ORGANOMETALLICS
Organometallics, 1998, 17(3), 296-307, DOI:10.1021/om9706626

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Supplementary Table 1.
Crystal data and structure refinement for monoclinic 1 at T = 323 K.

| | |
|---|---|
| Identification code | june |
| Empirical formula | C10 H10 Co F6 P |
| Formula weight | 334.08 |
| Temperature | 323(2) K |
| Wavelength | 0.71069 A |
| Crystal system | monoclinic |
| Space group | P2(1)/c |
| Unit cell dimensions | a = 13.426(5) A alpha = 90 deg.<br>b = 9.518(5) A beta = 90.17(4) deg.<br>c = 9.505(5) A gamma = 90 deg. |
| Volume | 1214.6(10) A^3 |
| Z | 4 |
| Density (calculated) | 1.827 Mg/m^3 |
| Absorption coefficient | 1.597 mm^-1 |
| F(000) | 664 |
| Crystal size | 0.16 x 0.14 x 0.14 mm |
| Theta range for data collection | 3.00 to 23.00 deg. |
| Index ranges | -14<=h<=14, -9<=k<=10, 0<=l<=10 |
| Reflections collected | 2534 |
| Independent reflections | 1550 [R(int) = 0.1108] |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 1550 / 0 / 142 |
| Goodness-of-fit on F^2 | 0.938 |
| Final R indices [I>2sigma(I)] | R1 = 0.0964, wR2 = 0.2566 |
| R indices (all data) | R1 = 0.2205, wR2 = 0.3823 |
| Largest diff. peak and hole | .508 and -.528 e.A^-3 |

Supplementary Table 2.
Atomic coordinates ( x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for monoclinic 1 at T = 333 K U(eq)
as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Co(1) | 0 | -5000 | 10000 | 73(1) |
| C(1) | 659(66) | -3038(96) | 9836(114) | 150 |
| C(2) | -636(54) | -3281(77) | 10519(83) | 150 |
| C(3) | -19(51) | -2679(66) | 9752(72) | 150 |
| C(4) | 984(87) | -5213(140) | 11523(136) | 150 |
| C(5) | 1239(52) | -3789(88) | 10780(95) | 150 |
| C(6) | 1231(54) | -6095(100) | 10719(106) | 150 |
| C(7) | -1360(108) | -5363(148) | 10398(191) | 150 |
| C(8) | -1134(50) | -4247(87) | 11288(84) | 150 |
| C(9) | 311(48) | -4154(76) | 11881(71) | 150 |
| C(10) | 162(65) | -5743(109) | 11994(93) | 150 |
| C(11) | 936 | -4200 | 11359 | 150 |
| C(12) | 695(120) | -6471(161) | 11216(185) | 150 |
| C(13) | -1015(68) | -6205(103) | 11071(109) | 150 |
| C(14) | -352 | -4439 | 12166 | 150 |
| C(15) | -360 | -5473 | 12184 | 150 |
| Co(2) | 5000 | 5000 | 10000 | 76(1) |
| C(16) | 6169(58) | 6274(77) | 9787(108) | 150 |
| C(17) | 4979(38) | 7074(50) | 10036(51) | 150 |
| C(18) | 4076(46) | 6720(66) | 10003(79) | 150 |
| C(19) | 3884(47) | 4948(84) | 11436(77) | 150 |
| C(20) | 5318(55) | 5655(88) | 11934(78) | 150 |
| C(21) | 5215(66) | 4119(110) | 11971(100) | 150 |
| C(22) | 6030(49) | 6002(72) | 11266(94) | 150 |
| C(23) | 5962(70) | 4166(116) | 11302(128) | 150 |
| C(24) | 4241(63) | 3676(85) | 11252(100) | 150 |
| C(25) | 4043(69) | 6143(109) | 11142(114) | 150 |
| C(26) | 4639 | 5525 | 12167 | 150 |
| C(27) | 4632 | 4532 | 12194 | 150 |
| C(28) | 6506 | 5062 | 10432 | 150 |
| C(29) | 6419 | 5629 | 9919 | 150 |
| C(30) | 3590 | 5628 | 10093 | 150 |
| P(1) | 2509(9) | 36(12) | 10005(13) | 135(2) |
| F(1) | 2443(16) | -1017(21) | 8826(28) | 212(9) |
| F(2) | 2509(13) | 1214(20) | 11111(26) | 193(8) |
| F(3) | 2524(14) | 1138(19) | 8866(19) | 161(7) |
| F(4) | 2478(14) | -1208(19) | 11203(23) | 193(8) |
| F(5) | 3655(14) | 91(16) | 9944(23) | 186(7) |
| F(6) | 1362(15) | -11(18) | 9949(21) | 185(7) |

Supplementary Table 3.
Selected bond lengths [A] and angles [deg]
for monoclinic 1 at T = 333 K.

| | |
|---|---|
| Co(1)-C(1) | 2.07(8) |
| Co(1)-C(2) | 1.91(7) |
| Co(1)-C(3) | 2.22(6) |
| Co(1)-C(4) | 1.97(12) |
| Co(1)-C(5) | 2.15(7) |
| Co(1)-C(6) | 2.07(8) |
| Co(1)-C(7) | 1.89(13) |
| Co(1)-C(8) | 2.08(6) |
| Co(1)-C(9) | 2.00(6) |
| Co(1)-C(10) | 2.03(9) |
| Co(1)-C(11) | 1.9540 |
| Co(1)-C(12) | 2.04(14) |
| Co(1)-C(13) | 2.05(8) |
| Co(1)-C(14) | 2.18 |
| Co(1)-C(15) | 2.17 |
| | |
| Co(2)-C(16) | 1.99(7) |
| Co(2)-C(17) | 1.97(5) |
| Co(2)-C(18) | 2.05(5) |
| Co(2)-C(19) | 2.03(6) |
| Co(2)-C(20) | 1.99(8) |
| Co(2)-C(21) | 2.07(10) |
| Co(2)-C(22) | 2.06(7) |
| Co(2)-C(23) | 1.96(11) |
| Co(2)-C(24) | 2.01(7) |
| Co(2)-C(25) | 2.00(8) |
| Co(2)-C(26) | 2.17 |
| Co(2)-C(27) | 2.19 |
| Co(2)-C(28) | 2.06 |
| Co(2)-C(29) | 1.99 |
| Co(2)-C(30) | 1.98 |
| | |
| P(1)-F(1) | 1.51(2) |
| P(1)-F(3) | 1.51(2) |
| P(1)-F(5) | 1.54(2) |
| P(1)-F(6) | 1.54(2) |
| P(1)-F(2) | 1.54(2) |
| P(1)-F(4) | 1.64(2) |
| | |
| F(1)-P(1)-F(3) | 86.0(13) |
| F(1)-P(1)-F(5) | 93.0(14) |
| F(3)-P(1)-F(5) | 86.2(12) |
| F(1)-P(1)-F(6) | 84.2(12) |
| F(3)-P(1)-F(6) | 90.6(13) |
| F(5)-P(1)-F(6) | 176(2) |
| F(1)-P(1)-F(2) | 173.9(14) |
| F(3)-P(1)-F(2) | 89.1(11) |
| F(5)-P(1)-F(2) | 90.2(12) |
| F(6)-P(1)-F(2) | 92.4(12) |
| F(1)-P(1)-F(4) | 92.0(12) |
| F(3)-P(1)-F(4) | 177.9(12) |
| F(5)-P(1)-F(4) | 94.5(12) |
| F(6)-P(1)-F(4) | 88.6(12) |
| F(2)-P(1)-F(4) | 93.0(13) |

