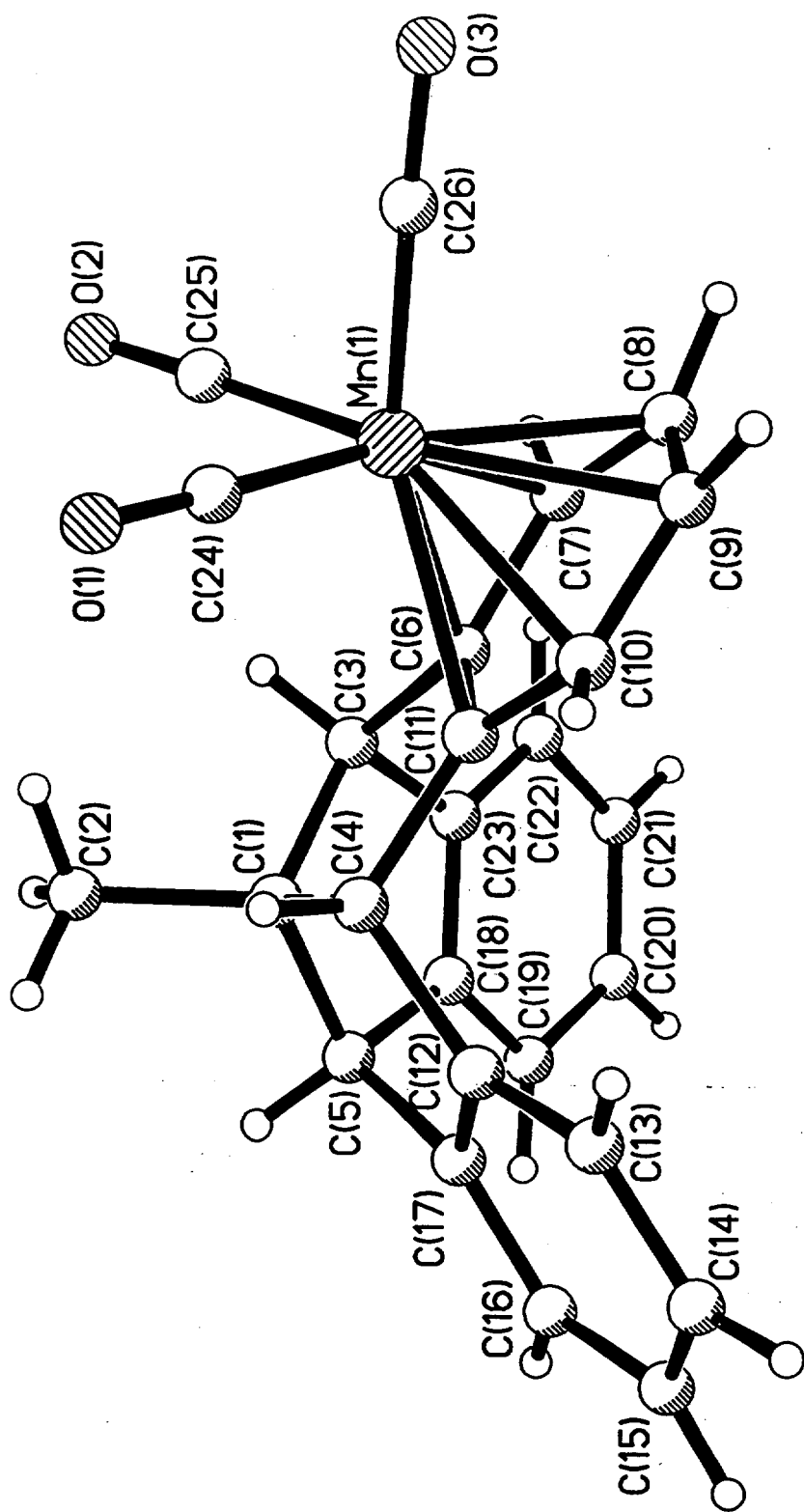
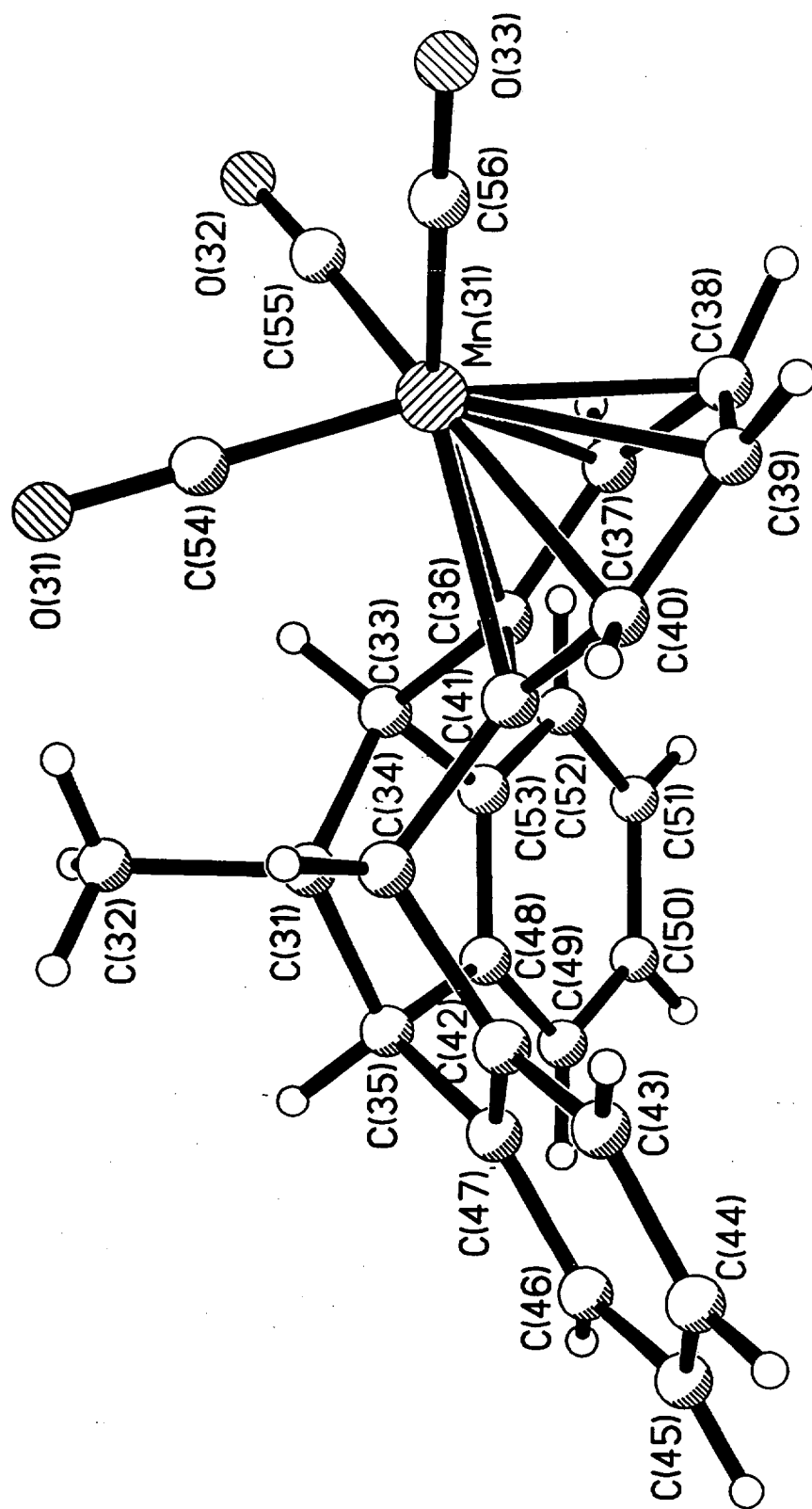
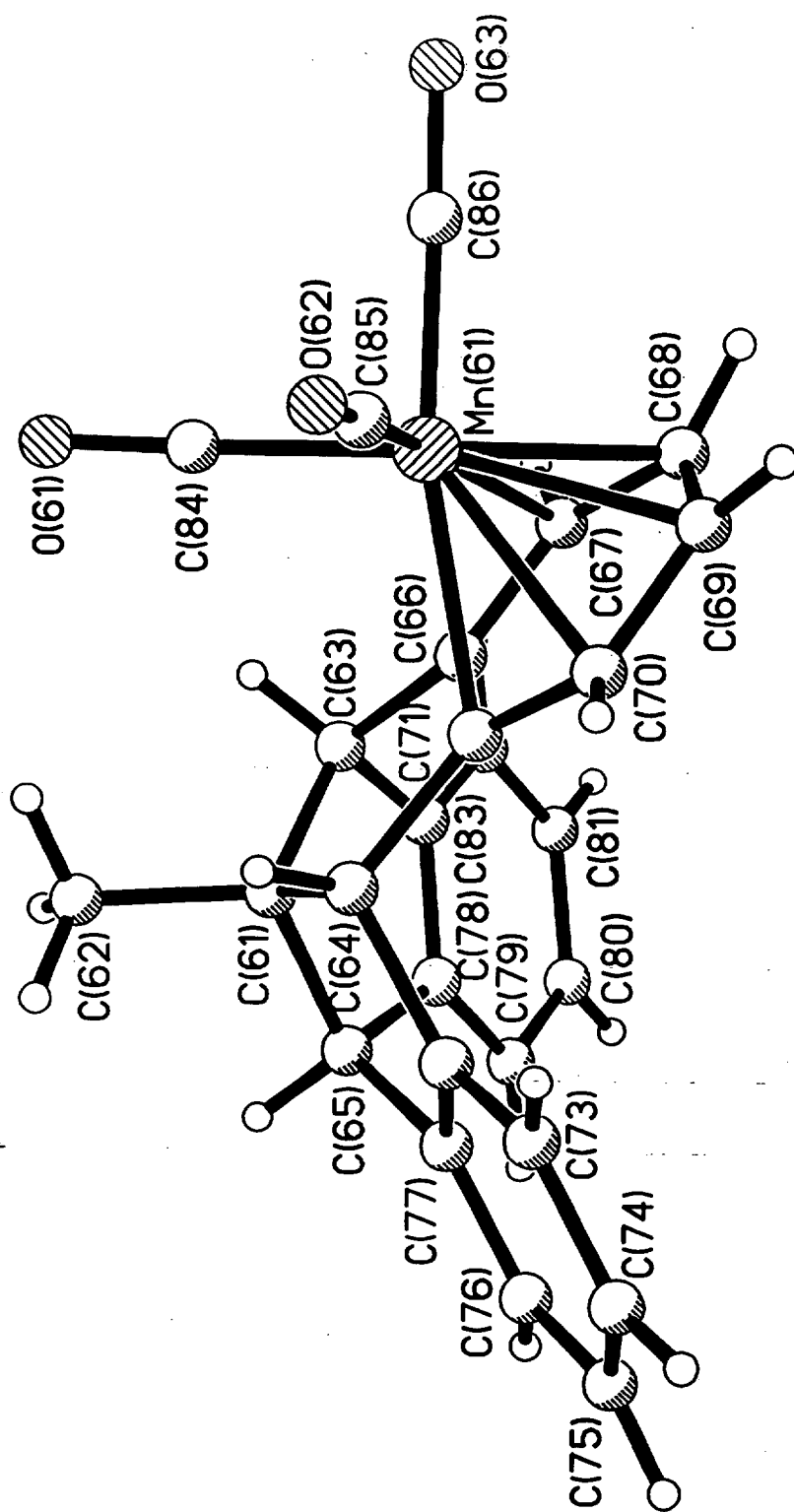
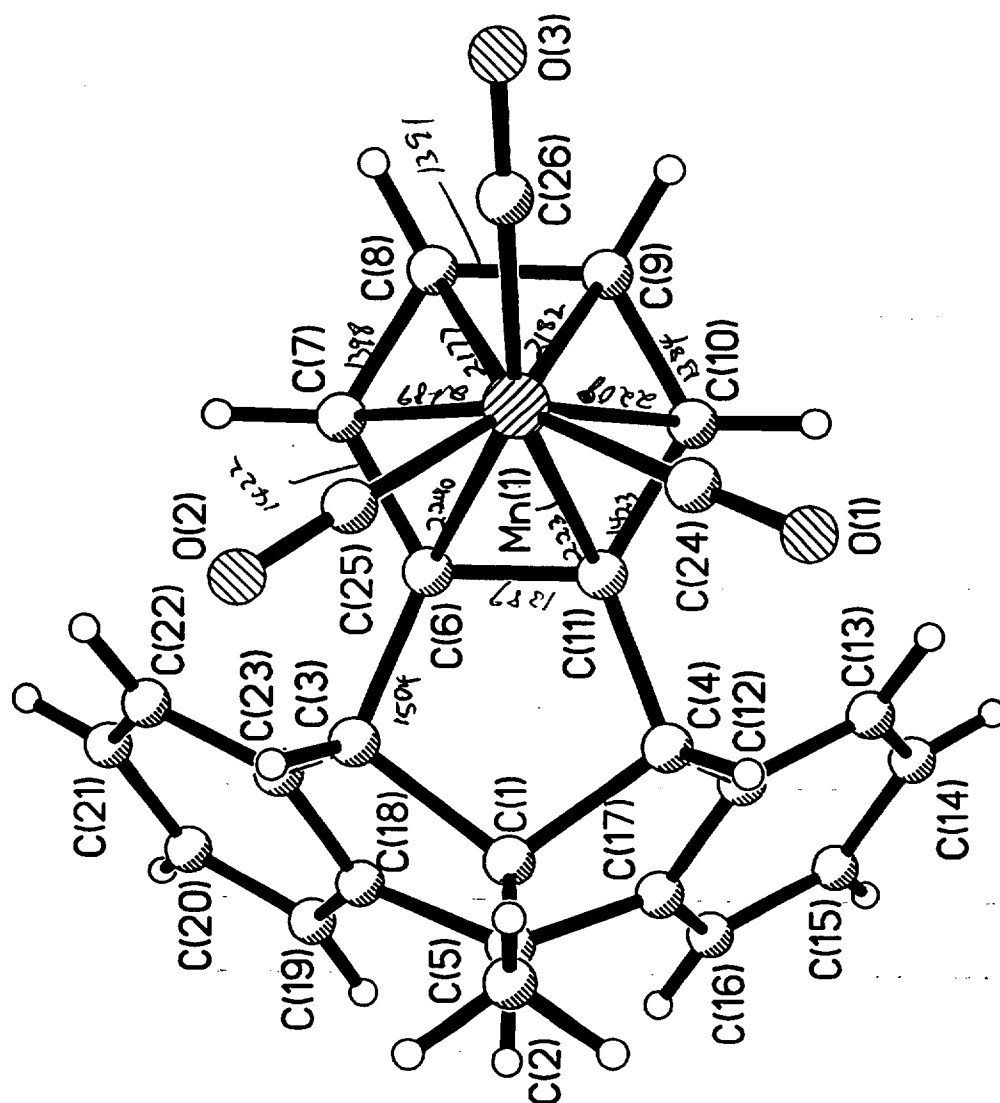


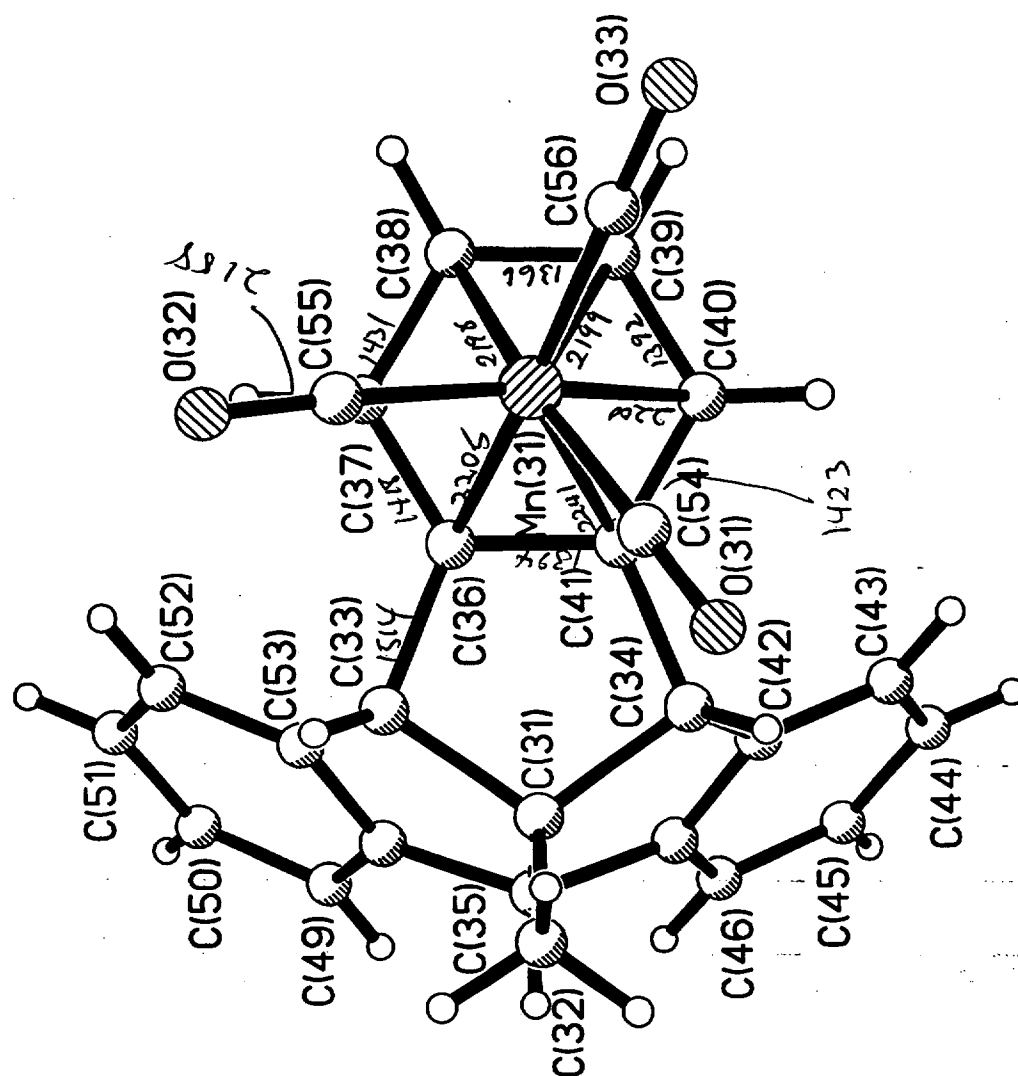
Identification code	cad13a
Empirical formula	$C_{26}H_{18}BF_4MnO_3$
