Inorganic Chemistry
including bioinorganic chemistry
Inorg. Chem., 1998, 37(12), 3122-3126, DOI:10.1021/ic971483j

Table S1

CRYSTAL DATA AND DATA COLLECTION PARAMETERS for

$[Re_2Br_3(dppm)_2(CO)(CNxyl)_2]PF_6 \cdot 2CH_2Cl_2$ 5b

| | |
|---|---|
| formula | $Re_2Br_3Cl_4P_5F_6ON_2C_{71}H_{66}$ |
| formula weight | 1986.13 |
| space group | P1 (No. 2) |
| a, Å | 13.800(5) |
| b, Å | 16.927(8) |
| c, Å | 17.556(5) |
| $\alpha$, deg | 87.05(7) |
| $\beta$, deg | 77.56(6) |
| $\gamma$, deg | 69.67(7) |
| V, Å$^3$ | 3753(7) |
| Z | 2 |
| $d_{calc}$, g cm$^{-3}$ | 1.757 |
| crystal dimensions, mm | 0.38x0.20x0.07 |
| temperature, K | 203. |
| radiation (wavelength) | Mo $K_\alpha$(0.71073Å) |
| monochromator | graphite |
| linear abs coef, mm$^{-1}$ | 5.153 |
| absorption correction applied | empirical[a] |
| transmission factors: min, max | 0.54, 0.91 |
| diffractometer | Enraf-Nonius CAD4 |
| scan method | $\omega$-2$\theta$ |
| h, k, l range | -13 to 13 0 to 18 -18 to 18 |
| 2$\theta$ range, deg | 5.52-45.12 |
| scan width, deg | 0.73 + 0.68tan($\theta$) |
| take-off angle, deg | 3.00 |
| programs used | SHELXL-93 |
| $F_{000}$ | 1932.0 |
| weighting | |
| $w=1/[\sigma^2(Fo^2)+(0.1596P)^2+26.4359P]$ where $P=(Fo^2+2Fc^2)/3$ | |
| data collected | 9589 |
| unique data | 9222 |
| $R_{int}$ | 0.058 |
| data used in refinement | 9222 |
| cutoff used in R-factor calculations | $F_o^2>2\sigma(F_o^2)$ |
| number of variables | 848 |
| largest shift/esd in final cycle | 0.00 |
| $R(F_o)$ | 0.065 |
| $R_w(F_o^2)$ | 0.185 |
| goodness of fit | 1.021 |

[a] Walker, N.; Stuart, D. Acta Crystallogr., Sect. A 1983, A39, 158.

Table S2

**Positional Parameters and Their Estimated Standard Deviations**

**for $[Re_2Br_3(dppm)_2(CO)(CNxyl)_2]PF_6 \cdot 2CH_2Cl_2$ 5b**

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| Re(1) | 0.09869(5) | 0.28774(4) | 0.24326(4) | 0.0232(2) |
| Re(2) | 0.28220(5) | 0.21501(4) | 0.32449(4) | 0.0261(3) |
| Br(1) | 0.26872(14) | 0.15846(11) | 0.19643(10) | 0.0359(6) |
| Br(2) | 0.12004(15) | 0.34548(11) | 0.37101(10) | 0.0375(6) |
| Br(3A) | 0.3440(4) | 0.2249(3) | 0.4499(4) | 0.0448(18) |
| Br(3B) | 0.4692(4) | 0.1065(4) | 0.3093(3) | 0.0539(19) |
| P(1) | 0.1791(3) | 0.3864(3) | 0.1757(2) | 0.0261(13) |
| P(2) | 0.3649(3) | 0.3137(3) | 0.2577(2) | 0.0251(13) |
| P(3) | 0.0164(4) | 0.1892(3) | 0.3085(3) | 0.0303(16) |
| P(4) | 0.2000(4) | 0.1180(3) | 0.3936(3) | 0.0282(15) |
| O(3A) | 0.347(3) | 0.232(3) | 0.478(2) | 0.0520(15)* |
| O(3B) | 0.487(2) | 0.069(2) | 0.2915(19) | 0.0410(15)* |
| N(10) | -0.0492(11) | 0.7517(8) | -0.0848(8) | 0.031(5) |
| N(20) | -0.1223(13) | 0.4335(10) | 0.2848(8) | 0.042(6) |
| C(10) | 0.0644(13) | 0.2612(10) | 0.1434(10) | 0.026(6) * |
| C(11) | -0.0369(14) | 0.7815(11) | -0.0138(9) | 0.032(6) |
| C(12) | -0.1155(16) | 0.8550(12) | 0.0241(11) | 0.041(7) |
| C(13) | 0.099(2) | 0.1177(13) | 0.9074(11) | 0.052(9) |
| C(14) | -0.013(3) | 0.8363(16) | 0.1233(14) | 0.076(12) |
| C(15) | 0.064(2) | 0.7647(17) | 0.0833(12) | 0.067(11) |
| C(16) | 0.0544(15) | 0.7375(14) | 0.0154(11) | 0.049(8) |
| C(17) | 0.2092(17) | 0.0962(13) | 0.0090(13) | 0.057(8) |
| C(18) | 0.1329(18) | 0.6512(13) | -0.0249(13) | 0.063(9) |
| C(1B) | 0.2670(13) | 0.4099(10) | 0.2273(10) | 0.029(6) |
| C(20) | 0.0421(16) | 0.6192(15) | 0.7328(9) | 0.048(8) |
| C(21) | -0.2248(13) | 0.4999(11) | 0.3130(10) | 0.033(6) |
| C(22) | -0.3082(14) | 0.5039(10) | 0.2778(10) | 0.034(7) |
| C(23) | 0.4052(16) | 0.4309(13) | 0.6965(14) | 0.056(8) |
| C(24) | -0.4153(19) | 0.6223(15) | 0.3682(17) | 0.075(11) |
| C(25) | -0.3304(18) | 0.6134(15) | 0.4006(15) | 0.074(10) |
| C(26) | 0.2315(16) | 0.4504(12) | 0.6252(13) | 0.049(8) |
| C(27) | -0.2968(16) | 0.4497(14) | 0.2139(11) | 0.053(8) |
| C(28) | -0.1402(17) | 0.5417(13) | 0.4133(13) | 0.055(9) |
| C(2B) | 0.1118(16) | 0.0935(12) | 0.3391(11) | 0.047(7) |
| C(3A) | 0.310(3) | 0.222(2) | 0.4242(19) | 0.016(7) * |
| C(3B) | 0.394(4) | 0.114(3) | 0.295(4) | 0.105(7) * |
| C(111) | 0.2563(13) | 0.3669(11) | 0.0736(10) | 0.030(6) |
| C(112) | 0.2743(16) | 0.2976(15) | 0.0331(12) | 0.057(8) |
| C(113) | 0.3315(15) | 0.2899(13) | -0.0448(11) | 0.049(7) |
| C(114) | 0.3727(16) | 0.3468(15) | 0.9182(12) | 0.053(8) |
| C(115) | 0.3509(16) | 0.4191(15) | -0.0375(12) | 0.057(8) |
| C(116) | 0.2968(15) | 0.4307(13) | 0.0397(10) | 0.045(7) |
| C(121) | 0.0755(14) | 0.4885(11) | 0.1663(10) | 0.035(6) |
| C(122) | 0.0136(13) | 0.4914(10) | 0.1140(10) | 0.033(6) |

Table S2 (continued)

**Positional Parameters and Their Estimated Standard Deviations (cont.)**

**for $[Re_2Br_3(dppm)_2(CO)(CNxyl)_2]PF_6 \cdot 2CH_2Cl_2$ 5b**

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| C(123) | -0.0742(16) | 0.5644(13) | 0.1110(12) | 0.049(8) |
| C(124) | -0.0983(15) | 0.6338(14) | 0.1573(12) | 0.050(8) |
| C(125) | 0.0353(16) | 0.3703(13) | 0.7927(12) | 0.047(8) * |
| C(126) | 0.0516(14) | 0.5594(11) | 0.2125(12) | 0.042(7) |
| C(211) | 0.4687(13) | 0.2823(11) | 0.1667(11) | 0.036(6) |
| C(212) | 0.5121(14) | 0.2034(12) | 0.1328(11) | 0.038(7) |
| C(213) | 0.5935(15) | 0.1843(16) | 0.0673(12) | 0.057(8) |
| C(214) | 0.6309(16) | 0.2416(14) | 0.0317(12) | 0.047(8) |
| C(215) | 0.5885(17) | 0.3267(15) | 0.0652(12) | 0.057(9) |
| C(216) | 0.5110(16) | 0.3429(14) | 0.1317(12) | 0.052(8) |
| C(221) | 0.4328(14) | 0.3544(10) | 0.3225(10) | 0.030(6) |
| C(222) | 0.3879(16) | 0.4294(12) | 0.3579(11) | 0.043(7) |
| C(223) | 0.441(2) | 0.4558(15) | 0.4063(14) | 0.078(11) |
| C(224) | 0.537(2) | 0.4045(16) | 0.4191(13) | 0.072(11) |
| C(225) | 0.5803(18) | 0.3259(16) | 0.3819(12) | 0.058(9) |
| C(226) | 0.5297(16) | 0.3009(12) | 0.3329(11) | 0.046(8) |
| C(311) | -0.0922(12) | 0.2181(13) | 0.3951(10) | 0.037(7) |
| C(312) | -0.1199(15) | 0.2929(13) | 0.4385(11) | 0.043(8) |
| C(313) | -0.1972(16) | 0.3119(15) | 0.5096(12) | 0.057(9) |
| C(314) | -0.2442(15) | 0.2528(14) | 0.5342(12) | 0.048(8) |
| C(315) | 0.218(2) | 0.8213(15) | 0.5061(16) | 0.079(10) |
| C(316) | -0.1432(15) | 0.1638(16) | 0.4270(13) | 0.061(8) |
| C(321) | -0.0472(15) | 0.1494(10) | 0.2407(11) | 0.039(7) |
| C(322) | -0.1453(16) | 0.1945(13) | 0.2317(12) | 0.048(8) |
| C(323) | -0.1935(19) | 0.1785(14) | 0.1785(14) | 0.059(9) |
| C(324) | -0.137(2) | 0.1112(15) | 0.1296(15) | 0.064(11) |
| C(325) | -0.032(2) | 0.0624(15) | 0.1370(15) | 0.076(11) |
| C(326) | 0.0110(16) | 0.0834(13) | 0.1920(12) | 0.044(8) |
| C(411) | 0.1196(15) | 0.1429(12) | 0.4938(11) | 0.042(7) |
| C(412) | 0.0968(17) | 0.2125(13) | 0.5311(12) | 0.054(8) |
| C(413) | 0.0262(13) | 0.2342(16) | 0.6075(13) | 0.061(9) |
| C(414) | 0.0163(19) | 0.8221(19) | 0.3577(12) | 0.075(12) |
| C(415) | 0.008(2) | 0.098(2) | 0.6038(14) | 0.084(13) |
| C(416) | 0.0752(17) | 0.0827(15) | 0.5324(13) | 0.057(9) |
| C(421) | 0.3000(14) | 0.0135(11) | 0.4057(11) | 0.036(7) |
| C(422) | 0.3316(18) | -0.0506(12) | 0.3522(11) | 0.052(8) |
| C(423) | 0.4123(18) | 0.8740(13) | 0.3600(12) | 0.058(8) |
| C(424) | 0.4605(15) | -0.1358(12) | 0.4211(13) | 0.050(8) |
| C(425) | 0.4277(15) | -0.0722(11) | 0.4766(13) | 0.047(8) |
| C(426) | 0.3458(16) | 0.0016(12) | 0.4686(12) | 0.046(8) |
| P(100) | 0.3186(4) | 0.6470(3) | 0.2117(3) | 0.0391(18) |
| F(101) | 0.2734(14) | 0.6061(10) | 0.1500(10) | 0.109(8) |
| F(102) | 0.3821(16) | 0.6820(12) | 0.1390(10) | 0.125(9) |
| F(103) | 0.4130(12) | 0.5596(9) | 0.2002(9) | 0.092(6) |
| F(104) | 0.2511(14) | 0.6133(11) | 0.2799(9) | 0.110(8) |

Table S2 (continued)

**Positional Parameters and Their Estimated Standard Deviations (cont.)**

**for $[Re_2Br_3(dppm)_2(CO)(CNxyl)_2]PF_6 \cdot 2CH_2Cl_2$ 5b**

| Atom | x | y | z | U(Å$^2$) |
|---|---|---|---|---|
| F(105) | 0.2202(12) | 0.7352(9) | 0.2155(9) | 0.096(6) |
| F(106) | 0.3643(12) | 0.6855(10) | 0.2672(11) | 0.111(8) |
| Cl(91) | 0.2770(8) | 0.9137(5) | 0.1440(5) | 0.130(4) |
| Cl(92) | 0.4699(13) | 0.9389(11) | 0.1099(15) | 0.307(13) |
| Cl(93) | 0.2395(7) | 0.0158(10) | 0.7079(6) | 0.154(6) |
| Cl(94) | 0.2940(15) | 0.1655(14) | 0.7389(13) | 0.304(13) |
| C(900) | 0.401(3) | 0.866(2) | 0.1383(15) | 0.108(15) |
| C(901) | 0.292(4) | 0.095(3) | 0.678(3) | 0.17(3) |

Starred atoms were refined isotropically

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a^*_i a^*_j a_i \cdot a_j$

Table S3

**Positional Parameters and Their Estimated Standard Deviations**

**for $[Re_2Br_3(dppm)_2(CO)(CNxyl)_2]PF_6 \cdot 2CH_2Cl_2$ 5b**

| Atom | x | y | z | U(Å$^2$) |
|---|---|---|---|---|
| H(13) | 0.147(2) | 0.0680(13) | 0.8823(11) | 0.068 |
| H(14) | -0.006(3) | 0.8529(16) | 0.1709(14) | 0.099 |
| H(15) | 0.123(2) | 0.7354(17) | 0.1039(12) | 0.087 |
| H(23) | 0.4616(16) | 0.4223(13) | 0.7208(14) | 0.072 |
| H(24) | -0.4803(19) | 0.6632(15) | 0.3883(17) | 0.098 |
| H(25) | -0.3381(18) | 0.6504(15) | 0.4406(15) | 0.096 |
| H(112) | 0.2499(16) | 0.2551(15) | 0.0553(12) | 0.074 |
| H(113) | 0.3418(15) | 0.2416(13) | -0.0730(11) | 0.064 |
| H(114) | 0.4122(16) | 0.3383(15) | 0.8673(12) | 0.069 |
| H(115) | 0.3739(16) | 0.4618(15) | -0.0608(12) | 0.075 |
| H(116) | 0.2871(15) | 0.4784(13) | 0.0685(10) | 0.058 |
| H(122) | 0.0295(13) | 0.4455(10) | 0.0808(10) | 0.043 |
| H(123) | -0.1172(16) | 0.5653(13) | 0.0765(12) | 0.063 |
| H(124) | -0.1559(15) | 0.6821(14) | 0.1543(12) | 0.065 |
| H(125) | 0.0509(16) | 0.3238(13) | 0.7602(12) | 0.062 |
| H(126) | 0.0941(14) | 0.5596(11) | 0.2469(12) | 0.054 |
| H(17A) | 0.1861(17) | 0.083(7) | 0.062(3) | 0.074 |
| H(17B) | 0.254(6) | 0.129(4) | 0.007(7) | 0.074 |
| H(17C) | 0.248(6) | 0.045(4) | -0.021(5) | 0.074 |
| H(18A) | 0.203(2) | 0.653(3) | -0.037(7) | 0.081 |
| H(18B) | 0.113(7) | 0.642(5) | -0.072(5) | 0.081 |
| H(18C) | 0.130(8) | 0.6061(15) | 0.010(4) | 0.081 |
| H(1B1) | 0.2252(13) | 0.4446(10) | 0.2732(10) | 0.038 |
| H(1B2) | 0.3044(13) | 0.4421(10) | 0.1938(10) | 0.038 |
| H(212) | 0.4864(14) | 0.1613(12) | 0.1543(11) | 0.050 |
| H(213) | 0.6228(15) | 0.1292(16) | 0.0476(12) | 0.074 |
| H(214) | 0.6831(16) | 0.2279(14) | -0.0138(12) | 0.062 |
| H(215) | 0.6133(17) | 0.3687(15) | 0.0423(12) | 0.074 |
| H(216) | 0.4851(16) | 0.3965(14) | 0.1547(12) | 0.068 |
| H(222) | 0.3218(16) | 0.4645(12) | 0.3509(11) | 0.056 |
| H(223) | 0.410(2) | 0.5091(15) | 0.4300(14) | 0.102 |
| H(224) | 0.571(2) | 0.4216(16) | 0.4514(13) | 0.094 |
| H(225) | 0.6450(18) | 0.2892(16) | 0.3901(12) | 0.075 |
| H(226) | 0.5607(16) | 0.2485(12) | 0.3073(11) | 0.059 |
| H(27A) | -0.3652(18) | 0.458(6) | 0.204(5) | 0.069 |
| H(27B) | -0.264(9) | 0.3920(15) | 0.227(3) | 0.069 |
| H(27C) | -0.253(8) | 0.463(6) | 0.168(2) | 0.069 |
| H(28A) | -0.122(7) | 0.489(4) | 0.440(6) | 0.072 |
| H(28B) | -0.161(4) | 0.588(5) | 0.450(6) | 0.072 |
| H(28C) | -0.080(4) | 0.543(8) | 0.3741(16) | 0.072 |
| H(2B1) | 0.1545(16) | 0.0589(12) | 0.2934(11) | 0.061 |
| H(2B2) | 0.0737(16) | 0.0614(12) | 0.3719(11) | 0.061 |
| H(312) | -0.0866(15) | 0.3315(13) | 0.4202(11) | 0.056 |
| H(313) | -0.2150(16) | 0.3616(15) | 0.5380(12) | 0.074 |

Table S3 (continued)

