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

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| Ir(1) | 0.51713(4) | 0.06275(3) | 0.75003(2) | 2.849(9) |
| Ir(2) | 0.50910(4) | 0.27649(3) | 0.81533(2) | 2.458(8) |
| W(3) | 0.23139(4) | 0.12051(4) | 0.71954(2) | 3.042(9) |
| W(4) | 0.36259(5) | 0.12301(3) | 0.88777(2) | 3.03(1) |
| Cl(01) | 0.135(1) | 0.3634(7) | 0.3983(6) | 18.8(4) |
| Cl(02) | 0.297(1) | 0.2149(8) | 0.4181(4) | 20.2(4) |
| P(1) | 0.6151(3) | 0.4042(2) | 0.7523(2) | 2.86(6) |
| O(11) | 0.640(1) | -0.1186(7) | 0.7902(5) | 5.7(3) |
| O(12) | 0.8328(8) | 0.2247(6) | 0.8165(5) | 5.5(2) |
| O(13) | 0.2355(9) | -0.1283(7) | 0.6691(5) | 5.5(2) |
| O(14) | 0.598(1) | 0.0115(7) | 0.5825(5) | 5.8(2) |
| O(21) | 0.6278(9) | 0.4326(7) | 0.9804(4) | 5.1(2) |
| O(23) | 0.2064(8) | 0.3509(6) | 0.8333(5) | 4.5(2) |
| O(31) | -0.0309(9) | 0.0154(7) | 0.7969(5) | 5.6(2) |
| O(41) | 0.704(1) | 0.1203(7) | 0.9547(5) | 5.7(2) |
| O(42) | 0.287(1) | -0.1304(7) | 0.8496(5) | 5.9(3) |
| C(01) | 0.148(3) | 0.239(1) | 0.3487(9) | 11.0(7) |
| C(11) | 0.598(1) | -0.049(1) | 0.7744(6) | 3.8(3) |
| C(12) | 0.697(1) | 0.2050(9) | 0.8035(6) | 3.5(3) |
| C(13) | 0.275(1) | -0.035(1) | 0.6962(6) | 3.6(3) |
| C(14) | 0.569(1) | 0.033(1) | 0.6468(7) | 3.9(3) |
| C(21) | 0.582(1) | 0.3737(8) | 0.9148(6) | 3.2(2) |
| C(23) | 0.276(1) | 0.2887(9) | 0.8073(7) | 3.6(3) |
| C(31) | 0.078(1) | 0.0609(9) | 0.7774(6) | 3.5(2) |

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

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| C(41) | 0.579(2) | 0.1200(9) | 0.9257(6) | 4.2(3) |
| C(42) | 0.315(1) | -0.038(1) | 0.8574(6) | 3.8(3) |
| C(211) | 0.710(1) | 0.3590(8) | 0.6643(6) | 3.0(2) |
| C(212) | 0.852(1) | 0.414(1) | 0.6537(7) | 5.1(3) |
| C(213) | 0.910(1) | 0.383(1) | 0.5855(7) | 5.8(3) |
| C(214) | 0.833(2) | 0.294(1) | 0.5229(7) | 5.5(4) |
| C(215) | 0.696(2) | 0.235(1) | 0.5336(7) | 6.2(4) |
| C(216) | 0.635(1) | 0.268(1) | 0.6035(7) | 5.2(3) |
| C(221) | 0.480(1) | 0.4789(9) | 0.7192(7) | 3.7(3) |
| C(222) | 0.397(1) | 0.530(1) | 0.7740(7) | 4.6(3) |
| C(223) | 0.303(2) | 0.596(1) | 0.753(1) | 6.1(4) |
| C(224) | 0.295(2) | 0.608(1) | 0.680(1) | 7.9(6) |
| C(225) | 0.372(2) | 0.557(1) | 0.624(1) | 7.4(5) |
| C(226) | 0.466(1) | 0.492(1) | 0.6446(8) | 5.2(3) |
| C(231) | 0.771(1) | 0.5168(8) | 0.8174(6) | 3.1(2) |
| C(232) | 0.887(1) | 0.493(1) | 0.8635(7) | 4.6(3) |
| C(233) | 1.011(1) | 0.574(1) | 0.9069(8) | 5.8(4) |
| C(234) | 1.022(2) | 0.679(1) | 0.9058(8) | 5.9(4) |
| C(235) | 0.909(2) | 0.704(1) | 0.8616(8) | 5.6(3) |
| C(236) | 0.783(1) | 0.623(1) | 0.8171(6) | 4.4(3) |
| C(301) | 0.102(3) | 0.031(1) | 0.593(1) | 8.2(5) |
| C(302) | 0.222(2) | 0.110(2) | 0.5847(7) | 6.3(4) |
| C(303) | 0.202(2) | 0.211(1) | 0.6256(9) | 5.9(4) |
| C(304) | 0.063(2) | 0.196(2) | 0.6585(9) | 7.3(5) |

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

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| C(305) | 0.008(2) | 0.090(3) | 0.631(1) | 10.4(8) |
| C(401) | 0.310(2) | 0.119(1) | 1.0121(7) | 5.8(4) |
| C(402) | 0.164(2) | 0.099(1) | 0.9615(7) | 5.6(4) |
| C(403) | 0.159(1) | 0.195(1) | 0.9443(7) | 4.6(3) |
| C(404) | 0.296(1) | 0.2732(9) | 0.9804(6) | 4.1(3) |
| C(405) | 0.391(2) | 0.227(1) | 1.0204(6) | 5.0(3) |
| H(01a) | 0.1811 | 0.2358 | 0.2983 | 13.2048 |
| H(01b) | 0.0522 | 0.1873 | 0.3408 | 13.2048 |
| H(212) | 0.9100 | 0.4746 | 0.6961 | 6.1640 |
| H(213) | 1.0071 | 0.4237 | 0.5802 | 6.9134 |
| H(214) | 0.8726 | 0.2744 | 0.4739 | 6.6551 |
| H(215) | 0.6424 | 0.1710 | 0.4924 | 7.4107 |
| H(216) | 0.5395 | 0.2257 | 0.6095 | 6.2684 |
| H(222) | 0.4032 | 0.5206 | 0.8260 | 5.5022 |
| H(223) | 0.2459 | 0.6320 | 0.7912 | 7.3513 |
| H(224) | 0.2323 | 0.6535 | 0.6671 | 9.5010 |
| H(225) | 0.3624 | 0.5659 | 0.5715 | 8.8488 |
| H(226) | 0.5212 | 0.4558 | 0.6058 | 6.2710 |
| H(232) | 0.8806 | 0.4207 | 0.8650 | 5.5674 |
| H(233) | 1.0908 | 0.5565 | 0.9380 | 6.9248 |
| H(234) | 1.1094 | 0.7341 | 0.9359 | 7.0822 |
| H(235) | 0.9162 | 0.7767 | 0.8613 | 6.6628 |
| H(236) | 0.7042 | 0.6408 | 0.7861 | 5.3332 |
| H(301) | 0.0894 | -0.0458 | 0.5749 | 9.8882 |