Formula weight	520.15
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$Pna2_1$
Unit cell dimensions	$a = 29.9759(3)$ Å $\alpha = 90^\circ$ $b = 9.8300(2)$ Å $\beta = 90^\circ$ $c = 23.6351(3)$ Å $\gamma = 90^\circ$
Volume, Z	$6964.4(2)$ Å ³ , 12
Density (calculated)	1.488 Mg/m ³
Absorption coefficient	0.627 mm ⁻¹
F(000)	3168
Crystal size	0.34 x 0.26 x 0.04 mm
θ range for data collection	1.36 to 23.49°
Limiting indices	$-32 \leq h \leq 33$, $-11 \leq k \leq 10$, $-26 \leq l \leq 22$
Reflections collected	25636
Independent reflections	8475 ($R_{int} = 0.0848$)
Absorption correction	Empirical (SADABS)
Max. and min. transmission	0.983 and 0.788
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8474 / 973 / 946
Goodness-of-fit on F^2	1.126
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0773$, $wR2 = 0.1265$
R indices (all data)	$R1 = 0.1277$, $wR2 = 0.1459$
Absolute structure parameter	0.05(3)
Largest diff. peak and hole	0.352 and -0.258 eÅ ⁻³

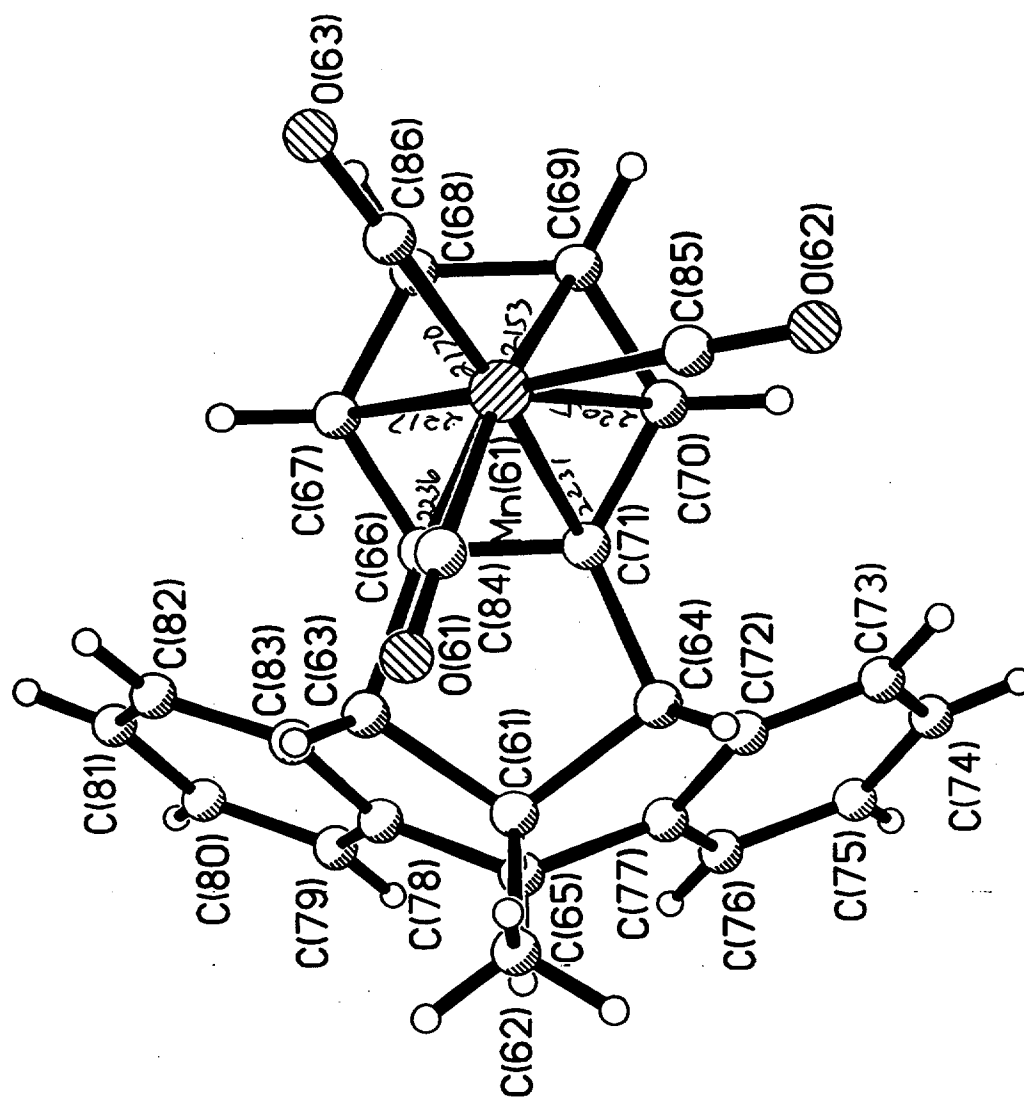




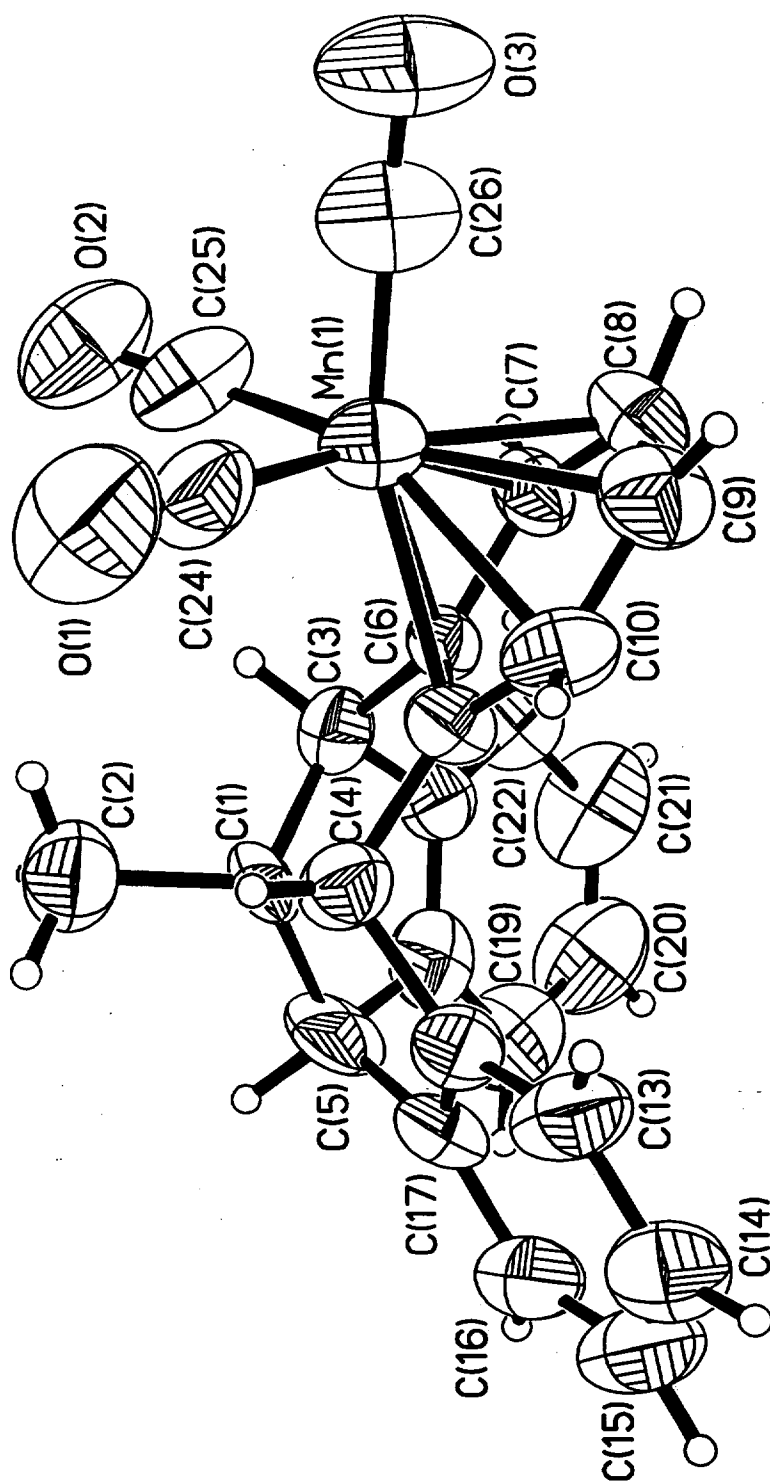