**Positional Parameters and Their Estimated Standard Deviations (cont.)**

**for $[Re_2Br_3(dppm)_2(CO)(CNxyl)_2]PF_6 \cdot 2CH_2Cl_2$ 5b**

| Atom | x | y | z | U(Å$^2$) |
|---|---|---|---|---|
| H(314) | -0.2957(15) | 0.2636(14) | 0.5801(12) | 0.062 |
| H(315) | 0.251(2) | 0.8603(15) | 0.4882(16) | 0.103 |
| H(316) | -0.1248(15) | 0.1126(16) | 0.4007(13) | 0.079 |
| H(322) | -0.1832(16) | 0.2408(13) | 0.2653(12) | 0.063 |
| H(323) | -0.2621(19) | 0.2119(14) | 0.1754(14) | 0.077 |
| H(324) | -0.166(2) | 0.0971(15) | 0.0916(15) | 0.083 |
| H(325) | 0.007(2) | 0.0159(15) | 0.1040(15) | 0.099 |
| H(326) | 0.0800(16) | 0.0524(13) | 0.1959(12) | 0.058 |
| H(412) | 0.1271(17) | 0.2514(13) | 0.5080(12) | 0.070 |
| H(413) | 0.0110(18) | 0.2860(16) | 0.6316(13) | 0.079 |
| H(414) | 0.0612(19) | 0.8097(19) | 0.3088(12) | 0.098 |
| H(415) | -0.022(2) | 0.059(2) | 0.6267(14) | 0.110 |
| H(416) | 0.0931(17) | 0.0307(15) | 0.5077(13) | 0.075 |
| H(422) | 0.2992(18) | -0.0441(12) | 0.3099(11) | 0.068 |
| H(423) | 0.4329(18) | 0.8305(13) | 0.3232(12) | 0.075 |
| H(424) | 0.5156(15) | -0.1854(12) | 0.4255(13) | 0.065 |
| H(425) | 0.4600(15) | -0.0786(11) | 0.5189(13) | 0.061 |
| H(426) | 0.3218(16) | 0.0438(12) | 0.5071(12) | 0.059 |
| H(90A) | 0.427(3) | 0.820(2) | 0.1001(15) | 0.140 |
| H(90B) | 0.413(3) | 0.842(2) | 0.1884(15) | 0.140 |
| H(90C) | 0.365(4) | 0.067(3) | 0.651(3) | 0.220 |
| H(90D) | 0.255(4) | 0.126(3) | 0.639(3) | 0.220 |

Hydrogens included in calculation of structure factors but not refined
$B_{iso}(H)=1.3*B_{iso}(C)$

Table S4

**Anisotropic Temperature Factor Coefficients - U's**

**for $[Re_2Br_3(dppm)_2(CO)(CNxyl)_2]PF_6 \cdot 2CH_2Cl_2$ 5b**

| Name | U(1,1) | U(2,2) | U(3,3) | U(1,2) | U(1,3) | U(2,3) |
|---|---|---|---|---|---|---|
| Re(1) | 0.0216(4) | 0.0226(4) | 0.0251(4) | -0.0062(3) | -0.0070(3) | 0.0024(3) |
| Re(2) | 0.0246(5) | 0.0248(4) | 0.0297(4) | -0.0072(3) | -0.0107(3) | 0.0045(3) |
| Br(1) | 0.0315(10) | 0.0326(10) | 0.0403(10) | -0.0041(8) | -0.0111(8) | -0.0042(8) |
| Br(2) | 0.0389(11) | 0.0354(10) | 0.0353(10) | -0.0069(9) | -0.0122(8) | 0.0019(8) |
| Br(3A) | 0.057(3) | 0.046(3) | 0.050(3) | -0.024(2) | -0.041(3) | 0.007(2) |
| Br(3B) | 0.056(3) | 0.053(3) | 0.051(3) | -0.019(3) | -0.008(2) | 0.003(3) |
| P(1) | 0.025(2) | 0.027(2) | 0.028(2) | -0.010(2) | -0.009(2) | 0.008(2) |
| P(2) | 0.023(2) | 0.026(2) | 0.030(2) | -0.013(2) | -0.007(2) | 0.006(2) |
| P(3) | 0.026(3) | 0.031(3) | 0.031(2) | -0.009(2) | -0.003(2) | 0.009(2) |
| P(4) | 0.030(3) | 0.025(2) | 0.031(2) | -0.010(2) | -0.010(2) | 0.008(2) |
| N(10) | 0.034(9) | 0.022(8) | 0.039(9) | -0.007(7) | -0.015(7) | 0.002(6) |
| N(20) | 0.038(11) | 0.041(10) | 0.030(9) | 0.000(9) | 0.003(7) | 0.014(7) |
| C(11) | 0.038(11) | 0.045(11) | 0.023(9) | -0.027(9) | -0.007(8) | 0.001(8) |
| C(12) | 0.044(12) | 0.049(12) | 0.043(11) | -0.030(10) | -0.012(10) | 0.000(10) |
| C(13) | 0.104(19) | 0.040(12) | 0.040(12) | -0.047(13) | -0.038(13) | 0.006(10) |
| C(14) | 0.13(3) | 0.069(17) | 0.041(14) | -0.054(18) | -0.015(16) | 0.001(13) |
| C(15) | 0.077(17) | 0.10(2) | 0.036(12) | -0.042(16) | -0.029(12) | 0.018(13) |
| C(16) | 0.033(12) | 0.084(16) | 0.040(12) | -0.033(11) | -0.011(9) | 0.015(11) |
| C(17) | 0.054(14) | 0.045(13) | 0.068(15) | -0.022(11) | 0.010(12) | -0.016(11) |
| C(18) | 0.061(15) | 0.050(14) | 0.058(14) | 0.008(11) | -0.021(12) | 0.011(11) |
| C(1B) | 0.035(10) | 0.022(9) | 0.028(9) | -0.013(8) | 0.000(8) | 0.017(7) |
| C(20) | 0.037(12) | 0.081(16) | 0.008(8) | -0.002(12) | -0.005(8) | 0.022(9) |
| C(21) | 0.017(9) | 0.029(10) | 0.041(11) | 0.004(8) | -0.001(8) | 0.008(8) |
| C(22) | 0.042(12) | 0.022(9) | 0.041(11) | -0.013(9) | -0.016(9) | 0.016(8) |
| C(23) | 0.032(12) | 0.051(14) | 0.077(16) | -0.010(10) | -0.004(11) | 0.002(12) |
| C(24) | 0.042(15) | 0.050(15) | 0.12(2) | 0.000(12) | -0.009(15) | -0.004(15) |
| C(25) | 0.051(15) | 0.067(17) | 0.090(19) | -0.005(13) | 0.002(14) | -0.054(14) |
| C(26) | 0.043(12) | 0.035(11) | 0.075(15) | -0.015(10) | -0.022(11) | -0.013(11) |
| C(27) | 0.041(12) | 0.080(16) | 0.037(11) | -0.026(12) | 0.002(10) | 0.006(11) |
| C(28) | 0.061(15) | 0.050(13) | 0.061(14) | -0.029(12) | -0.006(12) | -0.014(11) |
| C(2B) | 0.056(13) | 0.031(11) | 0.042(11) | -0.008(10) | -0.004(10) | 0.027(9) |
| C(111) | 0.028(10) | 0.039(11) | 0.032(10) | -0.016(9) | -0.013(8) | -0.008(9) |
| C(112) | 0.040(13) | 0.072(16) | 0.046(13) | -0.001(11) | -0.018(10) | 0.018(12) |
| C(113) | 0.041(12) | 0.051(13) | 0.034(11) | 0.008(10) | 0.000(9) | -0.014(10) |
| C(114) | 0.036(12) | 0.072(16) | 0.035(11) | -0.007(11) | 0.004(9) | 0.020(12) |
| C(115) | 0.044(13) | 0.060(15) | 0.042(13) | 0.009(11) | -0.003(10) | 0.012(11) |
| C(116) | 0.043(12) | 0.054(13) | 0.025(10) | -0.020(10) | 0.025(9) | -0.008(9) |
| C(121) | 0.033(11) | 0.026(10) | 0.036(10) | -0.006(8) | 0.005(9) | 0.005(8) |
| C(122) | 0.035(11) | 0.011(8) | 0.048(11) | 0.009(8) | -0.026(9) | -0.008(8) |
| C(123) | 0.048(13) | 0.060(14) | 0.049(12) | -0.029(12) | -0.018(10) | 0.018(11) |
| C(124) | 0.026(11) | 0.058(14) | 0.062(14) | -0.009(10) | -0.012(10) | 0.009(12) |
| C(126) | 0.031(11) | 0.020(10) | 0.073(14) | -0.003(8) | -0.020(10) | 0.008(9) |
| C(211) | 0.012(9) | 0.029(11) | 0.060(12) | 0.000(8) | -0.010(9) | 0.011(9) |
| C(212) | 0.032(11) | 0.042(12) | 0.046(11) | -0.015(9) | -0.013(9) | -0.004(9) |

Table S4 (continued)

**Anisotropic Temperature Factor Coefficients - U's (Continued)**

**for $[Re_2Br_3(dppm)_2(CO)(CNxyl)_2]PF_6 \cdot 2CH_2Cl_2$ 5b**

| Name | U(1,1) | U(2,2) | U(3,3) | U(1,2) | U(1,3) | U(2,3) |
|---|---|---|---|---|---|---|
| C(213) | 0.022(11) | 0.081(17) | 0.055(13) | -0.012(11) | 0.013(10) | -0.020(12) |
| C(214) | 0.034(12) | 0.075(16) | 0.052(13) | -0.037(12) | -0.017(10) | 0.001(12) |
| C(215) | 0.049(14) | 0.063(15) | 0.049(13) | -0.017(12) | 0.004(11) | 0.013(11) |
| C(216) | 0.046(13) | 0.047(13) | 0.052(13) | -0.009(10) | -0.002(11) | 0.016(10) |
| C(221) | 0.036(11) | 0.022(10) | 0.034(10) | -0.014(8) | -0.007(8) | 0.010(8) |
| C(222) | 0.042(12) | 0.040(12) | 0.058(13) | -0.019(10) | -0.024(10) | -0.002(10) |
| C(223) | 0.084(19) | 0.065(16) | 0.076(17) | 0.009(14) | -0.050(15) | -0.035(13) |
| C(224) | 0.084(19) | 0.082(18) | 0.052(14) | -0.009(15) | -0.046(14) | -0.009(13) |
| C(225) | 0.052(14) | 0.082(17) | 0.055(14) | -0.032(13) | -0.033(12) | 0.020(13) |
| C(226) | 0.048(13) | 0.044(12) | 0.055(13) | -0.024(11) | -0.014(11) | -0.020(10) |
| C(311) | 0.007(9) | 0.069(14) | 0.025(9) | -0.008(9) | 0.005(7) | 0.010(9) |
| C(312) | 0.042(12) | 0.064(14) | 0.042(11) | -0.044(11) | -0.002(10) | -0.004(10) |
| C(313) | 0.042(13) | 0.079(17) | 0.043(12) | -0.015(12) | -0.001(10) | -0.005(11) |
| C(314) | 0.030(11) | 0.067(15) | 0.059(13) | -0.038(12) | -0.004(10) | 0.014(12) |
| C(315) | 0.064(17) | 0.044(15) | 0.10(2) | 0.006(13) | 0.008(15) | 0.024(14) |
| C(316) | 0.020(11) | 0.084(17) | 0.064(14) | -0.019(11) | 0.020(10) | 0.013(13) |
| C(321) | 0.051(13) | 0.018(10) | 0.046(11) | -0.013(9) | -0.007(10) | 0.012(9) |
| C(322) | 0.047(13) | 0.042(12) | 0.056(13) | -0.008(10) | -0.025(11) | 0.010(10) |
| C(323) | 0.068(16) | 0.049(14) | 0.073(16) | -0.026(13) | -0.036(14) | 0.028(13) |
| C(324) | 0.075(18) | 0.071(17) | 0.085(18) | -0.056(15) | -0.050(15) | 0.015(14) |
| C(325) | 0.08(2) | 0.054(15) | 0.081(18) | -0.013(14) | -0.011(16) | -0.022(13) |
| C(326) | 0.041(12) | 0.053(13) | 0.060(13) | -0.036(11) | -0.021(11) | 0.003(11) |
| C(411) | 0.032(11) | 0.039(12) | 0.036(11) | 0.006(9) | 0.002(9) | 0.010(9) |
| C(412) | 0.061(15) | 0.039(13) | 0.052(13) | -0.007(11) | -0.009(11) | -0.001(11) |
| C(413) | 0.053(14) | 0.076(17) | 0.054(14) | -0.020(13) | -0.016(12) | 0.001(13) |
| C(414) | 0.066(17) | 0.13(3) | 0.025(12) | -0.051(18) | 0.022(11) | 0.001(14) |
| C(415) | 0.09(2) | 0.12(3) | 0.043(15) | -0.059(19) | 0.012(14) | -0.002(16) |
| C(416) | 0.054(14) | 0.071(16) | 0.064(15) | -0.045(13) | -0.015(12) | 0.033(12) |
| C(421) | 0.031(11) | 0.026(10) | 0.048(12) | -0.016(8) | 0.005(9) | 0.020(9) |
| C(422) | 0.073(15) | 0.031(11) | 0.037(11) | 0.003(11) | -0.014(11) | 0.005(9) |
| C(423) | 0.071(16) | 0.044(13) | 0.039(12) | 0.007(11) | -0.017(11) | 0.002(10) |
| C(424) | 0.022(11) | 0.032(12) | 0.083(16) | 0.000(9) | -0.004(11) | 0.018(11) |
| C(425) | 0.041(12) | 0.019(10) | 0.086(16) | -0.004(9) | -0.038(11) | 0.006(10) |
| C(426) | 0.053(13) | 0.042(12) | 0.062(13) | -0.025(10) | -0.040(11) | 0.007(10) |
| P(100) | 0.029(3) | 0.048(3) | 0.039(3) | -0.011(2) | -0.009(2) | 0.005(2) |
| F(101) | 0.114(13) | 0.101(12) | 0.120(13) | -0.021(10) | -0.064(11) | -0.026(10) |
| F(102) | 0.140(16) | 0.119(15) | 0.095(12) | -0.058(13) | 0.035(11) | 0.024(11) |
| F(103) | 0.079(10) | 0.064(9) | 0.110(12) | 0.013(8) | -0.031(9) | -0.014(9) |
| F(104) | 0.125(14) | 0.114(13) | 0.077(11) | -0.049(11) | 0.016(10) | 0.013(10) |
| F(105) | 0.079(10) | 0.075(10) | 0.102(12) | 0.010(8) | -0.013(9) | -0.013(9) |
| F(106) | 0.080(11) | 0.097(12) | 0.160(16) | -0.003(9) | -0.072(11) | -0.029(11) |
| Cl(91) | 0.149(8) | 0.091(6) | 0.095(6) | 0.028(6) | -0.020(6) | -0.023(5) |
| Cl(92) | 0.152(13) | 0.195(15) | 0.52(3) | 0.027(11) | -0.057(17) | -0.203(19) |
| Cl(93) | 0.079(6) | 0.265(15) | 0.102(7) | -0.038(8) | -0.009(5) | -0.050(8) |
| Cl(94) | 0.205(17) | 0.32(3) | 0.29(2) | -0.071(16) | 0.150(16) | -0.14(2) |

Table S4 (continued)

**Anisotropic Temperature Factor Coefficients - U's (Continued)**

**for $[Re_2Br_3(dppm)_2(CO)(CNxyl)_2]PF_6 \cdot 2CH_2Cl_2$ 5b**

| Name | U(1,1) | U(2,2) | U(3,3) | U(1,2) | U(1,3) | U(2,3) |
|---|---|---|---|---|---|---|
| C(900) | 0.12(3) | 0.14(3) | 0.046(15) | 0.00(2) | -0.033(16) | -0.032(17) |
| C(901) | 0.15(4) | 0.21(5) | 0.15(4) | -0.07(4) | -0.03(3) | 0.07(4) |

**The form of the anisotropic temperature factor is:**

**$\exp[-2\pi (h^2a^{*2}U(1,1) + k^2b^{*2}U(2,2) + l^2c^{*2}U(3,3) + 2hka^*b^*U(1,2) + 2hla^*c^*U(1,3)$**

**$+ 2klb^*c\ U(2,3))]$ where $a^*$, $b^*$, and $c^*$ are reciprocal lattice constants.**

Table S5

**Table of Bond Distances in Angstroms**

**for $[Re_2Br_3(dppm)_2(CO)(CNxyl)_2]PF_6 \cdot 2CH_2Cl_2$ 5b**

| Atom 1 | Atom 2 | Distance |
|---|---|---|
| Re(1) | C(20) | 2.00(2) |
| Re(1) | C(10) | 2.02(2) |
| Re(1) | P(3) | 2.437(5) |
| Re(1) | P(1) | 2.438(5) |
| Re(1) | Br(1) | 2.599(3) |
| Re(1) | Br(2) | 2.604(3) |
| Re(1) | Re(2) | 3.028(2) |
| Re(2) | C(3B) | 1.87(4) |
| Re(2) | C(3A) | 1.89(4) |
| Re(2) | P(4) | 2.439(5) |
| Re(2) | P(2) | 2.452(5) |
| Re(2) | Br(2) | 2.553(3) |
| Re(2) | Br(1) | 2.556(2) |
| Re(2) | Br(3A) | 2.559(6) |
| Re(2) | Br(3B) | 2.562(6) |
| Cl(91) | C(900) | 1.60(3) |
| Cl(92) | C(900) | 1.80(4) |
| Cl(93) | C(901) | 1.74(5) |
| Cl(94) | C(901) | 1.66(5) |
| P(1) | C(1B) | 1.81(2) |
| P(1) | C(121) | 1.85(2) |
| P(1) | C(111) | 1.86(2) |
| P(2) | C(1B) | 1.86(2) |
| P(2) | C(211) | 1.86(2) |
| P(2) | C(221) | 1.91(2) |
| P(3) | C(2B) | 1.84(2) |
| P(3) | C(311) | 1.84(2) |
| P(3) | C(321) | 1.89(2) |
| P(4) | C(411) | 1.85(2) |
| P(4) | C(2B) | 1.86(2) |
| P(4) | C(421) | 1.86(2) |
| P(100) | F(106) | 1.54(2) |
| P(100) | F(104) | 1.56(2) |
| P(100) | F(103) | 1.583(14) |
| P(100) | F(102) | 1.60(2) |
| P(100) | F(105) | 1.624(14) |
| P(100) | F(101) | 1.65(2) |
| N(10) | C(10) | 1.14(2) |
| N(10) | C(11) | 1.43(2) |
| N(20) | C(20) | 1.15(2) |
| N(20) | C(21) | 1.47(2) |
| C(11) | C(16) | 1.41(3) |
| C(11) | C(12) | 1.42(3) |
| C(12) | C(13) | 1.40(2) |
| C(12) | C(17) | 1.49(3) |
| C(13) | C(14) | 1.38(3) |
| C(13) | C(12) | 1.40(3) |
| C(14) | C(13) | 1.38(3) |
| C(14) | C(15) | 1.40(3) |
| C(15) | C(16) | 1.35(3) |
| C(16) | C(18) | 1.58(3) |
| C(17) | C(12) | 1.49(3) |
| C(21) | C(26) | 1.37(3) |
| C(21) | C(22) | 1.40(2) |
| C(22) | C(23) | 1.41(3) |
| C(22) | C(27) | 1.43(3) |
| C(23) | C(22) | 1.41(3) |
| C(23) | C(24) | 1.44(3) |
| C(24) | C(25) | 1.37(3) |
| C(24) | C(23) | 1.44(3) |
| C(25) | C(26) | 1.41(3) |
| C(26) | C(21) | 1.37(3) |
| C(26) | C(25) | 1.41(3) |
| C(26) | C(28) | 1.52(3) |
| C(28) | C(26) | 1.52(3) |
| C(411) | C(412) | 1.28(3) |
| C(411) | C(416) | 1.43(3) |
| C(111) | C(112) | 1.32(3) |
| C(111) | C(116) | 1.43(3) |
| C(112) | C(113) | 1.41(3) |
| C(113) | C(114) | 1.35(3) |
| C(114) | C(113) | 1.35(3) |
| C(114) | C(115) | 1.39(3) |
| C(115) | C(116) | 1.39(3) |
| C(115) | C(114) | 1.39(3) |
| C(121) | C(122) | 1.37(2) |
| C(121) | C(126) | 1.38(3) |
| C(122) | C(123) | 1.41(3) |
| C(123) | C(124) | 1.36(3) |
| C(124) | C(125) | 1.35(3) |
| C(125) | C(124) | 1.35(3) |
| C(125) | C(126) | 1.38(3) |
| C(126) | C(125) | 1.38(3) |
| C(211) | C(212) | 1.37(2) |
| C(211) | C(216) | 1.40(3) |