Supplementary Table 4.
Anisotropic displacement parameters (A^2 x 10^3)
for monoclinic 1 at T = 333 K.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Co(1) | 75(3) | 71(2) | 73(3) | -1(3) | -1(2) | -3(2) |
| Co(2) | 77(3) | 81(2) | 70(3) | 1(3) | -4(2) | 2(2) |
| P(1) | 128(4) | 134(5) | 143(6) | -25(10) | 6(4) | -14(7) |
| F(1) | 255(22) | 144(14) | 237(25) | -31(20) | -19(19) | -10(15) |
| F(2) | 170(15) | 174(17) | 233(23) | -31(19) | -2(15) | 38(13) |
| F(3) | 194(17) | 166(15) | 122(14) | 43(15) | 23(12) | 1(13) |
| F(4) | 226(19) | 185(17) | 169(18) | 62(17) | -3(15) | 7(15) |
| F(5) | 153(15) | 169(15) | 236(22) | -16(17) | -32(15) | -31(12) |
| F(6) | 152(16) | 213(18) | 190(19) | -17(18) | -27(14) | 12(14) |

Supplementary Table 1.
Crystal data and structure refinement for 2 at T = 143 K.

| | |
|---|---|
| Identification code | felt |
| Empirical formula | C10 H10 F6 Fe P |
| Formula weight | 331.00 |
| Temperature | 143(2) K |
| Wavelength | 0.71069 A |
| Crystal system | monoclinic |
| Space group | P2(1)/c |
| Unit cell dimensions | a = 13.431(10) A alpha = 90 deg.<br>b = 9.268(4) A beta = 96.91(6) deg.<br>c = 9.328(7) A gamma = 90 deg. |
| Volume | 1152.7(13) A^3 |
| Z | 4 |
| Density (calculated) | 1.907 Mg/m^3 |
| Absorption coefficient | 1.503 mm^-1 |
| F(000) | 660 |
| Crystal size | 0.12 x 0.10 x 0.10 mm |
| Theta range for data collection | 3.00 to 28.00 deg. |
| Index ranges | -17<=h<=17, 0<=k<=12, 0<=l<=8 |
| Reflections collected | 1457 |
| Independent reflections | 1198 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 1182 / 120 / 148 |
| Goodness-of-fit on F^2 | 1.140 |
| Final R indices [I>2sigma(I)] | R1 = 0.1244, wR2 = 0.2929 |
| R indices (all data) | R1 = 0.2023, wR2 = 0.3863 |
| Largest diff. peak and hole | 0.866 and -1.603 e.A^-3 |

Supplementary Table 2.
Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 2 at T = 143 K.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Fe(1) | 0 | -5000 | 10000 | 23(2) |
| C(1) | -1256(14) | -6324(18) | 9569(16) | 41(6) |
| C(2) | -598(14) | -6927(16) | 10719(20) | 44(6) |
| C(3) | -476(14) | -5905(20) | 11860(16) | 47(6) |
| C(4) | -1057(14) | -4669(17) | 11415(17) | 42(6) |
| C(5) | -1539(13) | -4928(18) | 9999(18) | 39(6) |
| Fe(2) | 5000 | 5000 | 10000 | 26(2) |
| C(6) | 5703(12) | 6475(24) | 11487(23) | 57(7) |
| C(7) | 5178(16) | 5408(22) | 12191(20) | 63(7) |
| C(8) | 4151(14) | 5474(22) | 11613(22) | 56(7) |
| C(9) | 4042(13) | 6580(23) | 10552(22) | 58(7) |
| C(10) | 5002(17) | 7199(20) | 10475(21) | 59(7) |
| P(1) | 2355(6) | 368(7) | 9799(7) | 35(2) |
| F(1) | 3539(10) | 266(17) | 9719(14) | 47(4) |
| F(2) | 2521(14) | 1744(15) | 10859(16) | 58(5) |
| F(3) | 2521(12) | -658(15) | 11189(14) | 43(4) |
| F(4) | 1192(13) | 434(21) | 9859(18) | 69(5) |
| F(5) | 2209(13) | -1024(16) | 8793(17) | 58(5) |
| F(6) | 2231(14) | 1361(15) | 8369(16) | 56(5) |

Supplementary Table 3.
Selected bond lengths [A] and angles [deg] for 2 at T = 143 K.

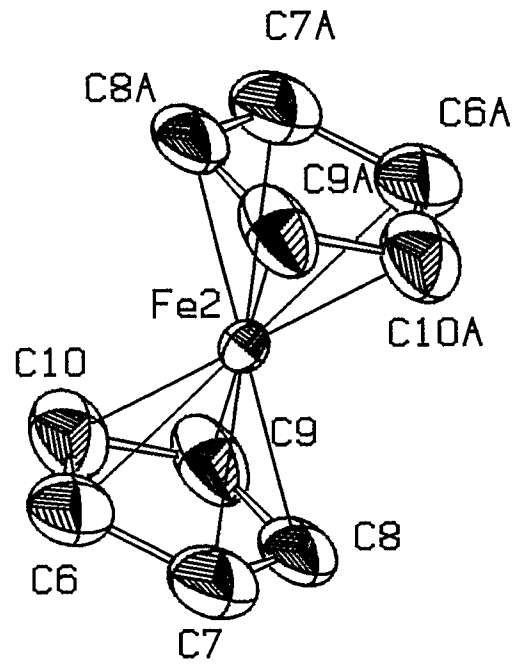
| | |
|---|---|
| Fe(1)-C(5) | 2.07(2) |
| Fe(1)-C(4) | 2.07(2) |
| Fe(1)-C(1) | 2.09(2) |
| Fe(1)-C(3) | 2.10(2) |
| Fe(1)-C(2) | 2.10(2) |
| | |
| Fe(2)-C(8) | 2.04(2) |
| Fe(2)-C(9) | 2.05(2) |
| Fe(2)-C(7) | 2.06(2) |
| Fe(2)-C(10) | 2.09(2) |
| Fe(2)-C(6) | 2.09(2) |
| | |
| C-C | 1.42 |
| | |
| P(1)-F(4) | 1.57(2) |
| P(1)-F(5) | 1.59(2) |
| P(1)-F(3) | 1.60(2) |
| P(1)-F(6) | 1.61(2) |
| P(1)-F(1) | 1.60(2) |
| P(1)-F(2) | 1.61(2) |
| | |
| C-C-C | 108.0 |
| | |
| F(4)-P(1)-F(5) | 90.0(10) |
| F(4)-P(1)-F(3) | 92.1(10) |
| F(5)-P(1)-F(3) | 89.5(9) |
| F(4)-P(1)-F(6) | 90.2(10) |
| F(5)-P(1)-F(6) | 89.0(8) |
| F(3)-P(1)-F(6) | 177.3(11) |
| F(4)-P(1)-F(1) | 178.7(10) |
| F(5)-P(1)-F(1) | 88.7(10) |
| F(3)-P(1)-F(1) | 87.8(8) |
| F(6)-P(1)-F(1) | 90.0(9) |
| F(4)-P(1)-F(2) | 90.7(11) |
| F(5)-P(1)-F(2) | 178.1(9) |
| F(3)-P(1)-F(2) | 88.7(8) |
| F(6)-P(1)-F(2) | 92.8(8) |
| F(1)-P(1)-F(2) | 90.6(9) |

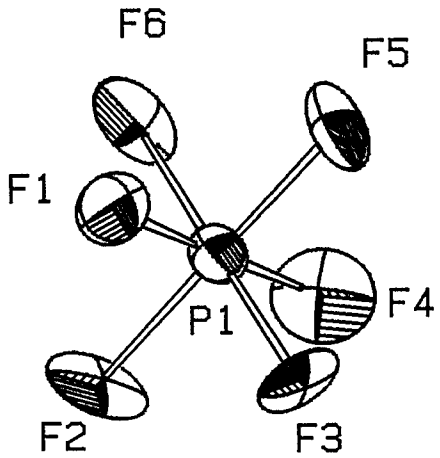
Supplementary Table 4.
Anisotropic displacement parameters (A^2 x 10^3) for 2 at T = 143 K.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