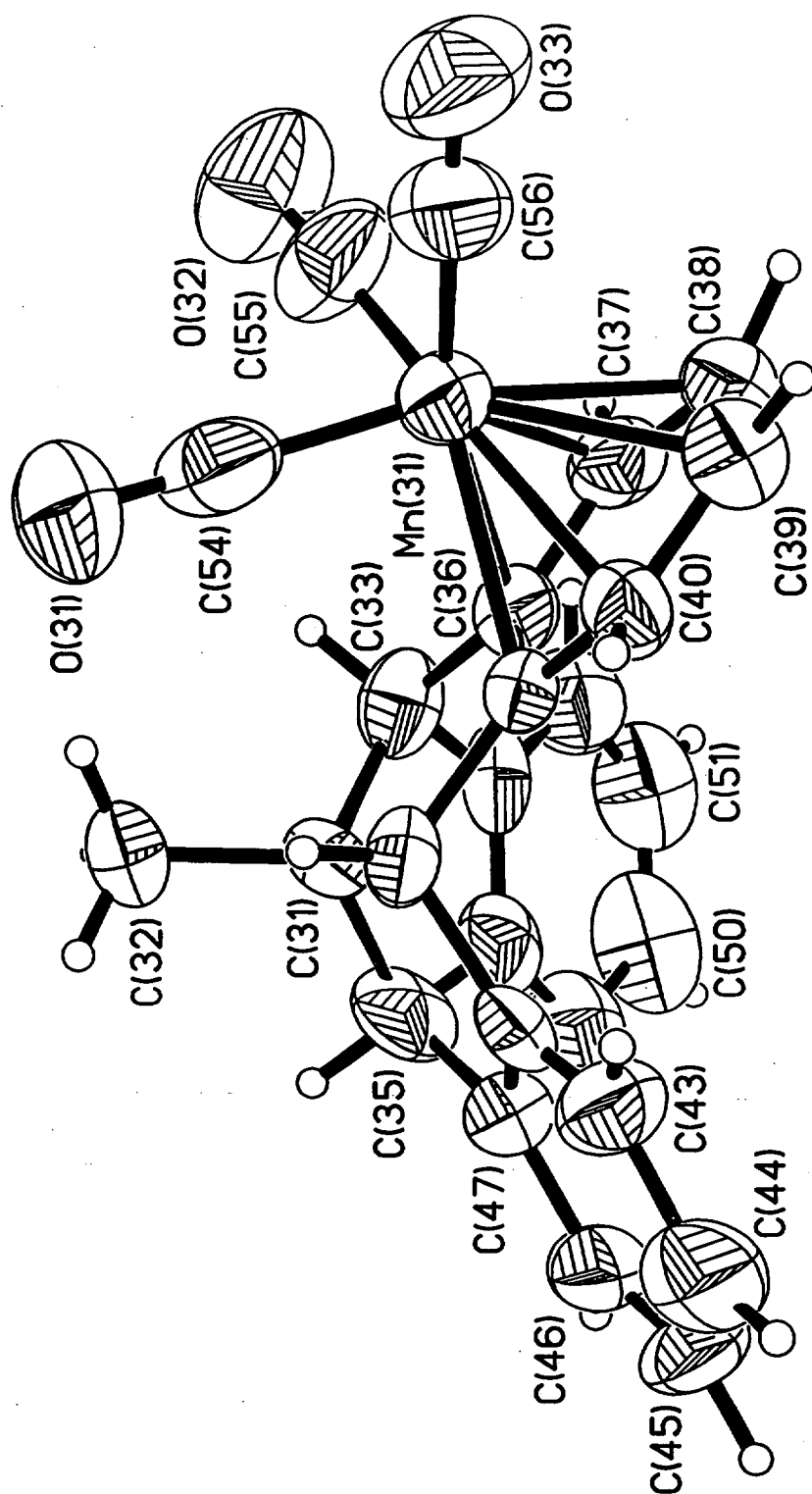


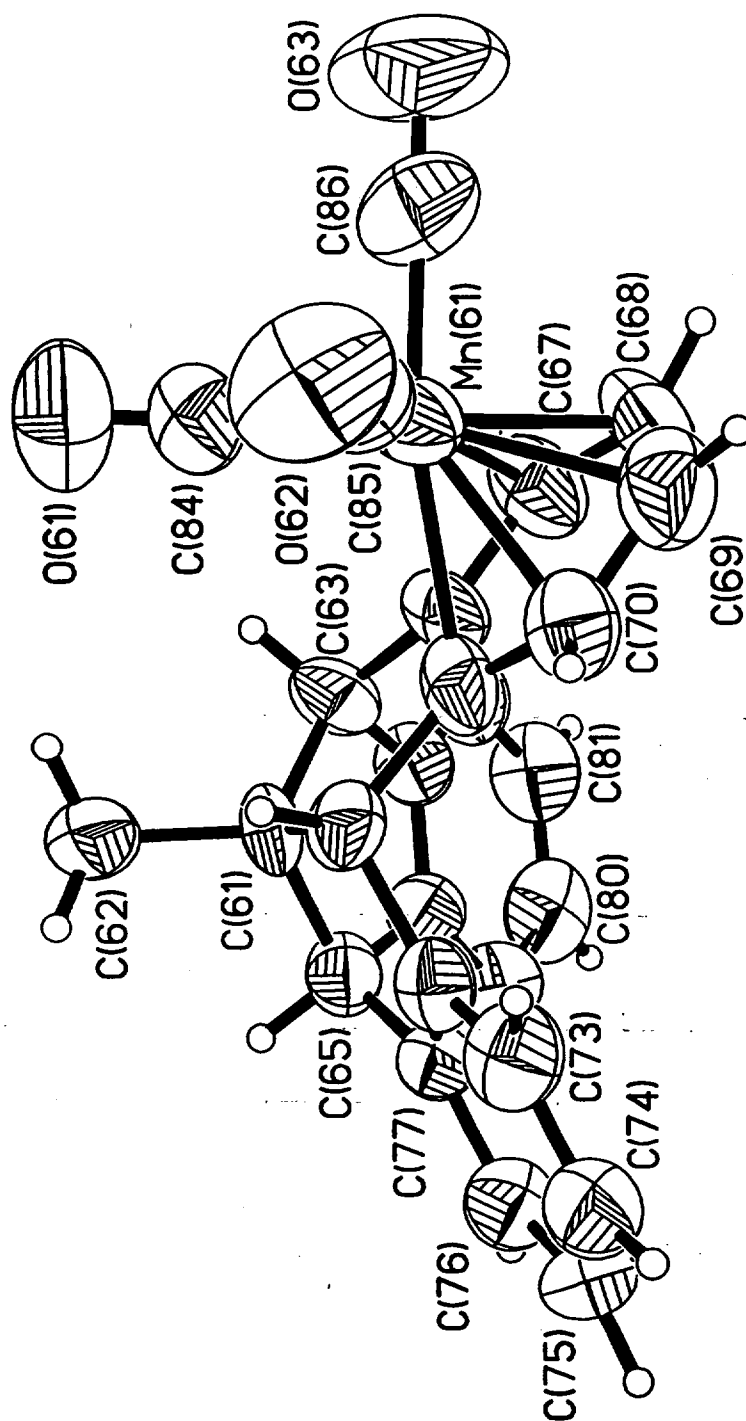




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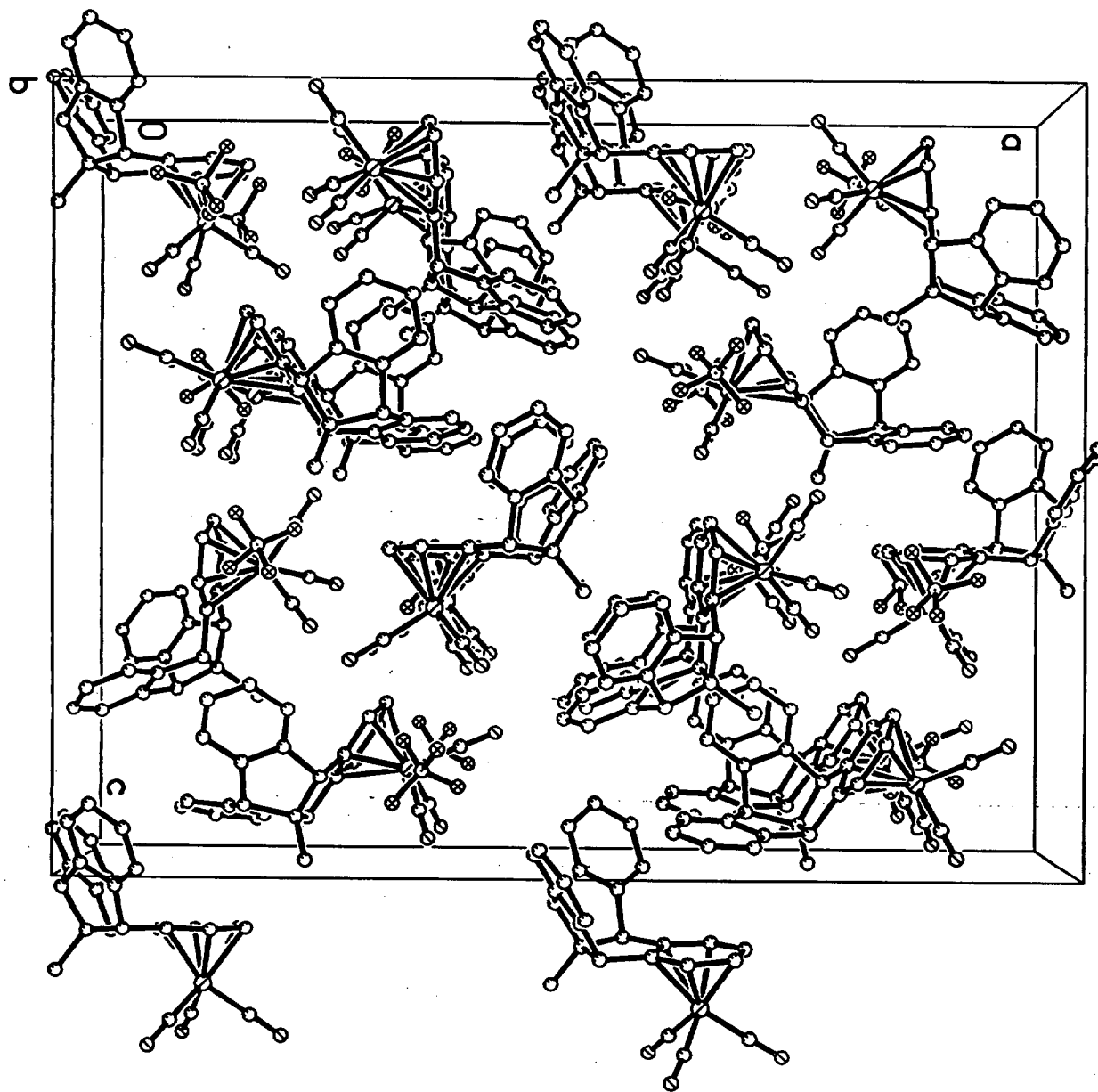
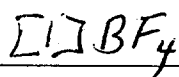


Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.