Table S5 (continued)

**Bond Distances (cont.)**

| Atom 1 | Atom 2 | Distance | Atom 1 | Atom 2 | Distance |
|---|---|---|---|---|---|
| C(212) | C(213) | 1.38(3) | C(322) | C(323) | 1.34(3) |
| C(213) | C(214) | 1.32(3) | C(323) | C(324) | 1.36(3) |
| C(214) | C(215) | 1.46(3) | C(324) | C(325) | 1.42(3) |
| C(215) | C(216) | 1.37(3) | C(325) | C(326) | 1.36(3) |
| C(221) | C(222) | 1.32(2) | C(412) | C(413) | 1.46(3) |
| C(221) | C(226) | 1.37(3) | C(413) | C(414) | 1.34(3) |
| C(222) | C(223) | 1.41(3) | C(414) | C(413) | 1.34(3) |
| C(223) | C(224) | 1.37(3) | C(414) | C(415) | 1.44(4) |
| C(224) | C(225) | 1.39(3) | C(415) | C(416) | 1.37(3) |
| C(225) | C(226) | 1.38(3) | C(415) | C(414) | 1.44(4) |
| C(311) | C(316) | 1.37(3) | C(421) | C(422) | 1.36(3) |
| C(311) | C(312) | 1.40(3) | C(421) | C(426) | 1.36(3) |
| C(312) | C(313) | 1.42(3) | C(422) | C(423) | 1.39(3) |
| C(313) | C(314) | 1.38(3) | C(423) | C(424) | 1.35(3) |
| C(314) | C(315) | 1.37(3) | C(423) | C(422) | 1.39(3) |
| C(315) | C(316) | 1.36(3) | C(424) | C(423) | 1.35(3) |
| C(315) | C(314) | 1.37(3) | C(424) | C(425) | 1.38(3) |
| C(316) | C(315) | 1.36(3) | C(425) | C(426) | 1.39(3) |
| C(321) | C(322) | 1.34(3) | O(3A) | C(3A) | 1.21(4) |
| C(321) | C(326) | 1.34(3) | C(3B) | O(3B) | 1.22(4) |

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table S6

**Table of Bond Angles in Degrees**

**for $[Re_2Br_3(dppm)_2(CO)(CNxyl)_2]PF_6 \cdot 2CH_2Cl_2$ 5b**

| Atom 1 | Atom 2 | Atom 3 | Angle |
|---|---|---|---|
| C(20) | Re(1) | C(10) | 89.2(7) |
| C(20) | Re(1) | P(3) | 89.5(6) |
| C(10) | Re(1) | P(3) | 88.1(5) |
| C(20) | Re(1) | P(1) | 90.1(6) |
| C(10) | Re(1) | P(1) | 90.8(5) |
| P(3) | Re(1) | P(1) | 178.78(14) |
| C(20) | Re(1) | Br(1) | 170.9(6) |
| C(10) | Re(1) | Br(1) | 82.1(5) |
| P(3) | Re(1) | Br(1) | 87.58(14) |
| P(1) | Re(1) | Br(1) | 92.64(14) |
| C(20) | Re(1) | Br(2) | 82.3(5) |
| C(10) | Re(1) | Br(2) | 170.8(4) |
| P(3) | Re(1) | Br(2) | 95.08(13) |
| P(1) | Re(1) | Br(2) | 86.01(13) |
| Br(1) | Re(1) | Br(2) | 106.58(9) |
| C(20) | Re(1) | Re(2) | 135.3(5) |
| C(10) | Re(1) | Re(2) | 135.4(5) |
| P(3) | Re(1) | Re(2) | 90.70(12) |
| P(1) | Re(1) | Re(2) | 90.40(12) |
| Br(1) | Re(1) | Re(2) | 53.36(7) |
| Br(2) | Re(1) | Re(2) | 53.25(7) |
| C(3B) | Re(2) | C(3A) | 95(2) |
| C(3B) | Re(2) | P(4) | 81(2) |
| C(3A) | Re(2) | P(4) | 80.6(11) |
| C(3B) | Re(2) | P(2) | 99(2) |
| C(3A) | Re(2) | P(2) | 98.2(11) |
| P(4) | Re(2) | P(2) | 178.75(14) |
| C(3B) | Re(2) | Br(2) | 175(2) |
| C(3A) | Re(2) | Br(2) | 84.5(10) |
| P(4) | Re(2) | Br(2) | 93.74(14) |
| P(2) | Re(2) | Br(2) | 85.82(13) |
| C(3B) | Re(2) | Br(1) | 71(2) |
| C(3A) | Re(2) | Br(1) | 162.8(10) |
| P(4) | Re(2) | Br(1) | 88.45(13) |
| P(2) | Re(2) | Br(1) | 92.80(13) |
| Br(2) | Re(2) | Br(1) | 109.50(9) |
| C(3B) | Re(2) | Br(3A) | 91(2) |
| P(4) | Re(2) | Br(3A) | 86.5(2) |
| P(2) | Re(2) | Br(3A) | 92.4(2) |
| Br(2) | Re(2) | Br(3A) | 88.87(14) |
| Br(1) | Re(2) | Br(3A) | 161.24(12) |
| C(3A) | Re(2) | Br(3B) | 78.6(10) |
| P(4) | Re(2) | Br(3B) | 93.1(2) |
| P(2) | Re(2) | Br(3B) | 87.0(2) |
| Br(2) | Re(2) | Br(3B) | 160.53(14) |
| Br(1) | Re(2) | Br(3B) | 88.9(2) |
| Br(3A) | Re(2) | Br(3B) | 73.4(2) |
| C(3B) | Re(2) | Re(1) | 125(2) |
| C(3A) | Re(2) | Re(1) | 137.8(10) |
| P(4) | Re(2) | Re(1) | 90.27(12) |
| P(2) | Re(2) | Re(1) | 90.42(12) |
| Br(2) | Re(2) | Re(1) | 54.84(7) |
| Br(1) | Re(2) | Re(1) | 54.69(7) |
| Br(3A) | Re(2) | Re(1) | 143.28(13) |
| Br(3B) | Re(2) | Re(1) | 143.34(13) |
| Re(2) | Br(1) | Re(1) | 71.95(9) |
| Re(2) | Br(2) | Re(1) | 71.91(9) |
| C(1B) | P(1) | C(121) | 105.8(8) |
| C(1B) | P(1) | C(111) | 103.1(8) |
| C(121) | P(1) | C(111) | 100.7(8) |
| C(1B) | P(1) | Re(1) | 113.3(5) |
| C(121) | P(1) | Re(1) | 110.0(6) |
| C(111) | P(1) | Re(1) | 122.2(6) |
| C(1B) | P(2) | C(211) | 101.8(7) |
| C(1B) | P(2) | C(221) | 104.9(8) |
| C(211) | P(2) | C(221) | 101.9(8) |
| C(1B) | P(2) | Re(2) | 112.3(6) |
| C(211) | P(2) | Re(2) | 121.4(6) |
| C(221) | P(2) | Re(2) | 112.7(5) |
| C(2B) | P(3) | C(311) | 102.6(8) |
| C(2B) | P(3) | C(321) | 104.6(9) |
| C(311) | P(3) | C(321) | 100.0(9) |
| C(2B) | P(3) | Re(1) | 113.0(7) |
| C(311) | P(3) | Re(1) | 123.3(7) |
| C(321) | P(3) | Re(1) | 111.2(6) |
| C(411) | P(4) | C(2B) | 103.7(9) |
| C(411) | P(4) | C(421) | 101.8(8) |
| C(2B) | P(4) | C(421) | 104.3(9) |
| C(411) | P(4) | Re(2) | 121.1(7) |
| C(2B) | P(4) | Re(2) | 112.4(6) |
| C(421) | P(4) | Re(2) | 111.8(6) |
| F(106) | P(100) | F(104) | 93.6(11) |
| F(106) | P(100) | F(103) | 94.8(8) |
| F(104) | P(100) | F(103) | 92.3(9) |

Table S6 (continued)

**Bond Angles (cont.)**

| Atom 1 | Atom 2 | Atom 3 | Angle | Atom 1 | Atom 2 | Atom 3 | Angle |
|---|---|---|---|---|---|---|---|
| F(106) | P(100) | F(102) | 89.5(11) | C(112) | C(111) | P(1) | 122.6(16) |
| F(104) | P(100) | F(102) | 176.4(11) | C(116) | C(111) | P(1) | 116.8(12) |
| F(103) | P(100) | F(102) | 89.2(10) | C(111) | C(112) | C(113) | 118(2) |
| F(106) | P(100) | F(105) | 90.0(9) | C(114) | C(113) | C(112) | 126(2) |
| F(104) | P(100) | F(105) | 89.9(9) | C(113) | C(114) | C(115) | 114.4(19) |
| F(103) | P(100) | F(105) | 174.6(9) | C(116) | C(115) | C(114) | 123(2) |
| F(102) | P(100) | F(105) | 88.3(10) | C(115) | C(116) | C(111) | 117.9(19) |
| F(106) | P(100) | F(101) | 177.9(11) | C(122) | C(121) | C(126) | 118.4(16) |
| F(104) | P(100) | F(101) | 88.3(10) | C(122) | C(121) | P(1) | 117.1(13) |
| F(103) | P(100) | F(101) | 84.4(8) | C(126) | C(121) | P(1) | 124.3(14) |
| F(102) | P(100) | F(101) | 88.5(11) | C(121) | C(122) | C(123) | 119.5(16) |
| F(105) | P(100) | F(101) | 90.7(8) | C(124) | C(123) | C(122) | 121.9(19) |
| C(10) | N(10) | C(11) | 171.2(17) | C(125) | C(124) | C(123) | 117.4(19) |
| C(20) | N(20) | C(21) | 176.0(16) | C(124) | C(125) | C(126) | 123(2) |
| N(10) | C(10) | Re(1) | 176.0(15) | C(125) | C(126) | C(121) | 120.0(18) |
| C(16) | C(11) | C(12) | 122.0(16) | C(212) | C(211) | C(216) | 116.5(18) |
| C(16) | C(11) | N(10) | 118.9(16) | C(212) | C(211) | P(2) | 125.6(15) |
| C(12) | C(11) | N(10) | 119.1(15) | C(216) | C(211) | P(2) | 117.8(14) |
| C(13) | C(12) | C(11) | 116.9(18) | C(211) | C(212) | C(213) | 122(2) |
| C(13) | C(12) | C(17) | 121.2(19) | C(214) | C(213) | C(212) | 122(2) |
| C(11) | C(12) | C(17) | 121.9(16) | C(213) | C(214) | C(215) | 118(2) |
| C(14) | C(13) | C(12) | 121(2) | C(216) | C(215) | C(214) | 118(2) |
| C(13) | C(14) | C(15) | 121(2) | C(215) | C(216) | C(211) | 123(2) |
| C(16) | C(15) | C(14) | 121(2) | C(222) | C(221) | C(226) | 121.2(17) |
| C(15) | C(16) | C(11) | 119(2) | C(222) | C(221) | P(2) | 122.0(14) |
| C(15) | C(16) | C(18) | 121.5(19) | C(226) | C(221) | P(2) | 116.8(13) |
| C(11) | C(16) | C(18) | 119.3(17) | C(221) | C(222) | C(223) | 119.7(19) |
| P(1) | C(1B) | P(2) | 113.0(9) | C(224) | C(223) | C(222) | 121(2) |
| N(20) | C(20) | Re(1) | 176.6(14) | C(223) | C(224) | C(225) | 117(2) |
| C(26) | C(21) | C(22) | 125.8(16) | C(226) | C(225) | C(224) | 122(2) |
| C(26) | C(21) | N(20) | 116.7(16) | C(221) | C(226) | C(225) | 119.1(19) |
| C(22) | C(21) | N(20) | 117.3(16) | C(316) | C(311) | C(312) | 115.1(17) |
| C(21) | C(22) | C(23) | 117.0(17) | C(316) | C(311) | P(3) | 122.3(17) |
| C(21) | C(22) | C(27) | 123.4(17) | C(312) | C(311) | P(3) | 122.2(15) |
| C(23) | C(22) | C(27) | 119.4(18) | C(311) | C(312) | C(313) | 122.4(19) |
| C(22) | C(23) | C(24) | 119(2) | C(314) | C(313) | C(312) | 117(2) |
| C(25) | C(24) | C(23) | 121(2) | C(315) | C(314) | C(313) | 123(2) |
| C(24) | C(25) | C(26) | 122(2) | C(316) | C(315) | C(314) | 118(3) |
| C(21) | C(26) | C(25) | 115.8(18) | C(315) | C(316) | C(311) | 125(3) |
| C(21) | C(26) | C(28) | 124.4(17) | C(322) | C(321) | C(326) | 118.9(19) |
| C(25) | C(26) | C(28) | 119.8(18) | C(322) | C(321) | P(3) | 120.2(15) |
| P(3) | C(2B) | P(4) | 112.2(11) | C(326) | C(321) | P(3) | 120.0(15) |
| C(412) | C(411) | C(416) | 117(2) | C(321) | C(322) | C(323) | 126(2) |
| C(412) | C(411) | P(4) | 124.5(17) | C(322) | C(323) | C(324) | 117(2) |
| C(416) | C(411) | P(4) | 118.7(16) | C(323) | C(324) | C(325) | 119(2) |
| C(112) | C(111) | C(116) | 120.6(18) | C(326) | C(325) | C(324) | 121(2) |

Table S6 (continued)

**Bond Angles (cont.)**

| Atom 1 | Atom 2 | Atom 3 | Angle | Atom 1 | Atom 2 | Atom 3 | Angle |
|---|---|---|---|---|---|---|---|
| C(321) | C(326) | C(325) | 119(2) | C(424) | C(425) | C(426) | 119.3(19) |
| C(411) | C(412) | C(413) | 124(2) | C(421) | C(426) | C(425) | 121.3(19) |
| C(414) | C(413) | C(412) | 119(2) | Cl(91) | C(900) | Cl(92) | 109(2) |
| C(413) | C(414) | C(415) | 120(2) | Cl(94) | C(901) | Cl(93) | 123(3) |
| C(416) | C(415) | C(414) | 118(3) | O(3B) | C(3B) | Re(2) | 151(5) |
| C(415) | C(416) | C(411) | 123(2) | | | | |
| C(422) | C(421) | C(426) | 118.7(18) | | | | |
| C(422) | C(421) | P(4) | 122.2(15) | | | | |
| C(426) | C(421) | P(4) | 119.1(15) | | | | |
| C(421) | C(422) | C(423) | 120.8(19) | | | | |
| C(424) | C(423) | C(422) | 120(2) | | | | |
| C(423) | C(424) | C(425) | 119.8(18) | | | | |