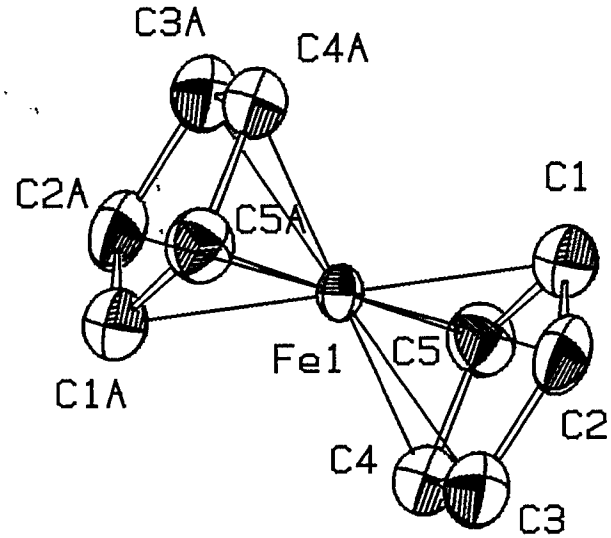
| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Fe(1) | 34(3) | 11(2) | 25(3) | 3(2) | 5(2) | -2(2) |
| C(1) | 48(11) | 36(10) | 40(11) | 1(10) | 8(10) | -6(10) |
| C(2) | 51(11) | 36(10) | 47(11) | 11(10) | 10(10) | -12(10) |
| C(3) | 48(11) | 52(11) | 42(11) | 1(10) | 5(10) | -16(10) |
| C(4) | 48(11) | 42(10) | 38(10) | 0(10) | 7(9) | -12(10) |
| C(5) | 42(10) | 33(10) | 43(10) | -1(10) | 7(9) | 1(10) |
| Fe(2) | 37(3) | 20(3) | 19(3) | 5(3) | 3(2) | -5(3) |
| C(6) | 63(12) | 58(12) | 52(12) | -20(10) | 21(10) | -2(10) |
| C(7) | 73(12) | 69(12) | 49(12) | -22(10) | 15(10) | -3(11) |
| C(8) | 55(11) | 66(12) | 51(11) | -33(10) | 23(10) | -13(11) |
| C(9) | 52(11) | 48(11) | 75(12) | -28(10) | 9(11) | -1(10) |
| C(10) | 64(11) | 43(11) | 72(12) | -18(10) | 15(11) | -1(10) |
| P(1) | 51(5) | 27(4) | 25(4) | -1(4) | 2(3) | -10(4) |
| F(1) | 45(10) | 58(11) | 38(9) | 3(8) | 5(7) | -9(9) |
| F(2) | 117(16) | 18(7) | 37(9) | -15(7) | 2(9) | 25(9) |
| F(3) | 76(12) | 26(8) | 30(9) | 22(7) | 22(8) | 12(8) |
| F(4) | 56(11) | 79(13) | 71(12) | -2(10) | 6(9) | 21(11) |
| F(5) | 78(13) | 34(9) | 60(11) | -16(8) | 3(10) | -21(9) |
| F(6) | 98(14) | 22(8) | 38(10) | 9(8) | -30(9) | 1(9) |

Supplementary Table 5.
Hydrogen coordinates ( x 10^4) and isotropic
displacement parameters (A^2 x 10^3) for 2 at T = 143 K.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1) | -1464(14) | -6765(18) | 8688(16) | 49 |
| H(2) | -301(20) | -7834(18) | 10725(29) | 53 |
| H(3) | -83(20) | -6023(29) | 12744(20) | 57 |
| H(4) | -1113(22) | -3836(21) | 11956(24) | 51 |
| H(5) | -1966(18) | -4294(24) | 9449(24) | 47 |
| H(6) | 6387(12) | 6665(24) | 11660(23) | 68 |
| H(7) | 5457(23) | 4778(30) | 12904(27) | 76 |
| H(8) | 3640(19) | 4893(31) | 11881(33) | 67 |
| H(9) | 3447(16) | 6852(34) | 10004(32) | 70 |
| H(10) | 5145(24) | 7947(26) | 9868(30) | 71 |


C7A
C8A
C6A
C9A
Fe2
C10A
C10
C9
C8
C6
C7


F6
F5
F1
P1
F4
F2
F3


C3A
C4A
C1
C2A
C5A
Fe1
C5
C1A
C2
C4
C3

Supplementary Table 1.
Crystal data and structure refinement for [(C6H6)2Cr][PF6].

| | |
|---|---|
| Identification code | 1t |
| Empirical formula | C12 H12 Cr F6 P |
| Formula weight | 354.18 |
| Temperature | 203(2) K |
| Wavelength | 0.71069 A |
| Crystal system | orthorhombic |
| Space group | Pna2(1) |
| Unit cell dimensions | a = 9.587(6) A alpha = 90 deg.<br>b = 9.661(4) A beta = 90 deg.<br>c = 27.510(10) A gamma = 90 deg. |
| Volume | 2548(2) A^3 |
| Z | 8 |
| Density (calculated) | 1.841 Mg/m^3 |
| Absorption coefficient | 1.081 mm^-1 |
| F(000) | 708 |
| Crystal size | 0.14 x 0.15 x 0.08 mm |
| Theta range for data collection | 3.00 to 30.00 deg. |
| Index ranges | 0<=h<=13, 0<=k<=13, 0<=l<=38 |
| Reflections collected | 4190 |
| Independent reflections | 3753 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 3753 / 13 / 316 |
| Goodness-of-fit on F^2 | 1.065 |
| Final R indices [I>2sigma(I)] | R1 = 0.0482, wR2 = 0.1145 |
| R indices (all data) | R1 = 0.1550, wR2 = 0.1584 |
| Absolute structure parameter | 0.10(11) |
| Extinction coefficient | 0.0005(2) |
| Largest diff. peak and hole | .535 and -.492 e.A^-3 |

Supplementary Table 2.
Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [(C6H6)2Cr][PF6].
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Cr(1) | 8(6) | 4987(4) | 4555(2) | 26(1) |
| C(1) | -28(12) | 5045(12) | 3801(4) | 36(4) |
| C(2) | -515(11) | 6314(12) | 3968(4) | 52(5) |
| C(3) | 275(14) | 7077(9) | 4297(4) | 45(5) |
| C(4) | 1551(13) | 6571(12) | 4458(4) | 48(5) |
| C(5) | 2038(10) | 5302(13) | 4291(4) | 44(5) |
| C(6) | 1248(12) | 4539(10) | 3963(4) | 39(4) |
| C(7) | -1596(12) | 3529(12) | 4644(4) | 42(5) |
| C(8) | -2055(10) | 4765(13) | 4847(4) | 44(5) |
| C(9) | -1254(14) | 5426(11) | 5199(4) | 47(5) |
| C(10) | 5(13) | 4851(12) | 5347(3) | 48(6) |
| C(11) | 464(10) | 3615(11) | 5143(4) | 38(5) |
| C(12) | -336(12) | 2954(9) | 4792(4) | 39(4) |
| Cr(2) | 465(1) | 5134(1) | 2052(2) | 27(1) |
| C(13) | 1259(18) | 3637(12) | 2542(4) | 94(9) |
| C(14) | 629(11) | 2964(7) | 2153(4) | 94(6) |
| C(15) | 1008(16) | 3297(12) | 1680(4) | 75(6) |
| C(16) | 2016(16) | 4302(13) | 1595(6) | 67(5) |
| C(17) | 2646(8) | 4975(11) | 1984(8) | 128(10) |
| C(18) | 2267(17) | 4642(13) | 2458(7) | 131(12) |
| C(19) | -1077(14) | 5950(15) | 2512(4) | 73(6) |
| C(20) | -1717(7) | 5319(10) | 2117(6) | 108(6) |
| C(21) | -1336(13) | 5688(14) | 1647(5) | 92(7) |
| C(22) | -315(14) | 6687(14) | 1572(4) | 65(5) |
| C(23) | 326(10) | 7318(7) | 1968(5) | 84(6) |
| C(24) | -55(15) | 6949(13) | 2438(4) | 92(8) |
| P(1) | 493(5) | 279(4) | 3405(1) | 35(1) |
| F(1) | 457(18) | 264(11) | 2834(4) | 53(4) |
| F(2) | -841(12) | -691(14) | 3415(5) | 64(4) |
| F(3) | 478(18) | 387(14) | 3986(3) | 61(4) |
| F(4) | 1825(13) | 1245(11) | 3413(5) | 65(4) |
| F(5) | -535(13) | 1566(11) | 3407(6) | 59(3) |
| F(6) | 1514(13) | -1024(11) | 3422(4) | 50(3) |
| P(2) | 494(6) | 283(5) | 709(1) | 34(1) |
| F(7) | -427(16) | 1642(10) | 720(6) | 66(4) |
| F(8) | -808(12) | -703(10) | 715(4) | 45(3) |
| F(9) | 1468(14) | -1046(10) | 719(5) | 61(4) |
| F(10) | 1831(13) | 1279(12) | 723(5) | 58(4) |
| F(11) | 538(17) | 281(14) | 1290(3) | 55(4) |
| F(12) | 491(21) | 212(13) | 137(4) | 63(4) |

