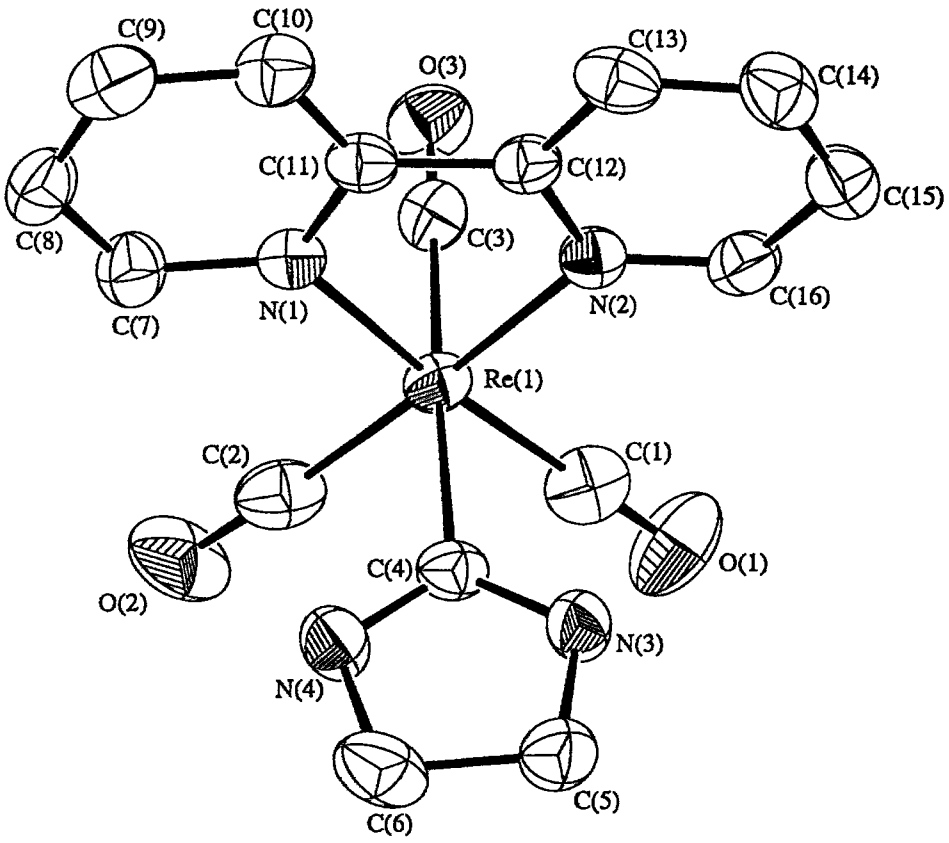
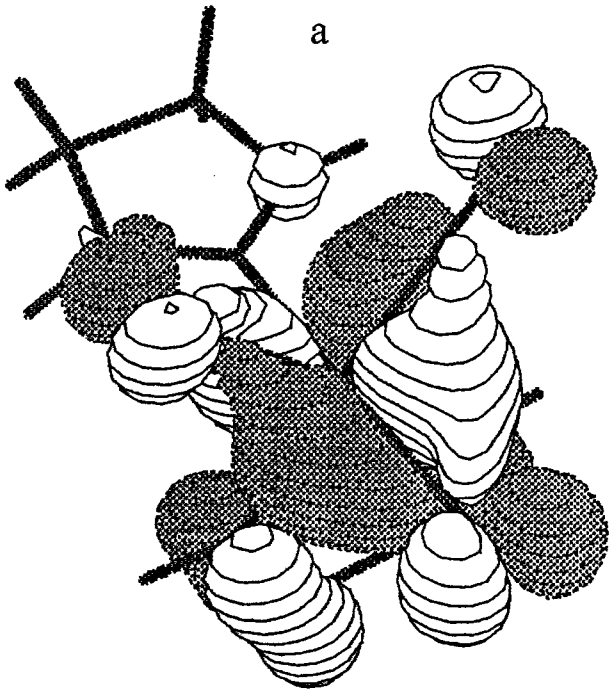
ORGANOMETALLICS
Organometallics, 1998, 17(8), 1622-1630, DOI:10.1021/om9709042

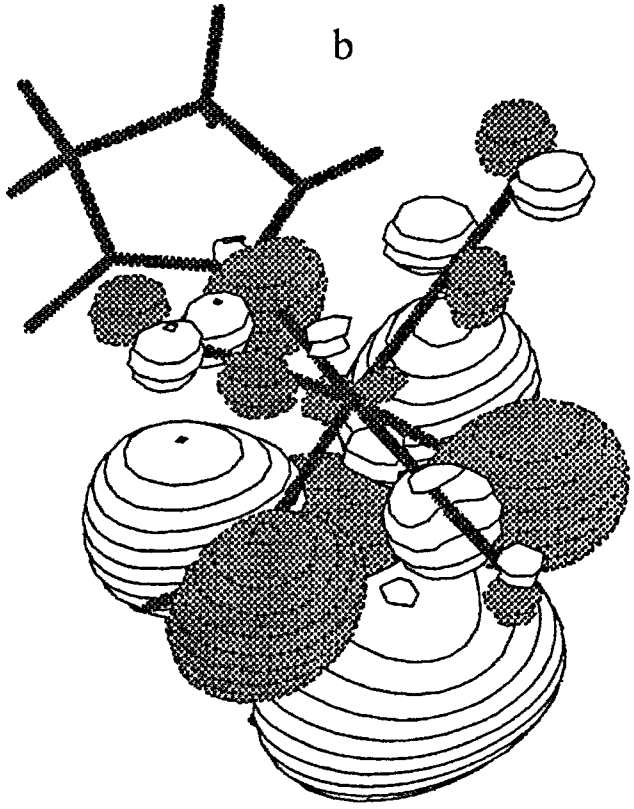
1. ORTEP plot of cation in complex **4** (40% probability ellipsoids).