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table S7

**Table of Torsion Angles in Degrees 5b**

| Atom 1 | Atom 2 | Atom 3 | Atom 4 | Angle |
|---|---|---|---|---|
| Br(2) | Re(1) | P(1) | C(1B) | 35.47 ( 0.65) |
| Br(2) | Re(1) | P(1) | C(111) | 149.92 ( 0.63) |
| Br(2) | Re(1) | P(1) | C(121) | -80.64 ( 0.51) |
| P(3) | Re(1) | P(1) | C(1B) | -177.43 ( 8.01) |
| P(3) | Re(1) | P(1) | C(111) | -62.98 ( 8.21) |
| P(3) | Re(1) | P(1) | C(121) | 66.46 ( 8.16) |
| C(10) | Re(1) | P(1) | C(1B) | -155.20 ( 0.84) |
| C(10) | Re(1) | P(1) | C(111) | -40.75 ( 0.82) |
| C(10) | Re(1) | P(1) | C(121) | 88.69 ( 0.73) |
| Br(2) | Re(1) | P(3) | C(2B) | -89.07 ( 0.60) |
| Br(2) | Re(1) | P(3) | C(311) | 46.58 ( 0.60) |
| Br(2) | Re(1) | P(3) | C(321) | 161.71 ( 0.69) |
| P(1) | Re(1) | P(3) | C(2B) | 123.79 ( 8.06) |
| P(1) | Re(1) | P(3) | C(311) | -100.56 ( 8.09) |
| P(1) | Re(1) | P(3) | C(321) | 14.57 ( 8.29) |
| C(10) | Re(1) | P(3) | C(2B) | 101.61 ( 0.80) |
| C(10) | Re(1) | P(3) | C(311) | -122.74 ( 0.79) |
| C(10) | Re(1) | P(3) | C(321) | -7.61 ( 0.86) |
| Br(1) | Re(2) | Br(3A) | O(3A) | -161.20 ( 14.66) |
| Br(1) | Re(2) | Br(3A) | C(3A) | -128.12 ( 6.95) |
| P(2) | Re(2) | Br(3A) | O(3A) | 100.93 ( 14.70) |
| P(2) | Re(2) | Br(3A) | C(3A) | 134.02 ( 6.96) |
| P(4) | Re(2) | Br(3A) | O(3A) | -78.50 ( 14.70) |
| P(4) | Re(2) | Br(3A) | C(3A) | -45.41 ( 6.96) |
| C(3A) | Re(2) | Br(3A) | O(3A) | -33.09 ( 16.18) |
| C(3B) | Re(2) | Br(3A) | O(3A) | -166.27 ( 14.77) |
| C(3B) | Re(2) | Br(3A) | C(3A) | -133.18 ( 7.11) |
| Br(1) | Re(2) | P(2) | C(1B) | 91.06 ( 0.52) |
| Br(1) | Re(2) | P(2) | C(211) | -41.77 ( 0.60) |
| Br(1) | Re(2) | P(2) | C(221) | -158.47 ( 0.66) |
| Br(3A) | Re(2) | P(2) | C(1B) | -111.67 ( 0.53) |
| Br(3A) | Re(2) | P(2) | C(211) | 115.50 ( 0.61) |
| Br(3A) | Re(2) | P(2) | C(221) | -1.19 ( 0.67) |
| P(4) | Re(2) | P(2) | C(1B) | -86.34 ( 7.88) |
| P(4) | Re(2) | P(2) | C(211) | 140.84 ( 7.80) |
| P(4) | Re(2) | P(2) | C(221) | 24.14 ( 8.00) |
| C(3A) | Re(2) | P(2) | C(1B) | -105.42 ( 1.28) |
| C(3A) | Re(2) | P(2) | C(211) | 121.76 ( 1.32) |
| C(3A) | Re(2) | P(2) | C(221) | 5.06 ( 1.35) |
| C(3B) | Re(2) | P(2) | C(1B) | 155.68 ( 1.68) |
| C(3B) | Re(2) | P(2) | C(211) | 22.85 ( 1.71) |
| C(3B) | Re(2) | P(2) | C(221) | -93.85 ( 1.73) |
| Br(1) | Re(2) | P(4) | C(2B) | -35.78 ( 0.76) |
| Br(1) | Re(2) | P(4) | C(411) | -149.54 ( 0.71) |
| Br(1) | Re(2) | P(4) | C(421) | 78.93 ( 0.56) |

Table S7 (continued)

**Table of Torsion Angles in Degrees (continued)**

| Atom 1 | Atom 2 | Atom 3 | Atom 4 | Angle |
|---|---|---|---|---|
| Br(3A) | Re(2) | P(4) | C(2B) | 167.03 ( 0.77) |
| Br(3A) | Re(2) | P(4) | C(411) | 53.28 ( 0.72) |
| Br(3A) | Re(2) | P(4) | C(421) | -78.25 ( 0.57) |
| P(2) | Re(2) | P(4) | C(2B) | 141.60 ( 7.77) |
| P(2) | Re(2) | P(4) | C(411) | 27.85 ( 8.08) |
| P(2) | Re(2) | P(4) | C(421) | -103.68 ( 7.84) |
| C(3A) | Re(2) | P(4) | C(2B) | 160.80 ( 1.41) |
| C(3A) | Re(2) | P(4) | C(411) | 47.05 ( 1.38) |
| C(3A) | Re(2) | P(4) | C(421) | -84.48 ( 1.30) |
| C(3B) | Re(2) | P(4) | C(2B) | -100.37 ( 1.77) |
| C(3B) | Re(2) | P(4) | C(411) | 145.88 ( 1.75) |
| C(3B) | Re(2) | P(4) | C(421) | 14.35 ( 1.69) |
| Br(1) | Re(2) | C(3A) | Br(3A) | 71.52 ( 8.49) |
| Br(1) | Re(2) | C(3A) | O(3A) | 88.41 ( 12.77) |
| Br(3A) | Re(2) | C(3A) | O(3A) | 16.88 ( 8.78) |
| P(2) | Re(2) | C(3A) | Br(3A) | -47.25 ( 7.08) |
| P(2) | Re(2) | C(3A) | O(3A) | -30.37 ( 12.74) |
| P(4) | Re(2) | C(3A) | Br(3A) | 133.20 ( 7.10) |
| P(4) | Re(2) | C(3A) | O(3A) | 150.08 ( 12.76) |
| C(3B) | Re(2) | C(3A) | Br(3A) | 47.37 ( 7.13) |
| C(3B) | Re(2) | C(3A) | O(3A) | 64.26 ( 12.66) |
| Br(1) | Re(2) | C(3B) | Br(3B) | 145.15 ( 6.16) |
| Br(1) | Re(2) | C(3B) | O(3B) | 142.98 ( 11.95) |
| Br(3A) | Re(2) | C(3B) | Br(3B) | -37.02 ( 5.64) |
| Br(3A) | Re(2) | C(3B) | O(3B) | -39.19 ( 11.48) |
| P(2) | Re(2) | C(3B) | Br(3B) | 61.86 ( 5.64) |
| P(2) | Re(2) | C(3B) | O(3B) | 59.69 ( 11.48) |
| P(4) | Re(2) | C(3B) | Br(3B) | -116.97 ( 5.63) |
| P(4) | Re(2) | C(3B) | O(3B) | -119.14 ( 11.47) |
| C(3A) | Re(2) | C(3B) | Br(3B) | -43.21 ( 5.85) |
| C(3A) | Re(2) | C(3B) | O(3B) | -45.39 ( 11.62) |
| Re(2) | Br(3A) | O(3A) | C(3A) | 19.67 ( 10.20) |
| Re(2) | Br(3A) | C(3A) | O(3A) | -164.44 ( 7.69) |
| O(3A) | Br(3A) | C(3A) | Re(2) | 164.44 ( 7.69) |
| O(3B) | Br(3B) | C(3B) | Re(2) | -178.35 ( 4.81) |
| Re(1) | P(1) | C(1B) | P(2) | 59.42 ( 0.99) |
| C(111) | P(1) | C(1B) | P(2) | -69.78 ( 1.04) |
| C(121) | P(1) | C(1B) | P(2) | 171.01 ( 0.83) |
| Re(1) | P(1) | C(111) | C(112) | -2.34 ( 2.22) |
| Re(1) | P(1) | C(111) | C(116) | 177.93 ( 1.29) |
| C(1B) | P(1) | C(111) | C(112) | 116.26 ( 2.00) |
| C(1B) | P(1) | C(111) | C(116) | -63.48 ( 1.66) |
| C(121) | P(1) | C(111) | C(112) | -127.24 ( 1.93) |
| C(121) | P(1) | C(111) | C(116) | 53.02 ( 1.73) |
| Re(1) | P(1) | C(121) | C(122) | -81.71 ( 1.52) |
| Re(1) | P(1) | C(121) | C(126) | 92.87 ( 1.81) |

Table S7 (continued)

**Table of Torsion Angles in Degrees (continued)**

| Atom 1 | Atom 2 | Atom 3 | Atom 4 | Angle |
|---|---|---|---|---|
| C(1B) | P(1) | C(121) | C(122) | 163.53 ( 1.52) |
| C(1B) | P(1) | C(121) | C(126) | -21.89 ( 2.05) |
| C(111) | P(1) | C(121) | C(122) | 53.31 ( 1.73) |
| C(111) | P(1) | C(121) | C(126) | -132.12 ( 1.77) |
| Re(2) | P(2) | C(1B) | P(1) | -58.58 ( 1.03) |
| C(211) | P(2) | C(1B) | P(1) | 77.46 ( 1.16) |
| C(221) | P(2) | C(1B) | P(1) | -170.51 ( 1.03) |
| Re(2) | P(2) | C(211) | C(212) | -4.84 ( 2.17) |
| Re(2) | P(2) | C(211) | C(216) | 179.20 ( 1.41) |
| C(1B) | P(2) | C(211) | C(212) | -134.26 ( 1.87) |
| C(1B) | P(2) | C(211) | C(216) | 49.79 ( 1.81) |
| C(221) | P(2) | C(211) | C(212) | 113.28 ( 1.96) |
| C(221) | P(2) | C(211) | C(216) | -62.67 ( 1.76) |
| Re(2) | P(2) | C(221) | C(222) | -93.28 ( 1.32) |
| Re(2) | P(2) | C(221) | C(226) | 85.08 ( 1.24) |
| C(1B) | P(2) | C(221) | C(222) | 19.00 ( 1.53) |
| C(1B) | P(2) | C(221) | C(226) | -162.63 ( 1.20) |
| C(211) | P(2) | C(221) | C(222) | 138.94 ( 1.35) |
| C(211) | P(2) | C(221) | C(226) | -42.70 ( 1.37) |
| Re(1) | P(3) | C(2B) | P(4) | 59.04 ( 1.15) |
| C(311) | P(3) | C(2B) | P(4) | -79.72 ( 1.30) |
| C(321) | P(3) | C(2B) | P(4) | 169.06 ( 1.15) |
| Re(1) | P(3) | C(311) | C(312) | -14.61 ( 2.04) |
| Re(1) | P(3) | C(311) | C(316) | 174.10 ( 1.52) |
| C(2B) | P(3) | C(311) | C(312) | 117.81 ( 1.86) |
| C(2B) | P(3) | C(311) | C(316) | -53.48 ( 1.93) |
| C(321) | P(3) | C(311) | C(312) | -130.62 ( 1.82) |
| C(321) | P(3) | C(311) | C(316) | 58.08 ( 1.86) |
| Re(1) | P(3) | C(321) | C(322) | -90.18 ( 1.38) |
| Re(1) | P(3) | C(321) | C(326) | 81.51 ( 1.33) |
| C(2B) | P(3) | C(321) | C(322) | 157.73 ( 1.37) |
| C(2B) | P(3) | C(321) | C(326) | -30.58 ( 1.56) |
| C(311) | P(3) | C(321) | C(322) | 37.51 ( 1.53) |
| C(311) | P(3) | C(321) | C(326) | -150.81 ( 1.36) |
| Re(2) | P(4) | C(2B) | P(3) | -60.89 ( 1.12) |
| C(411) | P(4) | C(2B) | P(3) | 67.18 ( 1.17) |
| C(421) | P(4) | C(2B) | P(3) | -172.66 ( 0.93) |
| Re(2) | P(4) | C(411) | C(412) | 4.75 ( 2.56) |
| Re(2) | P(4) | C(411) | C(416) | -178.32 ( 1.55) |
| C(2B) | P(4) | C(411) | C(412) | -112.54 ( 2.32) |
| C(2B) | P(4) | C(411) | C(416) | 64.39 ( 1.95) |
| C(421) | P(4) | C(411) | C(412) | 131.82 ( 2.18) |
| C(421) | P(4) | C(411) | C(416) | -51.25 ( 2.03) |
| Re(2) | P(4) | C(421) | C(422) | -80.57 ( 1.87) |
| Re(2) | P(4) | C(421) | C(426) | 97.14 ( 1.63) |
| C(2B) | P(4) | C(421) | C(422) | 33.08 ( 2.11) |

Table S7 (continued)

**Table of Torsion Angles in Degrees (continued)**

| Atom 1 | Atom 2 | Atom 3 | Atom 4 | Angle |
|---|---|---|---|---|
| C(2B) | P(4) | C(421) | C(426) | -149.22 ( 1.69) |
| C(411) | P(4) | C(421) | C(422) | 143.64 ( 1.82) |
| C(411) | P(4) | C(421) | C(426) | -38.66 ( 1.90) |
| Br(3A) | O(3A) | C(3A) | Re(2) | -31.18 ( 15.14) |
| Br(3B) | O(3B) | C(3B) | Re(2) | 3.46 ( 10.14) |
| N(10) | C(11) | C(16) | C(15) | -178.66 ( 1.82) |
| C(12) | C(11) | C(16) | C(15) | 2.43 ( 2.93) |
| C(14) | C(15) | C(16) | C(11) | -1.26 ( 3.10) |
| N(20) | C(21) | C(22) | C(27) | -2.56 ( 2.25) |
| P(1) | C(111) | C(112) | C(113) | 178.23 ( 1.57) |
| C(116) | C(111) | C(112) | C(113) | -2.03 ( 3.11) |
| P(1) | C(111) | C(116) | C(115) | -177.55 ( 1.40) |
| C(112) | C(111) | C(116) | C(115) | 2.66 ( 2.65) |
| P(1) | C(121) | C(122) | C(123) | 173.71 ( 1.26) |
| C(126) | C(121) | C(122) | C(123) | -2.13 ( 2.35) |
| C(121) | C(122) | C(123) | C(124) | 1.88 ( 3.23) |
| P(2) | C(211) | C(212) | C(213) | -176.24 ( 1.62) |
| C(216) | C(211) | C(212) | C(213) | -0.06 ( 3.04) |
| P(2) | C(211) | C(216) | C(215) | 179.37 ( 1.47) |
| C(212) | C(211) | C(216) | C(215) | 2.23 ( 2.61) |
| C(211) | C(212) | C(213) | C(214) | -3.12 ( 3.47) |
| C(212) | C(213) | C(214) | C(215) | 2.68 ( 2.74) |
| C(213) | C(214) | C(215) | C(216) | -0.65 ( 3.28) |
| C(214) | C(215) | C(216) | C(211) | -2.50 ( 3.51) |
| P(2) | C(221) | C(222) | C(223) | 178.84 ( 1.67) |
| C(226) | C(221) | C(222) | C(223) | 0.97 ( 3.13) |
| P(2) | C(221) | C(226) | C(225) | -177.29 ( 1.67) |
| C(222) | C(221) | C(226) | C(225) | 0.66 ( 3.14) |
| C(221) | C(222) | C(223) | C(224) | -1.29 ( 2.88) |
| C(222) | C(223) | C(224) | C(225) | 0.58 ( 3.77) |
| C(223) | C(224) | C(225) | C(226) | 1.07 ( 3.65) |
| C(224) | C(225) | C(226) | C(221) | -1.38 ( 2.75) |
| P(3) | C(311) | C(312) | C(313) | -173.81 ( 1.63) |
| C(316) | C(311) | C(312) | C(313) | -1.47 ( 2.95) |
| C(311) | C(312) | C(313) | C(314) | 0.00 ( 3.40) |
| P(3) | C(321) | C(322) | C(323) | 171.53 ( 1.88) |
| C(326) | C(321) | C(322) | C(323) | 1.68 ( 3.38) |
| P(3) | C(321) | C(326) | C(325) | -171.88 ( 1.82) |
| C(322) | C(321) | C(326) | C(325) | -2.22 ( 3.24) |
| C(321) | C(322) | C(323) | C(324) | -0.43 ( 2.94) |
| C(322) | C(323) | C(324) | C(325) | -0.08 ( 3.67) |
| C(323) | C(324) | C(325) | C(326) | -0.48 ( 3.85) |
| C(324) | C(325) | C(326) | C(321) | 1.31 ( 2.89) |
| P(4) | C(411) | C(412) | C(413) | 174.48 ( 1.82) |
| C(416) | C(411) | C(412) | C(413) | -2.71 ( 3.50) |
| P(4) | C(411) | C(416) | C(415) | -175.11 ( 1.78) |

Table S7 (continued)

**Table of Torsion Angles in Degrees (continued)**

| Atom 1 | Atom 2 | Atom 3 | Atom 4 | Angle |
|---|---|---|---|---|
| C(412) | C(411) | C(416) | C(415) | 2.60 ( 3.07) |
| P(4) | C(421) | C(426) | C(425) | -175.09 ( 1.35) |
| C(422) | C(421) | C(426) | C(425) | 3.06 ( 2.66) |
| C(424) | C(425) | C(426) | C(421) | -2.30 ( 3.23) |

Table S8

## CRYSTAL DATA AND DATA COLLECTION PARAMETERS for

$[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2 \cdot CH_2Cl_2]$ 7

| | |
|---|---|
| formula | $Re_2Br_3Cl_2P_4ON_2C_{70}H_{64}$ |
| formula weight | 1756.23 |
| space group | $P\bar{1}$ (No. 2) |
| a, Å | 13.330(4) |
| b, Å | 16.226(3) |
| c, Å | 16.327(6) |
| α ,deg | 99.29(2) |
| β, deg | 90.66(3) |
| γ, deg | 91.59(2) |
| V, Å$^3$ | 3483(3) |
| Z | 2 |
| $d_{calc}$, g cm$^{-3}$ | 1.674 |
| crystal dimensions, mm | 0.50x0.25x0.10 |
| temperature, K | 203. |
| radiation (wavelength) | Mo $K_\alpha$(0.71073Å) |
| monochromator | graphite |
| linear abs coef, mm$^{-1}$ | 5.434 |
| absorption correction applied | empirical[a] |
| transmission factors: min, max | 0.64, 0.88 |
| diffractometer | Enraf-Nonius CAD4 |
| scan method | ω-2θ |
| h, k, l range | -16 to 0 -20 to 20 -20 to 20 |
| 2θ range, deg | 5.52-52.64 |
| scan width, deg | 0.82 + 0.54tan(θ) |
| take-off angle, deg | 3.00 |
| programs used | SHELXL-93 |
| $F_{000}$ | 1710.0 |
| weighting | |
| $w=1/[\sigma^2(F_o^2)+(0.0768P)^2+4.1358P]$ where $P=(F_o^2+2F_c^2)/3$ | |
| data collected | 14104 |
| unique data | 14104 |
| $R_{int}$ | 0.023 |
| data used in refinement | 14104 |
| cutoff used in R-factor calculations | $F_o^2>2\sigma(F_o^2)$ |
| number of variables | 779 |
| largest shift/esd in final cycle | 0.04 |
| $R(F_o)$ | 0.040 |
| $R_w(F_o^2)$ | 0.112 |
| goodness of fit | 1.099 |

[a]Walker, N.; Stuart, D. Acta Crystallogr., Sect. A **1983**, A39,158.