Supplementary Table 3.
bond lengths [A] and angles [deg] for [(C6H6)2Cr][PF6].

| | |
|---|---|
| Cr(1)-C(6) | 2.063(12) |
| Cr(1)-C(5) | 2.099(12) |
| Cr(1)-C(12) | 2.095(10) |
| Cr(1)-C(1) | 2.075(11) |
| Cr(1)-C(11) | 2.137(9) |
| Cr(1)-C(7) | 2.099(12) |
| Cr(1)-C(4) | 2.145(11) |
| Cr(1)-C(2) | 2.121(11) |
| Cr(1)-C(3) | 2.156(11) |
| Cr(1)-C(10) | 2.182(11) |
| Cr(1)-C(8) | 2.145(12) |
| Cr(1)-C(9) | 2.187(11) |
| | |
| Cr(2)-C(16) | 2.106(10) |
| Cr(2)-C(20) | 2.107(7) |
| Cr(2)-C(19) | 2.099(11) |
| Cr(2)-C(17) | 2.104(8) |
| Cr(2)-C(15) | 2.115(11) |
| Cr(2)-C(18) | 2.111(13) |
| Cr(2)-C(21) | 2.124(12) |
| Cr(2)-C(24) | 2.109(11) |
| Cr(2)-C(14) | 2.121(7) |
| Cr(2)-C(13) | 2.119(12) |
| Cr(2)-C(22) | 2.134(12) |
| Cr(2)-C(23) | 2.126(7) |
| | |
| C-C | 1.39 |
| | |
| P(1)-F(1) | 1.571(11) |
| P(1)-F(5) | 1.587(10) |
| P(1)-F(2) | 1.586(12) |
| P(1)-F(4) | 1.582(11) |
| P(1)-F(6) | 1.595(10) |
| P(1)-F(3) | 1.602(10) |
| P(2)-F(8) | 1.570(10) |
| P(2)-F(12) | 1.576(12) |
| P(2)-F(9) | 1.588(11) |
| P(2)-F(7) | 1.582(10) |
| P(2)-F(10) | 1.603(11) |
| P(2)-F(11) | 1.598(10) |
| | |
| C(6)-Cr(1)-C(5) | 39.0(2) |
| C(6)-Cr(1)-C(12) | 98.0(5) |
| C(5)-Cr(1)-C(12) | 112.9(6) |
| C(6)-Cr(1)-C(1) | 39.3(2) |
| C(5)-Cr(1)-C(1) | 70.5(3) |
| C(12)-Cr(1)-C(1) | 109.5(5) |
| C(6)-Cr(1)-C(11) | 110.5(5) |
| C(5)-Cr(1)-C(11) | 99.4(5) |
| C(12)-Cr(1)-C(11) | 38.3(2) |
| C(1)-Cr(1)-C(11) | 141.0(6) |
| C(6)-Cr(1)-C(7) | 111.9(6) |
| C(5)-Cr(1)-C(7) | 144.7(6) |
| C(12)-Cr(1)-C(7) | 38.7(2) |
| C(1)-Cr(1)-C(7) | 97.0(5) |
| C(11)-Cr(1)-C(7) | 69.3(3) |
| C(6)-Cr(1)-C(4) | 69.8(3) |
| C(5)-Cr(1)-C(4) | 38.2(2) |
| C(12)-Cr(1)-C(4) | 144.7(7) |
| C(1)-Cr(1)-C(4) | 82.4(3) |

| | |
|---|---|
| C(11)-Cr(1)-C(4) | 113.3(6) |
| C(7)-Cr(1)-C(4) | 176.5(7) |
| C(6)-Cr(1)-C(2) | 70.2(3) |
| C(5)-Cr(1)-C(2) | 82.4(3) |
| C(12)-Cr(1)-C(2) | 140.0(6) |
| C(1)-Cr(1)-C(2) | 38.7(2) |
| C(11)-Cr(1)-C(2) | 177.9(6) |
| C(7)-Cr(1)-C(2) | 108.7(6) |
| C(4)-Cr(1)-C(2) | 68.7(3) |
| C(6)-Cr(1)-C(3) | 82.4(3) |
| C(5)-Cr(1)-C(3) | 68.9(3) |
| C(12)-Cr(1)-C(3) | 177.5(7) |
| C(1)-Cr(1)-C(3) | 69.3(3) |
| C(11)-Cr(1)-C(3) | 143.7(6) |
| C(7)-Cr(1)-C(3) | 138.9(6) |
| C(4)-Cr(1)-C(3) | 37.7(2) |
| C(2)-Cr(1)-C(3) | 37.9(2) |
| C(6)-Cr(1)-C(10) | 141.0(6) |
| C(5)-Cr(1)-C(10) | 110.8(6) |
| C(12)-Cr(1)-C(10) | 68.5(2) |
| C(1)-Cr(1)-C(10) | 177.8(6) |
| C(11)-Cr(1)-C(10) | 37.5(2) |
| C(7)-Cr(1)-C(10) | 80.9(3) |
| C(4)-Cr(1)-C(10) | 99.7(5) |
| C(2)-Cr(1)-C(10) | 142.7(6) |
| C(3)-Cr(1)-C(10) | 112.7(5) |
| C(6)-Cr(1)-C(8) | 143.7(6) |
| C(5)-Cr(1)-C(8) | 176.9(7) |
| C(12)-Cr(1)-C(8) | 69.2(3) |
| C(1)-Cr(1)-C(8) | 111.2(6) |
| C(11)-Cr(1)-C(8) | 81.0(3) |
| C(7)-Cr(1)-C(8) | 38.2(2) |
| C(4)-Cr(1)-C(8) | 138.9(6) |
| C(2)-Cr(1)-C(8) | 97.3(5) |
| C(3)-Cr(1)-C(8) | 109.0(6) |
| C(10)-Cr(1)-C(8) | 67.6(3) |
| C(6)-Cr(1)-C(9) | 178.0(6) |
| C(5)-Cr(1)-C(9) | 139.9(6) |
| C(12)-Cr(1)-C(9) | 80.9(3) |
| C(1)-Cr(1)-C(9) | 142.7(6) |
| C(11)-Cr(1)-C(9) | 67.7(3) |
| C(7)-Cr(1)-C(9) | 68.3(3) |
| C(4)-Cr(1)-C(9) | 110.1(6) |
| C(2)-Cr(1)-C(9) | 111.6(6) |
| C(3)-Cr(1)-C(9) | 98.7(5) |
| C(10)-Cr(1)-C(9) | 37.1(2) |
| C(8)-Cr(1)-C(9) | 37.4(2) |
| | |
| C(16)-Cr(2)-C(20) | 141.6(7) |
| C(16)-Cr(2)-C(19) | 179.5(5) |
| C(20)-Cr(2)-C(19) | 38.59(14) |
| C(16)-Cr(2)-C(17) | 38.55(13) |
| C(20)-Cr(2)-C(17) | 179.3(4) |
| C(19)-Cr(2)-C(17) | 141.3(7) |
| C(16)-Cr(2)-C(15) | 38.5(2) |
| C(20)-Cr(2)-C(15) | 110.9(6) |
| C(19)-Cr(2)-C(15) | 141.3(6) |
| C(17)-Cr(2)-C(15) | 69.6(2) |
| C(16)-Cr(2)-C(18) | 69.6(2) |
| C(20)-Cr(2)-C(18) | 141.9(8) |
| C(19)-Cr(2)-C(18) | 110.0(7) |
| C(17)-Cr(2)-C(18) | 38.5(2) |
| C(15)-Cr(2)-C(18) | 82.3(2) |
| C(16)-Cr(2)-C(21) | 110.9(7) |