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

| atom | x | y | z | $B_{eq}$ |
|---|---|---|---|---|
| H(302) | 0.3050 | 0.0971 | 0.5556 | 7.5781 |
| H(303) | 0.2690 | 0.2793 | 0.6309 | 7.0246 |
| H(304) | 0.0196 | 0.2488 | 0.6922 | 8.7583 |
| H(305) | -0.0920 | 0.0568 | 0.6387 | 12.5088 |
| H(401) | 0.3464 | 0.0691 | 1.0355 | 6.9739 |
| H(402) | 0.0863 | 0.0328 | 0.9436 | 6.6719 |
| H(403) | 0.0750 | 0.2067 | 0.9125 | 5.5118 |
| H(404) | 0.3193 | 0.3459 | 0.9778 | 4.9512 |
| H(405) | 0.4924 | 0.2618 | 1.0487 | 5.9906 |

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

Table 2. Anisotropic Displacement Parameters

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| Ir(1) | 0.0363(2) | 0.0336(2) | 0.0379(2) | 0.0091(2) | 0.0045(2) | 0.0096(2) |
| Ir(2) | 0.0312(2) | 0.0274(2) | 0.0338(2) | 0.0028(2) | 0.0014(2) | 0.0114(2) |
| W(3) | 0.0268(2) | 0.0470(3) | 0.0387(2) | 0.0015(2) | 0.0004(2) | 0.0138(2) |
| W(4) | 0.0529(3) | 0.0291(2) | 0.0336(2) | 0.0050(2) | 0.0096(2) | 0.0124(2) |
| Cl(01) | 0.247(9) | 0.211(9) | 0.35(1) | 0.105(7) | 0.179(8) | 0.158(8) |
| Cl(02) | 0.40(1) | 0.28(1) | 0.191(7) | 0.20(1) | 0.072(8) | 0.147(7) |
| P(1) | 0.035(1) | 0.031(2) | 0.041(1) | 0.002(1) | 0.004(1) | 0.013(1) |
| O(11) | 0.083(6) | 0.057(6) | 0.095(7) | 0.038(5) | 0.015(5) | 0.039(5) |
| O(12) | 0.031(4) | 0.049(5) | 0.113(7) | 0.005(4) | -0.002(4) | 0.006(5) |
| O(13) | 0.067(6) | 0.049(6) | 0.071(6) | -0.007(5) | -0.002(4) | -0.002(5) |
| O(14) | 0.083(6) | 0.086(7) | 0.048(5) | 0.022(5) | 0.026(5) | 0.009(5) |
| O(21) | 0.068(5) | 0.055(6) | 0.050(5) | 0.002(4) | -0.003(4) | -0.005(4) |
| O(23) | 0.047(4) | 0.048(5) | 0.085(6) | 0.021(4) | 0.025(4) | 0.024(4) |
| O(31) | 0.042(4) | 0.083(7) | 0.085(6) | -0.006(4) | 0.023(4) | 0.026(5) |
| O(41) | 0.079(6) | 0.063(6) | 0.066(6) | 0.010(5) | -0.028(5) | 0.024(5) |
| O(42) | 0.110(7) | 0.034(5) | 0.085(6) | 0.005(5) | 0.038(5) | 0.022(5) |
| C(01) | 0.30(3) | 0.07(1) | 0.08(1) | 0.07(2) | 0.06(1) | 0.034(9) |
| C(11) | 0.042(6) | 0.045(7) | 0.050(7) | 0.003(6) | 0.008(5) | 0.008(6) |
| C(12) | 0.043(6) | 0.039(7) | 0.048(6) | 0.003(5) | 0.012(5) | 0.009(5) |
| C(13) | 0.042(6) | 0.046(7) | 0.043(6) | 0.006(5) | 0.007(5) | 0.006(5) |
| C(14) | 0.036(6) | 0.055(8) | 0.051(7) | 0.010(5) | 0.004(5) | 0.009(6) |
| C(21) | 0.043(6) | 0.036(6) | 0.054(7) | 0.003(5) | 0.006(5) | 0.036(5) |
| C(23) | 0.036(6) | 0.040(7) | 0.063(7) | 0.013(5) | 0.005(5) | 0.015(6) |
| C(31) | 0.043(6) | 0.041(7) | 0.045(6) | 0.002(5) | 0.004(5) | 0.010(5) |

Table 2. Anisotropic Displacement Parameters (continued)

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| C(41) | 0.10(1) | 0.027(6) | 0.041(6) | 0.016(6) | 0.006(6) | 0.019(5) |
| C(42) | 0.057(7) | 0.046(8) | 0.039(6) | 0.004(6) | 0.019(5) | 0.010(5) |
| C(211) | 0.039(6) | 0.034(6) | 0.043(6) | 0.009(5) | 0.005(5) | 0.012(5) |
| C(212) | 0.053(7) | 0.065(9) | 0.064(8) | -0.003(6) | 0.017(6) | 0.005(7) |
| C(213) | 0.066(8) | 0.08(1) | 0.063(8) | -0.008(7) | 0.028(7) | 0.008(7) |
| C(214) | 0.076(9) | 0.09(1) | 0.047(7) | 0.013(8) | 0.025(7) | 0.018(7) |
| C(215) | 0.08(1) | 0.08(1) | 0.048(7) | -0.016(8) | 0.015(7) | 0.000(7) |
| C(216) | 0.054(7) | 0.067(9) | 0.056(7) | -0.010(7) | 0.017(6) | -0.003(7) |
| C(221) | 0.044(6) | 0.035(6) | 0.064(7) | -0.003(5) | 0.003(5) | 0.027(6) |
| C(222) | 0.067(8) | 0.041(7) | 0.078(8) | 0.020(6) | 0.029(7) | 0.025(6) |
| C(223) | 0.069(9) | 0.054(9) | 0.13(1) | 0.030(7) | 0.032(9) | 0.039(9) |
| C(224) | 0.07(1) | 0.09(1) | 0.17(2) | 0.034(9) | 0.01(1) | 0.08(1) |
| C(225) | 0.10(1) | 0.11(1) | 0.10(1) | 0.04(1) | 0.01(1) | 0.07(1) |
| C(226) | 0.069(8) | 0.07(1) | 0.074(9) | 0.024(7) | 0.011(7) | 0.039(8) |
| C(231) | 0.041(6) | 0.032(6) | 0.041(6) | -0.001(5) | 0.012(5) | 0.009(5) |
| C(232) | 0.042(6) | 0.047(8) | 0.077(8) | -0.007(6) | -0.002(6) | 0.017(6) |
| C(233) | 0.048(7) | 0.08(1) | 0.079(9) | -0.009(7) | -0.004(7) | 0.021(8) |
| C(234) | 0.058(8) | 0.07(1) | 0.063(8) | -0.022(8) | 0.010(7) | -0.010(8) |
| C(235) | 0.078(9) | 0.030(7) | 0.080(9) | -0.011(7) | 0.023(8) | -0.008(7) |
| C(236) | 0.064(8) | 0.046(8) | 0.050(7) | 0.000(6) | 0.014(6) | 0.007(6) |
| C(301) | 0.12(2) | 0.06(1) | 0.10(1) | 0.00(1) | -0.07(1) | 0.03(1) |
| C(302) | 0.071(9) | 0.13(2) | 0.034(7) | 0.02(1) | -0.010(6) | 0.032(9) |
| C(303) | 0.08(1) | 0.06(1) | 0.063(9) | -0.020(8) | -0.044(8) | 0.039(8) |
| C(304) | 0.09(1) | 0.13(2) | 0.07(1) | 0.08(1) | -0.01(1) | 0.03(1) |