Table S9

## Positional Parameters and Their Estimated Standard Deviations for $[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2\cdot CH_2Cl_2]$ 7

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| Re(1) | 0.18876(2) | 0 368318(14) | 0.288914(14) | 0.01794(7) |
| Re(2) | 0.34864(2) | 0 175619(14) | 0.261378(14) | 0.01613(7) |
| Br(1) | 0.25270(10) | 0.51710(9) | 0.30656(8) | 0.0348(4) |
| Br(2) | 0.37997(6) | 0.33802(4) | 0.29973(5) | 0.0336(2) |
| Br(3) | 0.15462(5) | 0.20879(4) | 0.26242(4) | 0.02636(16) |
| Br(4) | 0.0034(4) | 0.3988(3) | 0.2891(3) | 0.0370(12) |
| P(1) | 0.20082(12) | 0.34904(10) | 0.13778(10) | 0.0190(4) |
| P(2) | 0.34959(12) | 0.19510(10) | 0.11831(10) | 0.0182(4) |
| P(3) | 0.19037(12) | 0.35252(10) | 0.43574(10) | 0.0206(4) |
| P(4) | 0.33152(12) | 0.18234(10) | 0.40764(10) | 0.0198(4) |
| O(1) | -0.0297(10) | 0.4200(10) | 0.2882(10) | 0.057(4) |
| O(2) | 0.243(3) | 0.551(3) | 0.311(3) | 0.098(4)* |
| N(10) | 0.2919(6) | -0.0127(4) | 0.2255(4) | 0.048(2) |
| N(20) | 0.5694(5) | 0.1286(5) | 0.2675(4) | 0.046(2) |
| C(1) | 0.0576(11) | 0.4002(7) | 0.2879(7) | 0.026(3) |
| C(2) | 0.224(2) | 0.479(2) | 0.3054(16) | 0.031(3)* |
| C(10) | 0.3133(5) | 0.0580(4) | 0.2382(4) | 0.0246(19) |
| C(11) | 0.2621(6) | -0.0955(4) | 0.2259(4) | 0.0324(19) |
| C(12) | 0.1607(6) | -0.1156(5) | 0.2374(4) | 0.036(2) |
| C(13) | 0.1352(6) | -0.2006(5) | 0.2384(5) | 0.040(2) |
| C(14) | 0.2067(7) | -0.2603(5) | 0.2277(5) | 0.043(3) |
| C(15) | 0.3077(7) | -0.2387(5) | 0.2156(5) | 0.041(2) |
| C(16) | 0.3364(6) | -0.1557(4) | 0.2154(4) | 0.035(2) |
| C(17) | 0.0813(8) | -0.0512(6) | 0.2446(7) | 0.062(3) |
| C(18) | 0.4432(7) | -0.1300(6) | 0.2036(6) | 0.060(3) |
| C(1B) | 0.3172(4) | 0.3012(4) | 0.0977(4) | 0.0200(15) |
| C(20) | 0.4890(5) | 0.1498(4) | 0.2645(4) | 0.0240(17) |
| C(21) | 0.6739(5) | 0.1285(5) | 0.2764(4) | 0.033(2) |
| C(22) | 0.7169(5) | 0.0622(5) | 0.3070(4) | 0.0342(19) |
| C(23) | 0.8216(6) | 0.0623(5) | 0.3153(5) | 0.040(2) |
| C(24) | 0.8809(6) | 0.1239(6) | 0.2942(5) | 0.042(2) |
| C(25) | 0.8383(6) | 0.1916(6) | 0.2656(5) | 0.044(2) |
| C(26) | 0.7338(6) | 0.1949(5) | 0.2540(4) | 0.040(2) |
| C(27) | 0.6520(7) | -0.0066(7) | 0.3307(6) | 0.064(3) |
| C(28) | 0.6870(9) | 0.2652(6) | 0.2218(6) | 0.068(4) |
| C(2B) | 0.2309(5) | 0.2488(4) | 0.4577(4) | 0.0248(16) |
| C(111) | 0.1015(4) | 0.2896(4) | 0.0740(4) | 0.0206(16) |
| C(112) | 0.0120(5) | 0.2621(5) | 0.1070(4) | 0.0335(19) |
| C(113) | -0.0622(6) | 0.2209(5) | 0.0571(5) | 0.038(2) |
| C(114) | -0.0505(6) | 0.2043(5) | -0.0278(5) | 0.036(2) |
| C(115) | 0.0362(6) | 0.2304(5) | -0.0621(5) | 0.039(2) |

Table S9 (continued)

## Positional Parameters and Their Estimated Standard Deviations (cont.) for $[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2 \cdot CH_2Cl_2]$ 7

| Atom | x | y | z | U(Å$^2$) |
|---|---|---|---|---|
| C(116) | 0.1111(5) | 0.2734(5) | -0.0117(4) | 0.033(2) |
| C(121) | 0.2019(5) | 0.4456(4) | 0.0934(4) | 0.0276(19) |
| C(122) | 0.1138(6) | 0.4894(5) | 0.0970(6) | 0.048(3) |
| C(123) | 0.1073(7) | 0.5617(6) | 0.0636(7) | 0.057(3) |
| C(124) | 0.1885(7) | 0.5927(5) | 0.0273(6) | 0.051(3) |
| C(125) | 0.2781(8) | 0.5516(5) | 0.0245(6) | 0.057(3) |
| C(126) | 0.2825(6) | 0.4779(5) | 0.0583(5) | 0.041(2) |
| C(211) | 0.4719(5) | 0.1825(4) | 0.0692(4) | 0.0213(15) |
| C(212) | 0.5180(5) | 0.1065(4) | 0.0687(4) | 0.0274(19) |
| C(213) | 0.6099(5) | 0.0905(5) | 0.0326(4) | 0.033(2) |
| C(214) | 0.6592(5) | 0.1505(5) | -0.0045(4) | 0.0339(19) |
| C(215) | 0.6164(6) | 0.2273(5) | -0.0038(5) | 0.035(2) |
| C(216) | 0.5237(5) | 0.2435(4) | 0.0328(4) | 0.0258(17) |
| C(221) | 0.2724(5) | 0.1270(4) | 0.0390(4) | 0.0231(16) |
| C(222) | 0.1975(5) | 0.0759(4) | 0.0617(4) | 0.0275(19) |
| C(223) | 0.1407(6) | 0.0221(5) | 0.0023(5) | 0.037(2) |
| C(224) | 0.1585(6) | 0.0210(5) | -0.0792(5) | 0.043(3) |
| C(225) | 0.2334(6) | 0.0716(5) | -0.1037(5) | 0.039(2) |
| C(226) | 0.2902(6) | 0.1255(4) | -0.0448(4) | 0.0296(19) |
| C(311) | 0.2628(5) | 0.4322(4) | 0.5045(4) | 0.0261(17) |
| C(312) | 0.3613(6) | 0.4197(5) | 0.5281(5) | 0.036(2) |
| C(313) | 0.4145(6) | 0.4813(5) | 0.5803(5) | 0.040(2) |
| C(314) | 0.3707(6) | 0.5554(5) | 0.6099(5) | 0.039(2) |
| C(315) | 0.2722(6) | 0.5689(5) | 0.5882(5) | 0.043(2) |
| C(316) | 0.2206(6) | 0.5081(5) | 0.5337(5) | 0.038(2) |
| C(321) | 0.0690(5) | 0.3463(4) | 0.4881(4) | 0.0251(17) |
| C(322) | -0.0078(5) | 0.2997(5) | 0.4435(5) | 0.035(2) |
| C(323) | -0.0985(6) | 0.2817(5) | 0.4824(5) | 0.040(2) |
| C(324) | -0.1099(6) | 0.3149(6) | 0.5647(5) | 0.047(2) |
| C(325) | -0.0360(7) | 0.3643(6) | 0.6078(5) | 0.053(3) |
| C(326) | 0.0555(5) | 0.3781(5) | 0.5688(4) | 0.038(2) |
| C(411) | 0.2956(5) | 0.0808(4) | 0.4367(4) | 0.0288(19) |
| C(412) | 0.1994(6) | 0.0537(5) | 0.4472(6) | 0.046(3) |
| C(413) | 0.1776(8) | -0.0287(6) | 0.4600(7) | 0.060(3) |
| C(414) | 0.2542(8) | -0.0834(5) | 0.4586(6) | 0.055(3) |
| C(415) | 0.3519(7) | -0.0582(5) | 0.4473(6) | 0.053(3) |
| G(416) | 0.3716(7) | 0.0235(5) | 0.4356(5) | 0.041(2) |
| C(421) | 0.4376(5) | 0.2137(4) | 0.4804(4) | 0.0259(16) |
| C(422) | 0.4251(6) | 0.2128(5) | 0.5638(4) | 0.034(2) |
| C(423) | 0.4982(7) | 0.2467(5) | 0.6221(5) | 0.043(2) |
| C(424) | 0.5862(6) | 0.2824(5) | 0.5974(5) | 0.043(2) |

Table S9 (continued)

Positional Parameters and Their Estimated Standard Deviations (cont.)
for $[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2 \cdot CH_2Cl_2]$ 7

| Atom | x | y | z | U(Å$^2$) |
|---|---|---|---|---|
| C(425) | 0.5995(6) | 0.2819(5) | 0.5124(5) | 0.039(2) |
| C(426) | 0.5254(5) | 0.2467(4) | 0.4546(4) | 0.0283(19) |
| Cl(91) | 0.5524(2) | 0.4529(2) | 0.1649(2) | 0.0720(10) |
| Cl(92) | 0.5292(3) | 0.6210(2) | 0.1299(3) | 0.1010(14) |
| C(901) | 0.5120(10) | 0.5550(7) | 0.2012(7) | 0.082(4) |

Starred atoms were refined isotropically

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a^*_i a^*_j a_i \cdot a_j$

Table S10

## Positional Parameters and Their Estimated Standard Deviations for $[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2\cdot CH_2Cl_2]$ 7

| Atom | x | y | z | U(Å²) |
|---|---|---|---|---|
| H(13) | 0.0689(6) | -0.2163(5) | 0.2465(5) | 0.052 |
| H(14) | 0.1881(7) | -0.3159(5) | 0.2285(5) | 0.056 |
| H(15) | 0.3553(7) | -0.2799(5) | 0.2078(5) | 0.053 |
| H(23) | 0.8511(6) | 0.0184(5) | 0.3360(5) | 0.052 |
| H(24) | 0.9503(6) | 0.1212(6) | 0.2987(5) | 0.055 |
| H(25) | 0.8796(6) | 0.2352(6) | 0.2540(5) | 0.058 |
| H(112) | 0.0032(5) | 0.2723(5) | 0.1641(4) | 0.044 |
| H(113) | -0.1210(6) | 0.2038(5) | 0.0805(5) | 0.050 |
| H(114) | -0.1009(6) | 0.1756(5) | -0.0617(5) | 0.046 |
| H(115) | 0.0446(6) | 0.2192(5) | -0.1193(5) | 0.051 |
| H(116) | 0.1688(5) | 0.2918(5) | -0.0357(4) | 0.043 |
| H(122) | 0.0581(6) | 0.4695(5) | 0.1225(6) | 0.063 |
| H(123) | 0.0471(7) | 0.5895(6) | 0.0657(7) | 0.074 |
| H(124) | 0.1836(7) | 0.6415(5) | 0.0046(6) | 0.066 |
| H(125) | 0.3343(8) | 0.5726(5) | 0.0005(6) | 0.075 |
| H(126) | 0.3427(6) | 0.4501(5) | 0.0567(5) | 0.054 |
| H(17A) | 0.028(2) | -0.067(2) | 0.278(3) | 0.080 |
| H(17B) | 0.055(4) | -0.047(3) | 0.1903(8) | 0.080 |
| H(17C) | 0.1098(14) | 0.0020(10) | 0.270(4) | 0.080 |
| H(18A) | 0.4693(17) | -0.098(3) | 0.2541(14) | 0.079 |
| H(18B) | 0.4465(9) | -0.097(3) | 0.160(3) | 0.079 |
| H(18C) | 0.4824(12) | -0.1788(6) | 0.189(4) | 0.079 |
| H(1B1) | 0.3723(4) | 0.3392(4) | 0.1193(4) | 0.026 |
| H(1B2) | 0.3157(4) | 0.2990(4) | 0.0380(4) | 0.026 |
| H(212) | 0.4859(5) | 0.0654(4) | 0.0933(4) | 0.036 |
| H(213) | 0.6389(5) | 0.0391(5) | 0.0333(4) | 0.042 |
| H(214) | 0.7207(5) | 0.1393(5) | -0.0298(4) | 0.044 |
| H(215) | 0.6497(6) | 0.2683(5) | -0.0279(5) | 0.045 |
| H(216) | 0.4957(5) | 0.2954(4) | 0.0332(4) | 0.033 |
| H(222) | 0.1843(5) | 0.0771(4) | 0.1177(4) | 0.035 |
| H(223) | 0.0910(6) | -0.0128(5) | 0.0187(5) | 0.049 |
| H(224) | 0.1200(6) | -0.0141(5) | -0 1189(5) | 0.056 |
| H(225) | 0.2460(6) | 0.0697(5) | -0.1599(5) | 0.051 |
| H(226) | 0.3398(6) | 0.1603(4) | -0.0616(4) | 0.039 |
| H(27A) | 0.6901(16) | -0.038(3) | 0.365(3) | 0.083 |
| H(27B) | 0.629(4) | -0.043(2) | 0.2815(7) | 0.083 |
| H(27C) | 0.595(3) | 0.0168(7) | 0.361(4) | 0.083 |
| H(28A) | 0.634(3) | 0.287(3) | 0.258(2) | 0.088 |
| H(28B) | 0.660(5) | 0.2458(12) | 0.1673(18) | 0.088 |
| H(28C) | 0.7368(14) | 0.3085(19) | 0.219(4) | 0.088 |
| H(2B1) | 0.2474(5) | 0.2577(4) | 0.5165(4) | 0.032 |

Table S10 (continued)

Positional Parameters and Their Estimated Standard Deviations (cont.)
for $[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2 \cdot CH_2Cl_2]$ 7

| Atom | x | y | z | U(Å$^2$) |
|---|---|---|---|---|
| H(2B2) | 0.1706(5) | 0.2134(4) | 0.4510(4) | 0.032 |
| H(312) | 0.3913(6) | 0.3695(5) | 0.5084(5) | 0.046 |
| H(313) | 0.4803(6) | 0.4725(5) | 0.5955(5) | 0.052 |
| H(314) | 0.4071(6) | 0.5968(5) | 0.6448(5) | 0.051 |
| H(315) | 0.2415(6) | 0.6182(5) | 0.6101(5) | 0.056 |
| H(316) | 0.1561(6) | 0.5183(5) | 0.5163(5) | 0.049 |
| H(322) | 0.0001(5) | 0.2798(5) | 0.3873(5) | 0.046 |
| H(323) | -0.1490(6) | 0.2483(5) | 0.4531(5) | 0.051 |
| H(324) | -0.1687(6) | 0.3035(6) | 0.5913(5) | 0.061 |
| H(325) | -0.0460(7) | 0.3887(6) | 0.6626(5) | 0.069 |
| H(326) | 0.1071(5) | 0.4094(5) | 0.5990(4) | 0.049 |
| H(412) | 0.1473(6) | 0.0904(5) | 0.4460(6) | 0.060 |
| H(413) | 0.1121(8) | -0.0457(6) | 0.4691(7) | 0.077 |
| H(414) | 0.2401(8) | -0.1383(5) | 0.4655(6) | 0.072 |
| H(415) | 0.4038(7) | -0.0953(5) | 0.4474(6) | 0.069 |
| H(416) | 0.4373(7) | 0.0404(5) | 0.4269(5) | 0.054 |
| H(422) | 0.3666(6) | 0.1891(5) | 0.5815(4) | 0.043 |
| H(423) | 0.4879(7) | 0.2454(5) | 0.6782(5) | 0.056 |
| H(424) | 0.6349(6) | 0.3060(5) | 0.6360(5) | 0.056 |
| H(425) | 0.6581(6) | 0.3050(5) | 0.4941(5) | 0.050 |
| H(426) | 0.5358(5) | 0.2458(4) | 0.3982(4) | 0.036 |
| H(90A) | 0.4414(10) | 0.5524(7) | 0.2144(7) | 0.107 |
| H(90B) | 0.5488(10) | 0.5776(7) | 0.2518(7) | 0.107 |

Hydrogens included in calculation of structure factors but not refined $U_{iso}(H)=1.3*U_{iso}(C)$

 