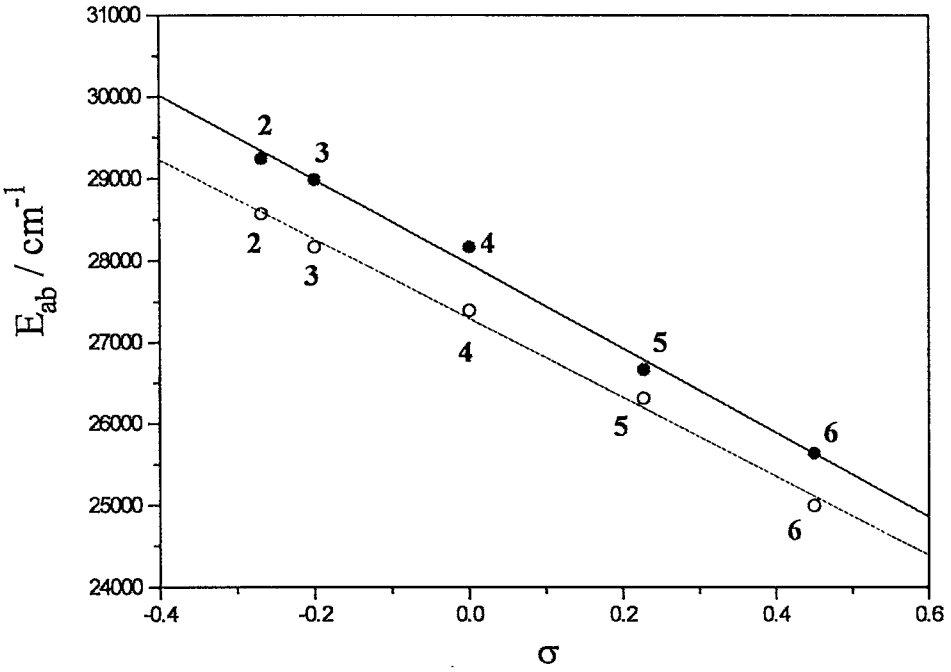


2. HOMO (a) and LUMO (b) of **4m**. Coefficients are derived from MP_2 calculation.

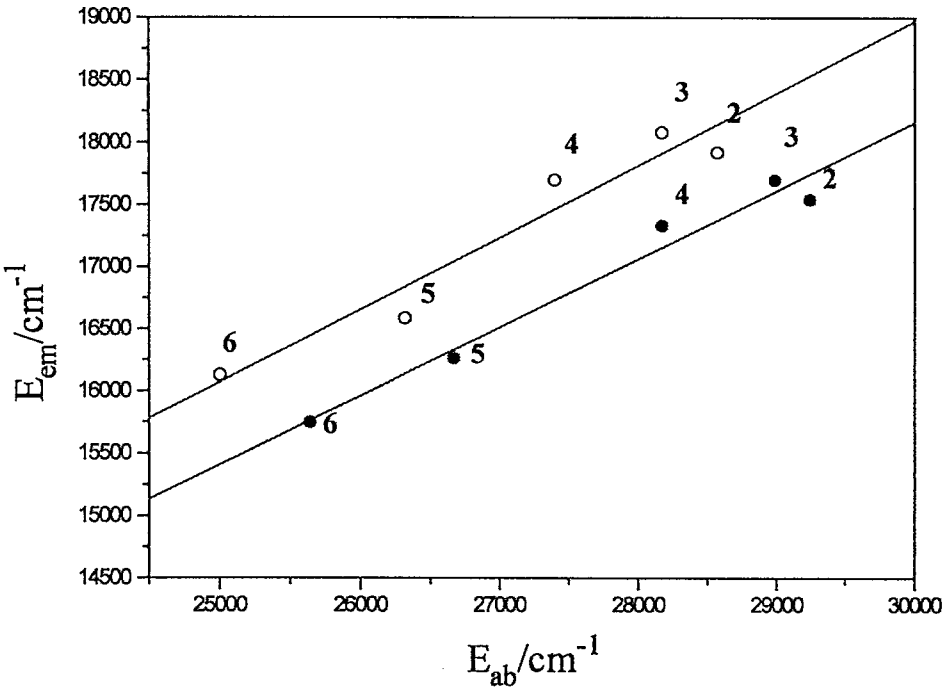


2. HOMO (a) and LUMO (b) of **4m**. Coefficients are derived from MP_2 calculation.



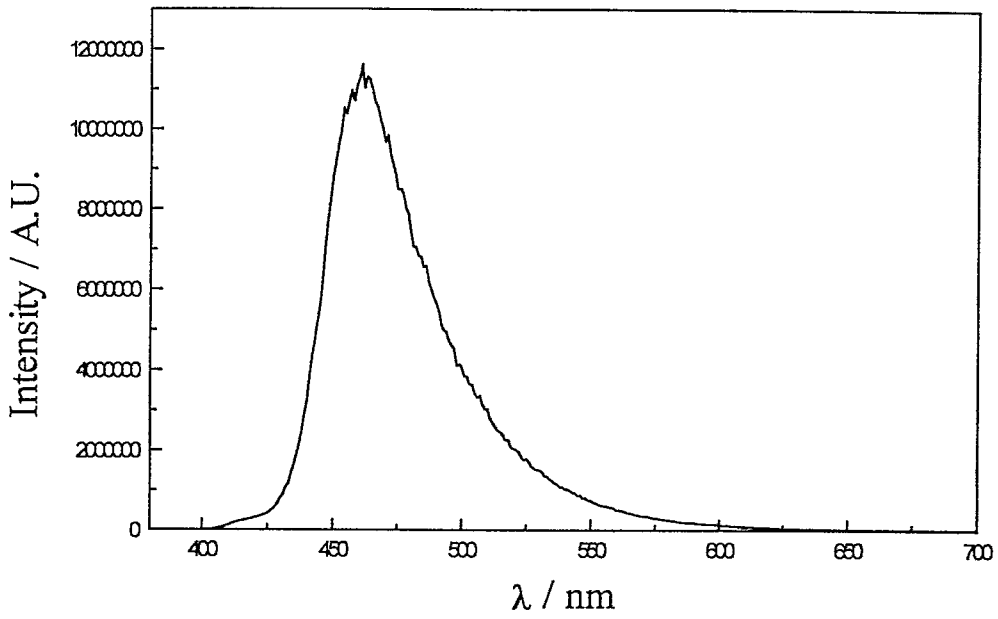


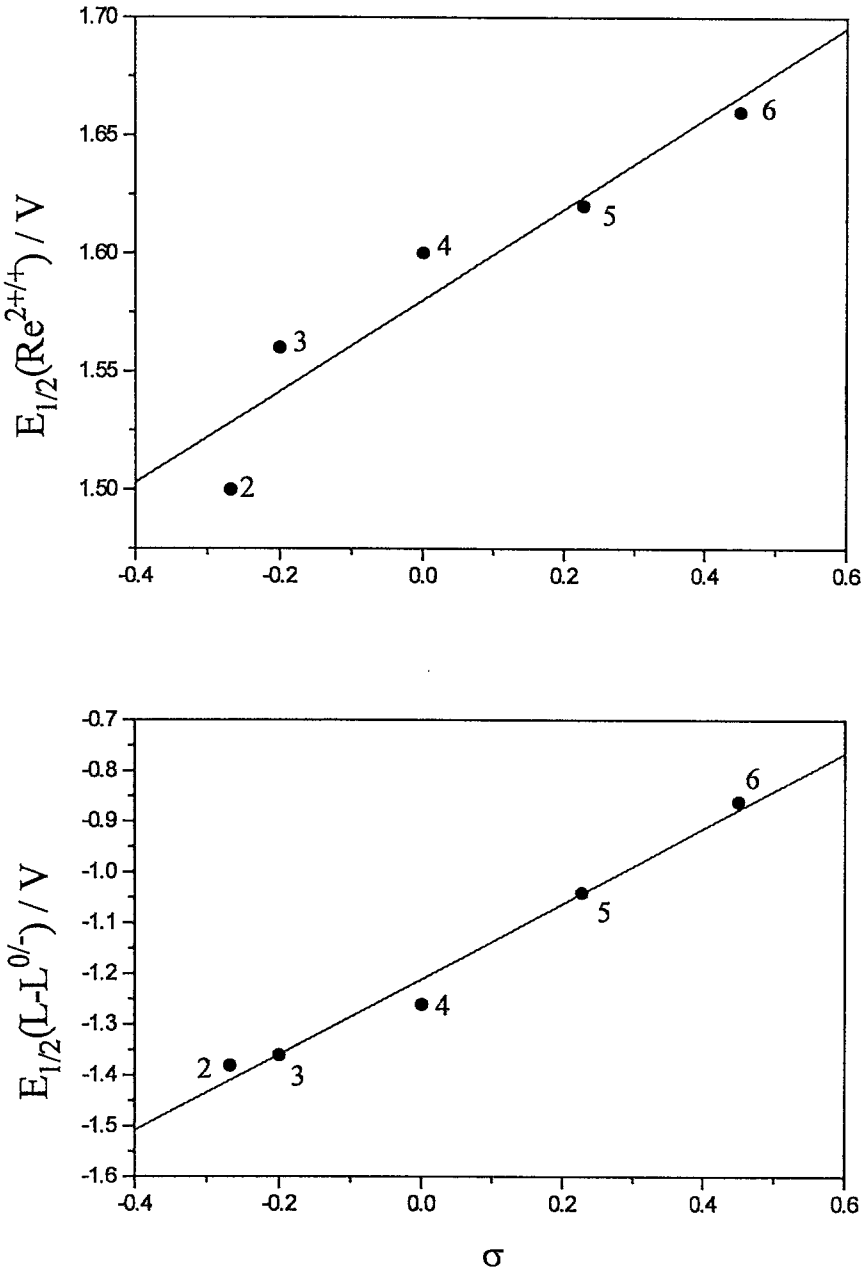
3. Absorption energies *vs* Hammett parameters correlation plots. Complexes are numbered as indicated in Scheme 1. Open circles indicate data in dichloromethane (correlation coefficient R = 0.99, slope = -(4.8±0.2) × 10^3), and closed circles represent data in acetonitrile (R = 0.99, slope = -(5.2±0.2) × 10^3).



4. Emission energies *vs* ^{1}MLCT absorption energies correlation plots. Complexes are numbered as indicated in Scheme 1. Open circles indicate data in dichloromethane (correlation coefficient R = 0.97, slope = 0.58 ± 0.08), and closed circles represent data in acetonitrile (R = 0.98, slope = 0.55 ± 0.05).

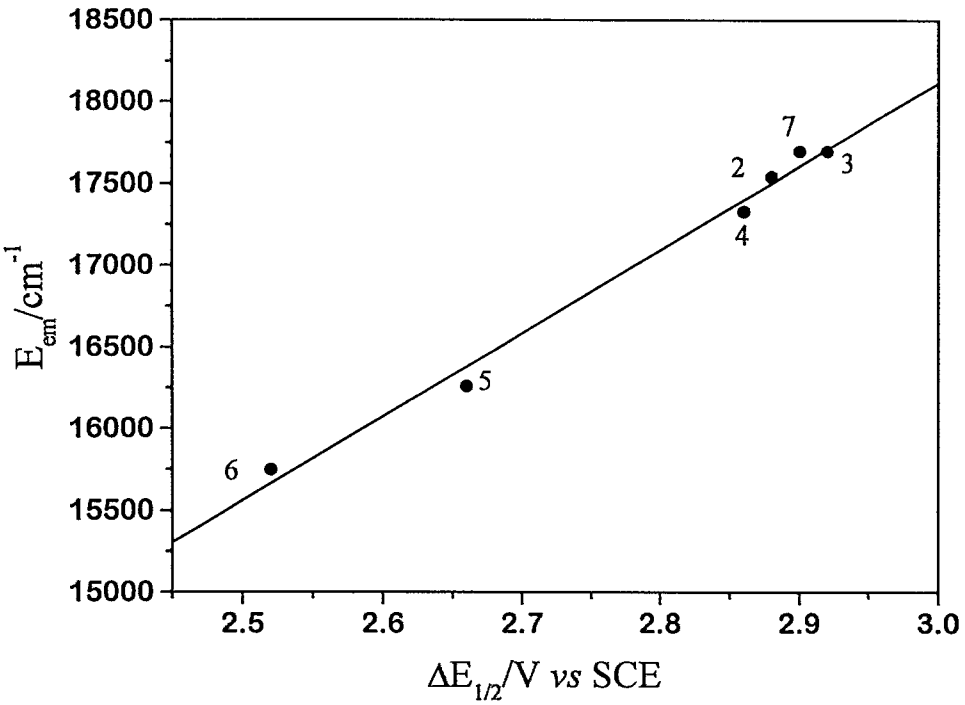
5. Emission spectrum of **8** in dichloromethane at 77K (λ_{ex} = 310 nm).