| | |
|---|---|
| C(20)-Cr(2)-C(21) | 38.3(2) |
| C(19)-Cr(2)-C(21) | 69.5(2) |
| C(17)-Cr(2)-C(21) | 141.2(8) |
| C(15)-Cr(2)-C(21) | 99.0(5) |
| C(18)-Cr(2)-C(21) | 178.4(5) |
| C(16)-Cr(2)-C(24) | 141.7(6) |
| C(20)-Cr(2)-C(24) | 69.6(2) |
| C(19)-Cr(2)-C(24) | 38.6(2) |
| C(17)-Cr(2)-C(24) | 109.9(6) |
| C(15)-Cr(2)-C(24) | 178.7(5) |
| C(18)-Cr(2)-C(24) | 96.6(5) |
| C(21)-Cr(2)-C(24) | 82.10(14) |
| C(16)-Cr(2)-C(14) | 69.4(2) |
| C(20)-Cr(2)-C(14) | 98.4(4) |
| C(19)-Cr(2)-C(14) | 110.1(5) |
| C(17)-Cr(2)-C(14) | 82.3(2) |
| C(15)-Cr(2)-C(14) | 38.3(2) |
| C(18)-Cr(2)-C(14) | 69.3(3) |
| C(21)-Cr(2)-C(14) | 112.2(5) |
| C(24)-Cr(2)-C(14) | 140.6(6) |
| C(16)-Cr(2)-C(13) | 82.3(2) |
| C(20)-Cr(2)-C(13) | 111.1(6) |
| C(19)-Cr(2)-C(13) | 97.2(5) |
| C(17)-Cr(2)-C(13) | 69.5(3) |
| C(15)-Cr(2)-C(13) | 69.3(2) |
| C(18)-Cr(2)-C(13) | 38.4(2) |
| C(21)-Cr(2)-C(13) | 142.9(6) |
| C(24)-Cr(2)-C(13) | 109.4(5) |
| C(14)-Cr(2)-C(13) | 38.3(2) |
| C(16)-Cr(2)-C(22) | 98.4(5) |
| C(20)-Cr(2)-C(22) | 69.2(3) |
| C(19)-Cr(2)-C(22) | 82.10(14) |
| C(17)-Cr(2)-C(22) | 110.2(6) |
| C(15)-Cr(2)-C(22) | 112.1(5) |
| C(18)-Cr(2)-C(22) | 140.6(6) |
| C(21)-Cr(2)-C(22) | 38.1(2) |
| C(24)-Cr(2)-C(22) | 69.1(2) |
| C(14)-Cr(2)-C(22) | 143.3(5) |
| C(13)-Cr(2)-C(22) | 178.4(5) |
| C(16)-Cr(2)-C(23) | 111.0(5) |
| C(20)-Cr(2)-C(23) | 82.10(14) |
| C(19)-Cr(2)-C(23) | 69.5(2) |
| C(17)-Cr(2)-C(23) | 97.2(4) |
| C(15)-Cr(2)-C(23) | 142.7(6) |
| C(18)-Cr(2)-C(23) | 109.4(4) |
| C(21)-Cr(2)-C(23) | 69.0(3) |
| C(24)-Cr(2)-C(23) | 38.32(13) |
| C(14)-Cr(2)-C(23) | 178.6(5) |
| C(13)-Cr(2)-C(23) | 140.3(5) |
| C(22)-Cr(2)-C(23) | 38.1(2) |
| | |
| C-C-C | 120.0 |
| | |
| F(1)-P(1)-F(5) | 89.8(8) |
| F(1)-P(1)-F(2) | 89.6(8) |
| F(5)-P(1)-F(2) | 87.8(7) |
| F(1)-P(1)-F(4) | 92.1(8) |
| F(5)-P(1)-F(4) | 92.2(7) |
| F(2)-P(1)-F(4) | 178.3(9) |
| F(1)-P(1)-F(6) | 92.0(7) |
| F(5)-P(1)-F(6) | 178.1(8) |
| F(2)-P(1)-F(6) | 91.6(7) |
| F(4)-P(1)-F(6) | 88.3(8) |
| F(1)-P(1)-F(3) | 176.3(7) |

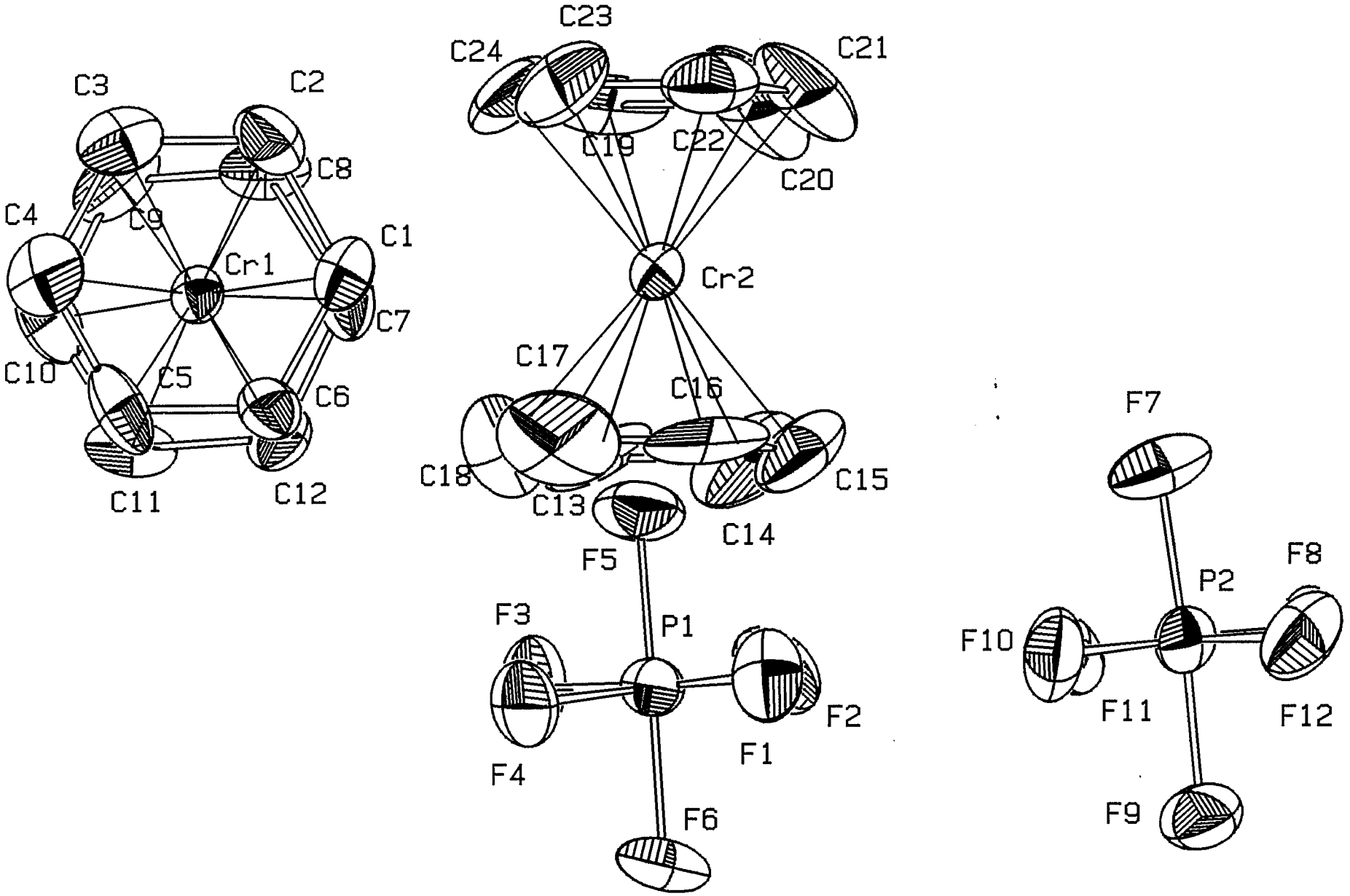
| | |
|---|---|
| F(5)-P(1)-F(3) | 86.6(8) |
| F(2)-P(1)-F(3) | 90.9(8) |
| F(4)-P(1)-F(3) | 87.5(8) |
| F(6)-P(1)-F(3) | 91.7(7) |
| | |
| F(8)-P(2)-F(12) | 89.0(9) |
| F(8)-P(2)-F(9) | 88.6(7) |
| F(12)-P(2)-F(9) | 89.0(8) |
| F(8)-P(2)-F(7) | 93.4(8) |
| F(12)-P(2)-F(7) | 93.1(8) |
| F(9)-P(2)-F(7) | 177.1(9) |
| F(8)-P(2)-F(10) | 178.0(7) |
| F(12)-P(2)-F(10) | 93.0(8) |
| F(9)-P(2)-F(10) | 90.8(8) |
| F(7)-P(2)-F(10) | 87.0(8) |
| F(8)-P(2)-F(11) | 90.6(7) |
| F(12)-P(2)-F(11) | 177.1(7) |
| F(9)-P(2)-F(11) | 88.1(8) |
| F(7)-P(2)-F(11) | 89.8(8) |
| F(10)-P(2)-F(11) | 87.5(8) |