Table S11

## Anisotropic Temperature Factor Coefficients - U's for $[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2 \cdot CH_2Cl_2]$ 7

| Name | U(1,1) | U(2,2) | U(3,3) | U(1,2) | U(1,3) | U(2,3) |
|---|---|---|---|---|---|---|
| Re(1) | 0.01790(13) | 0.01706(13) | 0.01849(13) | 0.00150(9) | 0.00073(9) | 0.00155(9) |
| Re(2) | 0.01568(13) | 0.01552(13) | 0.01734(13) | 0.00041(9) | 0.00043(9) | 0.00313(9) |
| Br(1) | 0.0410(7) | 0.0220(9) | 0.0399(7) | -0.0003(6) | 0.0020(5) | 0.0003(5) |
| Br(2) | 0.0353(4) | 0.0288(4) | 0.0362(4) | 0.0004(3) | -0.0021(3) | 0.0040(3) |
| Br(3) | 0.0224(3) | 0.0263(3) | 0.0297(3) | 0.0015(3) | 0.0001(3) | 0.0024(3) |
| Br(4) | 0.027(3) | 0.041(2) | 0.042(2) | 0.001(2) | -0.002(2) | 0.0041(15) |
| P(1) | 0.0185(8) | 0.0188(8) | 0.0196(8) | 0.0001(6) | 0.0004(6) | 0.0033(6) |
| P(2) | 0.0198(8) | 0.0169(7) | 0.0182(7) | 0.0023(6) | 0.0012(6) | 0.0036(6) |
| P(3) | 0.0214(8) | 0.0211(8) | 0.0182(8) | 0.0014(6) | 0.0014(6) | -0.0005(6) |
| P(4) | 0.0210(8) | 0.0200(8) | 0.0189(8) | -0.0005(6) | 0.0010(6) | 0.0052(6) |
| O(1) | 0.026(8) | 0.080(10) | 0.069(8) | 0.026(5) | 0.005(6) | 0.023(7) |
| N(10) | 0.082(6) | 0.021(3) | 0.040(4) | -0.007(3) | -0.014(4) | 0.003(3) |
| N(20) | 0.030(4) | 0.070(5) | 0.034(4) | 0.015(3) | -0.004(3) | -0.002(3) |
| C(1) | 0.012(6) | 0.030(6) | 0.036(6) | 0.002(5) | -0.001(5) | 0.005(4) |
| C(10) | 0.029(4) | 0.028(4) | 0.015(3) | 0.002(3) | -0.003(3) | -0.002(3) |
| C(11) | 0.054(5) | 0.019(3) | 0.024(3) | -0.004(3) | -0.011(3) | 0.005(3) |
| C(12) | 0.049(5) | 0.031(4) | 0.029(4) | -0.003(3) | -0.013(3) | 0.008(3) |
| C(13) | 0.048(5) | 0.039(4) | 0.035(4) | -0.011(4) | -0.008(4) | 0.011(3) |
| C(14) | 0.061(6) | 0.025(4) | 0.041(5) | -0.013(4) | -0.011(4) | 0.006(3) |
| C(15) | 0.063(6) | 0.022(4) | 0.038(4) | 0.009(4) | -0.009(4) | 0.007(3) |
| C(16) | 0.050(5) | 0.028(4) | 0.026(4) | -0.005(3) | -0.010(3) | 0.002(3) |
| C(17) | 0.061(6) | 0.051(6) | 0.075(7) | 0.017(5) | 0.000(5) | 0.014(5) |
| C(18) | 0.061(6) | 0.056(6) | 0.065(6) | -0.005(5) | -0.016(5) | 0.016(5) |
| C(1B) | 0.019(3) | 0.019(3) | 0.023(3) | 0.002(2) | 0.003(2) | 0.006(2) |
| C(20) | 0.025(4) | 0.028(3) | 0.018(3) | 0.002(3) | 0.002(3) | 0.000(3) |
| C(21) | 0.023(3) | 0.051(5) | 0.024(3) | 0.009(3) | 0.005(3) | -0.003(3) |
| C(22) | 0.030(4) | 0.045(4) | 0.024(3) | -0.006(3) | 0.000(3) | -0.004(3) |
| C(23) | 0.034(4) | 0.049(5) | 0.038(4) | 0.007(4) | -0.005(3) | 0.007(4) |
| C(24) | 0.023(4) | 0.058(5) | 0.044(5) | 0.000(4) | 0.000(3) | 0.001(4) |
| C(25) | 0.040(5) | 0.054(5) | 0.035(4) | -0.013(4) | 0.005(3) | -0.004(4) |
| C(26) | 0.055(5) | 0.042(5) | 0.018(3) | 0.010(4) | -0.003(3) | -0.007(3) |
| C(27) | 0.040(5) | 0.095(8) | 0.061(6) | -0.013(5) | -0.006(4) | 0.028(6) |
| C(28) | 0.102(9) | 0.055(6) | 0.041(5) | 0.014(6) | -0.017(5) | -0.007(4) |
| C(2B) | 0.027(3) | 0.023(3) | 0.024(3) | 0.002(3) | -0.002(3) | 0.003(3) |
| C(111) | 0.015(3) | 0.024(3) | 0.025(3) | -0.003(2) | -0.002(2) | 0.011(3) |
| C(112) | 0.031(4) | 0.046(4) | 0.024(3) | 0.000(3) | 0.001(3) | 0.007(3) |
| C(113) | 0.030(4) | 0.046(5) | 0.040(4) | -0.012(3) | -0.006(3) | 0.014(4) |
| C(114) | 0.033(4) | 0.037(4) | 0.035(4) | -0.001(3) | -0.015(3) | 0.001(3) |
| C(115) | 0.040(4) | 0.046(5) | 0.028(4) | -0.006(4) | -0.011(3) | -0.002(3) |
| C(116) | 0.029(4) | 0.041(4) | 0.030(4) | -0.004(3) | -0.002(3) | 0.008(3) |

Table S11 (continued)

## Anisotropic Temperature Factor Coefficients - U's (cont.) for $[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2 \cdot CH_2Cl_2]$

| Name | U(1,1) | U(2,2) | U(3,3) | U(1,2) | U(1,3) | U(2,3) |
|---|---|---|---|---|---|---|
| C(121) | 0.031(4) | 0.025(3) | 0.028(4) | 0.003(3) | 0.000(3) | 0.008(3) |
| C(122) | 0.035(4) | 0.042(5) | 0.074(6) | 0.009(4) | 0.012(4) | 0.024(4) |
| C(123) | 0.046(5) | 0.040(5) | 0.091(8) | 0.013(4) | -0.002(5) | 0.028(5) |
| C(124) | 0.069(6) | 0.028(4) | 0.061(6) | 0.004(4) | -0.006(5) | 0.024(4) |
| C(125) | 0.071(7) | 0.036(5) | 0.071(7) | 0.000(4) | 0.019(5) | 0.025(5) |
| C(126) | 0.038(4) | 0.032(4) | 0.059(5) | 0.011(3) | 0.021(4) | 0.022(4) |
| C(211) | 0.023(3) | 0.022(3) | 0.019(3) | 0.001(2) | 0.006(2) | 0.003(2) |
| C(212) | 0.026(4) | 0.035(4) | 0.021(3) | 0.007(3) | 0.001(3) | 0.003(3) |
| C(213) | 0.030(4) | 0.034(4) | 0.032(4) | 0.012(3) | 0.002(3) | -0.003(3) |
| C(214) | 0.021(3) | 0.044(4) | 0.033(4) | 0.001(3) | 0.014(3) | -0.006(3) |
| C(215) | 0.034(4) | 0.034(4) | 0.038(4) | -0.002(3) | 0.010(3) | 0.009(3) |
| C(216) | 0.024(3) | 0.029(4) | 0.025(3) | 0.006(3) | 0.008(3) | 0.005(3) |
| C(221) | 0.021(3) | 0.020(3) | 0.026(3) | 0.002(2) | -0.006(3) | -0.003(3) |
| C(222) | 0.028(4) | 0.020(3) | 0.033(4) | 0.003(3) | -0.002(3) | 0.000(3) |
| C(223) | 0.034(4) | 0.028(4) | 0.047(5) | -0.007(3) | -0.013(3) | -0.001(3) |
| C(224) | 0.041(5) | 0.045(5) | 0.040(5) | -0.004(4) | -0.024(4) | -0.004(4) |
| C(225) | 0.048(5) | 0.042(4) | 0.026(4) | 0.009(4) | -0.008(3) | -0.002(3) |
| C(226) | 0.039(4) | 0.028(4) | 0.020(3) | 0.005(3) | -0.003(3) | -0.002(3) |
| C(311) | 0.030(4) | 0.027(3) | 0.021(3) | -0.008(3) | -0.001(3) | 0.005(3) |
| C(312) | 0.034(4) | 0.033(4) | 0.037(4) | 0.003(3) | 0.000(3) | -0.005(3) |
| C(313) | 0.031(4) | 0.037(4) | 0.050(5) | -0.007(3) | -0.012(3) | 0.003(4) |
| C(314) | 0.050(5) | 0.028(4) | 0.034(4) | -0.020(3) | -0.011(3) | -0.004(3) |
| C(315) | 0.051(5) | 0.034(4) | 0.041(4) | 0.002(4) | -0.010(4) | -0.005(3) |
| C(316) | 0.035(4) | 0.030(4) | 0.047(5) | 0.003(3) | -0.001(3) | 0.004(3) |
| C(321) | 0.029(4) | 0.025(3) | 0.021(3) | 0.001(3) | 0.003(3) | 0.003(3) |
| C(322) | 0.028(4) | 0.043(4) | 0.030(4) | -0.005(3) | 0.006(3) | -0.007(3) |
| C(323) | 0.035(4) | 0.041(4) | 0.040(4) | -0.006(3) | 0.003(3) | -0.001(3) |
| C(324) | 0.036(4) | 0.059(5) | 0.046(5) | -0.007(4) | 0.019(4) | 0.009(4) |
| C(325) | 0.049(5) | 0.077(7) | 0.028(4) | -0.007(5) | 0.009(4) | -0.003(4) |
| C(326) | 0.027(4) | 0.058(5) | 0.024(4) | -0.010(3) | 0.001(3) | -0.003(3) |
| C(411) | 0.033(4) | 0.031(4) | 0.022(3) | -0.003(3) | -0.005(3) | 0.004(3) |
| C(412) | 0.040(5) | 0.040(5) | 0.059(5) | -0.006(4) | -0.002(4) | 0.013(4) |
| C(413) | 0.055(6) | 0.041(5) | 0.085(7) | -0.020(4) | 0.003(5) | 0.019(5) |
| C(414) | 0.083(7) | 0.029(4) | 0.056(6) | -0.009(5) | 0.007(5) | 0.016(4) |
| C(415) | 0.060(6) | 0.035(5) | 0.067(6) | 0.002(4) | 0.004(5) | 0.020(4) |
| C(416) | 0.047(5) | 0.029(4) | 0.052(5) | 0.008(3) | 0.005(4) | 0.016(4) |
| C(421) | 0.026(3) | 0.024(3) | 0.029(3) | -0.003(3) | -0.006(3) | 0.009(3) |
| C(422) | 0.031(4) | 0.041(4) | 0.030(4) | -0.003(3) | -0.008(3) | 0.011(3) |
| C(423) | 0.057(5) | 0.046(5) | 0.027(4) | 0.014(4) | 0.001(4) | 0.010(3) |
| C(424) | 0.041(5) | 0.053(5) | 0.037(4) | 0.004(4) | -0.021(4) | 0.012(4) |
| C(425) | 0.032(4) | 0.037(4) | 0.048(5) | -0.007(3) | -0.010(3) | 0.011(4) |

Table S11 (continued)

Anisotropic Temperature Factor Coefficients - U's (cont.)
for $[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2 \cdot CH_2Cl_2]$ 7

| Name | U(1,1) | U(2,2) | U(3,3) | U(1,2) | U(1,3) | U(2,3) |
|---|---|---|---|---|---|---|
| C(426) | 0.027(4) | 0.037(4) | 0.021(3) | 0.000(3) | -0.002(3) | 0.005(3) |
| Cl(91) | 0.075(2) | 0.066(2) | 0.076(2) | -0.0083(14) | 0.0063(14) | 0.0160(14) |
| Cl(92) | 0.104(3) | 0.084(2) | 0.123(3) | 0.024(2) | 0.019(2) | 0.036(2) |
| C(901) | 0.106(10) | 0.078(8) | 0.064(7) | 0.007(7) | 0.032(7) | 0.013(6) |

The form of the anisotropic temperature factor is:
$\exp[-2\pi \{h^2a^{*2}U(1,1) + k^2b^{*2}U(2,2) + l^2c^{*2}U(3,3) + 2hka^*b^*U(1,2) + 2hla^*c^*U(1,3) + 2klb^*c^* U(2,3)\}]$ where a*, b*, and c* are reciprocal lattice constants.

Table S12

Table of Bond Distances in Angstroms
for $[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2\cdot CH_2Cl_2]$

| Atom 1 | Atom 2 | Distance | Atom 1 | Atom 2 | Distance |
|---|---|---|---|---|---|
| Re(1) | Re(2) | 3.8023(2) | P(1) | C(111) | 1.828(6) |
| Re(1) | C(2) | 1.82(4) | P(1) | C(121) | 1.828(7) |
| Re(1) | C(1) | 1.838(14) | P(1) | C(1B) | 1.834(6) |
| Re(1) | P(1) | 2.444(2) | P(2) | C(211) | 1.826(6) |
| Re(1) | P(3) | 2.451(2) | P(2) | C(221) | 1.844(6) |
| Re(1) | Br(1) | 2.509(2) | P(2) | C(1B) | 1.868(6) |
| Re(1) | Br(4) | 2.533(5) | P(3) | C(311) | 1.817(7) |
| Re(1) | Br(3) | 2.5813(9) | P(3) | C(321) | 1.847(7) |
| Re(1) | Br(2) | 2.6184(11) | P(3) | C(2B) | 1.868(7) |
| Re(2) | C(10) | 1.929(7) | P(4) | C(411) | 1.839(7) |
| Re(2) | C(20) | 1.931(7) | P(4) | C(421) | 1.843(7) |
| Re(2) | P(4) | 2.387(2) | P(4) | C(2B) | 1.858(6) |
| Re(2) | P(2) | 2.407(2) | O(1) | C(1) | 1.22(2) |
| Re(2) | Br(2) | 2.6289(9) | N(10) | C(10) | 1.160(9) |
| Re(2) | Br(3) | 2.6560(11) | N(10) | C(11) | 1.391(9) |
| Br(1) | O(2) | 0.56(5) | N(20) | C(20) | 1.137(9) |
| Br(1) | C(2) | 0.71(4) | N(20) | C(21) | 1.399(9) |
| Br(4) | O(1) | 0.568(11) | O(2) | C(2) | 1.17(6) |
| Br(4) | C(1) | 0.723(13) | | | |

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table S12 (continued)

Table of Bond Distances in Angstroms
for $[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2 \cdot CH_2Cl_2]$ 7

| Atom 1 | Atom 2 | Distance | Atom 1 | Atom 2 | Distance |
|---|---|---|---|---|---|
| Cl(91) | C(901) | 1.768(12) | C(115) | C(116) | 1.385(10) |
| Cl(92) | C(901) | 1.717(12) | C(121) | C(126) | 1.356(10) |
| C(11) | C(16) | 1.403(11) | C(121) | C(122) | 1.385(10) |
| C(11) | C(12) | 1.404(11) | C(122) | C(123) | 1.376(12) |
| C(12) | C(13) | 1.414(10) | C(123) | C(124) | 1.363(13) |
| C(12) | C(17) | 1.500(11) | C(124) | C(125) | 1.381(13) |
| C(13) | C(14) | 1.369(11) | C(125) | C(126) | 1.399(11) |
| C(14) | C(15) | 1.407(12) | C(211) | C(212) | 1.391(9) |
| C(15) | C(16) | 1.389(10) | C(211) | C(216) | 1.404(9) |
| C(16) | C(18) | 1.496(12) | C(212) | C(213) | 1.379(9) |
| C(21) | C(22) | 1.392(11) | C(213) | C(214) | 1.383(10) |
| C(21) | C(26) | 1.421(11) | C(214) | C(215) | 1.384(10) |
| C(22) | C(23) | 1.400(10) | C(215) | C(216) | 1.393(9) |
| C(22) | C(27) | 1.497(12) | C(221) | C(222) | 1.373(9) |
| C(23) | C(24) | 1.349(12) | C(221) | C(226) | 1.388(9) |
| C(24) | C(25) | 1.392(12) | C(222) | C(223) | 1.396(9) |
| C(25) | C(26) | 1.407(11) | C(223) | C(224) | 1.350(12) |
| C(26) | C(28) | 1.479(12) | C(224) | C(225) | 1.380(12) |
| C(111) | C(116) | 1.390(9) | C(225) | C(226) | 1.392(10) |
| C(111) | C(112) | 1.406(9) | C(311) | C(316) | 1.385(10) |
| C(112) | C(113) | 1.362(10) | C(311) | C(312) | 1.392(10) |
| C(113) | C(114) | 1.382(11) | C(312) | C(313) | 1.378(10) |
| C(114) | C(115) | 1.376(11) | C(313) | C(314) | 1.370(11) |
| C(314) | C(315) | 1.388(11) | C(412) | C(413) | 1.409(12) |
| C(315) | C(316) | 1.379(10) | C(413) | C(414) | 1.369(13) |
| C(321) | C(326) | 1.352(9) | C(414) | C(415) | 1.378(13) |
| C(321) | C(322) | 1.383(9) | C(415) | C(416) | 1.387(11) |
| C(322) | C(323) | 1.417(10) | C(421) | C(426) | 1.372(9) |
| C(323) | C(324) | 1.376(11) | C(421) | C(422) | 1.376(10) |
| C(324) | C(325) | 1.366(12) | C(422) | C(423) | 1.393(11) |
| C(325) | C(326) | 1.412(11) | C(423) | C(424) | 1.388(12) |
| C(411) | C(412) | 1.366(11) | C(424) | C(425) | 1.399(11) |
| C(411) | C(416) | 1.392(10) | C(425) | C(426) | 1.402(10) |