Table 2. Anisotropic Displacement Parameters (continued)

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| C(305) | 0.044(9) | 0.23(3) | 0.13(2) | -0.02(1) | -0.04(1) | 0.13(2) |
| C(401) | 0.14(1) | 0.055(9) | 0.035(6) | 0.028(9) | 0.040(8) | 0.019(6) |
| C(402) | 0.10(1) | 0.055(9) | 0.048(7) | -0.007(8) | 0.040(7) | 0.007(7) |
| C(403) | 0.068(8) | 0.054(8) | 0.056(7) | 0.018(7) | 0.031(6) | 0.013(6) |
| C(404) | 0.077(8) | 0.036(7) | 0.039(6) | 0.007(6) | 0.025(6) | 0.005(5) |
| C(405) | 0.11(1) | 0.051(8) | 0.035(6) | 0.027(8) | 0.016(6) | 0.014(6) |

The general temperature factor expression:

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

Table 3. Bond Lengths(Å)

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| Ir(1) | Ir(2) | 2.7348(6) | Ir(1) | W(3) | 2.8294(7) |
| Ir(1) | W(4) | 2.8833(6) | Ir(1) | C(11) | 1.88(1) |
| Ir(1) | C(12) | 2.13(1) | Ir(1) | C(13) | 2.25(1) |
| Ir(1) | C(14) | 1.86(1) | Ir(2) | W(3) | 2.9146(6) |
| Ir(2) | W(4) | 2.8381(6) | Ir(2) | P(1) | 2.348(3) |
| Ir(2) | C(12) | 2.07(1) | Ir(2) | C(21) | 1.83(1) |
| Ir(2) | C(23) | 2.11(1) | W(3) | W(4) | 3.0604(6) |
| W(3) | C(13) | 2.08(1) | W(3) | C(23) | 2.25(1) |
| W(3) | C(31) | 1.94(1) | W(3) | C(301) | 2.29(1) |
| W(3) | C(302) | 2.32(1) | W(3) | C(303) | 2.30(1) |
| W(3) | C(304) | 2.28(1) | W(3) | C(305) | 2.30(1) |
| W(4) | C(41) | 1.98(1) | W(4) | C(42) | 1.98(1) |
| W(4) | C(401) | 2.28(1) | W(4) | C(402) | 2.31(1) |
| W(4) | C(403) | 2.37(1) | W(4) | C(404) | 2.39(1) |
| W(4) | C(405) | 2.31(1) | Cl(01) | C(01) | 1.66(2) |
| Cl(02) | C(01) | 1.84(2) | P(1) | C(211) | 1.83(1) |
| P(1) | C(221) | 1.84(1) | P(1) | C(231) | 1.842(9) |
| O(11) | C(11) | 1.14(1) | O(12) | C(12) | 1.17(1) |
| O(13) | C(13) | 1.16(1) | O(14) | C(14) | 1.15(1) |
| O(21) | C(21) | 1.18(1) | O(23) | C(23) | 1.13(1) |
| O(31) | C(31) | 1.17(1) | O(41) | C(41) | 1.18(1) |
| O(42) | C(42) | 1.15(1) | C(211) | C(212) | 1.38(1) |
| C(211) | C(216) | 1.37(1) | C(212) | C(213) | 1.34(2) |
| C(213) | C(214) | 1.37(2) | C(214) | C(215) | 1.37(2) |

Table 3. Bond Lengths(Å) (continued)

| atom | atom | distance |
|---|---|---|
| C(215) | C(216) | 1.38(2) |
| C(221) | C(226) | 1.36(2) |
| C(223) | C(224) | 1.33(2) |
| C(225) | C(226) | 1.40(2) |
| C(231) | C(236) | 1.38(2) |
| C(233) | C(234) | 1.36(2) |
| C(235) | C(236) | 1.38(1) |
| C(301) | C(305) | 1.35(3) |
| C(303) | C(304) | 1.41(2) |
| C(401) | C(402) | 1.44(2) |
| C(402) | C(403) | 1.39(2) |
| C(404) | C(405) | 1.37(2) |
| C(221) | C(222) | 1.37(2) |
| C(222) | C(223) | 1.40(2) |
| C(224) | C(225) | 1.35(2) |
| C(231) | C(232) | 1.39(1) |
| C(232) | C(233) | 1.36(1) |
| C(234) | C(235) | 1.36(2) |
| C(301) | C(302) | 1.38(2) |
| C(302) | C(303) | 1.37(2) |
| C(304) | C(305) | 1.31(3) |
| C(401) | C(405) | 1.42(2) |
| C(403) | C(404) | 1.39(2) |

Table 4. Bond Lengths(Å)

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| C(01) | H(01a) | 0.95 | C(01) | H(01b) | 0.95 |
| C(212) | H(212) | 0.95 | C(213) | H(213) | 0.95 |
| C(214) | H(214) | 0.95 | C(215) | H(215) | 0.95 |
| C(216) | H(216) | 0.95 | C(222) | H(222) | 0.95 |
| C(223) | H(223) | 0.95 | C(224) | H(224) | 0.95 |
| C(225) | H(225) | 0.95 | C(226) | H(226) | 0.95 |
| C(232) | H(232) | 0.95 | C(233) | H(233) | 0.95 |
| C(234) | H(234) | 0.95 | C(235) | H(235) | 0.95 |
| C(236) | H(236) | 0.95 | C(301) | H(301) | 0.95 |
| C(302) | H(302) | 0.95 | C(303) | H(303) | 0.95 |
| C(304) | H(304) | 0.95 | C(305) | H(305) | 0.95 |
| C(401) | H(401) | 0.95 | C(402) | H(402) | 0.95 |
| C(403) | H(403) | 0.95 | C(404) | H(404) | 0.95 |
| C(405) | H(405) | 0.95 | | | |