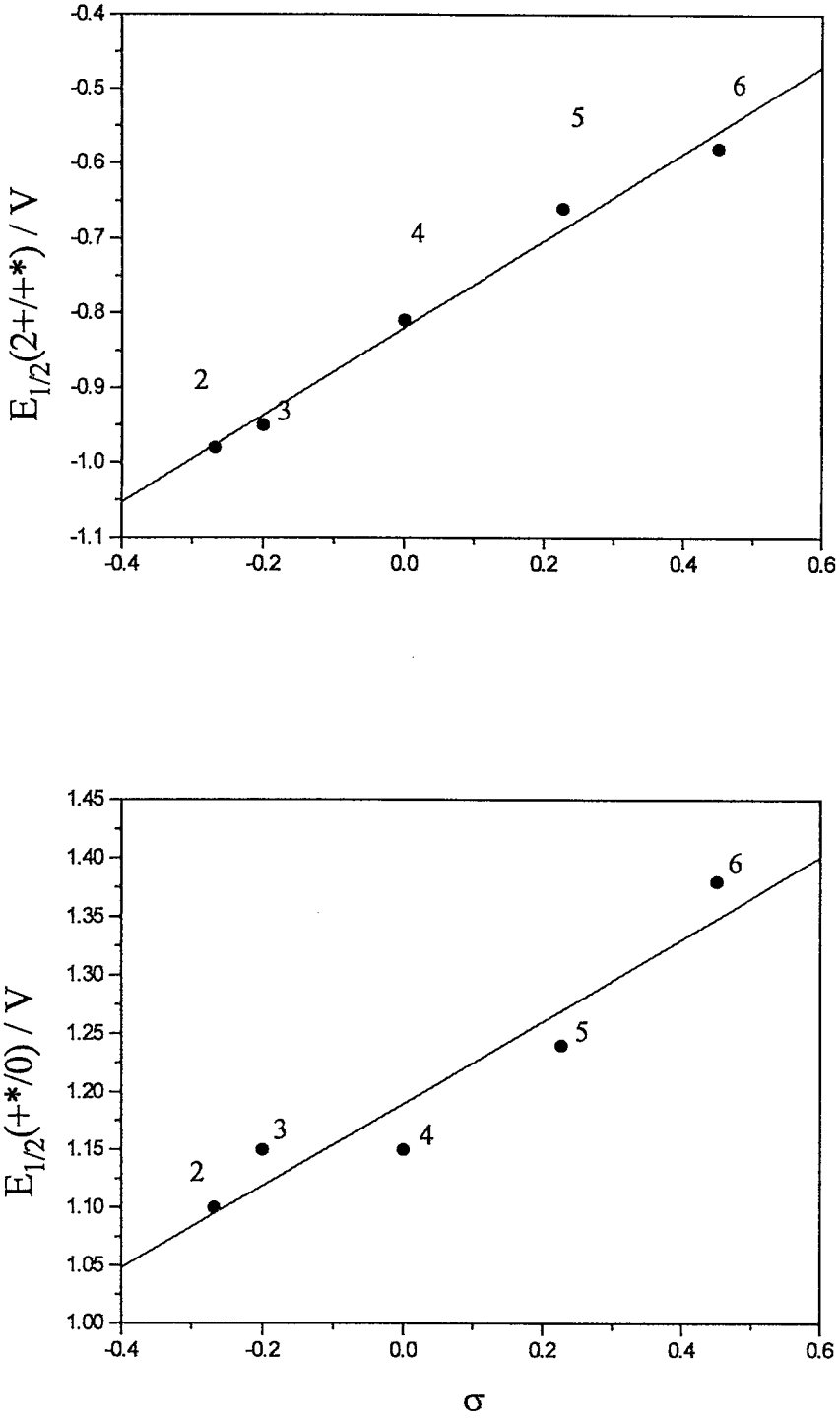




6. Plots of Ground state redox potential vs Hammett parameters, measured in acetonitrile at room temperature. Complexes are numbered as indicated in Scheme 1. (top): R = 0.94, slope = 0.19 ± 0.03; (bottom): R = 0.99, slope = 0.74 ± 0.05.

7. Correlation of emission energies with redox potential differences [$\Delta E_{1/2}$ = ($E_{1/2}(Re^{2+/+}) - E_{1/2}(L\text{-}L^{0/-})$)], measured in acetonitrile at room temperature, (R = 0.98, slope = $(5.1 \pm 0.2) \times 10^3$). Complexes are numbered as indicated in Scheme 1.





8. Excited state redox potentials *vs* Hammett parameters correlation plots. Complexes are numbered as indicated in Scheme 1. Upper: R = 0.95, slope = 0.35 ± 0.06; Lower: R = 0.99, slope = 0.58 ± 0.03.

Crystal data for $[HNCH_2CH_2NHCRe(bpy)(CO)_3]Br{\cdot}CH_3CN{\cdot}0.5H_2O$ (**4**)

$\{[Re N_4 O_3 C_{16} H_{14}]^+ Br^-.\ CH_3CN\ .\ 0.5\ H_2O\ \}$, formula weight = 626.49, orthorhombic, space group *Ccca* (No. 68), a = 19.512(8) Å, b =29.865(8) Å, c = 14.523(8) Å, V = 8462(5) Å^3, Z = 16, D_c = 1.967 g cm^{-3}, μ(Mo-Kα) = 76.71 cm^{-1}, F(000) = 4784, T = 301 K. A pale yellow crystal of dimensions 0.25 × 0.20 × 0.30 mm in a glass capillary was used for data collection at 301 K on a Rigaku AFC7R diffractometer with graphite monochromatized Mo-Kα radiation (λ = 0.71073 Å) using ω-2θ scans with ω-scan angle $(0.63 + 0.35 \tan\theta)^\circ$ at a scan speed of 16.0 deg min^{-1} (up to 6 scans for reflection $I < 15\ \sigma(I)$). Intensity data (in the range of $2\theta_{max} = 50^\circ$; h: 0 to 23; k: 0 to 35; l: 0 to 19 and 3 standard reflections measured after every 300 reflections showed decay of 2.30 %), were corrected for decay and for Lorentz and polarization effects, and empirical absorption corrections based on the ψ-scan of six strong reflections (minimum and maximum transmission factors 0.641and 1.000). 4088 unique reflections were measured, of which 2584 reflections with $I > 3\ \sigma(I)$ were considered observed and used in the structural analysis. The space group was uniquely determined from systematic absences and the structure was solved by direct methods (*SIR92*) and expanded by Fourier methods and refined by full-matrix least-squares using the software package *TeXsan* on a Silicon Graphics Indy computer. One formula unit constitutes a crystallographic asymmetric unit with the 2 Br atoms and the O atom of the water molecule at special positions with occupation number of 1/2. All 30 non-H atoms were refined anisotropically. The hydrogen atoms of the water molecule were not located. 17 H atoms were included in the calculation, and these comprised of 2 H atoms bonded to N(3) and N(4) atoms located in the difference Fourier synthesis and 15 H atoms at calculated positions with thermal parameters equal to 1.3 times that of the attached C atoms, but their positional parameters were not refined. Convergence for 259 variable parameters by least-squares refinement on F with $w = 4F_o^2 / \sigma^2(F_o^2)$, where $\sigma^2(F_o^2) = [\sigma^2(I) + (0.023\ F_o^2)^2]$ for 2584 reflections with $I > 3\ \sigma(I)$ was reached at R = 0.028 and wR = 0.039 with a goodness-of-fit of 1.89. $(\Delta / \sigma)_{max}$ = 0.02 for atoms of the complex cation and Br atoms. The final difference Fourier map was featureless, with maximum positive and negative peaks of 1.13 and 0.67 e Å^{-3} respectively.

Crystal data for $[HNCH_2CH_2NHCRe(bpy)(CO)_3]Br{\cdot}CH_3CN{\cdot}0.5H_2O$ (**4**)

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Re(1)	0.14854(2)	0.37511(1)	0.11959(2)	3.182(7)
Br(1)	0.0000	0.2500	-0.03887(9)	5.08(3)
Br(2)	0.2500	0.5000	-0.0868(1)	5.96(4)
O(1)	0.1199(4)	0.4761(2)	0.1172(4)	6.9(2)
O(2)	-0.0058(3)	0.3570(2)	0.1402(4)	6.4(2)
O(3)	0.1625(3)	0.3832(2)	0.3320(4)	5.1(2)
O(4)	0.4330(9)	0.2500	0.2500	21.9(9)
N(1)	0.1820(3)	0.3055(2)	0.1169(4)	3.4(1)
N(2)	0.2586(3)	0.3769(2)	0.0964(4)	3.3(1)
N(3)	0.1712(3)	0.3988(2)	-0.0881(4)	4.4(2)
N(4)	0.1019(3)	0.3433(2)	-0.0770(4)	4.3(2)
N(5)	0.0201(4)	0.0514(4)	0.598(1)	20.9(5)
C(1)	0.1300(4)	0.4381(3)	0.1177(5)	4.1(2)
C(2)	0.0519(5)	0.3641(3)	0.1327(5)	4.3(2)
C(3)	0.1584(4)	0.3792(2)	0.2540(6)	3.9(2)
C(4)	0.1401(3)	0.3714(2)	-0.0293(5)	3.4(2)
C(5)	0.1526(4)	0.3899(3)	-0.1849(6)	5.4(2)
C(6)	0.1030(5)	0.3521(4)	-0.1760(6)	5.2(3)
C(7)	0.1385(4)	0.2698(3)	0.1248(5)	4.1(2)
C(8)	0.1619(4)	0.2261(3)	0.1278(5)	4.3(2)
C(9)	0.2310(5)	0.2189(3)	0.1225(5)	5.1(2)
C(10)	0.2764(4)	0.2552(3)	0.1136(5)	4.3(2)
C(11)	0.2504(4)	0.2974(2)	0.1092(4)	3.2(2)
C(12)	0.2928(4)	0.3380(2)	0.0955(5)	3.0(2)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(13)	0.3631(4)	0.3367(3)	0.0801(6)	4.4(2)
C(14)	0.3987(4)	0.3739(3)	0.0676(6)	4.7(2)
C(15)	0.3643(4)	0.4160(3)	0.0698(5)	4.1(2)
C(16)	0.2946(4)	0.4154(2)	0.0843(5)	3.6(2)
C(17)	0.0403(6)	0.0163(4)	0.631(1)	12.9(6)
C(18)	0.0665(6)	-0.0217(4)	0.6466(8)	8.8(4)
H(1)	0.1889	0.4237	-0.0788	5.4525
H(2)	0.0707	0.3189	-0.0499	5.4525
H(3)	0.1314	0.4153	-0.2129	6.3817
H(4)	0.1915	0.3815	-0.2205	6.3817
H(5)	0.1183	0.3263	-0.2089	6.5920
H(6)	0.0586	0.3601	-0.1972	6.5920
H(7)	0.0910	0.2748	0.1282	4.9798
H(8)	0.1312	0.2021	0.1330	5.1953
H(9)	0.2480	0.1896	0.1259	6.1477
H(10)	0.3242	0.2499	0.1112	5.0948
H(11)	0.3857	0.3082	0.0789	5.1642
H(12)	0.4471	0.3732	0.0574	5.5693
H(13)	0.3887	0.4429	0.0613	4.9756
H(14)	0.2710	0.4430	0.0859	4.4914
H(15)	0.0533	-0.0305	0.7069	10.6579
H(16)	0.0505	-0.0441	0.6039	10.6579
H(17)	0.1150	-0.0204	0.6429	10.6579