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table S13

## Table of Bond Angles in Degrees for $[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2\cdot CH_2Cl_2]$ 7

| Atom 1 | Atom 2 | Atom 3 | Angle | Atom 1 | Atom 2 | Atom 3 | Angle |
|---|---|---|---|---|---|---|---|
| C(2) | Re(1) | C(1) | 87.0(9) | P(1) | Re(1) | Br(2) | 89.67(5) |
| C(2) | Re(1) | P(1) | 95.3(8) | P(3) | Re(1) | Br(2) | 83.29(5) |
| C(1) | Re(1) | P(1) | 93.3(4) | Br(1) | Re(1) | Br(2) | 82.81(4) |
| C(2) | Re(1) | P(3) | 96.5(8) | Br(4) | Re(1) | Br(2) | 176.12(10) |
| C(1) | Re(1) | P(3) | 94.8(4) | Br(3) | Re(1) | Br(2) | 87.75(3) |
| P(1) | Re(1) | P(3) | 166.02(5) | C(10) | Re(2) | C(20) | 90.1(3) |
| C(2) | Re(1) | Br(1) | 5.3(9) | C(10) | Re(2) | P(4) | 93.2(2) |
| C(1) | Re(1) | Br(1) | 91.9(4) | C(20) | Re(2) | P(4) | 93.1(2) |
| P(1) | Re(1) | Br(1) | 93.11(5) | C(10) | Re(2) | P(2) | 95.4(2) |
| P(3) | Re(1) | Br(1) | 97.95(5) | C(20) | Re(2) | P(2) | 94.4(2) |
| C(2) | Re(1) | Br(4) | 92.0(9) | P(4) | Re(2) | P(2) | 168.58(5) |
| C(1) | Re(1) | Br(4) | 5.2(4) | C(10) | Re(2) | Br(2) | 174.5(2) |
| P(1) | Re(1) | Br(4) | 94.21(11) | C(20) | Re(2) | Br(2) | 94.7(2) |
| P(3) | Re(1) | Br(4) | 92.90(11) | P(4) | Re(2) | Br(2) | 83.90(5) |
| Br(1) | Re(1) | Br(4) | 97.00(11) | P(2) | Re(2) | Br(2) | 86.89(5) |
| C(2) | Re(1) | Br(3) | 175.2(9) | C(10) | Re(2) | Br(3) | 89.1(2) |
| C(1) | Re(1) | Br(3) | 97.7(4) | C(20) | Re(2) | Br(3) | 177.8(2) |
| P(1) | Re(1) | Br(3) | 83.20(5) | P(4) | Re(2) | Br(3) | 84.89(5) |
| P(3) | Re(1) | Br(3) | 84.46(5) | P(2) | Re(2) | Br(3) | 87.74(5) |
| Br(1) | Re(1) | Br(3) | 169.90(4) | Br(2) | Re(2) | Br(3) | 85.99(3) |
| Br(4) | Re(1) | Br(3) | 92.66(10) | O(2) | Br(1) | C(2) | 134(5) |
| C(2) | Re(1) | Br(2) | 87.6(9) | O(2) | Br(1) | Re(1) | 147(4) |
| C(1) | Re(1) | Br(2) | 174.0(4) | C(2) | Br(1) | Re(1) | 14(2) |
| Re(1) | Br(2) | Re(2) | 92.87(3) | C(321) | P(3) | Re(1) | 118.3(2) |
| Re(1) | Br(3) | Re(2) | 93.09(3) | C(2B) | P(3) | Re(1) | 115.3(2) |
| O(1) | Br(4) | C(1) | 140(3) | C(411) | P(4) | C(421) | 100.3(3) |
| O(1) | Br(4) | Re(1) | 154(2) | C(411) | P(4) | C(2B) | 100.9(3) |
| C(1) | Br(4) | Re(1) | 13.4(10) | C(421) | P(4) | C(2B) | 101.3(3) |
| C(111) | P(1) | C(121) | 100.0(3) | C(411) | P(4) | Re(2) | 112.7(2) |
| C(111) | P(1) | C(1B) | 104.4(3) | C(421) | P(4) | Re(2) | 121.8(2) |
| C(121) | P(1) | C(1B) | 102.0(3) | C(2B) | P(4) | Re(2) | 116.7(2) |
| C(111) | P(1) | Re(1) | 119.2(2) | Br(4) | O(1) | C(1) | 22.4(15) |
| C(121) | P(1) | Re(1) | 114.9(2) | C(10) | N(10) | C(11) | 169.4(8) |
| C(1B) | P(1) | Re(1) | 114.1(2) | C(20) | N(20) | C(21) | 162.8(9) |
| C(211) | P(2) | C(221) | 99.2(3) | Br(4) | C(1) | O(1) | 17.4(11) |
| C(211) | P(2) | C(1B) | 101.0(3) | Br(4) | C(1) | Re(1) | 161.3(14) |
| C(221) | P(2) | C(1B) | 101.7(3) | O(1) | C(1) | Re(1) | 178.6(13) |
| C(211) | P(2) | Re(2) | 114.5(2) | Br(1) | O(2) | C(2) | 26(3) |
| C(221) | P(2) | Re(2) | 121.1(2) | Br(1) | C(2) | O(2) | 20(2) |
| C(1B) | P(2) | Re(2) | 116.2(2) | Br(1) | C(2) | Re(1) | 161(3) |

Table S13 (continued)

Table of Bond Angles in Degrees (cont.)
for $[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2\cdot CH_2Cl_2]$ 7

| Atom 1 | Atom 2 | Atom 3 | Angle | Atom 1 | Atom 2 | Atom 3 | Angle |
|---|---|---|---|---|---|---|---|
| C(311) | P(3) | C(321) | 104.2(3) | O(2) | C(2) | Re(1) | 176(3) |
| C(311) | P(3) | C(2B) | 107.2(3) | N(10) | C(10) | Re(2) | 179.0(6) |
| C(321) | P(3) | C(2B) | 93.9(3) | N(20) | C(20) | Re(2) | 174.7(7) |
| C(311) | P(3) | Re(1) | 115.3(2) | | | | |

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table S13 (continued)

## Table of Bond Angles in Degrees

for $[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2 \cdot CH_2Cl_2]$ 7

| Atom 1 | Atom 2 | Atom 3 | Angle | Atom 1 | Atom 2 | Atom 3 | Angle |
|---|---|---|---|---|---|---|---|
| N(10) | C(11) | C(16) | 117.7(7) | C(25) | C(26) | C(28) | 122.1(9) |
| N(10) | C(11) | C(12) | 119.6(7) | C(21) | C(26) | C(28) | 120.8(8) |
| C(16) | C(11) | C(12) | 122.7(7) | P(4) | C(2B) | P(3) | 128.6(4) |
| C(11) | C(12) | C(13) | 117.0(7) | C(116) | C(111) | C(112) | 117.2(6) |
| C(11) | C(12) | C(17) | 122.1(7) | C(116) | C(111) | P(1) | 119.6(5) |
| C(13) | C(12) | C(17) | 120.8(8) | C(112) | C(111) | P(1) | 123.1(5) |
| C(14) | C(13) | C(12) | 121.1(8) | C(113) | C(112) | C(111) | 121.5(7) |
| C(13) | C(14) | C(15) | 120.8(7) | C(112) | C(113) | C(114) | 120.3(7) |
| C(16) | C(15) | C(14) | 120.1(7) | C(115) | C(114) | C(113) | 119.6(7) |
| C(15) | C(16) | C(11) | 118.3(7) | C(114) | C(115) | C(116) | 120.2(7) |
| C(15) | C(16) | C(18) | 121.7(8) | C(115) | C(116) | C(111) | 121.1(7) |
| C(11) | C(16) | C(18) | 119.9(7) | C(126) | C(121) | C(122) | 117.8(7) |
| P(1) | C(1B) | P(2) | 120.3(3) | C(126) | C(121) | P(1) | 124.9(5) |
| C(22) | C(21) | N(20) | 118.6(7) | C(122) | C(121) | P(1) | 117.3(6) |
| C(22) | C(21) | C(26) | 121.4(7) | C(123) | C(122) | C(121) | 121.2(8) |
| N(20) | C(21) | C(26) | 120.0(7) | C(124) | C(123) | C(122) | 120.4(8) |
| C(21) | C(22) | C(23) | 118.3(7) | C(123) | C(124) | C(125) | 119.8(8) |
| C(21) | C(22) | C(27) | 120.3(7) | C(124) | C(125) | C(126) | 118.7(8) |
| C(23) | C(22) | C(27) | 121.4(8) | C(121) | C(126) | C(125) | 122.1(8) |
| C(24) | C(23) | C(22) | 122.0(8) | C(212) | C(211) | C(216) | 117.3(6) |
| C(23) | C(24) | C(25) | 120.0(7) | C(212) | C(211) | P(2) | 117.3(5) |
| C(24) | C(25) | C(26) | 121.1(8) | C(216) | C(211) | P(2) | 125.4(5) |
| C(25) | C(26) | C(21) | 117.1(7) | C(213) | C(212) | C(211) | 121.9(7) |
| C(212) | C(213) | C(214) | 120.3(7) | C(321) | C(322) | C(323) | 120.7(7) |
| C(213) | C(214) | C(215) | 119.4(6) | C(324) | C(323) | C(322) | 118.3(7) |
| C(214) | C(215) | C(216) | 120.2(7) | C(325) | C(324) | C(323) | 121.0(7) |
| C(215) | C(216) | C(211) | 120.9(6) | C(324) | C(325) | C(326) | 119.6(7) |
| C(222) | C(221) | C(226) | 118.8(6) | C(321) | C(326) | C(325) | 120.7(7) |
| C(222) | C(221) | P(2) | 120.7(5) | C(412) | C(411) | C(416) | 118. 0(7) |
| C(226) | C(221) | P(2) | 120.5(5) | C(412) | C(411) | P(4) | 125.0(6) |
| C(221) | C(222) | C(223) | 121.2(7) | C(416) | C(411) | P(4) | 116.3(6) |
| C(224) | C(223) | C(222) | 119.7(7) | C(411) | C(412) | C(413) | 121.3(8) |
| C(223) | C(224) | C(225) | 120.3(7) | C(414) | C(413) | C(412) | 119.1(9) |
| C(224) | C(225) | C(226) | 120.3(7) | C(413) | C(414) | C(415) | 120.9(8) |
| C(221) | C(226) | C(225) | 119.7(7) | C(414) | C(415) | C(416) | 118.9(9) |
| C(316) | C(311) | C(312) | 118.4(6) | C(415) | C(416) | C(411) | 121.8(8) |
| C(316) | C(311) | P(3) | 119.8(6) | C(426) | C(421) | C(422) | 118.9(6) |
| C(312) | C(311) | P(3) | 121.8(5) | C(426) | C(421) | P(4) | 121.3(5) |
| C(313) | C(312) | C(311) | 120.6(7) | C(422) | C(421) | P(4) | 119.5(5) |
| C(314) | C(313) | C(312) | 120.1(7) | C(421) | C(422) | C(423) | 121.3(7) |

Table S13 (continued)

Table of Bond Angles in Degrees (cont.)

for $[Re_2(\mu\text{-}Br)_2Br(\mu\text{-}dppm)_2(CO)(CNxyl)_2 \cdot CH_2Cl_2]$ 7

| Atom 1 | Atom 2 | Atom 3 | Angle | Atom 1 | Atom 2 | Atom 3 | Angle |
|---|---|---|---|---|---|---|---|
| C(313) | C(314) | C(315) | 120.4(7) | C(424) | C(423) | C(422) | 120.5(7) |
| C(316) | C(315) | C(314) | 119.0(7) | C(423) | C(424) | C(425) | 117.9(7) |
| C(315) | C(316) | C(311) | 121.3(7) | C(424) | C(425) | C(426) | 120.6(7) |
| C(326) | C(321) | C(322) | 119.5(7) | C(421) | C(426) | C(425) | 120.6(7) |
| C(326) | C(321) | P(3) | 123.1(5) | Cl(92) | C(901) | Cl(91) | 112.6(6) |
| C(322) | C(321) | P(3) | 117.1(5) | | | | |

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table S14

**Table of Torsion Angles in Degrees** 7

| Atom 1 | Atom 2 | Atom 3 | Atom 4 | Angle |
|---|---|---|---|---|
| Br(2) | Re(1) | Br(1) | O(2) | -173.14 ( 7.77) |
| Br(2) | Re(1) | Br(1) | C(2) | -155.91 ( 9.35) |
| Br(3) | Re(1) | Br(1) | O(2) | 165.88 ( 7.77) |
| Br(3) | Re(1) | Br(1) | C(2) | -176.90 ( 9.34) |
| Br(4) | Re(1) | Br(1) | O(2) | 2.93 ( 7.77) |
| Br(4) | Re(1) | Br(1) | C(2) | 20.16 ( 9.35) |
| P(1) | Re(1) | Br(1) | O(2) | 98.50 ( 7.77) |
| P(1) | Re(1) | Br(1) | C(2) | 115.72 ( 9.35) |
| P(3) | Re(1) | Br(1) | O(2) | -90.05 ( 7.77) |
| P(3) | Re(1) | Br(1) | C(2) | -72.83 ( 9.35) |
| C(1) | Re(1) | Br(1) | O(2) | 4.10 ( 7.78) |
| C(1) | Re(1) | Br(1) | C(2) | 21.33 ( 9.36) |
| C(2) | Re(1) | Br(1) | O(2) | -17.22 ( 12.15) |
| Br(1) | Re(1) | Br(2) | Re(2) | -172.96 ( 0.04) |
| Br(3) | Re(1) | Br(2) | Re(2) | 3.71 ( 0.02) |
| Br(4) | Re(1) | Br(2) | Re(2) | 113.13 ( 1.63) |
| P(1) | Re(1) | Br(2) | Re(2) | -66.30 ( 0.04) |
| P(3) | Re(1) | Br(2) | Re(2) | 101.15 ( 0.04) |
| C(1) | Re(1) | Br(2) | Re(2) | 163.45 ( 3.04) |
| C(2) | Re(1) | Br(2) | Re(2) | -174.96 ( 0.78) |
| Br(1) | Re(1) | Br(3) | Re(2) | 16.51 ( 0.21) |
| Br(2) | Re(1) | Br(3) | Re(2) | -4.01 ( 0.02) |
| Br(4) | Re(1) | Br(3) | Re(2) | 179.78 ( 0.13) |
| P(1) | Re(1) | Br(3) | Re(2) | 86.79 ( 0.04) |
| P(3) | Re(1) | Br(3) | Re(2) | -86.48 ( 0.04) |
| C(1) | Re(1) | Br(3) | Re(2) | 178.37 ( 0.36) |
| C(2) | Re(1) | Br(3) | Re(2) | 13.15 ( 10.08) |
| Br(1) | Re(1) | Br(4) | O(1) | 9.70 ( 3.89) |
| Br(1) | Re(1) | Br(4) | C(1) | 12.70 ( 4.09) |
| Br(2) | Re(1) | Br(4) | O(1) | 82.81 ( 4.27) |
| Br(2) | Re(1) | Br(4) | C(1) | 85.80 ( 4.43) |
| Br(3) | Re(1) | Br(4) | O(1) | -167.57 ( 3.88) |
| Br(3) | Re(1) | Br(4) | C(1) | -164.58 ( 4.09) |
| P(1) | Re(1) | Br(4) | O(1) | -97.76 ( 3.88) |
| P(1) | Re(1) | Br(4) | C(1) | -94.77 ( 4.09) |
| P(3) | Re(1) | Br(4) | O(1) | 94.70 ( 3.88) |
| P(3) | Re(1) | Br(4) | C(1) | 97.70 ( 4.09) |
| C(1) | Re(1) | Br(4) | O(1) | -2.99 ( 5.35) |
| C(2) | Re(1) | Br(4) | O(1) | 11.39 ( 3.96) |
| C(2) | Re(1) | Br(4) | C(1) | 14.38 ( 4.16) |
| Br(1) | Re(1) | P(1) | C(1B) | 91.30 ( 0.24) |
| Br(1) | Re(1) | P(1) | C(111) | -143.05 ( 0.23) |
| Br(1) | Re(1) | P(1) | C(121) | -21.15 ( 0.25) |
| Br(2) | Re(1) | P(1) | C(1B) | 13.60 ( 0.24) |
| Br(2) | Re(1) | P(1) | C(111) | 139.24 ( 0.23) |

Table S14 (continued)

**Table of Torsion Angles in Degrees (continued)**

| Atom 1 | Atom 2 | Atom 3 | Atom 4 | Angle |
|---|---|---|---|---|
| Br(2) | Re(1) | P(1) | C(121) | -98.85 ( 0.25) |
| Br(3) | Re(1) | P(1) | C(1B) | -79.55 ( 0.24) |
| Br(3) | Re(1) | P(1) | C(111) | 46.10 ( 0.23) |
| Br(3) | Re(1) | P(1) | C(121) | 168.00 ( 0.25) |
| Br(4) | Re(1) | P(1) | C(1B) | -166.36 ( 0.26) |
| Br(4) | Re(1) | P(1) | C(111) | -40.72 ( 0.26) |
| Br(4) | Re(1) | P(1) | C(121) | 81.19 ( 0.27) |
| P(3) | Re(1) | P(1) | C(1B) | -50.50 ( 0.35) |
| P(3) | Re(1) | P(1) | C(111) | 75.15 ( 0.33) |
| P(3) | Re(1) | P(1) | C(121) | -162.95 ( 0.30) |
| C(1) | Re(1) | P(1) | C(1B) | -171.65 ( 0.44) |
| C(1) | Re(1) | P(1) | C(111) | -46.00 ( 0.44) |
| C(1) | Re(1) | P(1) | C(121) | 75.90 ( 0.45) |
| C(2) | Re(1) | P(1) | C(1B) | 95.92 ( 0.97) |
| C(2) | Re(1) | P(1) | C(111) | -138.43 ( 0.97) |
| C(2) | Re(1) | P(1) | C(121) | -16.53 ( 0.98) |
| Br(1) | Re(1) | P(3) | C(2B) | -142.96 ( 0.24) |
| Br(1) | Re(1) | P(3) | C(311) | -14.13 ( 0.23) |
| Br(1) | Re(1) | P(3) | C(321) | 112.70 ( 0.24) |
| Br(2) | Re(1) | P(3) | C(2B) | -64.68 ( 0.23) |
| Br(2) | Re(1) | P(3) | C(311) | 64.15 ( 0.23) |
| Br(2) | Re(1) | P(3) | C(321) | -169.02 ( 0.24) |
| Br(3) | Re(1) | P(3) | C(2B) | 27.92 ( 0.24) |
| Br(3) | Re(1) | P(3) | C(311) | 156.75 ( 0.23) |
| Br(3) | Re(1) | P(3) | C(321) | -76.42 ( 0.24) |
| Br(4) | Re(1) | P(3) | C(2B) | 116.16 ( 0.26) |
| Br(4) | Re(1) | P(3) | C(311) | -115.01 ( 0.26) |
| Br(4) | Re(1) | P(3) | C(321) | 11.82 ( 0.27) |
| P(1) | Re(1) | P(3) | C(2B) | 0.51 ( 0.36) |
| P(1) | Re(1) | P(3) | C(311) | 129.34 ( 0.30) |
| P(1) | Re(1) | P(3) | C(321) | -103.83 ( 0.32) |
| C(1) | Re(1) | P(3) | C(2B) | 121.42 ( 0.44) |
| C(1) | Re(1) | P(3) | C(311) | -109.75 ( 0.44) |
| C(1) | Re(1) | P(3) | C(321) | 17.08 ( 0.45) |
| C(2) | Re(1) | P(3) | C(2B) | -147.63 ( 0.93) |
| C(2) | Re(1) | P(3) | C(311) | -18.80 ( 0.93) |
| C(2) | Re(1) | P(3) | C(321) | 108.03 ( 0.93) |
| Br(1) | Re(1) | C(1) | Br(4) | -167.48 ( 4.04) |
| Br(1) | Re(1) | C(1) | O(1) | -137.31 ( 54.42) |
| Br(2) | Re(1) | C(1) | Br(4) | -144.33 ( 2.63) |
| Br(2) | Re(1) | C(1) | O(1) | -114.16 ( 53.55) |
| Br(3) | Re(1) | C(1) | Br(4) | 15.43 ( 4.09) |
| Br(3) | Re(1) | C(1) | O(1) | 45.59 ( 54.45) |
| Br(4) | Re(1) | C(1) | O(1) | 30.17 ( 51.91) |
| P(1) | Re(1) | C(1) | Br(4) | 85.44 ( 4.08) |
| P(1) | Re(1) | C(1) | O(1) | 115.61 ( 54.44) |