Table 5. Bond Angles(°)

| atom | atom | atom | angle |
|---|---|---|---|
| Ir(2) | Ir(1) | W(3) | 63.15(1) |
| Ir(2) | Ir(1) | C(11) | 141.2(3) |
| Ir(2) | Ir(1) | C(13) | 109.0(3) |
| W(3) | Ir(1) | W(4) | 64.78(2) |
| W(3) | Ir(1) | C(12) | 110.5(3) |
| W(3) | Ir(1) | C(14) | 99.0(3) |
| W(4) | Ir(1) | C(12) | 89.0(3) |
| W(4) | Ir(1) | C(14) | 163.8(3) |
| C(11) | Ir(1) | C(13) | 98.1(4) |
| C(12) | Ir(1) | C(13) | 157.0(4) |
| C(13) | Ir(1) | C(14) | 88.4(4) |
| Ir(1) | Ir(2) | W(4) | 62.28(1) |
| Ir(1) | Ir(2) | C(12) | 50.3(3) |
| Ir(1) | Ir(2) | C(23) | 108.5(3) |
| W(3) | Ir(2) | P(1) | 113.01(6) |
| W(3) | Ir(2) | C(21) | 142.2(3) |
| W(4) | Ir(2) | P(1) | 176.49(6) |
| W(4) | Ir(2) | C(21) | 89.6(3) |
| P(1) | Ir(2) | C(12) | 91.6(3) |
| P(1) | Ir(2) | C(23) | 101.4(3) |
| C(12) | Ir(2) | C(23) | 158.8(4) |
| Ir(1) | W(3) | Ir(2) | 56.84(2) |
| Ir(1) | W(3) | C(13) | 51.9(3) |
| Ir(1) | W(3) | C(31) | 111.1(3) |

| atom | atom | atom | angle |
|---|---|---|---|
| Ir(2) | Ir(1) | W(4) | 60.62(1) |
| Ir(2) | Ir(1) | C(12) | 48.4(3) |
| Ir(2) | Ir(1) | C(14) | 113.0(4) |
| W(3) | Ir(1) | C(11) | 141.2(3) |
| W(3) | Ir(1) | C(13) | 46.5(3) |
| W(4) | Ir(1) | C(11) | 98.8(3) |
| W(4) | Ir(1) | C(13) | 80.5(3) |
| C(11) | Ir(1) | C(12) | 103.7(4) |
| C(11) | Ir(1) | C(14) | 94.4(5) |
| C(12) | Ir(1) | C(14) | 97.0(4) |
| Ir(1) | Ir(2) | W(3) | 60.01(2) |
| Ir(1) | Ir(2) | P(1) | 118.74(7) |
| Ir(1) | Ir(2) | C(21) | 132.7(3) |
| W(3) | Ir(2) | W(4) | 64.26(1) |
| W(3) | Ir(2) | C(12) | 109.3(3) |
| W(3) | Ir(2) | C(23) | 50.2(3) |
| W(4) | Ir(2) | C(12) | 91.5(3) |
| W(4) | Ir(2) | C(23) | 75.2(3) |
| P(1) | Ir(2) | C(21) | 91.7(3) |
| C(12) | Ir(2) | C(21) | 97.6(4) |
| C(21) | Ir(2) | C(23) | 98.7(4) |
| Ir(1) | W(3) | W(4) | 58.46(1) |
| Ir(1) | W(3) | C(23) | 101.3(3) |
| Ir(1) | W(3) | C(301) | 113.0(6) |

Table 5. Bond Angles(°) (continued)

| atom | atom | atom | angle |
|---|---|---|---|
| Ir(1) | W(3) | C(302) | 100.9(4) |
| Ir(1) | W(3) | C(304) | 155.1(6) |
| Ir(2) | W(3) | W(4) | 56.66(1) |
| Ir(2) | W(3) | C(23) | 45.9(3) |
| Ir(2) | W(3) | C(301) | 145.3(6) |
| Ir(2) | W(3) | C(303) | 95.6(3) |
| Ir(2) | W(3) | C(305) | 147.2(8) |
| W(4) | W(3) | C(23) | 68.7(3) |
| W(4) | W(3) | C(301) | 151.7(4) |
| W(4) | W(3) | C(303) | 149.8(3) |
| W(4) | W(3) | C(305) | 144.8(5) |
| C(13) | W(3) | C(31) | 81.9(4) |
| C(13) | W(3) | C(302) | 90.9(6) |
| C(13) | W(3) | C(304) | 134.1(6) |
| C(23) | W(3) | C(31) | 92.4(4) |
| C(23) | W(3) | C(302) | 116.5(6) |
| C(23) | W(3) | C(304) | 79.1(6) |
| C(31) | W(3) | C(301) | 97.6(7) |
| C(31) | W(3) | C(303) | 129.3(5) |
| C(31) | W(3) | C(305) | 79.5(6) |
| C(301) | W(3) | C(303) | 58.5(5) |
| C(301) | W(3) | C(305) | 34.2(7) |
| C(302) | W(3) | C(304) | 58.5(6) |
| C(303) | W(3) | C(304) | 35.8(6) |

| atom | atom | atom | angle |
|---|---|---|---|
| Ir(1) | W(3) | C(303) | 119.3(5) |
| Ir(1) | W(3) | C(305) | 147.1(9) |
| Ir(2) | W(3) | C(13) | 108.1(3) |
| Ir(2) | W(3) | C(31) | 117.0(3) |
| Ir(2) | W(3) | C(302) | 110.9(4) |
| Ir(2) | W(3) | C(304) | 114.3(6) |
| W(4) | W(3) | C(13) | 78.9(3) |
| W(4) | W(3) | C(31) | 65.7(3) |
| W(4) | W(3) | C(302) | 159.1(3) |
| W(4) | W(3) | C(304) | 140.1(4) |
| C(13) | W(3) | C(23) | 146.4(4) |
| C(13) | W(3) | C(301) | 76.0(5) |
| C(13) | W(3) | C(303) | 125.3(6) |
| C(13) | W(3) | C(305) | 102.0(9) |
| C(23) | W(3) | C(301) | 137.5(5) |
| C(23) | W(3) | C(303) | 83.5(5) |
| C(23) | W(3) | C(305) | 109.5(9) |
| C(31) | W(3) | C(302) | 131.4(5) |
| C(31) | W(3) | C(304) | 93.7(7) |
| C(301) | W(3) | C(302) | 34.8(6) |
| C(301) | W(3) | C(304) | 59.2(6) |
| C(302) | W(3) | C(303) | 34.5(5) |
| C(302) | W(3) | C(305) | 55.0(6) |
| C(303) | W(3) | C(305) | 55.2(6) |

