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Complex 20d

Table 2S. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Co(1)	53.0(8)	1108.1(5)	2372.0(4)	20(1)
O(1)	-2413(4)	1859(3)	4011(2)	33(1)
O(2)	-461(4)	1204(3)	408(2)	28(1)
O(3)	598(4)	1049(3)	4335(2)	35(1)
O(4)	2515(4)	278(3)	737(2)	28(1)
O(5)	1637(5)	4829(3)	1579(3)	51(1)
O(6)	2055(4)	4101(3)	109(2)	36(1)
N(1)	-2122(5)	1761(3)	3042(2)	25(1)
N(2)	-1191(4)	1440(3)	1315(2)	22(1)
N(3)	1318(5)	786(3)	3426(2)	25(1)
N(4)	2227(4)	422(3)	1699(2)	22(1)
N(5)	-390(4)	-512(3)	2549(2)	21(1)
C(1)	-5181(6)	2639(4)	2948(4)	39(1)
C(2)	-3382(5)	2094(4)	2535(3)	24(1)
C(3)	-2834(5)	1897(4)	1508(3)	21(1)
C(4)	-4001(6)	2176(4)	747(3)	36(1)
C(5)	4057(6)	-100(5)	4002(4)	42(1)
C(6)	2913(6)	241(4)	3241(3)	29(1)
C(7)	3473(5)	22(4)	2209(3)	26(1)
C(8)	5224(6)	-594(4)	1786(4)	36(1)
C(9)	-105(6)	-1221(4)	1810(3)	29(1)
C(10)	-378(6)	-2304(4)	1899(4)	38(1)
C(11)	-970(7)	-2698(4)	2794(4)	41(1)
C(12)	-1263(6)	-1981(4)	3564(3)	35(1)
C(13)	-955(6)	-905(4)	3428(3)	27(1)
C(14)	503(5)	2649(4)	2211(3)	25(1)
C(15)	1179(5)	2958(4)	1344(3)	27(1)
C(16)	1614(6)	4065(4)	1074(3)	30(1)
C(17)	2581(6)	5115(4)	-283(4)	38(1)
C(18)	3242(8)	4879(5)	-1322(4)	58(2)
C(19)	54(6)	3410(4)	3067(3)	36(1)
Cl(1)	3544(3)	-2782(2)	3171(1)	85(1)
Cl(2)	2530(3)	-5506(2)	5070(1)	89(1)
C(102)	3447(11)	-4159(7)	3635(6)	105(3)
C(101)	2496(12)	-4111(7)	4532(6)	104(3)

Complex 2cd

Table 4S. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Co(1)	24(1)	21(1)	16(1)	-2(1)	-3(1)	-6(1)
O(1)	36(2)	42(2)	21(2)	-8(2)	2(1)	-10(2)
O(2)	34(2)	34(2)	14(2)	-7(1)	-3(1)	-7(2)
O(3)	48(2)	45(2)	14(2)	-5(2)	-4(1)	-16(2)
O(4)	30(2)	33(2)	18(2)	-5(1)	-1(1)	-5(2)
O(5)	89(3)	32(2)	41(2)	-4(2)	0(2)	-34(2)
O(6)	46(2)	34(2)	30(2)	6(2)	-3(2)	-20(2)
N(1)	35(2)	23(2)	16(2)	-5(2)	2(2)	-8(2)
N(2)	28(2)	20(2)	18(2)	-3(2)	-2(2)	-7(2)
N(3)	33(2)	26(2)	20(2)	-2(2)	-7(2)	-12(2)
N(4)	26(2)	22(2)	18(2)	-1(2)	-3(2)	-8(2)
N(5)	23(2)	20(2)	21(2)	-2(2)	-4(1)	-6(2)
C(1)	30(3)	35(3)	48(3)	-4(2)	2(2)	-7(2)
C(2)	23(2)	17(2)	32(3)	-2(2)	1(2)	-9(2)
C(3)	26(2)	16(2)	24(2)	-1(2)	-8(2)	-7(2)
C(4)	30(3)	39(3)	40(3)	-2(2)	-16(2)	-6(2)
C(5)	42(3)	55(4)	35(3)	4(3)	-19(2)	-14(3)
C(6)	28(3)	30(3)	33(3)	4(2)	-11(2)	-12(2)
C(7)	22(2)	21(2)	35(3)	1(2)	-3(2)	-5(2)
C(8)	28(3)	38(3)	43(3)	3(2)	-9(2)	-7(2)
C(9)	37(3)	28(3)	21(2)	-5(2)	1(2)	-10(2)
C(10)	51(3)	31(3)	31(3)	-11(2)	-4(2)	-10(2)
C(11)	59(4)	22(3)	44(3)	3(2)	-7(3)	-17(3)
C(12)	47(3)	27(3)	32(3)	3(2)	1(2)	-12(2)
C(13)	37(3)	24(3)	19(2)	0(2)	-3(2)	-8(2)
C(14)	25(2)	23(2)	27(3)	-4(2)	-3(2)	-6(2)
C(15)	31(3)	20(2)	30(3)	-2(2)	-3(2)	-9(2)
C(16)	27(3)	24(3)	37(3)	0(2)	-4(2)	-5(2)
C(17)	42(3)	27(3)	45(3)	10(2)	-1(2)	-14(2)
C(18)	65(4)	52(4)	55(4)	10(3)	10(3)	-24(3)
C(19)	49(3)	25(3)	35(3)	-10(2)	3(2)	-14(2)
Cl(1)	104(2)	51(1)	98(2)	11(1)	0(1)	-26(1)
Cl(2)	133(2)	54(1)	68(1)	-5(1)	28(1)	-26(1)
C(102)	109(7)	63(5)	119(7)	15(5)	7(6)	4(5)
C(101)	124(7)	85(6)	68(5)	4(5)	13(5)	19(5)