Supplementary Table 4.
Anisotropic displacement parameters (A^2 x 10^3)
for [(C6H6)2Cr][PF6]. The anisotropic displacement factor exponent
takes the form: -2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Cr(1) | 28(1) | 23(1) | 27(1) | 2(1) | -1(1) | -2(1) |
| C(1) | 47(12) | 32(6) | 30(6) | -3(5) | 4(7) | -7(7) |
| C(2) | 31(10) | 52(10) | 74(12) | -1(9) | -14(9) | 1(9) |
| C(3) | 66(14) | 33(9) | 36(8) | 17(7) | 10(9) | 7(9) |
| C(4) | 32(10) | 39(9) | 74(13) | 2(8) | 14(9) | -20(8) |
| C(5) | 30(10) | 61(11) | 41(9) | 22(8) | -12(7) | -24(8) |
| C(6) | 41(11) | 43(9) | 31(6) | -1(6) | -7(6) | 10(8) |
| C(7) | 52(12) | 34(8) | 39(9) | 8(7) | -15(8) | -17(8) |
| C(8) | 29(10) | 54(10) | 48(9) | 4(8) | 28(7) | 16(8) |
| C(9) | 69(15) | 40(10) | 33(7) | -4(6) | 37(8) | -3(9) |
| C(10) | 49(14) | 73(12) | 22(6) | 12(7) | -11(8) | -4(10) |
| C(11) | 47(11) | 40(8) | 28(6) | 31(6) | 15(7) | 14(8) |
| C(12) | 42(10) | 21(7) | 55(9) | -1(7) | -1(8) | -5(7) |
| Cr(2) | 29(1) | 25(1) | 26(1) | -2(2) | 1(2) | 0(1) |
| C(13) | 204(27) | 41(9) | 37(7) | -8(7) | -26(11) | 73(12) |
| C(14) | 145(13) | 19(4) | 117(18) | 18(8) | 4(14) | -5(6) |
| C(15) | 148(18) | 33(7) | 43(8) | -3(7) | -14(10) | 26(9) |
| C(16) | 73(11) | 72(10) | 55(9) | 15(8) | 49(8) | 57(9) |
| C(17) | 20(5) | 135(15) | 229(31) | -42(28) | 19(15) | 14(8) |
| C(18) | 120(20) | 109(18) | 164(31) | -39(18) | -81(19) | 22(16) |
| C(19) | 91(14) | 107(14) | 21(5) | 14(7) | 33(7) | 72(11) |
| C(20) | 23(5) | 220(18) | 81(12) | -18(19) | 7(9) | 25(8) |
| C(21) | 18(6) | 144(19) | 114(16) | 6(14) | -11(8) | 7(10) |
| C(22) | 83(13) | 60(9) | 52(8) | 5(8) | -3(9) | 39(9) |
| C(23) | 113(11) | 24(4) | 114(17) | -6(7) | -12(12) | 0(6) |
| C(24) | 150(21) | 60(10) | 66(11) | -42(9) | -36(12) | 51(12) |
| P(1) | 25(3) | 24(2) | 55(3) | 4(2) | -3(2) | -4(2) |
| F(1) | 73(10) | 42(6) | 45(7) | 14(5) | -10(6) | -19(6) |
| F(2) | 29(6) | 85(8) | 77(9) | 7(8) | 1(7) | -4(6) |
| F(3) | 72(9) | 82(7) | 28(5) | -15(5) | 0(5) | -10(7) |
| F(4) | 40(7) | 50(6) | 106(9) | -10(7) | -21(7) | -17(6) |
| F(5) | 33(5) | 49(6) | 96(8) | 2(6) | 4(6) | 12(5) |
| F(6) | 43(7) | 62(7) | 45(5) | 16(5) | 6(5) | 28(6) |
| P(2) | 44(3) | 38(2) | 21(2) | -2(2) | 0(2) | 4(2) |
| F(7) | 89(9) | 34(5) | 76(7) | 4(6) | 14(8) | 23(6) |
| F(8) | 45(7) | 33(4) | 58(6) | 2(5) | -7(6) | -19(5) |
| F(9) | 47(8) | 32(5) | 103(9) | -5(6) | -6(7) | 2(5) |
| F(10) | 48(8) | 65(7) | 61(7) | -26(6) | -1(6) | -14(7) |
| F(11) | 53(8) | 78(8) | 33(6) | -3(5) | -9(5) | 9(7) |
| F(12) | 91(12) | 49(5) | 48(6) | -12(4) | 8(6) | 4(6) |

Supplementary Table 5.
Hydrogen coordinates ( x 10^4) and isotropic
displacement parameters (A^2 x 10^3) for [(C6H6)2Cr][PF6].

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1) | -556 | 4534 | 3582 | 43 |
| H(2) | -1368 | 6652 | 3860 | 63 |
| H(3) | -51 | 7926 | 4408 | 54 |
| H(4) | 2079 | 7082 | 4678 | 58 |
| H(5) | 2891 | 4964 | 4399 | 53 |
| H(6) | 1574 | 3690 | 3851 | 46 |
| H(7) | -2131 | 3087 | 4408 | 50 |
| H(8) | -2897 | 5150 | 4748 | 52 |
| H(9) | -1562 | 6253 | 5335 | 57 |
| H(10) | 540 | 5293 | 5582 | 58 |
| H(11) | 1306 | 3231 | 5243 | 46 |
| H(12) | -29 | 2128 | 4656 | 47 |
| H(13) | 1006 | 3414 | 2859 | 113 |
| H(14) | -45 | 2291 | 2210 | 112 |
| H(15) | 587 | 2847 | 1420 | 90 |
| H(16) | 2269 | 4525 | 1279 | 80 |
| H(17) | 3320 | 5648 | 1928 | 154 |
| H(18) | 2688 | 5092 | 2718 | 157 |
| H(19) | -1331 | 5703 | 2827 | 88 |
| H(20) | -2400 | 4651 | 2166 | 130 |
| H(21) | -1764 | 5266 | 1382 | 111 |
| H(22) | -60 | 6934 | 1258 | 78 |
| H(23) | 1009 | 7986 | 1918 | 100 |
| H(24) | 373 | 7370 | 2703 | 111 |


C3
C2
C8
C4
C9
C1
Cr1
C7
C10
C5
C6
C11
C12
C23
C24
C21
C19
C22
C20
Cr2
C17
C16
C18
C15
C13
C14
F5
F8
P2
F3
P1
F10
F2
F1
F4
F11
F12
F6
F7
F9

Supplementary Table 1.
Crystal data and structure refinement for [(C6H5Me)2Cr][PF6].