Table 5. Bond Angles(°) (continued)

| atom | atom | atom | angle |
|---|---|---|---|
| C(304) | W(3) | C(305) | 33.2(7) |
| Ir(1) | W(4) | W(3) | 56.76(1) |
| Ir(1) | W(4) | C(42) | 76.6(3) |
| Ir(1) | W(4) | C(402) | 153.7(3) |
| Ir(1) | W(4) | C(404) | 143.9(3) |
| Ir(2) | W(4) | W(3) | 59.08(1) |
| Ir(2) | W(4) | C(42) | 133.3(3) |
| Ir(2) | W(4) | C(402) | 139.9(4) |
| Ir(2) | W(4) | C(404) | 86.8(3) |
| W(3) | W(4) | C(41) | 126.7(3) |
| W(3) | W(4) | C(401) | 146.4(4) |
| W(3) | W(4) | C(403) | 92.0(3) |
| W(3) | W(4) | C(405) | 140.3(3) |
| C(41) | W(4) | C(401) | 86.8(5) |
| C(41) | W(4) | C(403) | 137.0(4) |
| C(41) | W(4) | C(405) | 79.7(5) |
| C(42) | W(4) | C(402) | 81.8(4) |
| C(42) | W(4) | C(404) | 139.2(4) |
| C(401) | W(4) | C(402) | 36.6(5) |
| C(401) | W(4) | C(404) | 57.8(4) |
| C(402) | W(4) | C(403) | 34.4(4) |
| C(402) | W(4) | C(405) | 59.9(4) |
| C(403) | W(4) | C(405) | 57.3(4) |
| Ir(2) | P(1) | C(211) | 119.1(3) |

| atom | atom | atom | angle |
|---|---|---|---|
| Ir(1) | W(4) | Ir(2) | 57.10(1) |
| Ir(1) | W(4) | C(41) | 71.5(3) |
| Ir(1) | W(4) | C(401) | 152.9(4) |
| Ir(1) | W(4) | C(403) | 148.5(3) |
| Ir(1) | W(4) | C(405) | 145.5(4) |
| Ir(2) | W(4) | C(41) | 83.8(3) |
| Ir(2) | W(4) | C(401) | 138.2(4) |
| Ir(2) | W(4) | C(403) | 105.5(3) |
| Ir(2) | W(4) | C(405) | 102.1(3) |
| W(3) | W(4) | C(42) | 92.2(3) |
| W(3) | W(4) | C(402) | 110.0(4) |
| W(3) | W(4) | C(404) | 106.7(3) |
| C(41) | W(4) | C(42) | 87.1(4) |
| C(41) | W(4) | C(402) | 122.5(5) |
| C(41) | W(4) | C(404) | 107.9(4) |
| C(42) | W(4) | C(401) | 86.5(4) |
| C(42) | W(4) | C(403) | 112.0(4) |
| C(42) | W(4) | C(405) | 121.1(4) |
| C(401) | W(4) | C(403) | 58.0(5) |
| C(401) | W(4) | C(405) | 36.1(4) |
| C(402) | W(4) | C(404) | 58.0(4) |
| C(403) | W(4) | C(404) | 34.1(4) |
| C(404) | W(4) | C(405) | 33.8(4) |
| Ir(2) | P(1) | C(221) | 115.4(4) |

Table 5. Bond Angles(°) (continued)

| atom | atom | atom | angle |
|---|---|---|---|
| Ir(2) | P(1) | C(231) | 114.0(3) |
| C(211) | P(1) | C(231) | 100.8(4) |
| Cl(01) | C(01) | Cl(02) | 101(1) |
| Ir(1) | C(12) | Ir(2) | 81.3(4) |
| Ir(2) | C(12) | O(12) | 142.6(9) |
| Ir(1) | C(13) | O(13) | 126.7(9) |
| Ir(1) | C(14) | O(14) | 178(1) |
| Ir(2) | C(23) | W(3) | 83.9(4) |
| W(3) | C(23) | O(23) | 138.2(8) |
| W(4) | C(41) | O(41) | 174(1) |
| P(1) | C(211) | C(212) | 124.0(8) |
| C(212) | C(211) | C(216) | 117(1) |
| C(212) | C(213) | C(214) | 122(1) |
| C(214) | C(215) | C(216) | 121(1) |
| P(1) | C(221) | C(222) | 118.1(9) |
| C(222) | C(221) | C(226) | 119(1) |
| C(222) | C(223) | C(224) | 119(1) |
| C(224) | C(225) | C(226) | 118(1) |
| P(1) | C(231) | C(232) | 119.3(8) |
| C(232) | C(231) | C(236) | 118.4(9) |
| C(232) | C(233) | C(234) | 120(1) |
| C(234) | C(235) | C(236) | 120(1) |
| W(3) | C(301) | C(302) | 74.1(8) |
| C(302) | C(301) | C(305) | 103(2) |
| C(211) | P(1) | C(221) | 103.6(5) |
| C(221) | P(1) | C(231) | 101.5(5) |
| Ir(1) | C(11) | O(11) | 176(1) |
| Ir(1) | C(12) | O(12) | 136.1(9) |
| Ir(1) | C(13) | W(3) | 81.6(4) |
| W(3) | C(13) | O(13) | 151.5(9) |
| Ir(2) | C(21) | O(21) | 176.9(9) |
| Ir(2) | C(23) | O(23) | 137.9(9) |
| W(3) | C(31) | O(31) | 166.4(9) |
| W(4) | C(42) | O(42) | 172(1) |
| P(1) | C(211) | C(216) | 119.2(8) |
| C(211) | C(212) | C(213) | 122(1) |
| C(213) | C(214) | C(215) | 118(1) |
| C(211) | C(216) | C(215) | 121(1) |
| P(1) | C(221) | C(226) | 123(1) |
| C(221) | C(222) | C(223) | 120(1) |
| C(223) | C(224) | C(225) | 123(2) |
| C(221) | C(226) | C(225) | 122(1) |
| P(1) | C(231) | C(236) | 122.1(8) |
| C(231) | C(232) | C(233) | 121(1) |
| C(233) | C(234) | C(235) | 120(1) |
| C(231) | C(236) | C(235) | 120(1) |
| W(3) | C(301) | C(305) | 73(1) |
| W(3) | C(302) | C(301) | 71.1(9) |