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Re(1)	0.0403(2)	0.0436(2)	0.0369(2)	0.0073(1)	0.0025(1)	0.0024(1)
Br(1)	0.0512(7)	0.0591(7)	0.0827(10)	-0.0032(7)	0.0000	0.0000
Br(2)	0.0702(9)	0.0596(8)	0.097(1)	-0.0067(7)	0.0000	0.0000
O(1)	0.112(5)	0.050(3)	0.100(5)	0.029(4)	0.027(4)	0.006(3)
O(2)	0.037(3)	0.113(5)	0.092(5)	0.002(4)	0.015(3)	0.005(4)
O(3)	0.073(4)	0.083(4)	0.037(3)	0.007(3)	0.003(3)	-0.003(3)
O(4)	0.22(2)	0.31(2)	0.31(3)	0.0000	0.0000	-0.03(2)
N(1)	0.042(3)	0.050(4)	0.038(4)	0.005(3)	-0.002(3)	0.005(3)
N(2)	0.043(3)	0.043(3)	0.038(3)	0.001(3)	-0.002(3)	0.000(3)
N(3)	0.054(4)	0.074(4)	0.040(4)	-0.020(4)	0.000(3)	0.005(3)
N(4)	0.063(5)	0.059(5)	0.041(4)	-0.017(4)	-0.004(3)	-0.001(3)
N(5)	0.071(5)	0.13(1)	0.60(2)	-0.008(6)	-0.086(9)	0.06(1)
C(1)	0.061(5)	0.049(6)	0.046(5)	0.011(4)	0.011(4)	0.009(4)
C(2)	0.059(5)	0.058(6)	0.047(5)	0.014(5)	-0.001(4)	0.002(4)
C(3)	0.049(4)	0.051(4)	0.049(5)	0.007(3)	0.004(4)	-0.006(4)
C(4)	0.039(4)	0.052(5)	0.039(4)	0.005(4)	0.002(3)	0.006(4)
C(5)	0.068(6)	0.100(5)	0.037(5)	-0.002(4)	-0.005(4)	0.001(4)
C(6)	0.078(6)	0.069(8)	0.050(6)	0.001(6)	-0.007(5)	-0.001(6)
C(7)	0.049(5)	0.049(5)	0.059(5)	-0.004(4)	-0.003(4)	0.002(4)
C(8)	0.075(6)	0.034(5)	0.053(5)	-0.007(4)	-0.008(4)	0.004(4)
C(9)	0.096(7)	0.036(5)	0.062(6)	0.008(5)	-0.008(5)	-0.003(4)
C(10)	0.058(5)	0.053(4)	0.054(5)	0.015(4)	0.002(4)	-0.002(4)
C(11)	0.042(4)	0.047(4)	0.034(4)	0.006(4)	-0.001(3)	0.000(3)
C(12)	0.037(4)	0.043(4)	0.036(4)	0.006(3)	-0.005(3)	0.001(3)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(13)	0.045(5)	0.069(6)	0.052(5)	0.020(4)	-0.004(4)	-0.014(4)
C(14)	0.043(5)	0.073(6)	0.062(5)	0.004(4)	0.008(4)	-0.002(5)
C(15)	0.050(5)	0.055(5)	0.050(5)	-0.008(4)	0.006(4)	-0.002(4)
C(16)	0.052(5)	0.043(5)	0.044(5)	0.004(4)	-0.001(4)	0.006(4)
C(17)	0.056(7)	0.091(9)	0.34(3)	-0.005(6)	-0.06(1)	0.09(1)
C(18)	0.070(9)	0.141(9)	0.12(1)	0.023(7)	0.014(8)	0.011(8)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Crystal data for $[HNCH_2CH_2NHCRe(bpy)(CO)_3]Br{\cdot}CH_3CN{\cdot}0.5H_2O$ (**4**)

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Re(1)	N(1)	2.178(6)	Re(1)	N(2)	2.175(6)
Re(1)	C(1)	1.917(9)	Re(1)	C(2)	1.924(9)
Re(1)	C(3)	1.965(9)	Re(1)	C(4)	2.171(7)
O(1)	C(1)	1.15(1)	O(2)	C(2)	1.15(1)
O(3)	C(3)	1.14(1)	N(1)	C(7)	1.368(10)
N(1)	C(11)	1.362(10)	N(2)	C(12)	1.339(9)
N(2)	C(16)	1.358(9)	N(3)	C(4)	1.329(10)
N(3)	C(5)	1.48(1)	N(4)	C(4)	1.320(10)
N(4)	C(6)	1.46(1)	N(5)	C(17)	1.22(2)
C(5)	C(6)	1.49(1)	C(7)	C(8)	1.38(1)
C(8)	C(9)	1.37(1)	C(9)	C(10)	1.41(1)
C(10)	C(11)	1.36(1)	C(11)	C(12)	1.480(10)
C(12)	C(13)	1.39(1)	C(13)	C(14)	1.32(1)
C(14)	C(15)	1.43(1)	C(15)	C(16)	1.38(1)
C(17)	C(18)	1.27(2)			

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Re(1)	N(2)	74.0(2)	N(1)	Re(1)	C(1)	173.2(3)
N(1)	Re(1)	C(2)	97.6(3)	N(1)	Re(1)	C(3)	92.7(2)
N(1)	Re(1)	C(4)	87.5(2)	N(2)	Re(1)	C(1)	99.2(3)
N(2)	Re(1)	C(2)	171.0(3)	N(2)	Re(1)	C(3)	93.2(3)
N(2)	Re(1)	C(4)	85.5(2)	C(1)	Re(1)	C(2)	89.1(4)
C(1)	Re(1)	C(3)	88.4(3)	C(1)	Re(1)	C(4)	91.2(3)
C(2)	Re(1)	C(3)	90.5(3)	C(2)	Re(1)	C(4)	90.9(3)
C(3)	Re(1)	C(4)	178.6(3)	Re(1)	N(1)	C(7)	123.8(5)
Re(1)	N(1)	C(11)	117.7(4)	C(7)	N(1)	C(11)	118.4(6)
Re(1)	N(2)	C(12)	118.1(4)	Re(1)	N(2)	C(16)	123.5(5)
C(12)	N(2)	C(16)	118.4(6)	C(4)	N(3)	C(5)	112.9(6)
C(4)	N(4)	C(6)	113.1(7)	Re(1)	C(1)	O(1)	178.9(7)
Re(1)	C(2)	O(2)	179.2(8)	Re(1)	C(3)	O(3)	177.1(6)
Re(1)	C(4)	N(3)	125.1(5)	Re(1)	C(4)	N(4)	126.7(5)
N(3)	C(4)	N(4)	108.2(6)	N(3)	C(5)	C(6)	102.3(7)
N(4)	C(6)	C(5)	103.4(7)	N(1)	C(7)	C(8)	122.3(7)
C(7)	C(8)	C(9)	118.0(8)	C(8)	C(9)	C(10)	120.5(8)
C(9)	C(10)	C(11)	118.9(7)	N(1)	C(11)	C(10)	121.8(7)
N(1)	C(11)	C(12)	114.4(6)	C(10)	C(11)	C(12)	123.9(7)
N(2)	C(12)	C(11)	115.6(6)	N(2)	C(12)	C(13)	121.1(7)
C(11)	C(12)	C(13)	123.3(7)	C(12)	C(13)	C(14)	121.2(7)
C(13)	C(14)	C(15)	119.3(7)	C(14)	C(15)	C(16)	117.2(7)
N(2)	C(16)	C(15)	122.8(7)	N(5)	C(17)	C(18)	166(1)

Crystal data for $[HNCH_2CH_2NHCRe(4,4'\text{-}(CO_2Me)_2\text{-}bpy)(CO)_3]ClO_4 \cdot H_2O$ (**6**)