| | |
|---|---|
| Identification code | tol |
| Empirical formula | C14 H16 Cr1 F6 P1 |
| Formula weight | 381.24 |
| Temperature | 273(2) K |
| Wavelength | 0.71069 A |
| Crystal system | monoclinic |
| Space group | P2(1)/n |
| Unit cell dimensions | a = 6.793(2) A alpha = 90 deg.<br>b = 11.056(2) A beta = 104.97(3) deg.<br>c = 10.740(5) A gamma = 90 deg. |
| Volume | 779.2(5) A^3 |
| Z | 2 |
| Density (calculated) | 1.625 Mg/m^3 |
| Absorption coefficient | 0.891 mm^-1 |
| F(000) | 772 |
| Crystal size | 0.16 x 0.12 x 0.10 mm |
| Theta range for data collection | 3.00 to 25.00 deg. |
| Index ranges | -8<=h<=7, 0<=k<=13, 0<=l<=7 |
| Reflections collected | 1167 |
| Independent reflections | 1028 [R(int) = 0.0203] |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 1028 / 0 / 93 |
| Goodness-of-fit on F^2 | 1.087 |
| Final R indices [I>2sigma(I)] | R1 = 0.0446, wR2 = 0.1143 |
| R indices (all data) | R1 = 0.0803, wR2 = 0.1391 |
| Extinction coefficient | 0.001(2) |
| Largest diff. peak and hole | .347 and -.259 e.A^-3 |

Supplementary Table 2.
Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [(C6H5Me)2Cr][PF6]. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Cr(1) | 0 | 0 | 0 | 39(1) |
| C(1) | 3104(5) | 342(3) | 942(3) | 66(2) |
| C(2) | 2517(5) | 1127(2) | -99(4) | 58(2) |
| C(3) | 1631(5) | 675(3) | -1323(4) | 48(1) |
| C(4) | 1332(5) | -563(3) | -1506(3) | 57(2) |
| C(5) | 1919(5) | -1348(2) | -465(4) | 62(2) |
| C(6) | 2805(5) | -896(3) | 759(4) | 72(2) |
| C(7) | 985(10) | 1537(6) | -2456(6) | 88(2) |
| P(1) | 5000 | 0 | 5000 | 69(1) |
| F(1) | 4387(7) | -1005(3) | 3934(4) | 117(2) |
| F(2) | 3263(7) | 849(3) | 4193(4) | 118(2) |
| F(3) | 3497(9) | -542(5) | 5731(5) | 149(2) |

Supplementary Table 3.
Bond lengths [A] and angles [deg] for [(C6H5Me)2Cr][PF6].

| | |
|---|---|
| Cr(1)-C(1) | 2.124(3) |
| Cr(1)-C(2) | 2.141(3) |
| Cr(1)-C(3) | 2.148(3) |
| Cr(1)-C(4) | 2.140(3) |
| Cr(1)-C(5) | 2.123(3) |
| Cr(1)-C(6) | 2.115(3) |
| | |
| C-C | 1.39 |
| | |
| P(1)-F(1) | 1.572(3) |
| P(1)-F(2) | 1.580(3) |
| P(1)-F(3) | 1.560(5) |
| | |
| C(6)-Cr(1)-C(6)#1 | 180.0(3) |
| C(6)-Cr(1)-C(5)#1 | 141.7(2) |
| C(6)#1-Cr(1)-C(5)#1 | 38.3 |
| C(6)-Cr(1)-C(5) | 38.3 |
| C(6)#1-Cr(1)-C(5) | 141.7(2) |
| C(5)#1-Cr(1)-C(5) | 180.0(3) |
| C(6)-Cr(1)-C(1)#1 | 141.7 |
| C(6)#1-Cr(1)-C(1)#1 | 38.3(2) |
| C(5)#1-Cr(1)-C(1)#1 | 69.1(2) |
| C(5)-Cr(1)-C(1)#1 | 110.93(7) |
| C(6)-Cr(1)-C(1) | 38.3 |
| C(6)#1-Cr(1)-C(1) | 141.7(2) |
| C(5)#1-Cr(1)-C(1) | 110.9(2) |
| C(5)-Cr(1)-C(1) | 69.07(7) |
| C(1)#1-Cr(1)-C(1) | 180.0 |
| C(6)-Cr(1)-C(4) | 68.92(7) |
| C(6)#1-Cr(1)-C(4) | 111.1(2) |
| C(5)#1-Cr(1)-C(4) | 141.9(2) |
| C(5)-Cr(1)-C(4) | 38.06(5) |
| C(1)#1-Cr(1)-C(4) | 98.61(7) |
| C(1)-Cr(1)-C(4) | 81.39(7) |
| C(6)-Cr(1)-C(4)#1 | 111.1(2) |
| C(6)#1-Cr(1)-C(4)#1 | 68.92(7) |
| C(5)#1-Cr(1)-C(4)#1 | 38.06(5) |
| C(5)-Cr(1)-C(4)#1 | 141.9(2) |
| C(1)#1-Cr(1)-C(4)#1 | 81.4(2) |
| C(1)-Cr(1)-C(4)#1 | 98.6(2) |
| C(4)-Cr(1)-C(4)#1 | 180.0(3) |
| C(6)-Cr(1)-C(2)#1 | 111.1(2) |
| C(6)#1-Cr(1)-C(2)#1 | 68.90(7) |
| C(5)#1-Cr(1)-C(2)#1 | 81.39(7) |
| C(5)-Cr(1)-C(2)#1 | 98.6(2) |
| C(1)#1-Cr(1)-C(2)#1 | 38.0(2) |
| C(1)-Cr(1)-C(2)#1 | 142.0(2) |
| C(4)-Cr(1)-C(2)#1 | 111.5(2) |
| C(4)#1-Cr(1)-C(2)#1 | 68.45(7) |
| C(6)-Cr(1)-C(2) | 68.90(7) |
| C(6)#1-Cr(1)-C(2) | 111.1(2) |
| C(5)#1-Cr(1)-C(2) | 98.6(2) |
| C(5)-Cr(1)-C(2) | 81.39(7) |
| C(1)#1-Cr(1)-C(2) | 142.0 |
| C(1)-Cr(1)-C(2) | 38.0 |
| C(4)-Cr(1)-C(2) | 68.46(7) |
| C(4)#1-Cr(1)-C(2) | 111.5(2) |
| C(2)#1-Cr(1)-C(2) | 180.0(3) |
| C(6)-Cr(1)-C(3) | 81.39(7) |

| | |
|---|---|
| C(6)#1-Cr(1)-C(3) | 98.6(2) |
| C(5)#1-Cr(1)-C(3) | 111.4(2) |
| C(5)-Cr(1)-C(3) | 68.61(8) |
| C(1)#1-Cr(1)-C(3) | 111.40(7) |
| C(1)-Cr(1)-C(3) | 68.60(7) |
| C(4)-Cr(1)-C(3) | 37.83(6) |
| C(4)#1-Cr(1)-C(3) | 142.2(2) |
| C(2)#1-Cr(1)-C(3) | 142.2(2) |
| C(2)-Cr(1)-C(3) | 37.8 |
| C(6)-Cr(1)-C(3)#1 | 98.6(2) |
| C(6)#1-Cr(1)-C(3)#1 | 81.39(7) |
| C(5)#1-Cr(1)-C(3)#1 | 68.61(8) |
| C(5)-Cr(1)-C(3)#1 | 111.4(2) |
| C(1)#1-Cr(1)-C(3)#1 | 68.6(2) |
| C(1)-Cr(1)-C(3)#1 | 111.4(2) |
| C(4)-Cr(1)-C(3)#1 | 142.2(2) |
| C(4)#1-Cr(1)-C(3)#1 | 37.83(5) |
| C(2)#1-Cr(1)-C(3)#1 | 37.8 |
| C(2)-Cr(1)-C(3)#1 | 142.2(2) |
| C(3)-Cr(1)-C(3)#1 | 180.0(3) |
| C(2)-C(1)-C(6) | 120.0 |
| C(2)-C(1)-Cr(1) | 71.63(10) |
| C(6)-C(1)-Cr(1) | 70.51(9) |
| C(3)-C(2)-C(1) | 120.0 |
| C(3)-C(2)-Cr(1) | 71.40(12) |
| C(1)-C(2)-Cr(1) | 70.33(11) |
| C(2)-C(3)-C(4) | 120.0 |
| C(2)-C(3)-C(7) | 119.8(4) |
| C(4)-C(3)-C(7) | 120.2(4) |
| C(2)-C(3)-Cr(1) | 70.78(11) |
| C(4)-C(3)-Cr(1) | 70.74(10) |
| C(7)-C(3)-Cr(1) | 131.0(3) |
| C(5)-C(4)-C(3) | 120.0 |
| C(5)-C(4)-Cr(1) | 70.32(10) |
| C(3)-C(4)-Cr(1) | 71.43(9) |
| C(4)-C(5)-C(6) | 120.0 |
| C(4)-C(5)-Cr(1) | 71.62(11) |
| C(6)-C(5)-Cr(1) | 70.55(11) |
| C(5)-C(6)-C(1) | 120.0 |
| C(5)-C(6)-Cr(1) | 71.16(11) |
| C(1)-C(6)-Cr(1) | 71.20(9) |
| | |
| F(3)#2-P(1)-F(3) | 180.0 |
| F(3)#2-P(1)-F(1) | 89.4(3) |
| F(3)-P(1)-F(1) | 90.6(3) |
| F(3)#2-P(1)-F(1)#2 | 90.6(3) |
| F(3)-P(1)-F(1)#2 | 89.4(3) |
| F(1)-P(1)-F(1)#2 | 180.0 |
| F(3)#2-P(1)-F(2)#2 | 90.6(3) |
| F(3)-P(1)-F(2)#2 | 89.4(3) |
| F(1)-P(1)-F(2)#2 | 89.9(2) |
| F(1)#2-P(1)-F(2)#2 | 90.1(2) |
| F(3)#2-P(1)-F(2) | 89.4(3) |
| F(3)-P(1)-F(2) | 90.6(3) |
| F(1)-P(1)-F(2) | 90.1(2) |
| F(1)#2-P(1)-F(2) | 89.9(2) |
| F(2)#2-P(1)-F(2) | 180.0 |