Table 5. Bond Angles(°) (continued)

| atom | atom | atom | angle |
|---|---|---|---|
| W(3) | C(302) | C(303) | 71.9(7) |
| W(3) | C(303) | C(302) | 73.6(8) |
| C(302) | C(303) | C(304) | 108(1) |
| W(3) | C(304) | C(305) | 74(1) |
| W(3) | C(305) | C(301) | 72.5(9) |
| C(301) | C(305) | C(304) | 116(2) |
| W(4) | C(401) | C(405) | 73.1(7) |
| W(4) | C(402) | C(401) | 70.8(7) |
| C(401) | C(402) | C(403) | 106(1) |
| W(4) | C(403) | C(404) | 73.9(7) |
| W(4) | C(404) | C(403) | 72.0(6) |
| C(403) | C(404) | C(405) | 109(1) |
| W(4) | C(405) | C(404) | 76.3(6) |

| atom | atom | atom | angle |
|---|---|---|---|
| C(301) | C(302) | C(303) | 109(2) |
| W(3) | C(303) | C(304) | 71.2(8) |
| W(3) | C(304) | C(303) | 73.0(8) |
| C(303) | C(304) | C(305) | 103(2) |
| W(3) | C(305) | C(304) | 72.8(9) |
| W(4) | C(401) | C(402) | 72.6(6) |
| C(402) | C(401) | C(405) | 107(1) |
| W(4) | C(402) | C(403) | 75.2(7) |
| W(4) | C(403) | C(402) | 70.3(7) |
| C(402) | C(403) | C(404) | 110(1) |
| W(4) | C(404) | C(405) | 69.9(7) |
| W(4) | C(405) | C(401) | 70.8(6) |
| C(401) | C(405) | C(404) | 108(1) |

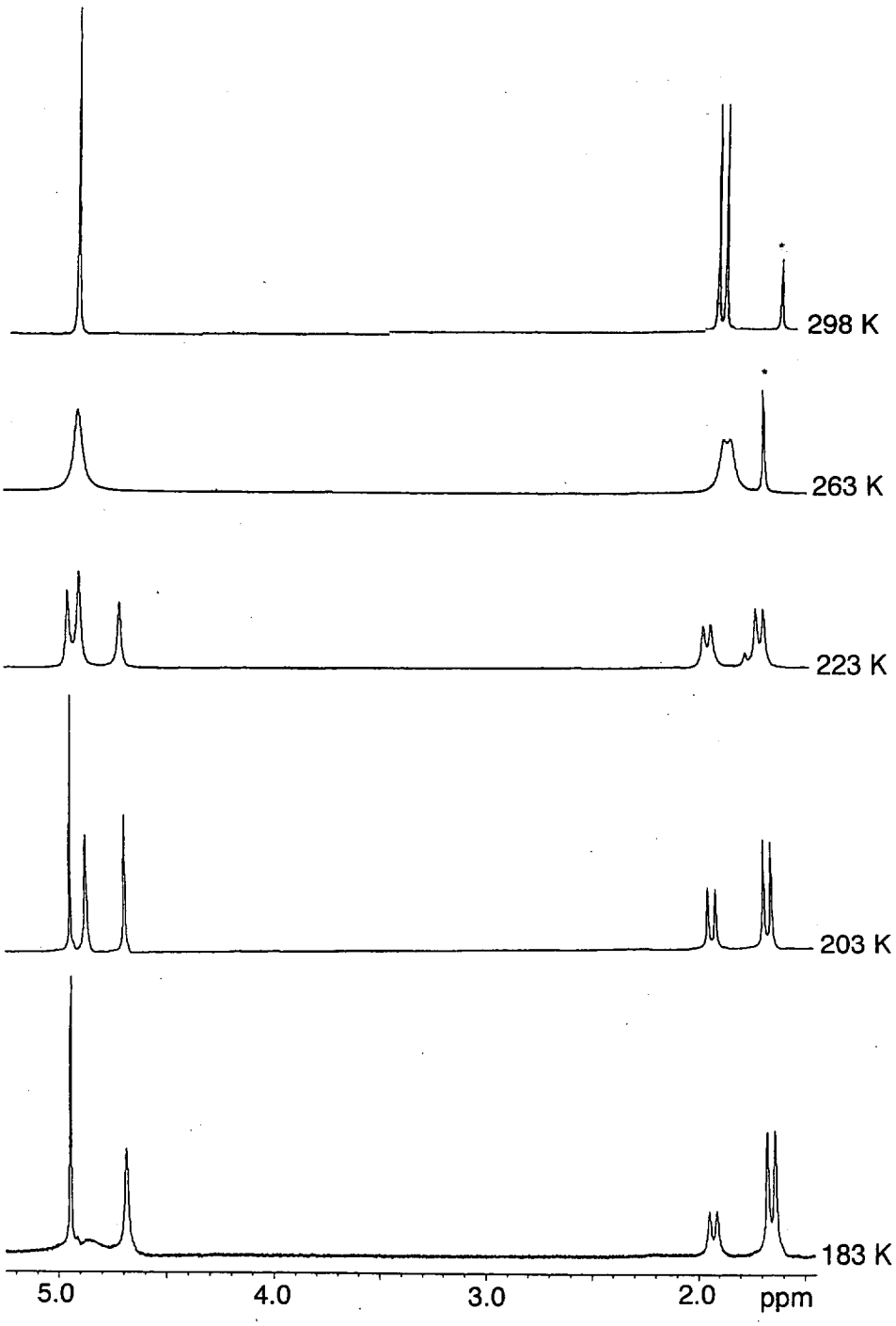


Figure 1: Variable temperature $^1H$ NMR spectroscopic study of $Cp_2W_2Ir_2(\mu\text{-}CO)_3(CO)_6(PMe_3)$ (**4**) in $CD_2Cl_2$.