Complex 20d.

Table 5S. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(1A)	-1498(4)	1615(3)	4237(2)	50
H(4A)	1619(4)	571(3)	502(2)	41
H(1B)	-5251(6)	2683(4)	3641(4)	58
H(1C)	-5914(6)	2177(4)	2801(4)	58
H(1D)	-5550(6)	3412(4)	2672(4)	58
H(4B)	-3343(6)	1969(4)	122(3)	54
H(4C)	-4563(6)	2997(4)	745(3)	54
H(4D)	-4854(6)	1742(4)	882(3)	54
H(5A)	3408(6)	132(5)	4624(4)	64
H(5B)	4976(6)	278(5)	3870(4)	64
H(5C)	4532(6)	-932(5)	4007(4)	64
H(8A)	5271(6)	-627(4)	1094(4)	55
H(8B)	5518(6)	-1373(4)	2059(4)	55
H(8C)	6027(6)	-185(4)	1930(4)	55
H(9A)	302(6)	-964(4)	1198(3)	34
H(10A)	-166(6)	-2772(4)	1359(4)	45
H(11A)	-1166(7)	-3436(4)	2876(4)	49
H(12A)	-1671(6)	-2225(4)	4181(3)	42
H(13A)	-1143(6)	-428(4)	3961(3)	32
H(15A)	1401(5)	2417(4)	854(3)	32
H(17A)	3476(6)	5241(4)	57(4)	46
H(17B)	1610(6)	5804(4)	-221(4)	46
H(18A)	3614(8)	5534(5)	-1621(4)	87
H(18B)	2342(8)	4755(5)	-1647(4)	87
H(18C)	4197(8)	4194(5)	-1370(4)	87
H(19A)	-414(6)	3011(4)	3617(3)	54
H(19B)	-786(6)	4118(4)	2926(3)	54
H(19C)	1072(6)	3594(4)	3212(3)	54
H(10B)	2944(11)	-4527(7)	3191(6)	126
H(10C)	4608(11)	-4639(7)	3678(6)	126
H(10D)	1311(12)	-3690(7)	4475(6)	125
H(10E)	2935(12)	-3676(7)	4957(6)	125

complex 22b

Table 2S. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Co	8671.3(8)	6279.5(5)	7993.0(7)	24(1)
O(1)	5312(5)	6848(3)	7275(5)	52(1)
O(2)	10913(7)	5295(3)	6115(6)	49(1)
O(3)	6395(6)	7203(3)	9953(6)	52(1)
O(4)	12075(5)	5755(3)	8690(5)	46(1)
O(5)	7514(5)	8163(3)	5648(5)	45(1)
O(6)	8198(6)	8581(3)	8079(5)	53(1)
N(1)	6677(5)	6413(4)	6776(5)	33(1)
N(2)	9403(6)	5657(3)	6223(5)	33(1)
N(3)	7990(6)	6889(3)	9777(6)	36(1)
N(4)	10703(5)	6205(4)	9184(5)	34(1)
N(5)	7702(6)	5206(3)	8989(5)	28(1)
C(1)	6682(7)	6047(4)	5417(7)	38(2)
C(2)	8273(8)	5595(4)	5076(6)	37(2)
C(3)	5202(8)	6094(5)	4296(8)	64(3)
C(4)	8613(11)	5109(5)	3612(8)	66(2)
C(5)	9113(9)	6990(4)	10883(6)	41(2)
C(6)	10711(7)	6565(4)	10522(6)	39(2)
C(7)	8780(11)	7479(6)	12347(8)	70(2)
C(8)	12232(9)	6547(6)	11599(8)	65(3)
C(9)	6027(7)	5131(4)	9333(7)	35(2)
C(10)	5345(8)	4432(4)	10018(7)	48(2)
C(11)	6409(9)	3767(4)	10406(7)	47(2)
C(12)	8130(9)	3829(4)	10085(7)	44(2)
C(13)	8719(8)	4561(4)	9377(6)	36(1)
C(14)	9564(8)	7326(4)	7035(6)	32(1)
C(15)	11079(10)	7417(6)	6448(9)	52(2)
C(16)	8370(8)	8085(4)	7015(7)	36(1)
C(17)	6264(10)	8833(5)	5573(9)	69(2)
C(18)	5311(14)	8798(8)	4120(11)	118(5)

