)	0.003(7)	0.002(7)	-0.002(6)

Table IV. Bond Lengths (A)

Re	N(1)	2.17(1)	N(4)	C(6)	1.36(2)
Re	N(3)	2.12(1)	N(4)	B	1.57(2)
Re	N(5)	2.15(1)	N(5)	N(6)	1.39(1)
Re	N(7)	1.98(1)	N(5)	C(7)	1.33(2)
Re	C(10)	1.91(2)	N(6)	C(9)	1.33(2)
Re	C(11)	1.90(2)	N(6)	B	1.52(2)
O(1)	C(10)	1.15(2)	N(7)	N(7)	1.15(2)
O(2)	C(11)	1.16(2)	C(1)	C(2)	1.37(2)
N(1)	N(2)	1.34(1)	C(2)	C(3)	1.34(2)
N(1)	C(1)	1.35(2)	C(4)	C(5)	1.39(2)
N(2)	C(3)	1.35(2)	C(5)	C(6)	1.34(2)
N(2)	B	1.51(2)	C(7)	C(8)	1.35(2)
N(3)	N(4)	1.35(1)	C(8)	C(9)	1.40(2)
N(3)	C(4)	1.37(2)			

Table V. Bond Angles (deg)

N(1)	Re	N(3)	83.7(4)	N(3)	N(4)	C(6)	109(1)
N(1)	Re	N(5)	82.0(4)	N(3)	N(4)	B	120(1)
N(1)	Re	N(7)	91.2(5)	C(6)	N(4)	B	131(1)
N(1)	Re	C(10)	176.7(5)	Re	N(5)	N(6)	120.5(7)
N(1)	Re	C(11)	92.7(5)	Re	N(5)	C(7)	135(1)
N(3)	Re	N(5)	84.3(4)	N(6)	N(5)	C(7)	105(1)
N(3)	Re	N(7)	170.8(4)	N(5)	N(6)	C(9)	111(1)
N(3)	Re	C(10)	93.4(5)	N(5)	N(6)	B	119(1)
N(3)	Re	C(11)	93.9(5)	C(9)	N(6)	B	130(1)
N(5)	Re	N(7)	87.5(4)	Re	N(7)	N(7)	176(1)
N(5)	Re	C(10)	96.2(5)	N(1)	C(1)	C(2)	110(1)
N(5)	Re	C(11)	174.5(5)	C(1)	C(2)	C(3)	105(1)
N(7)	Re	C(10)	91.5(6)	N(2)	C(3)	C(2)	110(1)
N(7)	Re	C(11)	93.9(6)	N(3)	C(4)	C(5)	108(1)
C(10)	Re	C(11)	89.1(6)	C(4)	C(5)	C(6)	106(1)
C(12)	Cl(1)	C(12)	85(1)	N(4)	C(6)	C(5)	109(1)
Re	N(1)	N(2)	120.7(8)	N(5)	C(7)	C(8)	112(1)
Re	N(1)	C(1)	132(1)	C(7)	C(8)	C(9)	106(1)
N(2)	N(1)	C(1)	107(1)	N(6)	C(9)	C(8)	106(1)
N(1)	N(2)	C(3)	108(1)	Re	C(10)	O(1)	178(1)
N(1)	N(2)	B	120(1)	Re	C(11)	O(2)	177(1)
C(3)	N(2)	B	132(1)	Cl(1)	C(12)	Cl(1)	95(1)
Re	N(3)	N(4)	121.1(7)	N(2)	B	N(4)	107(1)
Re	N(3)	C(4)	132.2(8)	N(2)	B	N(6)	109(1)
N(4)	N(3)	C(4)	107(1)	N(4)	B	N(6)	108(1)