{$[Re\ N_4O_7C_{20}H_{18}]^+\ ClO_4^-\ .\ H_2O$}; formula weight = 730.07, triclinic, space group $P\bar{1}$ (No. 2), a = 11.826(6) Å, b = 12.012(6) Å, c = 11.694(5) Å, α = 117.45(3)°, β = 97.33(4)°, γ = 60.61(3)°, V = 1274(1) Å^3, Z = 2, D_c = 1.903 g cm^{-3}, μ(Mo-Kα)= 49.45 cm^{-1}, $F(000)$ = 712, T = 301 K. A yellow crystal of dimensions 0.20 × 0.20 × 0.35 mm in a glass capillary was used for data collection at 28°C on a Rigaku AFC7R diffractometer with graphite monochromatized Mo-Kα radiation (λ = 0.71073 Å) using ω-2θ scans with ω-scan angle $(0.79 + 0.35 \tan\theta)^\circ$ at a scan speed of 16.0 deg min^{-1} (up to 6 scans for reflection $I < 15\ \sigma(I)$). Intensity data (in the range of $2\theta_{max} = 50^\circ$; h: 0 to 14; k:-14 to 14; l: -13 to 13 and 3 standard reflections measured after every 300 reflections showed no decay), were corrected for Lorentz and polarization effects, and empirical absorption corrections based on the ψ-scan of six strong reflections (minimum and maximum transmission factors 0.680 and 1.000). 4725 reflections were measured, of which 4485 were unique and R_{int} = 0.016. 4036 reflections with $I > 3\ \sigma(I)$ were considered observed and used in the structural analysis. The space group was determined based on a statistical analysis of intensity distribution and the successful refinement of the structure solved by Patterson methods and expanded by Fourier methods (*PATTY*) and refinement by full-matrix least-squares using the software package *TeXsan* on a Silicon Graphics Indy computer. A crystallographic asymmetric unit consists of atoms in one formula unit. All 38 non-H atoms were refined anisotropically. The two H atoms bonded to N(3) and N(4) were located in difference Fourier synthesis and their positional parameters were refined. The H atoms of the water molecule were not located. The other 16 H atoms at calculated positions with thermal parameters equal to 1.3 times that of the attached C atoms were not refined. Convergence for 349 variable parameters by least-squares refinement on F with $w = 4\ F_o^2 / \sigma^2(F_o^2)$, where $\sigma^2(F_o^2) = [\sigma^2(I) + (0.016\ F_o^2)^2]$ for 4036 reflections with $I > 3\ \sigma(I)$ was reached at R = 0.023 and wR = 0.026 with a goodness-of-fit of 1.45. $(\Delta / \sigma)_{max}$ = 0.02 for atoms of the complex cation. The final difference Fourier map was featureless, with maximum positive and negative peaks of 0.62 and 0.54 e Å^{-3} respectively.

Crystal data for $[HNCH_2CH_2NHCRe(4,4'\text{-}(CO_2Me)_2\text{-}bpy)(CO)_3]ClO_4 \cdot H_2O$ (**6**)

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Re(1)	0.20145(2)	0.06874(2)	0.19200(2)	2.965(4)
Cl(1)	0.2891(2)	0.4527(1)	0.6758(1)	5.42(3)
O(1)	0.1544(4)	0.3664(4)	0.2525(4)	6.2(1)
O(2)	0.2993(4)	-0.0419(4)	-0.0906(3)	5.77(9)
O(3)	-0.0809(3)	0.1505(4)	0.1204(3)	5.18(9)
O(4)	0.4380(4)	-0.6457(3)	0.0948(3)	5.71(9)
O(5)	0.3827(3)	-0.5155(3)	0.3099(3)	5.03(8)
O(6)	0.0496(3)	0.0955(4)	0.7782(3)	5.14(9)
O(7)	0.0070(3)	0.3218(3)	0.8530(3)	4.80(8)
O(8)	0.2141(7)	0.4791(6)	0.7732(5)	13.4(2)
O(9)	0.3483(5)	0.5353(6)	0.7259(7)	12.9(2)
O(10)	0.3756(8)	0.3106(5)	0.6094(6)	14.8(2)
O(11)	0.2128(8)	0.491(1)	0.5872(7)	17.1(3)
O(12)	0.7955(4)	0.2288(4)	0.4026(4)	7.6(1)
N(1)	0.2442(3)	-0.1348(3)	0.1802(3)	2.98(7)
N(2)	0.1441(3)	0.1210(3)	0.3872(3)	3.04(7)
N(3)	0.4352(4)	0.0750(5)	0.3512(4)	4.66(10)
N(4)	0.5066(4)	-0.1077(4)	0.1659(4)	4.81(10)
C(1)	0.1712(4)	0.2539(5)	0.2285(5)	4.0(1)
C(2)	0.2626(4)	-0.0014(5)	0.0145(5)	3.8(1)
C(3)	0.0226(4)	0.1189(5)	0.1474(4)	3.57(10)
C(4)	0.3989(4)	0.0069(4)	0.2409(4)	3.24(9)
C(5)	0.5762(5)	0.0081(6)	0.3553(6)	5.5(1)
C(6)	0.6273(5)	-0.1256(6)	0.2246(6)	5.1(1)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(7)	0.2951(4)	-0.2623(4)	0.0713(4)	3.40(9)
C(8)	0.3382(4)	-0.3900(4)	0.0721(4)	3.73(10)
C(9)	0.3321(4)	-0.3906(4)	0.1895(4)	3.45(9)
C(10)	0.2764(4)	-0.2604(4)	0.3014(4)	3.34(9)
C(11)	0.2312(4)	-0.1340(4)	0.2945(4)	2.90(9)
C(12)	0.1675(4)	0.0096(4)	0.4074(4)	2.81(8)
C(13)	0.1321(4)	0.0308(4)	0.5276(4)	3.05(9)
C(14)	0.0735(4)	0.1698(4)	0.6306(4)	3.20(9)
C(15)	0.0498(4)	0.2822(4)	0.6088(4)	3.93(10)
C(16)	0.0843(4)	0.2556(4)	0.4874(4)	3.8(1)
C(17)	0.3898(4)	-0.5319(5)	0.1915(5)	4.1(1)
C(18)	0.4485(6)	-0.6451(6)	0.3252(6)	6.7(2)
C(19)	0.0423(4)	0.1889(5)	0.7602(4)	3.53(10)
C(20)	-0.0189(6)	0.3506(6)	0.9839(5)	6.1(2)
H(1)	0.381(5)	0.147(5)	0.407(5)	5.0214
H(2)	0.510(4)	-0.173(5)	0.091(5)	5.0214
H(3)	0.6088	0.0689	0.3630	6.6636
H(4)	0.5984	-0.0165	0.4243	6.6636
H(5)	0.6690	-0.2104	0.2349	6.1588
H(6)	0.6862	-0.1271	0.1752	6.1588
H(7)	0.3014	-0.2629	-0.0092	4.0756
H(8)	0.3716	-0.4775	-0.0070	4.4786
H(9)	0.2696	-0.2578	0.3828	4.0370
H(10)	0.1480	-0.0483	0.5395	3.7133

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(11)	0.0100	0.3779	0.6774	4.7212
H(12)	0.0657	0.3345	0.4735	4.6256
H(13)	0.4119	-0.7058	0.2755	8.0477
H(14)	0.5389	-0.6948	0.2952	8.0477
H(15)	0.4372	-0.6208	0.4140	8.0477
H(16)	0.0575	0.2891	1.0069	7.3672
H(17)	-0.0430	0.4483	1.0420	7.3672
H(18)	-0.0883	0.3340	0.9889	7.3672

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Crystal data for $[HNCH_2CH_2NHCRe(4,4'\text{-}(CO_2Me)_2\text{-}bpy)(CO)_3]ClO_4 \cdot H_2O$ (**6**)

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Re(1)	0.0375(1)	0.0339(1)	0.0356(1)	-0.01382(8)	-0.00421(7)	0.01562(8)
Cl(1)	0.099(1)	0.0627(8)	0.0437(7)	-0.0478(8)	0.0047(7)	0.0115(6)
O(1)	0.093(3)	0.046(2)	0.100(3)	-0.034(2)	-0.024(2)	0.038(2)
O(2)	0.077(2)	0.077(3)	0.047(2)	-0.019(2)	0.010(2)	0.030(2)
O(3)	0.045(2)	0.064(2)	0.065(2)	-0.019(2)	-0.014(2)	0.023(2)
O(4)	0.095(3)	0.035(2)	0.058(2)	-0.020(2)	0.005(2)	0.009(2)
O(5)	0.075(2)	0.040(2)	0.061(2)	-0.013(2)	0.014(2)	0.024(2)
O(6)	0.084(3)	0.057(2)	0.051(2)	-0.031(2)	0.005(2)	0.023(2)
O(7)	0.087(2)	0.055(2)	0.034(2)	-0.038(2)	0.007(2)	0.009(2)
O(8)	0.248(7)	0.147(5)	0.102(4)	-0.101(5)	0.081(4)	0.019(4)
O(9)	0.119(4)	0.107(4)	0.222(7)	-0.079(4)	0.005(4)	0.011(4)
O(10)	0.277(8)	0.067(3)	0.136(5)	-0.045(4)	0.091(5)	-0.002(3)
O(11)	0.240(8)	0.34(1)	0.143(6)	-0.169(8)	-0.106(6)	0.156(7)
O(12)	0.126(4)	0.082(3)	0.076(3)	-0.037(3)	0.006(2)	0.044(2)
N(1)	0.038(2)	0.031(2)	0.035(2)	-0.014(1)	-0.003(1)	0.011(1)
N(2)	0.041(2)	0.035(2)	0.033(2)	-0.016(2)	-0.004(1)	0.013(2)
N(3)	0.048(2)	0.054(3)	0.052(3)	-0.018(2)	-0.012(2)	0.015(2)
N(4)	0.041(2)	0.052(3)	0.063(3)	-0.016(2)	-0.003(2)	0.013(2)
C(1)	0.051(3)	0.047(3)	0.053(3)	-0.022(2)	-0.012(2)	0.025(2)
C(2)	0.045(2)	0.042(3)	0.053(3)	-0.015(2)	-0.006(2)	0.025(2)
C(3)	0.046(3)	0.045(2)	0.038(2)	-0.018(2)	-0.003(2)	0.017(2)
C(4)	0.043(2)	0.040(2)	0.044(2)	-0.020(2)	-0.007(2)	0.024(2)
C(5)	0.055(3)	0.084(4)	0.085(4)	-0.038(3)	-0.031(3)	0.051(3)
C(6)	0.041(3)	0.069(3)	0.090(4)	-0.022(2)	-0.010(3)	0.046(3)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(7)	0.047(2)	0.040(2)	0.034(2)	-0.020(2)	-0.001(2)	0.011(2)
C(8)	0.046(3)	0.034(2)	0.043(3)	-0.015(2)	0.001(2)	0.008(2)
C(9)	0.039(2)	0.035(2)	0.048(3)	-0.015(2)	-0.002(2)	0.015(2)
C(10)	0.042(2)	0.038(2)	0.039(2)	-0.016(2)	-0.001(2)	0.014(2)
C(11)	0.035(2)	0.035(2)	0.035(2)	-0.015(2)	-0.005(2)	0.014(2)
C(12)	0.035(2)	0.034(2)	0.035(2)	-0.015(2)	-0.004(2)	0.015(2)
C(13)	0.038(2)	0.036(2)	0.041(2)	-0.018(2)	-0.006(2)	0.018(2)
C(14)	0.038(2)	0.038(2)	0.036(2)	-0.016(2)	-0.003(2)	0.013(2)
C(15)	0.058(3)	0.033(2)	0.039(2)	-0.016(2)	0.003(2)	0.007(2)
C(16)	0.061(3)	0.033(2)	0.041(2)	-0.017(2)	0.001(2)	0.014(2)
C(17)	0.050(3)	0.037(3)	0.056(3)	-0.015(2)	0.003(2)	0.018(2)
C(18)	0.102(5)	0.055(3)	0.094(5)	-0.018(3)	0.011(4)	0.047(3)
C(19)	0.040(2)	0.048(3)	0.038(2)	-0.020(2)	-0.003(2)	0.015(2)
C(20)	0.109(5)	0.083(4)	0.033(3)	-0.052(4)	0.004(3)	0.012(3)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Crystal data for $[HNCH_2CH_2NHCRe(4,4'\text{-}(CO_2Me)_2\text{-}bpy)(CO)_3]ClO_4 \cdot H_2O$ (**6**)

