

**Table 1** Selected Distances, Angles, and Torsions for **1**

Selected Distances (Å)	
Re(1)-C(16)	1.89(1)
Re(1)-C(17)	1.934(8)
Re(1)-C(18)	1.90(1)
Re(1)-N(1)	2.162(6)
Re(1)-N(2)	2.236(9)
Re(1)-Cl(1)	2.496(2)
Selected Angles (deg)	
C(16)-Re(1)-C(17)	87.6(4)
C(16)-Re(1)-C(18)	88.3(4)
C(17)-Re(1)-C(18)	87.3(4)
C(16)-Re(1)-N(1)	96.4(3)
C(17)-Re(1)-N(1)	174.9(3)
C(18)-Re(1)-N(1)	95.9(3)
C(16)-Re(1)-N(2)	169.3(3)
C(17)-Re(1)-N(2)	101.1(3)
C(18)-Re(1)-N(2)	98.3(3)
N(2)-Re(1)-N(1)	74.5(3)
C(16)-Re(1)-Cl(1)	91.7(3)
C(17)-Re(1)-Cl(1)	91.7(3)
C(18)-Re(1)-Cl(1)	179.9(3)
N(1)-Re(1)-Cl(1)	84.0(2)
N(2)-Re(1)-Cl(1)	81.6(2)
O(1)-C(16)-Re(1)	179.6(9)
O(2)-C(17)-Re(1)	176.0(8)
O(3)-C(18)-Re(1)	177.3(9)
Selected Torsions (deg)	
N(1)-C(5)-C(6)-N(2)	16(1)
N(2)-C(10)-C(11)-N(3)	41(1)

**Table 2** Selected Distances, Angles, and Torsions for **2**

Selected Distances (Å)	
Re(1)-C(16)	1.926(9)
Re(1)-C(17)	1.975(10)
Re(1)-N(1)	2.119(7)
Re(1)-N(2)	2.080(7)
Re(1)-N(3)	2.126(7)
Re(1)-Cl(1)	2.489(3)
N(1)-N(3)	4.14(1)
Selected Angles (deg)	
C(16)-Re(1)-C(17)	91.5(4)
C(16)-Re(1)-N(2)	173.7(4)
C(17)-Re(1)-N(2)	94.6(3)
C(16)-Re(1)-N(1)	103.9(3)
C(17)-Re(1)-N(1)	92.7(3)
N(2)-Re(1)-N(1)	77.3(3)
C(16)-Re(1)-N(3)	101.8(3)
C(17)-Re(1)-N(3)	91.7(3)
N(2)-Re(1)-N(3)	76.6(3)
N(1)-Re(1)-N(3)	153.7(3)
C(16)-Re(1)-Cl(1)	91.8(3)
C(17)-Re(1)-Cl(1)	176.5(2)
N(2)-Re(1)-Cl(1)	82.1(2)
N(1)-Re(1)-Cl(1)	85.4(2)
N(3)-Re(1)-Cl(1)	88.7(2)
O(1)-C(16)-Re(1)	177.9(9)
O(2)-C(17)-Re(1)	173.2(8)
Selected Torsions (deg)	
N(1)-C(5)-C(6)-N(2)	1(1)
N(2)-C(10)-C(11)-N(3)	-4(1)