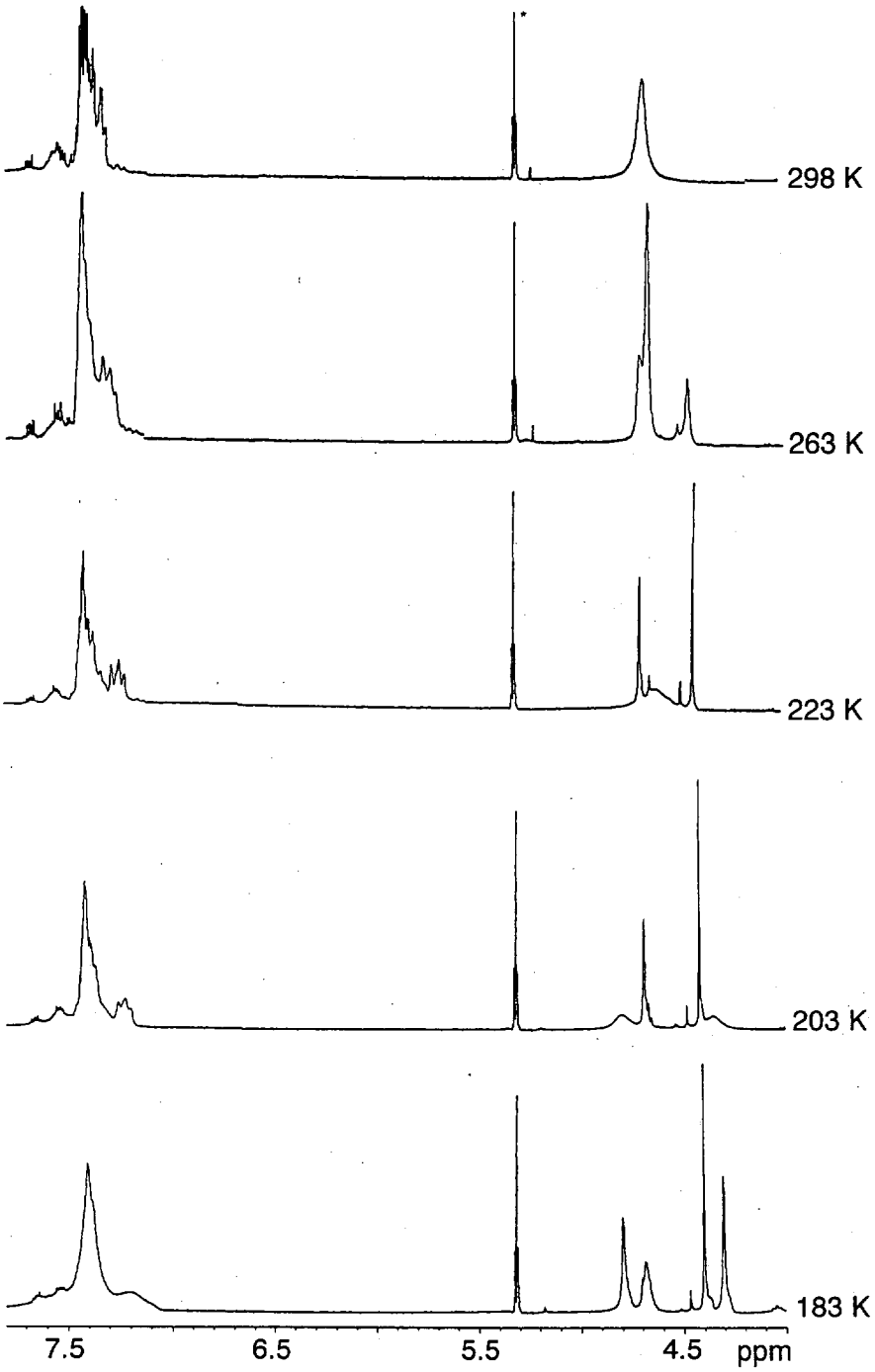


Figure 2: Variable temperature $^1H$ NMR spectroscopic study of $Cp_2W_2Ir_2(\mu\text{-}CO)_3(CO)_6(PPh_3)$ (**2**) in $CD_2Cl_2$.

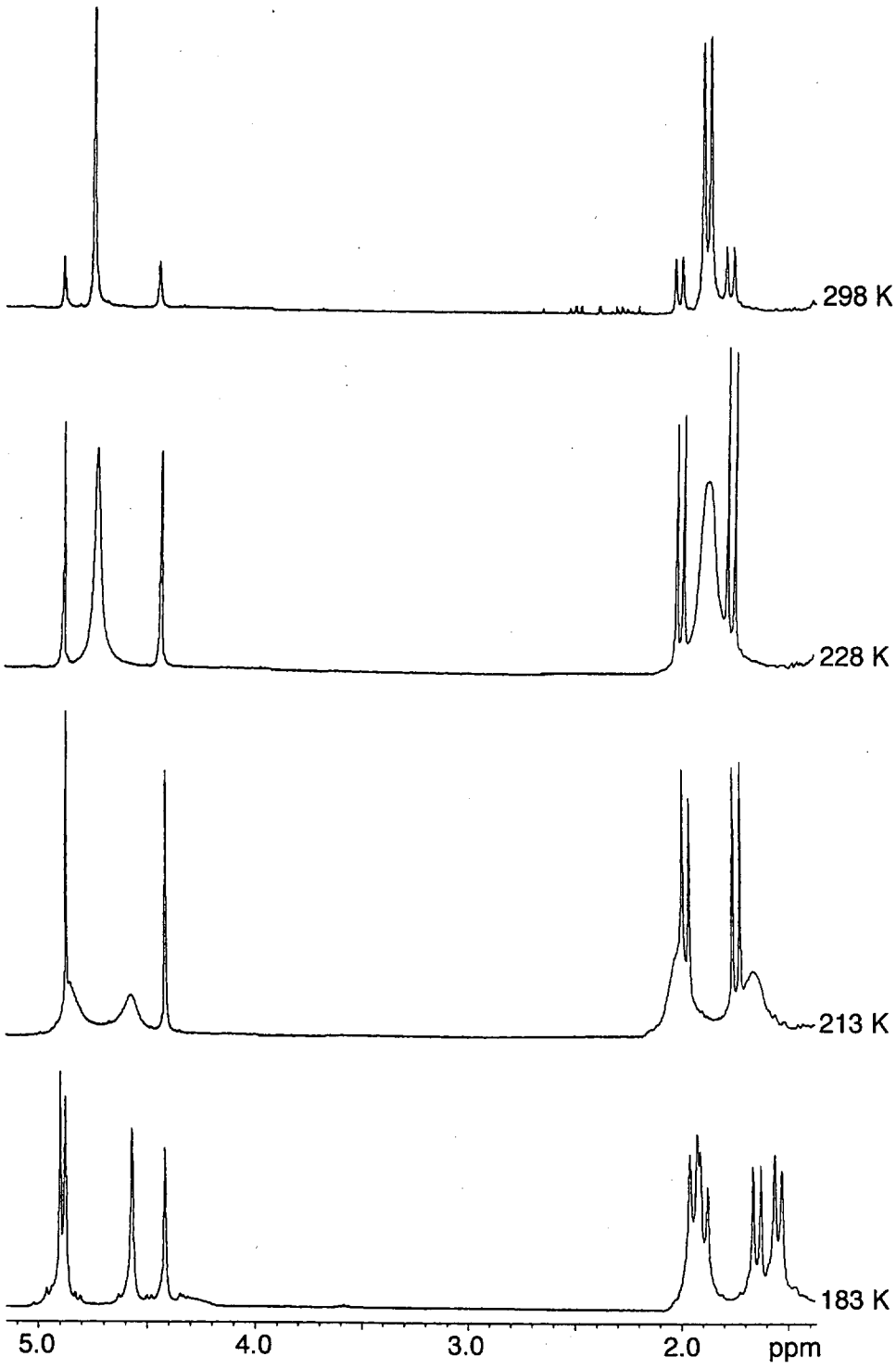


Figure 3: Variable temperature $^1H$ NMR spectroscopic study of $Cp_2W_2Ir_2(\mu\text{-}CO)_3(CO)_5(PMe_3)_2$ (**5**) in $CD_2Cl_2$.