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Re(1)	N(1)	2.178(3)	Re(1)	N(2)	2.172(3)
Re(1)	C(1)	1.908(5)	Re(1)	C(2)	1.928(5)
Re(1)	C(3)	1.966(5)	Re(1)	C(4)	2.163(4)
Cl(1)	O(8)	1.355(5)	Cl(1)	O(9)	1.364(5)
Cl(1)	O(10)	1.352(5)	Cl(1)	O(11)	1.377(6)
O(1)	C(1)	1.159(5)	O(2)	C(2)	1.146(5)
O(3)	C(3)	1.140(5)	O(4)	C(17)	1.203(5)
O(5)	C(17)	1.314(6)	O(5)	C(18)	1.446(6)
O(6)	C(19)	1.195(5)	O(7)	C(19)	1.328(5)
O(7)	C(20)	1.444(6)	N(1)	C(7)	1.350(5)
N(1)	C(11)	1.360(5)	N(2)	C(12)	1.355(5)
N(2)	C(16)	1.353(5)	N(3)	C(4)	1.321(5)
N(3)	C(5)	1.459(6)	N(4)	C(4)	1.318(5)
N(4)	C(6)	1.464(6)	C(5)	C(6)	1.516(8)
C(7)	C(8)	1.363(6)	C(8)	C(9)	1.388(6)
C(9)	C(10)	1.384(5)	C(9)	C(17)	1.497(6)
C(10)	C(11)	1.380(6)	C(11)	C(12)	1.471(5)
C(12)	C(13)	1.390(6)	C(13)	C(14)	1.394(5)
C(14)	C(15)	1.377(6)	C(14)	C(19)	1.491(6)
C(15)	C(16)	1.373(6)			

Crystal data for $[HNCH_2CH_2NHCRe(4,4'\text{-}(CO_2Me)_2\text{-}bpy)(CO)_3]ClO_4 \cdot H_2O$ (**6**)

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Re(1)	N(2)	75.0(1)	N(1)	Re(1)	C(1)	171.3(2)
N(1)	Re(1)	C(2)	98.4(2)	N(1)	Re(1)	C(3)	94.5(2)
N(1)	Re(1)	C(4)	83.5(1)	N(2)	Re(1)	C(1)	97.7(2)
N(2)	Re(1)	C(2)	173.2(1)	N(2)	Re(1)	C(3)	91.9(2)
N(2)	Re(1)	C(4)	87.5(1)	C(1)	Re(1)	C(2)	88.8(2)
C(1)	Re(1)	C(3)	90.5(2)	C(1)	Re(1)	C(4)	91.5(2)
C(2)	Re(1)	C(3)	90.1(2)	C(2)	Re(1)	C(4)	90.3(2)
C(3)	Re(1)	C(4)	178.0(2)	O(8)	Cl(1)	O(9)	109.1(4)
O(8)	Cl(1)	O(10)	111.0(4)	O(8)	Cl(1)	O(11)	110.5(5)
O(9)	Cl(1)	O(10)	112.7(4)	O(9)	Cl(1)	O(11)	107.0(5)
O(10)	Cl(1)	O(11)	106.4(5)	C(17)	O(5)	C(18)	116.8(4)
C(19)	O(7)	C(20)	116.5(4)	Re(1)	N(1)	C(7)	124.9(3)
Re(1)	N(1)	C(11)	116.5(2)	C(7)	N(1)	C(11)	118.2(3)
Re(1)	N(2)	C(12)	116.7(2)	Re(1)	N(2)	C(16)	124.9(3)
C(12)	N(2)	C(16)	118.4(3)	C(4)	N(3)	C(5)	114.6(4)
C(4)	N(4)	C(6)	114.8(4)	Re(1)	C(1)	O(1)	178.7(4)
Re(1)	C(2)	O(2)	179.3(4)	Re(1)	C(3)	O(3)	178.1(4)
Re(1)	C(4)	N(3)	127.1(3)	Re(1)	C(4)	N(4)	126.2(3)
N(3)	C(4)	N(4)	106.7(4)	N(3)	C(5)	C(6)	102.1(4)
N(4)	C(6)	C(5)	101.6(4)	N(1)	C(7)	C(8)	122.9(4)
C(7)	C(8)	C(9)	119.1(4)	C(8)	C(9)	C(10)	118.7(4)
C(8)	C(9)	C(17)	119.0(4)	C(10)	C(9)	C(17)	122.3(4)
C(9)	C(10)	C(11)	119.6(4)	N(1)	C(11)	C(10)	121.3(4)
N(1)	C(11)	C(12)	115.1(3)	C(10)	C(11)	C(12)	123.6(4)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(2)	C(12)	C(11)	116.0(3)	N(2)	C(12)	C(13)	121.6(3)
C(11)	C(12)	C(13)	122.4(4)	C(12)	C(13)	C(14)	119.2(4)
C(13)	C(14)	C(15)	118.6(4)	C(13)	C(14)	C(19)	118.2(4)
C(15)	C(14)	C(19)	123.2(4)	C(14)	C(15)	C(16)	119.8(4)
N(2)	C(16)	C(15)	122.3(4)	O(4)	C(17)	O(5)	125.0(4)
O(4)	C(17)	C(9)	122.9(5)	O(5)	C(17)	C(9)	112.1(4)
O(6)	C(19)	O(7)	124.3(4)	O(6)	C(19)	C(14)	124.0(4)
O(7)	C(19)	C(14)	111.6(4)				

Crystal data for $[HNCH_2CH_2NHCRe(pdpp)(CO)_3]Br$ (**8**)

$\{[Re\,P_2\,O_3\,N_2\,C_{36}\,H_{30}]^+\,Br^-\}$; formula weight = 866.71, triclinic, space group $P\bar{1}$ (No. 2), a = 12.027(8) Å, b = 16.75(1) Å, c = 9.582(3) Å, α = 105.26(4)°, β = 109.93(4)°, γ = 73.23(5)°, V = 1708(1) Å^3, Z = 2, D_c = 1.685 g cm^{-3}, μ(Mo-Kα)= 48.62 cm^{-1}, $F(000)$ = 848, T = 301 K. A colorless crystal of dimensions 0.15 × 0.05 × 0.20 mm in a glass capillary was used for data collection at 28°C on a Rigaku AFC7R diffractometer with graphite monochromatized Mo-Kα radiation (λ = 0.71073 Å) using ω-2θ scans with ω-scan angle $(0.63 + 0.35 \tan\theta)^\circ$ at a scan speed of 16.0 deg min^{-1} (up to 6 scans for reflection $I < 15\,\sigma(I)$). Intensity data (in the range of $2\theta_{max}$ = 50° ; h: 0 to 14; k:-19 to 19; l: -11 to 11 and 3 standard reflections measured after every 300 reflections showed decay of 2.09 %), were corrected for Lorentz and polarization effects, and empirical absorption corrections based on the ψ-scan of six strong reflections (minimum and maximum transmission factors 0.655 and 1.000). 6326 reflections were measured, of which 6008 were unique and R_{int} = 0.038. 4776 reflections with $I > 3\,\sigma(I)$ were considered observed and used in the structural analysis. The space group was determined based on a statistical analysis of intensity distribution and the successful refinement of the structure solved by Patterson methods and expanded by Fourier methods (*PATTY*) and refinement by full-matrix least-squares using the software package *TeXsan* on a Silicon Graphics Indy computer. A crystallographic asymmetric unit consists of atoms in one formula unit. All 45 non-H atoms were refined anisotropically. The two H atoms bonded to N(1) and N(2) were located in difference Fourier synthesis and their positional parameters were refined. The other 28 H atoms at calculated positions with thermal parameters equal to 1.3 times that of the attached C atoms were not refined. Convergence for 412 variable parameters by least-squares refinement on F with $w = 4\,F_o^2 / \sigma^2(F_o^2)$, where $\sigma^2(F_o^2) = [\sigma^2(I) + (0.023\,F_o^2)^2]$ for 4776 reflections with $I > 3\,\sigma(I)$ was reached at R = 0.030 and wR = 0.034 with a goodness-of-fit of 1.25. $(\Delta/\sigma)_{max}$ = 0.01 for non-H atoms. The final difference Fourier map was featureless, with maximum positive and negative peaks of 0.80 and 1.01 e Å^{-3} respectively.