**Table 3** Selected Distances, Angles, and Torsions for **3**

Selected Distances (Å)	
Re(1)-C(16)	1.911(3)
Re(1)-C(17)	1.890(3)
Re(1)-C(18)	1.921(4)
Re(1)-N(1)	2.173(3)
Re(1)-N(2)	2.232(2)
Re(1)-Br(1)	2.6410(4)
Selected Angles (deg)	
C(16)-Re(1)-C(17)	89.1(1)
C(16)-Re(1)-C(18)	85.9(1)
C(16)-Re(1)-N(1)	97.9(1)
C(17)-Re(1)-N(1)	92.5(1)
C(18)-Re(1)-N(1)	175.4(1)
C(16)-Re(1)-N(2)	171.2(1)
C(17)-Re(1)-N(2)	96.0(1)
C(18)-Re(1)-N(2)	101.3(1)
N(1)-Re(1)-N(2)	74.7(1)
C(16)-Re(1)-Br(1)	92.7(1)
C(17)-Re(1)-Br(1)	177.6(1)
C(18)-Re(1)-Br(1)	91.6(1)
N(1)-Re(1)-Br(1)	85.74(7)
N(2)-Re(1)-Br(1)	82.07(7)
O(1)-C(16)-Re(1)	178.6(3)
O(2)-C(17)-Re(1)	179.5(3)
O(3)-C(18)-Re(1)	179.9(3)
Selected Torsions (deg)	
N(1)-C(6)-C(1)-N(2)	-15.4(4)
N(2)-C(5)-C(11)-N(3)	141.1(3)

**Table 4** Selected Distances and Angles for **5**

Selected Distances (Å)	
Re(2)-C(35)	1.138(9)
Re(2)-C(36)	1.926(6)
Re(2)-C(37)	1.954(7)
Re(2)-C(38)	1.902(9)
Re(2)-N(5)	2.242(7)
Re(2)-N(6)	2.168(5)
C(35)-N(8)	1.138(9)
C(36)-O(4)	1.145(8)
C(37)-O(5)	1.151(9)
C(38)-O(6)	1.17(1)
Selected Angles (deg)	
C(16)-Re(1)-C(17)	91.5(4)
C(16)-Re(1)-N(2)	173.7(4)
C(17)-Re(1)-N(2)	94.6(3)
C(16)-Re(1)-N(1)	103.9(3)
C(17)-Re(1)-N(1)	92.7(3)
N(2)-Re(1)-N(1)	77.3(3)
C(16)-Re(1)-N(3)	101.8(3)
C(17)-Re(1)-N(3)	91.7(3)
N(2)-Re(1)-N(3)	76.6(3)
N(1)-Re(1)-N(3)	153.7(3)
C(16)-Re(1)-Cl(1)	91.8(3)
C(17)-Re(1)-Cl(1)	176.5(2)
N(2)-Re(1)-Cl(1)	82.1(2)
N(1)-Re(1)-Cl(1)	85.4(2)
N(3)-Re(1)-Cl(1)	88.7(2)
O(1)-C(16)-Re(1)	177.9(9)
O(2)-C(17)-Re(1)	173.2(8)

**Table 5** Selected Distances and Angles for **8.CH<sub>3</sub>CN**

Selected Distances (Å)	
Re(1)-C(16)	1.889(4)
Re(1)-C(17)	1.885(3)
Re(1)-N(1)	2.091(3)
Re(1)-N(2)	2.135(3)
Re(1)-N(3)	2.131(3)
Re(1)-N(4)	2.160(3)
Selected Angles (deg)	
C(16)-Re(1)-C(17)	87.69(16)
C(16)-Re(1)-N(1)	175.95(12)
C(17)-Re(1)-N(1)	96.35(12)
C(16)-Re(1)-N(3)	103.81(13)
C(17)-Re(1)-N(3)	94.03(12)
N(1)-Re(1)-N(3)	76.20(10)
C(16)-Re(1)-N(2)	103.58(13)
C(17)-Re(1)-N(2)	93.73(12)
N(1)-Re(1)-N(2)	75.99(10)
N(3)-Re(1)-N(2)	151.77(11)
C(16)-Re(1)-N(4)	90.50(14)
C(17)-Re(1)-N(4)	178.10(12)
N(1)-Re(1)-N(4)	85.46(10)
N(3)-Re(1)-N(4)	86.94(10)
N(2)-Re(1)-N(4)	86.15(10)
O(1)-C(16)-Re(1)	179.1(3)
O(2)-C(17)-Re(1)	178.0(3)

**Table 6** Selected Distances, Angles, and Torsions for  $\kappa^2(\text{terpy})\text{Mn}(\text{CO})_3\text{Br}$  from Compain et. al.