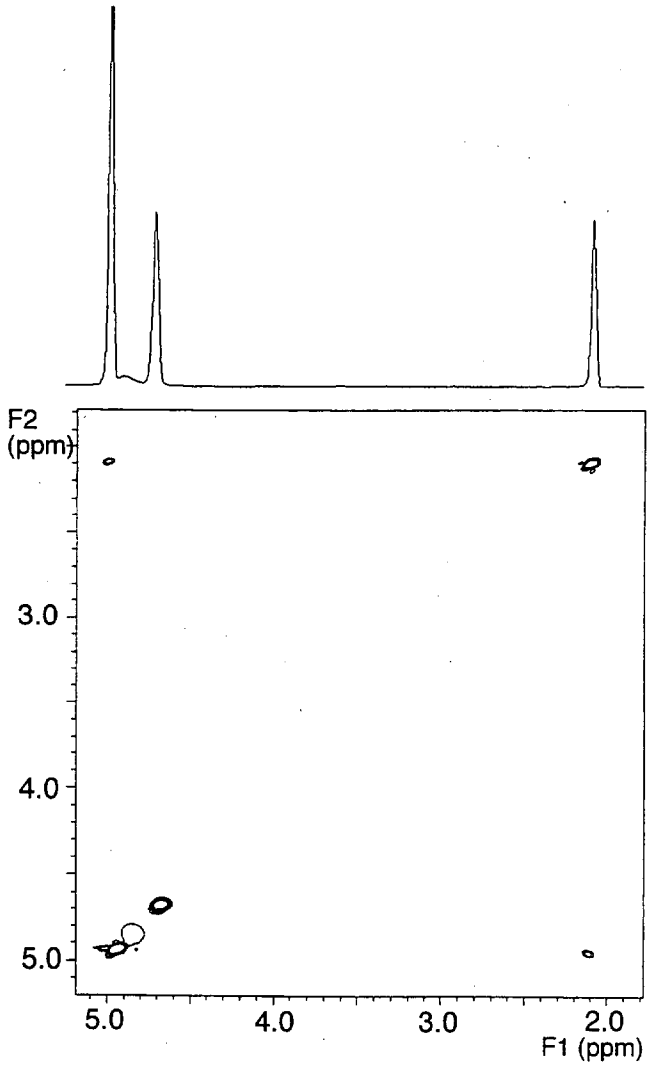


Figure 4: $^{1}H$ NOESY spectrum of $Cp_2W_2Ir_2(\mu\text{-}CO)_3(CO)_6(PMe_3)$ (**4**) in $CD_2Cl_2$ at 183 K.

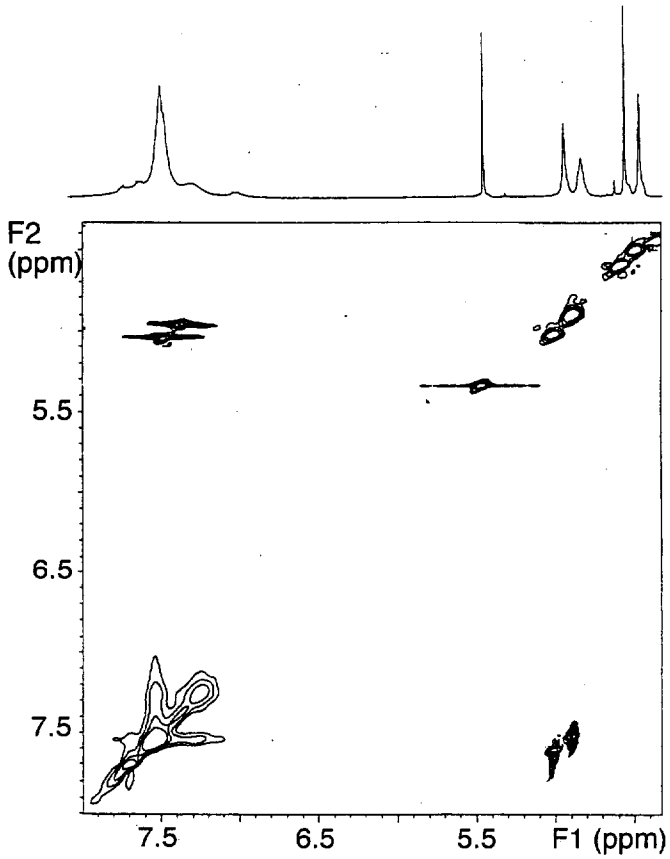


Figure 5: $^{1}H$ NOESY spectrum of $Cp_2W_2Ir_2(\mu\text{-}CO)_3(CO)_6(PPh_3)$ (**2**) in $CD_2Cl_2$ at 183 K.

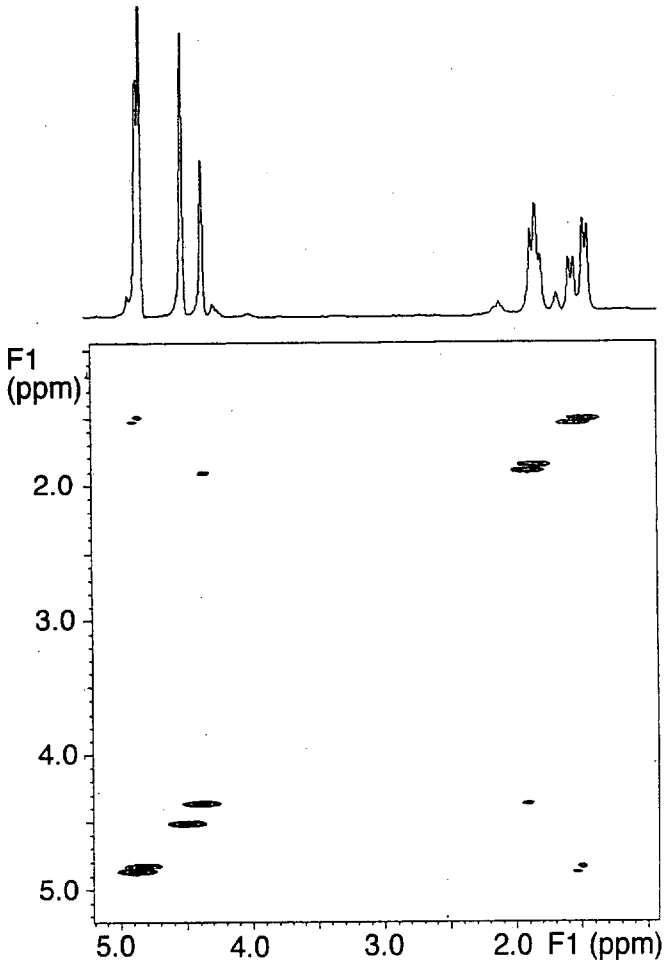


Figure 6: $^1$H NOESY spectrum of $Cp_2W_2Ir_2(\mu\text{-}CO)_3(CO)_5(PMe_3)_2$ (**5**) in $CD_2Cl_2$ at 183 K.