	x	y	z	U(eq)
Mn(1)	3101(1)	9895(1)	1126(1)	54(1)
C(1)	3645(3)	8227(9)	2495(3)	52(3)
C(2)	3227(3)	8080(11)	2858(5)	78(4)
C(3)	3603(3)	7435(8)	1923(3)	52(3)
C(4)	3727(3)	9752(9)	2332(3)	54(3)
C(5)	4081(3)	7738(9)	2785(4)	66(3)
C(6)	3629(3)	8516(8)	1474(3)	39(2)
C(7)	3592(3)	8357(9)	878(4)	51(3)
C(8)	3635(4)	9489(11)	524(4)	63(3)
C(9)	3703(3)	10773(11)	756(5)	68(3)
C(10)	3731(3)	10949(9)	1336(4)	60(3)
C(11)	3690(3)	9805(8)	1702(3)	43(2)
C(12)	4188(3)	10061(10)	2544(4)	52(3)
C(13)	4424(3)	11243(11)	2495(5)	71(4)
C(14)	4850(4)	11351(11)	2716(5)	73(4)
C(15)	5034(4)	10287(14)	3001(5)	87(4)
C(16)	4801(3)	9081(12)	3054(5)	74(4)
C(17)	4378(3)	8967(10)	2822(4)	60(3)
C(18)	4258(3)	6629(9)	2387(4)	59(3)
C(19)	4643(4)	5856(12)	2458(5)	88(4)
C(20)	4774(4)	4965(14)	2032(7)	102(5)
C(21)	4513(4)	4841(11)	1563(6)	95(4)
C(22)	4128(3)	5583(10)	1499(5)	62(3)
C(23)	4009(3)	6500(9)	1910(4)	51(3)
C(24)	2790(3)	11007(11)	1599(5)	68(3)
O(1)	2591(3)	11699(10)	1884(4)	127(4)
C(25)	2679(3)	8620(11)	1268(5)	77(4)
O(2)	2424(3)	7797(8)	1366(4)	101(3)
C(26)	2771(4)	10527(12)	550(5)	83(4)
O(3)	2570(3)	10938(9)	172(4)	106(3)
Mn(31)	3707(1)	81(2)	6614(1)	54(1)
C(31)	4857(3)	902(8)	5884(4)	51(3)
C(32)	5152(3)	1300(11)	6385(4)	74(3)
C(33)	4681(3)	-584(9)	5963(4)	58(3)
C(34)	4448(3)	1866(9)	5810(4)	54(3)
C(35)	5112(3)	908(9)	5317(4)	68(3)
C(36)	4179(3)	-422(8)	5930(4)	48(3)
C(37)	3848(3)	-1451(9)	5967(4)	59(3)
C(38)	3388(3)	-1080(10)	5929(4)	58(3)
C(39)	3272(3)	255(10)	5868(4)	58(3)
C(40)	3591(3)	1282(9)	5842(4)	53(3)
C(41)	4051(2)	927(8)	5849(4)	42(2)
C(42)	4499(3)	2449(10)	5223(4)	53(3)
C(43)	4243(4)	3423(10)	4968(5)	63(3)
C(44)	4359(4)	3864(11)	4431(5)	82(4)
C(45)	4724(4)	3330(12)	4154(4)	75(4)
C(46)	4982(4)	2367(12)	4411(4)	72(3)

C(48)	5109 (3)	-553 (10)	5109 (5)	65 (3)
C(49)	5312 (3)	-1084 (13)	4632 (5)	82 (4)
C(50)	5260 (4)	-2445 (15)	4523 (6)	101 (5)
C(51)	5021 (5)	-3273 (13)	4876 (6)	97 (5)
C(52)	4823 (4)	-2741 (12)	5354 (5)	80 (4)
C(53)	4870 (3)	-1369 (11)	5470 (4)	60 (3)
C(54)	3998 (4)	1340 (11)	7032 (5)	73 (4)
O(31)	4186 (3)	2133 (8)	7302 (4)	105 (3)
C(55)	3875 (4)	-1213 (11)	7104 (5)	88 (4)
O(32)	4005 (4)	-2044 (9)	7403 (4)	122 (4)
C(56)	3219 (3)	439 (12)	7010 (5)	75 (4)
O(33)	2898 (3)	682 (9)	7261 (3)	97 (3)
Mn(61)	6633 (1)	5207 (2)	3772 (1)	67 (1)
C(61)	7725 (3)	3295 (8)	4341 (3)	51 (3)
C(62)	7610 (3)	2493 (11)	4871 (4)	70 (3)
C(63)	7472 (3)	2817 (8)	3812 (4)	56 (3)
C(64)	7647 (2)	4866 (9)	4404 (4)	55 (3)
C(65)	8237 (3)	3141 (9)	4195 (4)	54 (3)
C(66)	7261 (3)	4079 (10)	3570 (4)	60 (3)
C(67)	7014 (4)	4225 (12)	3079 (4)	77 (4)
C(68)	6863 (4)	5526 (14)	2912 (4)	91 (4)
C(69)	6969 (4)	6667 (12)	3243 (6)	93 (5)
C(70)	7227 (3)	6523 (10)	3728 (5)	68 (3)
C(71)	7371 (3)	5226 (10)	3893 (4)	58 (3)
C(72)	8107 (3)	5491 (9)	4396 (4)	51 (3)
C(73)	8224 (3)	6811 (10)	4498 (4)	69 (3)
C(74)	8666 (4)	7183 (11)	4465 (5)	73 (3)
C(75)	8987 (3)	6274 (12)	4336 (5)	70 (3)
C(76)	8873 (3)	4920 (11)	4221 (5)	63 (3)
C(77)	8432 (3)	4544 (9)	4258 (4)	55 (3)
C(78)	8243 (3)	2469 (10)	3621 (4)	55 (3)
C(79)	8609 (3)	2048 (10)	3311 (5)	62 (3)
C(80)	8543 (4)	1358 (10)	2806 (5)	77 (4)
C(81)	8121 (4)	1118 (11)	2615 (5)	76 (4)
C(82)	7762 (4)	1538 (11)	2929 (4)	66 (3)
C(83)	7820 (3)	2234 (10)	3427 (4)	56 (3)
