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Table : Anisotropic thermal parameters for [Ir(cp*)(C₁₈H₂₃O₂)](BF₄)

Atom	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Ir(1)	0.0281(3)	0.0282(3)	0.0276(3)	-0.0008(4)	0.0028(4)	-0.0035(5)
O(1)	0.05(1)	0.05(1)	0.08(1)	-0.015(9)	0.03(1)	0.01(1)
O(2)	0.07(1)	0.036(8)	0.065(9)	-0.005(7)	0.00(1)	0.01(1)
C(1)	0.04(1)	0.036(9)	0.024(9)	-0.004(9)	0.02(1)	0.00(1)
C(2)	0.05(2)	0.03(1)	0.05(1)	-0.00(1)	0.00(1)	-0.01(1)
C(3)	0.04(1)	0.03(1)	0.05(1)	-0.01(1)	0.02(1)	-0.01(1)
C(4)	0.04(1)	0.03(1)	0.03(1)	0.001(9)	0.002(8)	-0.00(1)
C(5)	0.05(1)	0.02(1)	0.03(1)	0.004(8)	0.01(1)	-0.01(1)
C(6)	0.05(1)	0.04(1)	0.02(1)	0.003(9)	-0.01(1)	-0.00(1)
C(7)	0.03(1)	0.05(1)	0.04(1)	-0.01(1)	-0.02(1)	0.00(1)
C(8)	0.05(1)	0.05(1)	0.03(1)	0.007(9)	-0.04(1)	-0.02(1)
C(9)	0.03(1)	0.020(9)	0.05(1)	-0.005(9)	-0.02(1)	0.003(8)
C(10)	0.03(1)	0.05(1)	0.018(9)	-0.002(8)	0.003(8)	-0.020(9)
C(11)	0.04(1)	0.04(1)	0.06(2)	-0.02(1)	-0.02(1)	-0.02(1)
C(12)	0.03(1)	0.04(1)	0.11(2)	-0.03(1)	-0.03(1)	0.01(1)
C(13)	0.04(1)	0.03(1)	0.03(1)	-0.012(9)	0.02(1)	-0.011(9)
C(14)	0.03(1)	0.05(1)	0.024(9)	0.001(9)	0.002(9)	-0.01(1)
C(15)	0.03(1)	0.05(2)	0.10(2)	-0.01(2)	-0.03(2)	-0.00(1)
C(16)	0.04(1)	0.03(1)	0.05(1)	0.00(1)	-0.01(1)	0.01(1)
C(17)	0.03(1)	0.04(1)	0.05(1)	0.01(1)	-0.01(1)	-0.00(1)
C(18)	0.06(1)	0.04(1)	0.05(1)	0.01(1)	0.01(1)	-0.02(1)
C(21)	0.03(1)	0.06(1)	0.02(1)	0.002(9)	-0.011(9)	-0.01(1)
C(22)	0.03(1)	0.04(1)	0.03(1)	0.026(9)	-0.002(9)	0.01(1)
C(23)	0.05(1)	0.03(1)	0.03(1)	0.019(8)	0.02(1)	0.01(1)
C(24)	0.04(1)	0.05(1)	0.09(2)	0.01(1)	0.04(1)	-0.01(1)
C(25)	0.04(1)	0.04(1)	0.03(1)	0.004(9)	0.01(1)	0.00(1)
C(26)	0.06(2)	0.06(2)	0.04(1)	0.01(1)	0.01(1)	-0.04(2)
C(27)	0.07(2)	0.06(2)	0.07(2)	0.01(1)	0.00(2)	0.01(2)
C(28)	0.09(2)	0.03(1)	0.08(2)	-0.01(1)	0.06(2)	0.00(1)
C(29)	0.07(2)	0.06(2)	0.05(2)	-0.00(1)	-0.01(1)	-0.06(1)
C(30)	0.03(1)	0.08(2)	0.04(1)	0.00(1)	0.01(1)	0.00(1)
B(1)	0.05(2)	0.06(2)	0.06(2)	-0.02(2)	0.01(2)	0.00(2)
F(1)	0.15(2)	0.17(2)	0.15(2)	-0.02(2)	0.01(2)	-0.10(2)
F(2)	0.07(1)	0.12(1)	0.11(1)	-0.07(1)	-0.02(1)	0.04(1)
F(3)	0.17(2)	0.09(1)	0.05(1)	0.014(9)	0.00(1)	0.01(1)
F(4)	0.17(2)	0.09(1)	0.09(1)	-0.03(1)	-0.03(1)	0.08(2)

Table : Fractional parameters for $[\text{Ir}(\text{cp}^*)(\text{C}_{18}\text{H}_{23}\text{O}_2)](\text{BF}_4)$

Atom	x/a	y/b	z/c	U(eq)
Ir(1)	0.94982(9)	0.85665(6)	0.11997(3)	0.0277
O(1)	1.269(2)	0.828(1)	0.0277(7)	0.0513
O(2)	0.430(2)	1.465(1)	0.1423(6)	0.0541
C(1)	1.068(3)	1.017(1)	0.1158(8)	0.0281
C(2)	1.185(3)	0.935(2)	0.1008(9)	0.0447
C(3)	1.168(3)	0.875(2)	0.0483(9)	0.0352
C(4)	0.996(2)	0.873(2)	0.0346(7)	0.0337
C(5)	0.876(3)	0.951(2)	0.0479(8)	0.0291
C(6)	0.718(3)	0.948(2)	0.0221(7)	0.0342
C(7)	0.584(2)	1.009(2)	0.0510(8)	0.0336
C(8)	0.648(3)	1.120(2)	0.0664(7)	0.0105
C(9)	0.784(2)	1.106(1)	0.1098(9)	0.0290
C(10)	0.909(2)	1.026(2)	0.0906(7)	0.0241
C(11)	0.853(2)	1.214(2)	0.125(1)	0.0248
C(12)	0.722(3)	1.292(2)	0.147(1)	0.0390
C(13)	0.589(2)	1.302(2)	0.1106(8)	0.0300
C(14)	0.519(3)	1.193(2)	0.0946(7)	0.0320
C(15)	0.364(3)	1.217(2)	0.067(1)	0.0467
C(16)	0.300(3)	1.319(2)	0.0947(9)	0.0392
C(17)	0.431(3)	1.352(2)	0.1340(7)	0.0382
C(18)	0.635(3)	1.375(2)	0.0612(9)	0.0463
C(21)	0.921(3)	0.814(2)	0.2042(7)	0.0336
C(22)	1.016(2)	0.738(2)	0.1788(8)	0.0226
C(23)	0.935(4)	0.686(2)	0.1275(8)	0.0288
C(24)	0.775(3)	0.732(2)	0.136(1)	0.0449
C(25)	0.763(3)	0.814(2)	0.1794(8)	0.0341
C(26)	0.960(3)	0.882(2)	0.2500(8)	0.0456
C(27)	1.186(4)	0.709(2)	0.195(1)	0.0638
C(28)	0.983(4)	0.596(2)	0.104(1)	0.0487
C(29)	0.631(3)	0.701(2)	0.1043(9)	0.0396
C(30)	0.624(3)	0.871(2)	0.1958(8)	0.0443
B(1)	0.323(4)	0.076(3)	0.241(1)	0.0566
F(1)	0.470(3)	0.129(2)	0.2402(9)	0.1310
F(2)	0.326(2)	-0.004(1)	0.2047(7)	0.0744
F(3)	0.301(3)	0.041(1)	0.2899(6)	0.0905
F(4)	0.197(3)	0.142(2)	0.2273(7)	0.0930