Selected Distances (Å)	
Mn(1)-N(1)	2.045(1)
Mn(1)-N(2)	2.105(2)
N(1)-N(2)	2.636(2)
Selected Angles (deg)	
N(1)-Mn(1)-N(2)	78.84(6)
Selected Torsions (deg)	
N(1)-C(8)-C(9)-N(2)	-16.5(2)
N(2)-C(13)-C(14)-N(3)	143.2(2)

**Table 7** Crystal data and structure refinement for compounds **1**, **3**, **5**, and **7**

Compound	<b>1</b>	<b>3</b>	<b>5</b>	<b>7</b>
Empirical formula	C <sub>19</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> ReCl	C <sub>19</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> ReBr	C <sub>20</sub> H <sub>11</sub> N <sub>4</sub> O <sub>3</sub> Re	C <sub>22</sub> H <sub>14</sub> N <sub>4</sub> O <sub>6</sub> F <sub>3</sub> SRe
Formula weight (g/mol)	538.96	583.41	530.04	693.63
Temperature (K)	200(2)	200	200	200
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal System	Triclinic	Monoclinic	Triclinic	
Space Group	P-1	C2/c	P-1	
a (Å)	9.8736(4)	31.1537(7)	9.9196(9)	
b (Å)	14.8202(4)	7.1176(2)	14.9902(14)	
c (Å)	16.3472(4)	16.8519(4)	16.5187(15)	
$\alpha$ (deg)	69.2890(10)	90.000	68.363(2)	
$\beta$ (deg)	80.801(2)	111.0230(10)	80.929(2)	
$\gamma$ (deg)	79.836(2)	90.000	79.975(2)	
Volume (Å <sup>3</sup> )	2190.00(12)	3488.00	2236.6(4)	
Z, r (calc) (Mg/m <sup>3</sup> )	2, 1.997	8, 2.222	2, 1.927	
Absorption coefficient (mm <sup>-1</sup> )	6.063	9.282	5.821	
Absorption correction	Semi-empirical from equivalents			
Final R indices [ $I \geq 2\sigma(I)$ ]	R1 = 0.0397, wR2 = 0.0839	R1 = 0.0232, wR2 = 0.0614	R1 = 0.0390, wR2 = 0.0921	
R indices (all data)	R1 = 0.0604, WR2 = 0.0951	R1 = 0.0285, wR2 = 0.0642	R1 = 0.0500, wR2 = 0.0961	

**Table 8** Crystal data and structure refinement for compounds **2**, **4**, **6**, and **8**

Compound	<b>2</b>	<b>4</b>	<b>6</b>	<b>8</b>
Empirical formula	C <sub>18</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> ReCl	C <sub>18</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> ReBr	C <sub>19</sub> H <sub>11</sub> N <sub>4</sub> O <sub>2</sub> Re	C <sub>21</sub> H <sub>14</sub> N <sub>4</sub> O <sub>5</sub> F <sub>3</sub> SRe
Formula weight (g/mol)	510.95	530.04	502.04	665.61
Temperature (K)	200(2)	200	200	200
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal System	Triclinic			Triclinic
Space Group	P-1			P-1
a (Å)	8.5275(3)			8.5745(4)
b (Å)	14.2421(5)			11.9805(5)
c (Å)	17.4637(6)			13.0970(5)
α (deg)	77.948(2)			79.748(2)
β (deg)	85.684(2)			81.106(2)
γ (deg)	79.890			88.091(2)
Volume (Å <sup>3</sup> )	2041.79(12)			1307.99(10)
Z, r (calc) (Mg/m <sup>3</sup> )	4, 2.050			2, 1.993
Absorption coefficient (mm <sup>-1</sup> )	6.494			5.094
Absorption correction		Semi-empirical from equivalents		
Final R indices [I ≥ 2σ(I)]	R1 = 0.0636, wR2 = 0.1018			R1 = 0.0294, wR2 = 0.0673
R indices (all data)	R1 = 0.0985, wR2 = 0.1110			R1 = 0.0366, wR2 = 0.0700