Complex 22b

Table 4.5 Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Co	20(1)	27(1)	26(1)	-1(1)	1(1)	1(1)
O(1)	24(2)	61(3)	71(3)	18(3)	4(2)	11(2)
O(2)	41(3)	52(3)	54(3)	-11(3)	14(2)	11(3)
O(3)	43(3)	48(3)	64(3)	-3(3)	20(3)	17(2)
O(4)	22(2)	64(3)	52(2)	-1(2)	0(2)	8(2)
O(5)	48(3)	44(3)	42(2)	0(2)	3(2)	8(2)
O(6)	66(3)	42(3)	51(3)	-17(2)	4(2)	11(2)
N(1)	29(3)	27(4)	41(3)	12(3)	-7(2)	-5(3)
N(2)	38(3)	29(3)	32(3)	-5(2)	9(2)	1(2)
N(3)	39(3)	31(3)	38(3)	6(2)	9(2)	1(3)
N(4)	20(2)	48(3)	33(2)	1(3)	-1(2)	0(3)
N(5)	28(3)	26(3)	31(2)	4(2)	0(2)	-1(2)
C(1)	40(3)	37(4)	38(3)	12(3)	-14(3)	-10(3)
C(2)	55(4)	33(4)	23(3)	-4(3)	-10(3)	-14(3)
C(3)	53(4)	76(7)	65(4)	31(4)	-32(3)	-22(4)
C(4)	97(6)	59(5)	40(4)	-17(4)	-2(4)	-7(5)
C(5)	58(4)	41(4)	25(3)	5(3)	5(3)	-8(4)
C(6)	47(3)	48(4)	23(3)	10(3)	-7(2)	-12(3)
C(7)	106(7)	62(5)	42(4)	-17(4)	17(4)	-10(5)
C(8)	65(4)	85(7)	46(3)	1(4)	-26(3)	-4(4)
C(9)	23(3)	38(4)	42(4)	2(3)	5(3)	2(3)
C(10)	39(4)	49(4)	54(4)	5(3)	10(3)	-17(3)
C(11)	68(5)	32(4)	41(4)	5(3)	0(3)	-19(4)
C(12)	64(5)	26(3)	42(4)	1(3)	-2(3)	-2(3)
C(13)	37(3)	34(4)	36(3)	2(3)	1(3)	4(3)
C(14)	38(3)	33(4)	25(3)	-5(3)	-1(3)	-5(3)
C(15)	56(5)	41(4)	60(5)	5(4)	8(4)	-17(4)
C(16)	42(4)	35(3)	30(3)	1(3)	9(3)	-7(3)
C(17)	76(6)	54(5)	76(5)	21(4)	9(4)	27(4)
C(18)	132(9)	150(12)	74(6)	-8(7)	-39(6)	82(9)

complex 22b

Table 5S. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(3A)	5817(6)	7092(3)	9160(6)	78
H(4A)	11879(5)	5560(3)	7803(5)	69
H(3B)	4288(8)	6424(5)	4764(8)	97
H(3C)	4790(8)	5530(5)	4074(8)	97
H(3D)	5570(8)	6360(5)	3327(8)	97
H(4B)	9753(11)	4867(5)	3660(8)	98
H(4C)	8533(11)	5482(5)	2711(8)	98
H(4D)	7776(11)	4660(5)	3510(8)	98
H(7A)	7625(11)	7704(6)	12320(8)	105
H(7B)	9593(11)	7940(6)	12424(8)	105
H(7C)	8906(11)	7111(6)	13251(8)	105
H(8A)	13148(9)	6227(6)	11113(8)	98
H(8B)	11914(9)	6283(6)	12585(8)	98
H(8C)	12618(9)	7118(6)	11796(8)	98
H(9A)	5294(7)	5583(4)	9089(7)	42
H(10A)	4165(8)	4402(4)	10225(7)	57
H(11A)	5963(9)	3280(4)	10882(7)	56
H(12A)	8885(9)	3387(4)	10337(7)	53
H(13A)	9895(8)	4606(4)	9158(6)	43
H(15A)	11414(10)	7939(6)	6026(9)	63
H(15B)	11847(10)	6960(6)	6443(9)	63
H(17A)	5474(10)	8784(5)	6462(9)	83
H(17B)	6847(10)	9379(5)	5654(9)	83
H(18A)	4481(14)	9253(8)	4096(11)	178
H(18B)	4719(14)	8262(8)	4048(11)	178
H(18C)	6091(14)	8856(8)	3240(11)	178