Crystal data for $[HNCH_2CH_2NHCRe(pdpp)(CO)_3]Br$ (**8**)

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Re(1)	0.20549(2)	0.23296(1)	0.45399(2)	2.782(5)
Br(1)	0.39916(7)	0.31132(5)	-0.02473(8)	5.42(2)
P(1)	0.2772(1)	0.13320(9)	0.2504(2)	2.96(3)
P(2)	0.0900(1)	0.31488(9)	0.2534(2)	2.99(3)
O(1)	0.1075(4)	0.3694(3)	0.6973(5)	4.7(1)
O(2)	0.3616(4)	0.1183(3)	0.6875(5)	4.9(1)
O(3)	-0.0001(4)	0.1465(3)	0.4190(5)	5.6(1)
N(1)	0.4014(5)	0.3128(4)	0.4103(6)	4.0(1)
N(2)	0.4184(5)	0.3224(4)	0.6435(6)	5.0(1)
C(1)	0.1448(5)	0.3203(4)	0.6088(6)	3.3(1)
C(2)	0.3060(5)	0.1617(4)	0.6026(6)	3.4(1)
C(3)	0.0756(6)	0.1794(4)	0.4263(6)	3.8(1)
C(4)	0.3565(5)	0.2950(4)	0.5046(7)	3.5(1)
C(5)	0.5009(7)	0.3561(5)	0.4854(10)	6.6(2)
C(6)	0.5148(7)	0.3609(6)	0.6491(10)	6.8(2)
C(7)	0.4376(5)	0.1186(3)	0.2656(6)	3.2(1)
C(8)	0.5225(5)	0.0985(4)	0.3990(7)	4.0(1)
C(9)	0.6443(6)	0.0887(4)	0.4210(7)	4.7(2)
C(10)	0.6836(6)	0.1017(5)	0.3103(9)	5.2(2)
C(11)	0.6006(7)	0.1219(5)	0.1792(9)	5.5(2)
C(12)	0.4773(6)	0.1303(4)	0.1542(7)	4.2(2)
C(13)	0.2567(5)	0.0243(4)	0.2092(6)	3.2(1)
C(14)	0.3521(5)	-0.0460(4)	0.2051(7)	3.8(1)
C(15)	0.3324(7)	-0.1270(4)	0.1753(7)	4.6(2)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(16)	0.2197(7)	-0.1399(4)	0.1475(7)	4.9(2)
C(17)	0.1238(6)	-0.0703(5)	0.1484(8)	5.2(2)
C(18)	0.1410(6)	0.0102(4)	0.1762(7)	4.4(2)
C(19)	0.1886(5)	0.1691(4)	0.0707(6)	3.1(1)
C(20)	0.1960(5)	0.1169(4)	-0.0667(7)	3.7(1)
C(21)	0.1217(6)	0.1419(4)	-0.2004(6)	3.8(1)
C(22)	0.0401(6)	0.2187(4)	-0.1996(6)	4.2(2)
C(23)	0.0330(5)	0.2714(4)	-0.0650(6)	3.7(1)
C(24)	0.1062(5)	0.2479(3)	0.0730(6)	3.1(1)
C(25)	-0.0759(5)	0.3512(4)	0.2128(6)	3.3(1)
C(26)	-0.1450(6)	0.2935(4)	0.1925(7)	4.2(2)
C(27)	-0.2704(6)	0.3191(4)	0.1563(8)	4.9(2)
C(28)	-0.3266(6)	0.4020(5)	0.1410(7)	4.8(2)
C(29)	-0.2583(6)	0.4581(4)	0.1600(7)	4.7(2)
C(30)	-0.1332(6)	0.4342(4)	0.1954(7)	3.9(1)
C(31)	0.1384(5)	0.4121(3)	0.2712(6)	3.3(1)
C(32)	0.1710(6)	0.4300(4)	0.1600(7)	4.5(2)
C(33)	0.2074(7)	0.5051(5)	0.1845(8)	5.3(2)
C(34)	0.2108(7)	0.5625(4)	0.3167(8)	5.1(2)
C(35)	0.1801(6)	0.5443(4)	0.4276(7)	4.3(2)
C(36)	0.1434(6)	0.4697(4)	0.4054(6)	3.8(1)
H(1)	0.378(6)	0.305(4)	0.320(7)	5.2765
H(2)	0.407(6)	0.322(4)	0.732(7)	5.2765
H(3)	0.5721	0.3240	0.4590	7.8640

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(4)	0.4803	0.4108	0.4614	7.8640
H(5)	0.5038	0.4178	0.7003	8.1394
H(6)	0.5918	0.3294	0.6963	8.1394
H(7)	0.4959	0.0912	0.4766	4.7632
H(8)	0.7015	0.0733	0.5116	5.5846
H(9)	0.7676	0.0965	0.3254	6.2586
H(10)	0.6280	0.1303	0.1034	6.5828
H(11)	0.4211	0.1438	0.0619	5.0263
H(12)	0.4313	-0.0383	0.2228	4.5170
H(13)	0.3984	-0.1744	0.1743	5.5255
H(14)	0.2069	-0.1955	0.1276	5.8152
H(15)	0.0446	-0.0785	0.1292	6.2446
H(16)	0.0737	0.0569	0.1732	5.2058
H(17)	0.2523	0.0637	-0.0685	4.5313
H(18)	0.1267	0.1058	-0.2939	4.5401
H(19)	-0.0113	0.2352	-0.2921	5.0321
H(20)	-0.0227	0.3248	-0.0656	4.4526
H(21)	-0.1063	0.2365	0.2032	5.0593
H(22)	-0.3174	0.2794	0.1427	5.8818
H(23)	-0.4122	0.4196	0.1174	5.7050
H(24)	-0.2972	0.5150	0.1487	5.6129
H(25)	-0.0868	0.4741	0.2075	4.7018
H(26)	0.1687	0.3910	0.0675	5.4430
H(27)	0.2305	0.5171	0.1083	6.4146

Crystal data for $[HNCH_2CH_2NHCRe(pdpp)(CO)_3]Br$ (**8**)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(28)	0.2339	0.6144	0.3311	6.0950
H(29)	0.1838	0.5831	0.5203	5.1643
H(30)	0.1216	0.4579	0.4830	4.6049

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Crystal data for $[HNCH_2CH_2NHCRe(pdpp)(CO)_3]Br$ (**8**)