---

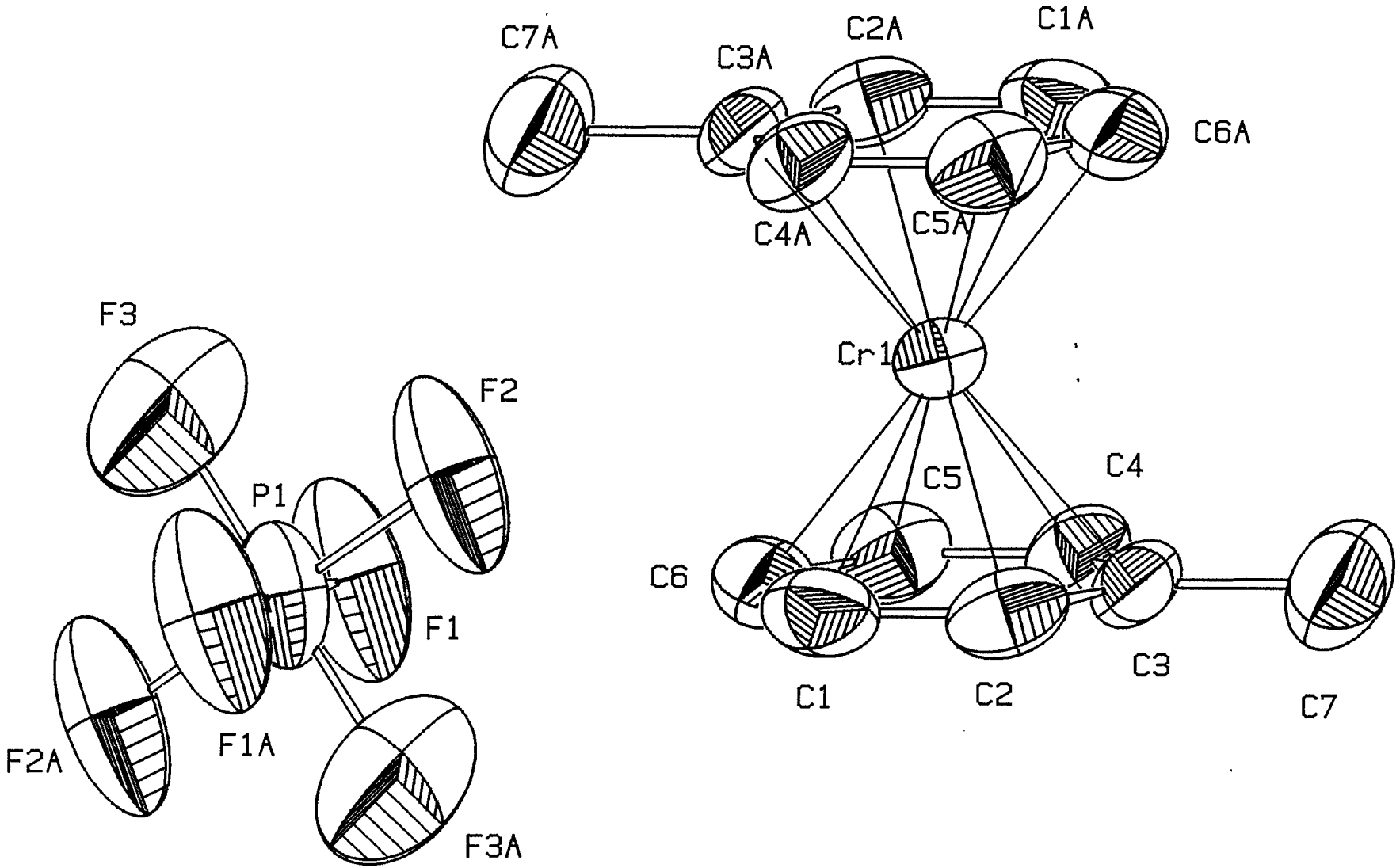
Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z  #2 -x+1,-y,-z+1

Supplementary Table 4.
Anisotropic displacement parameters (A^2 x 10^3) for [(C6H5Me)2Cr][PF6].
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Cr(1) | 38(1) | 36(1) | 47(1) | -2(1) | 16(1) | -2(1) |
| C(1) | 39(3) | 100(4) | 58(5) | -15(3) | 9(3) | -13(3) |
| C(2) | 53(3) | 54(3) | 75(5) | -12(3) | 30(3) | -18(2) |
| C(3) | 50(3) | 53(3) | 49(5) | 8(3) | 26(3) | 0(2) |
| C(4) | 61(3) | 65(3) | 51(5) | -8(3) | 28(3) | -6(3) |
| C(5) | 66(3) | 47(3) | 84(6) | -3(3) | 37(3) | 5(2) |
| C(6) | 51(3) | 86(4) | 88(6) | 34(4) | 32(3) | 27(3) |
| C(7) | 103(5) | 88(4) | 84(6) | 28(4) | 43(4) | 7(4) |
| P(1) | 101(2) | 44(1) | 53(2) | -2(1) | 1(1) | 10(1) |
| F(1) | 176(4) | 69(2) | 72(3) | -21(2) | -29(3) | 27(2) |
| F(2) | 161(4) | 79(3) | 81(3) | -9(2) | -28(3) | 51(3) |
| F(3) | 178(5) | 137(4) | 154(5) | 18(4) | 83(4) | -15(4) |

Supplementary Table 5.
Hydrogen coordinates ( x 10^4) and isotropic
displacement parameters (A^2 x 10^3) for [(C6H5Me)2Cr][PF6].

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1) | 3697 | 645 | 1761 | 79 |
| H(2) | 2717 | 1955 | 24 | 69 |
| H(4) | 739 | -866 | -2325 | 68 |
| H(5) | 1719 | -2176 | -588 | 75 |
| H(6) | 3198 | -1421 | 1455 | 87 |
| H(7A) | 1292 | 2353 | -2163 | 132 |
| H(7B) | -454 | 1460 | -2833 | 132 |
| H(7C) | 1708 | 1344 | -3089 | 132 |


C7A
C3A
C2A
C1A
C6A
C4A
C5A
Cr1
C5
C4
C6
C1
C2
C3
C7
F3
F2
P1
F1
F2A
F1A
F3A