Table S14 (continued)

**Table of Torsion Angles in Degrees (continued)**

| Atom 1 | Atom 2 | Atom 3 | Atom 4 | Angle |
|---|---|---|---|---|
| P(3) | Re(1) | C(1) | Br(4) | -82.71 ( 4.08) |
| P(3) | Re(1) | C(1) | O(1) | -52.54 ( 54.46) |
| C(2) | Re(1) | C(1) | Br(4) | -165.71 ( 4.14) |
| C(2) | Re(1) | C(1) | O(1) | -135.55 ( 54.44) |
| Br(1) | Re(1) | C(2) | O(2) | 101.67 ( 40.72) |
| Br(2) | Re(1) | C(2) | Br(1) | 23.74 ( 9.22) |
| Br(2) | Re(1) | C(2) | O(2) | 125.41 ( 39.27) |
| Br(3) | Re(1) | C(2) | Br(1) | 6.45 ( 19.31) |
| Br(3) | Re(1) | C(2) | O(2) | 108.12 ( 39.08) |
| Br(4) | Re(1) | C(2) | Br(1) | -160.10 ( 9.23) |
| Br(4) | Re(1) | C(2) | O(2) | -58.43 ( 39.26) |
| P(1) | Re(1) | C(2) | Br(1) | -65.69 ( 9.46) |
| P(1) | Re(1) | C(2) | O(2) | 35.99 ( 39.42) |
| P(3) | Re(1) | C(2) | Br(1) | 106.65 ( 9.36) |
| P(3) | Re(1) | C(2) | O(2) | -151.68 ( 39.30) |
| C(1) | Re(1) | C(2) | Br(1) | -158.79 ( 9.30) |
| C(1) | Re(1) | C(2) | O(2) | -57.12 ( 39.24) |
| Br(3) | Re(2) | Br(2) | Re(1) | -3.88 ( 0.02) |
| P(2) | Re(2) | Br(2) | Re(1) | 83.09 ( 0.04) |
| P(4) | Re(2) | Br(2) | Re(1) | -89.87 ( 0.05) |
| C(10) | Re(2) | Br(2) | Re(1) | -29.50 ( 2.08) |
| C(20) | Re(2) | Br(2) | Re(1) | 178.13 ( 0.20) |
| Br(2) | Re(2) | Br(3) | Re(1) | 3.66 ( 0.02) |
| P(2) | Re(2) | Br(3) | Re(1) | -95.96 ( 0.04) |
| P(4) | Re(2) | Br(3) | Re(1) | 74.73 ( 0.04) |
| C(10) | Re(2) | Br(3) | Re(1) | -178.50 ( 0.18) |
| C(20) | Re(2) | Br(3) | Re(1) | 102.05 ( 5.60) |
| Br(2) | Re(2) | P(2) | C(1B) | -23.39 ( 0.20) |
| Br(2) | Re(2) | P(2) | C(211) | 88.59 ( 0.24) |
| Br(2) | Re(2) | P(2) | C(221) | -151.22 ( 0.24) |
| Br(3) | Re(2) | P(2) | C(1B) | 67.09 ( 0.19) |
| Br(3) | Re(2) | P(2) | C(211) | 179.07 ( 0.24) |
| Br(3) | Re(2) | P(2) | C(221) | -60.74 ( 0.24) |
| P(4) | Re(2) | P(2) | C(1B) | 12.47 ( 0.38) |
| P(4) | Re(2) | P(2) | C(211) | 124.45 ( 0.35) |
| P(4) | Re(2) | P(2) | C(221) | -115.36 ( 0.35) |
| C(10) | Re(2) | P(2) | C(1B) | 151.97 ( 0.27) |
| C(10) | Re(2) | P(2) | C(211) | -96.06 ( 0.30) |
| C(10) | Re(2) | P(2) | C(221) | 24.13 ( 0.30) |
| C(20) | Re(2) | P(2) | C(1B) | -113.54 ( 0.28) |
| C(20) | Re(2) | P(2) | C(211) | -1.56 ( 0.31) |
| C(20) | Re(2) | P(2) | C(221) | 118.63 ( 0.31) |
| Br(2) | Re(2) | P(4) | C(2B) | 63.20 ( 0.25) |
| Br(2) | Re(2) | P(4) | C(411) | 175.93 ( 0.23) |
| Br(2) | Re(2) | P(4) | C(421) | -59.77 ( 0.24) |
| Br(3) | Re(2) | P(4) | C(2B) | -29.04 ( 0.25) |

Table S14 (continued)

**Table of Torsion Angles in Degrees (continued)**

| Atom 1 | Atom 2 | Atom 3 | Atom 4 | Angle | |
|---|---|---|---|---|---|
| Br(3) | Re(2) | P(4) | C(411) | 83.69 | ( 0.23) |
| Br(3) | Re(2) | P(4) | C(421) | -152.01 | ( 0.25) |
| P(2) | Re(2) | P(4) | C(2B) | 25.60 | ( 0.42) |
| P(2) | Re(2) | P(4) | C(411) | 138.33 | ( 0.34) |
| P(2) | Re(2) | P(4) | C(421) | -97.36 | ( 0.37) |
| C(10) | Re(2) | P(4) | C(2B) | -112.29 | ( 0.32) |
| C(10) | Re(2) | P(4) | C(411) | 0.44 | ( 0.30) |
| C(10) | Re(2) | P(4) | C(421) | 124.75 | ( 0.31) |
| C(20) | Re(2) | P(4) | C(2B) | 151.88 | ( 0.32) |
| C(20) | Re(2) | P(4) | C(411) | -95.38 | ( 0.30) |
| C(20) | Re(2) | P(4) | C(421) | 28.92 | ( 0.32) |
| Br(2) | Re(2) | C(10) | N(10) | -59.21 | ( 40.04) |
| Br(3) | Re(2) | C(10) | N(10) | -84.95 | ( 39.13) |
| P(2) | Re(2) | C(10) | N(10) | -172.50 | ( 39.15) |
| P(4) | Re(2) | C(10) | N(10) | -0.20 | ( 39.17) |
| C(20) | Re(2) | C(10) | N(10) | 93.05 | ( 39.13) |
| Br(2) | Re(2) | C(20) | N(20) | 156.69 | ( 6.74) |
| Br(3) | Re(2) | C(20) | N(20) | 58.27 | ( 10.47) |
| P(2) | Re(2) | C(20) | N(20) | -103.67 | ( 6.73) |
| P(4) | Re(2) | C(20) | N(20) | 85.54 | ( 6.74) |
| C(10) | Re(2) | C(20) | N(20) | -20.99 | ( 6.75) |
| Re(1) | Br(1) | O(2) | C(2) | 5.34 | ( 3.75) |
| Re(1) | Br(1) | C(2) | O(2) | -167.01 | ( 9.27) |
| O(2) | Br(1) | C(2) | Re(1) | 167.01 | ( 9.27) |
| Re(1) | Br(4) | O(1) | C(1) | 1.04 | ( 1.87) |
| Re(1) | Br(4) | C(1) | O(1) | -177.87 | ( 3.80) |
| O(1) | Br(4) | C(1) | Re(1) | 177.87 | ( 3.80) |
| Re(1) | P(1) | C(1B) | P(2) | 72.45 | ( 0.41) |
| C(111) | P(1) | C(1B) | P(2) | -65.99 | ( 0.43) |
| C(121) | P(1) | C(1B) | P(2) | -174.68 | ( 0.40) |
| Re(1) | P(1) | C(111) | C(112) | 7.52 | ( 0.70) |
| Re(1) | P(1) | C(111) | C(116) | -175.56 | ( 0.51) |
| C(1B) | P(1) | C(111) | C(112) | 139.75 | ( 0.62) |
| C(1B) | P(1) | C(111) | C(116) | -43.33 | ( 0.65) |
| C(121) | P(1) | C(111) | C(112) | -113.61 | ( 0.63) |
| C(121) | P(1) | C(111) | C(116) | 63.32 | ( 0.66) |
| Re(1) | P(1) | C(121) | C(122) | -73.60 | ( 0.62) |
| Re(1) | P(1) | C(121) | C(126) | 105.43 | ( 0.64) |
| C(1B) | P(1) | C(121) | C(122) | 164.97 | ( 0.61) |
| C(1B) | P(1) | C(121) | C(126) | -15.99 | ( 0.72) |
| C(111) | P(1) | C(121) | C(122) | 61.13 | ( 0.66) |
| C(111) | P(1) | C(121) | C(126) | -119.83 | ( 0.65) |
| Re(2) | P(2) | C(1B) | P(1) | -58.55 | ( 0.40) |
| C(211) | P(2) | C(1B) | P(1) | -177.25 | ( 0.39) |
| C(221) | P(2) | C(1B) | P(1) | 79.30 | ( 0.44) |
| Re(2) | P(2) | C(211) | C(212) | 70.71 | ( 0.58) |

Table S14 (continued)

**Table of Torsion Angles in Degrees (continued)**

| Atom 1 | Atom 2 | Atom 3 | Atom 4 | Angle |
|---|---|---|---|---|
| Re(2) | P(2) | C(211) | C(216) | -108.39 ( 0.58) |
| C(1B) | P(2) | C(211) | C(212) | -176.28 ( 0.54) |
| C(1B) | P(2) | C(211) | C(216) | 4.62 ( 0.68) |
| C(221) | P(2) | C(211) | C(212) | -64.69 ( 0.58) |
| C(221) | P(2) | C(211) | C(216) | 116.21 ( 0.61) |
| Re(2) | P(2) | C(221) | C(222) | 14.66 ( 0.71) |
| Re(2) | P(2) | C(221) | C(226) | -164.21 ( 0.51) |
| C(1B) | P(2) | C(221) | C(222) | -111.66 ( 0.61) |
| C(1B) | P(2) | C(221) | C(226) | 69.47 ( 0.66) |
| C(211) | P(2) | C(221) | C(222) | 141.21 ( 0.62) |
| C(211) | P(2) | C(221) | C(226) | -37.66 ( 0.66) |
| Re(1) | P(3) | C(2B) | P(4) | 42.31 ( 0.52) |
| C(311) | P(3) | C(2B) | P(4) | -92.72 ( 0.51) |
| C(321) | P(3) | C(2B) | P(4) | 159.78 ( 0.49) |
| Re(1) | P(3) | C(311) | C(312) | -92.54 ( 0.62) |
| Re(1) | P(3) | C(311) | C(316) | 86.50 ( 0.63) |
| C(2B) | P(3) | C(311) | C(312) | 33.08 ( 0.70) |
| C(2B) | P(3) | C(311) | C(316) | -147.87 ( 0.61) |
| C(321) | P(3) | C(311) | C(312) | 135.98 ( 0.62) |
| C(321) | P(3) | C(311) | C(316) | -44.98 ( 0.67) |
| Re(1) | P(3) | C(321) | C(322) | 36.02 ( 0.56) |
| Re(1) | P(3) | C(321) | C(326) | -149.05 ( 0.48) |
| C(2B) | P(3) | C(321) | C(322) | -73.31 ( 0.54) |
| C(2B) | P(3) | C(321) | C(326) | 101.62 ( 0.57) |
| C(311) | P(3) | C(321) | C(322) | 172.17 ( 0.49) |
| C(311) | P(3) | C(321) | C(326) | -12.89 ( 0.60) |
| Re(2) | P(4) | C(2B) | P(3) | -47.77 ( 0.58) |
| C(411) | P(4) | C(2B) | P(3) | -158.28 ( 0.48) |
| C(421) | P(4) | C(2B) | P(3) | 89.52 ( 0.51) |
| Re(2) | P(4) | C(411) | C(412) | -90.99 ( 0.71) |
| Re(2) | P(4) | C(411) | C(416) | 78.15 ( 0.56) |
| C(2B) | P(4) | C(411) | C(412) | 35.02 ( 0.77) |
| C(2B) | P(4) | C(411) | C(416) | -155.84 ( 0.56) |
| C(421) | P(4) | C(411) | C(412) | 134.39 ( 0.70) |
| C(421) | P(4) | C(411) | C(416) | -56.48 ( 0.63) |
| Re(2) | P(4) | C(421) | C(422) | -176.85 ( 0.53) |
| Re(2) | P(4) | C(421) | C(426) | 10.84 ( 0.72) |
| C(2B) | P(4) | C(421) | C(422) | 48.88 ( 0.66) |
| C(2B) | P(4) | C(421) | C(426) | -123.42 ( 0.62) |
| C(411) | P(4) | C(421) | C(422) | -57.32 ( 0.69) |
| C(411) | P(4) | C(421) | C(426) | 130.38 ( 0.61) |
| Br(4) | O(1) | C(1) | Re(1) | -32.19 ( 55.00) |
| Br(1) | O(2) | C(2) | Re(1) | -114.02 ( 38.74) |
| C(11) | N(10) | C(10) | Re(2) | 8.18 ( 42.90) |
| C(10) | N(10) | C(11) | C(12) | 69.55 ( 4.76) |
| C(10) | N(10) | C(11) | C(16) | -109.82 ( 4.55) |

Table S14 (continued)

**Table of Torsion Angles in Degrees (continued)**

| Atom 1 | Atom 2 | Atom 3 | Atom 4 | Angle |
|---|---|---|---|---|
| C(21) | N(20) | C(20) | Re(2) | -158.55 ( 5.28) |
| C(20) | N(20) | C(21) | C(22) | 147.66 ( 2.13) |
| C(20) | N(20) | C(21) | C(26) | -32.70 ( 2.60) |
| N(10) | C(11) | C(12) | C(13) | -179.11 ( 0.65) |
| N(10) | C(11) | C(12) | C(17) | 3.61 ( 1.07) |
| C(16) | C(11) | C(12) | C(13) | 0.24 ( 0.99) |
| C(16) | C(11) | C(12) | C(17) | -177.03 ( 0.75) |
| N(10) | C(11) | C(16) | C(15) | -179.96 ( 0.72) |
| N(10) | C(11) | C(16) | C(18) | -0.49 ( 0.95) |
| C(12) | C(11) | C(16) | C(15) | 0.67 ( 0.98) |
| C(12) | C(11) | C(16) | C(18) | -179.87 ( 0.66) |
| C(11) | C(12) | C(13) | C(14) | -0.68 ( 1.11) |
| C(17) | C(12) | C(13) | C(14) | 176.62 ( 0.82) |
| C(12) | C(13) | C(14) | C(15) | 0.15 ( 1.20) |
| C(13) | C(14) | C(15) | C(16) | 0.81 ( 1.22) |
| C(14) | C(15) | C(16) | C(11) | -1.22 ( 1.10) |
| C(14) | C(15) | C(16) | C(18) | 179.35 ( 0.77) |
| N(20) | C(21) | C(22) | C(23) | 179.63 ( 0.65) |
| N(20) | C(21) | C(22) | C(27) | -0.81 ( 1.01) |
| C(26) | C(21) | C(22) | C(23) | -0.02 ( 1.00) |
| C(26) | C(21) | C(22) | C(27) | 179.53 ( 0.69) |
| N(20) | C(21) | C(26) | C(25) | 179.00 ( 0.70) |
| N(20) | C(21) | C(26) | C(28) | 0.62 ( 1.10) |
| C(22) | C(21) | C(26) | C(25) | -1.37 ( 1.07) |
| C(22) | C(21) | C(26) | C(28) | -179.75 ( 0.74) |
| C(21) | C(22) | C(23) | C(24) | -0.47 ( 1.24) |
| C(27) | C(22) | C(23) | C(24) | -179.97 ( 0.63) |
| C(22) | C(23) | C(24) | C(25) | 2.41 ( 1.33) |
| C(23) | C(24) | C(25) | C(26) | -3.58 ( 1.21) |
| C(24) | C(25) | C(26) | C(21) | 3.35 ( 1.19) |
| C(24) | C(25) | C(26) | C(28) | -178.32 ( 0.83) |
| P(1) | C(111) | C(112) | C(113) | 177.65 ( 0.55) |
| C(116) | C(111) | C(112) | C(113) | 0.25 ( 0.99) |
| P(1) | C(111) | C(116) | C(115) | -178.50 ( 0.57) |
| C(112) | C(111) | C(116) | C(115) | -1.17 ( 1.04) |
| C(111) | C(112) | C(113) | C(114) | 0.70 ( 1.28) |
| C(112) | C(113) | C(114) | C(115) | -0.65 ( 1.18) |
| C(113) | C(114) | C(115) | C(116) | -0.23 ( 1.11) |
| C(114) | C(115) | C(116) | C(111) | 1.29 ( 1.27) |
| P(1) | C(121) | C(122) | C(123) | -178.35 ( 0.81) |
| C(126) | C(121) | C(122) | C(123) | 2.59 ( 1.36) |
| P(1) | C(121) | C(126) | C(125) | 179.04 ( 0.70) |
| C(122) | C(121) | C(126) | C(125) | -1.97 ( 1.27) |
| C(121) | C(122) | C(123) | C(124) | -1.31 ( 1.54) |
| C(122) | C(123) | C(124) | C(125) | -0.52 ( 1.65) |
| C(123) | C(124) | C(125) | C(126) | 1.12 ( 1.53) |