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Re(1)	0.0336(1)	0.0399(1)	0.0327(1)	-0.00602(9)	0.01033(9)	0.00775(9)
Br(1)	0.0570(4)	0.0757(5)	0.0688(5)	-0.0081(4)	0.0131(4)	0.0178(4)
P(1)	0.0352(8)	0.0418(8)	0.0351(7)	-0.0042(6)	0.0112(6)	0.0090(6)
P(2)	0.0389(8)	0.0405(8)	0.0335(7)	-0.0038(6)	0.0121(6)	0.0080(6)
O(1)	0.068(3)	0.054(3)	0.054(3)	-0.002(2)	0.029(2)	0.001(2)
O(2)	0.057(3)	0.067(3)	0.063(3)	0.003(2)	0.017(2)	0.030(2)
O(3)	0.063(3)	0.108(4)	0.061(3)	-0.046(3)	0.015(2)	0.018(3)
N(1)	0.046(3)	0.064(3)	0.053(3)	-0.022(3)	0.016(3)	0.011(3)
N(2)	0.054(3)	0.090(4)	0.052(3)	-0.041(3)	0.008(3)	0.003(3)
C(1)	0.042(3)	0.049(4)	0.036(3)	-0.007(3)	0.009(3)	0.013(3)
C(2)	0.042(3)	0.045(3)	0.042(3)	-0.005(3)	0.017(3)	0.007(3)
C(3)	0.049(4)	0.068(4)	0.027(3)	-0.003(3)	0.010(3)	0.017(3)
C(4)	0.032(3)	0.050(4)	0.047(3)	-0.007(3)	0.010(3)	0.009(3)
C(5)	0.078(6)	0.097(6)	0.090(6)	-0.046(5)	0.027(5)	0.008(5)
C(6)	0.073(6)	0.101(7)	0.092(6)	-0.047(5)	0.016(5)	0.007(5)
C(7)	0.039(3)	0.042(3)	0.042(3)	-0.008(3)	0.013(3)	0.009(3)
C(8)	0.040(3)	0.063(4)	0.046(3)	-0.007(3)	0.011(3)	0.013(3)
C(9)	0.040(4)	0.070(5)	0.058(4)	-0.007(3)	0.008(3)	0.008(3)
C(10)	0.042(4)	0.078(5)	0.079(5)	-0.011(4)	0.024(4)	0.007(4)
C(11)	0.061(5)	0.088(6)	0.080(5)	-0.024(4)	0.037(4)	0.016(4)
C(12)	0.046(4)	0.065(4)	0.055(4)	-0.014(3)	0.018(3)	0.016(3)
C(13)	0.043(3)	0.047(3)	0.034(3)	-0.009(3)	0.013(2)	0.009(2)
C(14)	0.044(4)	0.041(3)	0.056(4)	-0.001(3)	0.016(3)	0.011(3)
C(15)	0.070(5)	0.041(4)	0.061(4)	-0.002(3)	0.021(4)	0.011(3)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(16)	0.077(5)	0.049(4)	0.055(4)	-0.024(4)	0.011(4)	0.003(3)
C(17)	0.059(5)	0.074(5)	0.068(5)	-0.034(4)	0.010(4)	0.005(4)
C(18)	0.046(4)	0.053(4)	0.063(4)	-0.011(3)	0.016(3)	0.003(3)
C(19)	0.043(3)	0.045(3)	0.035(3)	-0.010(3)	0.017(2)	0.006(2)
C(20)	0.047(4)	0.049(4)	0.047(3)	-0.005(3)	0.022(3)	0.006(3)
C(21)	0.050(4)	0.057(4)	0.036(3)	-0.013(3)	0.013(3)	0.005(3)
C(22)	0.060(4)	0.065(4)	0.034(3)	-0.010(3)	0.011(3)	0.015(3)
C(23)	0.054(4)	0.047(3)	0.038(3)	-0.001(3)	0.013(3)	0.014(3)
C(24)	0.039(3)	0.044(3)	0.036(3)	-0.010(3)	0.013(2)	0.005(2)
C(25)	0.037(3)	0.050(4)	0.034(3)	-0.005(3)	0.010(2)	0.007(2)
C(26)	0.047(4)	0.048(4)	0.060(4)	-0.009(3)	0.011(3)	0.006(3)
C(27)	0.047(4)	0.064(5)	0.068(4)	-0.022(3)	0.007(3)	0.005(4)
C(28)	0.035(4)	0.070(5)	0.058(4)	0.000(3)	0.003(3)	0.007(3)
C(29)	0.050(4)	0.051(4)	0.063(4)	0.008(3)	0.014(3)	0.012(3)
C(30)	0.051(4)	0.043(3)	0.054(4)	-0.001(3)	0.019(3)	0.011(3)
C(31)	0.038(3)	0.041(3)	0.045(3)	-0.002(3)	0.014(3)	0.012(3)
C(32)	0.069(5)	0.061(4)	0.053(4)	-0.020(4)	0.026(3)	0.009(3)
C(33)	0.075(5)	0.077(5)	0.072(5)	-0.023(4)	0.033(4)	0.024(4)
C(34)	0.067(5)	0.057(4)	0.074(5)	-0.022(4)	0.015(4)	0.015(4)
C(35)	0.064(4)	0.049(4)	0.049(4)	-0.021(3)	0.011(3)	0.001(3)
C(36)	0.054(4)	0.050(4)	0.044(3)	-0.010(3)	0.017(3)	0.011(3)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Crystal data for $[HNCH_2CH_2NHCRe(pdpp)(CO)_3]Br$ (**8**)

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Re(1)	P(1)	2.437(1)	Re(1)	P(2)	2.444(1)
Re(1)	C(1)	1.963(6)	Re(1)	C(2)	1.950(6)
Re(1)	C(3)	1.928(7)	Re(1)	C(4)	2.199(6)
P(1)	C(7)	1.833(6)	P(1)	C(13)	1.832(6)
P(1)	C(19)	1.841(5)	P(2)	C(24)	1.836(5)
P(2)	C(25)	1.843(6)	P(2)	C(31)	1.832(6)
O(1)	C(1)	1.130(6)	O(2)	C(2)	1.140(6)
O(3)	C(3)	1.168(7)	N(1)	C(4)	1.328(7)
N(1)	C(5)	1.454(9)	N(2)	C(4)	1.318(7)
N(2)	C(6)	1.460(9)	C(5)	C(6)	1.50(1)
C(7)	C(8)	1.389(8)	C(7)	C(12)	1.384(7)
C(8)	C(9)	1.374(8)	C(9)	C(10)	1.385(9)
C(10)	C(11)	1.365(10)	C(11)	C(12)	1.390(9)
C(13)	C(14)	1.390(7)	C(13)	C(18)	1.394(8)
C(14)	C(15)	1.385(8)	C(15)	C(16)	1.358(9)
C(16)	C(17)	1.384(10)	C(17)	C(18)	1.367(9)
C(19)	C(20)	1.391(7)	C(19)	C(24)	1.403(7)
C(20)	C(21)	1.379(8)	C(21)	C(22)	1.375(8)
C(22)	C(23)	1.372(8)	C(23)	C(24)	1.400(7)
C(25)	C(26)	1.384(8)	C(25)	C(30)	1.388(8)
C(26)	C(27)	1.388(9)	C(27)	C(28)	1.380(9)
C(28)	C(29)	1.359(9)	C(29)	C(30)	1.384(9)
C(31)	C(32)	1.378(8)	C(31)	C(36)	1.383(8)
C(32)	C(33)	1.386(9)	C(33)	C(34)	1.370(9)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(34)	C(35)	1.364(9)	C(35)	C(36)	1.385(8)

Crystal data for $[HNCH_2CH_2NHCRe(pdpp)(CO)_3]Br$ (**8**)

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	Re(1)	P(2)	82.57(5)	P(1)	Re(1)	C(1)	175.5(2)
P(1)	Re(1)	C(2)	92.7(2)	P(1)	Re(1)	C(3)	94.1(2)
P(1)	Re(1)	C(4)	89.1(2)	P(2)	Re(1)	C(1)	93.3(2)
P(2)	Re(1)	C(2)	175.1(2)	P(2)	Re(1)	C(3)	93.9(2)
P(2)	Re(1)	C(4)	89.5(2)	C(1)	Re(1)	C(2)	91.4(2)
C(1)	Re(1)	C(3)	87.9(2)	C(1)	Re(1)	C(4)	89.1(2)
C(2)	Re(1)	C(3)	87.7(2)	C(2)	Re(1)	C(4)	89.1(2)
C(3)	Re(1)	C(4)	175.6(2)	Re(1)	P(1)	C(7)	116.2(2)
Re(1)	P(1)	C(13)	118.3(2)	Re(1)	P(1)	C(19)	108.8(2)
C(7)	P(1)	C(13)	103.2(3)	C(7)	P(1)	C(19)	107.1(2)
C(13)	P(1)	C(19)	101.8(2)	Re(1)	P(2)	C(24)	108.3(2)
Re(1)	P(2)	C(25)	120.3(2)	Re(1)	P(2)	C(31)	115.1(2)
C(24)	P(2)	C(25)	102.0(2)	C(24)	P(2)	C(31)	107.0(2)
C(25)	P(2)	C(31)	102.6(3)	C(4)	N(1)	C(5)	113.8(6)
C(4)	N(2)	C(6)	113.0(6)	Re(1)	C(1)	O(1)	178.1(5)
Re(1)	C(2)	O(2)	177.5(5)	Re(1)	C(3)	O(3)	175.7(5)
Re(1)	C(4)	N(1)	129.3(4)	Re(1)	C(4)	N(2)	122.8(4)
N(1)	C(4)	N(2)	107.9(5)	N(1)	C(5)	C(6)	102.0(6)
N(2)	C(6)	C(5)	103.2(6)	P(1)	C(7)	C(8)	117.7(4)
P(1)	C(7)	C(12)	123.3(4)	C(8)	C(7)	C(12)	118.9(5)
C(7)	C(8)	C(9)	121.3(6)	C(8)	C(9)	C(10)	119.6(6)
C(9)	C(10)	C(11)	119.3(6)	C(10)	C(11)	C(12)	121.7(6)
C(7)	C(12)	C(11)	119.1(6)	P(1)	C(13)	C(14)	122.5(5)
P(1)	C(13)	C(18)	119.5(4)	C(14)	C(13)	C(18)	117.9(6)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(13)	C(14)	C(15)	120.4(6)	C(14)	C(15)	C(16)	121.1(6)
C(15)	C(16)	C(17)	118.9(6)	C(16)	C(17)	C(18)	121.0(6)
C(13)	C(18)	C(17)	120.6(6)	P(1)	C(19)	C(20)	120.9(4)
P(1)	C(19)	C(24)	119.1(4)	C(20)	C(19)	C(24)	119.8(5)
C(19)	C(20)	C(21)	120.2(5)	C(20)	C(21)	C(22)	120.5(5)
C(21)	C(22)	C(23)	119.9(5)	C(22)	C(23)	C(24)	121.2(5)
P(2)	C(24)	C(19)	120.2(4)	P(2)	C(24)	C(23)	121.4(4)
C(19)	C(24)	C(23)	118.4(5)	P(2)	C(25)	C(26)	119.3(4)
P(2)	C(25)	C(30)	121.3(5)	C(26)	C(25)	C(30)	119.4(5)
C(25)	C(26)	C(27)	120.0(6)	C(26)	C(27)	C(28)	120.3(6)
C(27)	C(28)	C(29)	119.5(6)	C(28)	C(29)	C(30)	121.4(6)
C(25)	C(30)	C(29)	119.5(6)	P(2)	C(31)	C(32)	123.7(5)
P(2)	C(31)	C(36)	117.3(4)	C(32)	C(31)	C(36)	119.0(6)
C(31)	C(32)	C(33)	119.5(6)	C(32)	C(33)	C(34)	121.4(6)
C(33)	C(34)	C(35)	119.2(6)	C(34)	C(35)	C(36)	120.3(6)
C(31)	C(36)	C(35)	120.6(6)				