C(84)	6496 (4)	3862 (12)	4274 (5)	75 (4)
O(61)	6397 (3)	3067 (10)	4600 (4)	128 (4)
C(85)	6432 (4)	6434 (13)	4284 (6)	95 (5)
O(62)	6320 (3)	7198 (10)	4606 (5)	128 (4)
C(86)	6095 (4)	5108 (15)	3485 (6)	107 (5)
O(63)	5736 (3)	5011 (16)	3300 (5)	184 (6)
B(1)	3031 (4)	4353 (13)	832 (6)	60 (4)
F(1)	3325 (3)	3663 (7)	1124 (4)	135 (3)
F(2)	3218 (4)	5081 (14)	437 (5)	223 (7)
F(3)	2692 (3)	3709 (8)	638 (5)	172 (5)
F(4)	2889 (4)	5335 (12)	1174 (6)	233 (7)
B(31)	1449 (5)	38 (14)	1347 (7)	105 (7)
F(31)	1473 (3)	-1116 (7)	1655 (4)	147 (3)
F(32)	1622 (3)	1048 (7)	1649 (4)	154 (4)
F(33)	1680 (4)	-115 (13)	870 (5)	222 (6)
F(34)	1025 (3)	315 (9)	1221 (5)	167 (4)
B(61)	1419 (5)	4828 (17)	3648 (8)	112 (7)
F(61)	1609 (3)	3921 (12)	3314 (4)	190 (5)
F(62)	1252 (4)	5853 (9)	3364 (5)	185 (5)
F(63)	1072 (3)	4163 (12)	3873 (5)	220 (6)
F(64)	1698 (4)	5179 (11)	4047 (5)	235 (7)

Table 3. Bond lengths [Å] and angles [°] for [1]BF₄

Mn(1) - C(26)	1.794 (11)	Mn(1) - C(25)	1.812 (10)
Mn(1) - C(24)	1.822 (10)	Mn(1) - C(8)	2.177 (10)
Mn(1) - C(9)	2.182 (10)	Mn(1) - C(7)	2.189 (8)
Mn(1) - C(10)	2.209 (9)	Mn(1) - C(11)	2.231 (8)
Mn(1) - C(6)	2.240 (7)	C(1) - C(2)	1.524 (11)
C(1) - C(5)	1.552 (11)	C(1) - C(3)	1.565 (10)
C(1) - C(4)	1.568 (10)	C(3) - C(6)	1.504 (9)
C(3) - C(23)	1.525 (10)	C(4) - C(11)	1.496 (10)
C(4) - C(12)	1.499 (10)	C(5) - C(17)	1.505 (11)
C(5) - C(18)	1.535 (11)	C(6) - C(11)	1.389 (10)
C(6) - C(7)	1.422 (10)	C(7) - C(8)	1.398 (11)
C(8) - C(9)	1.391 (12)	C(9) - C(10)	1.384 (11)
C(10) - C(11)	1.423 (10)	C(12) - C(13)	1.365 (11)
C(12) - C(17)	1.383 (11)	C(13) - C(14)	1.383 (12)
C(14) - C(15)	1.362 (13)	C(15) - C(16)	1.381 (13)
C(16) - C(17)	1.385 (11)	C(18) - C(23)	1.359 (11)
C(18) - C(19)	1.390 (12)	C(19) - C(20)	1.392 (13)
C(20) - C(21)	1.363 (14)	C(21) - C(22)	1.372 (12)
C(22) - C(23)	1.374 (11)	C(24) - O(1)	1.128 (10)
C(25) - O(2)	1.138 (10)	C(26) - O(3)	1.150 (11)
Mn(31) - C(56)	1.771 (11)	Mn(31) - C(55)	1.793 (11)
Mn(31) - C(54)	1.808 (11)	Mn(31) - C(37)	2.188 (9)
Mn(31) - C(38)	2.198 (9)	Mn(31) - C(39)	2.199 (9)
Mn(31) - C(40)	2.200 (9)	Mn(31) - C(36)	2.205 (8)
Mn(31) - C(41)	2.241 (8)	C(31) - C(32)	1.528 (11)
C(31) - C(35)	1.544 (12)	C(31) - C(34)	1.559 (10)
C(31) - C(33)	1.565 (11)	C(33) - C(53)	1.508 (11)
C(33) - C(36)	1.514 (10)	C(34) - C(42)	1.509 (10)
C(34) - C(41)	1.510 (10)	C(35) - C(47)	1.511 (11)
C(35) - C(48)	1.518 (11)	C(36) - C(41)	1.394 (11)
C(36) - C(37)	1.418 (10)	C(37) - C(38)	1.431 (11)
C(38) - C(39)	1.366 (11)	C(39) - C(40)	1.392 (11)
C(40) - C(41)	1.423 (10)	C(42) - C(43)	1.367 (11)
C(42) - C(47)	1.382 (11)	C(43) - C(44)	1.386 (12)
C(44) - C(45)	1.379 (12)	C(45) - C(46)	1.364 (12)
C(46) - C(47)	1.387 (11)	C(48) - C(53)	1.373 (11)
C(48) - C(49)	1.383 (12)	C(49) - C(50)	1.372 (13)
C(50) - C(51)	1.368 (14)	C(51) - C(52)	1.379 (13)
C(52) - C(53)	1.384 (12)	C(54) - O(31)	1.155 (10)
C(55) - O(32)	1.149 (11)	C(56) - O(33)	1.155 (10)
Mn(61) - C(86)	1.752 (13)	Mn(61) - C(85)	1.812 (13)
Mn(61) - C(84)	1.824 (12)	Mn(61) - C(69)	2.153 (11)
Mn(61) - C(68)	2.170 (10)	Mn(61) - C(70)	2.205 (10)
Mn(61) - C(67)	2.217 (9)	Mn(61) - C(71)	2.231 (9)
Mn(61) - C(66)	2.236 (9)	C(61) - C(62)	1.520 (11)
C(61) - C(63)	1.536 (10)	C(61) - C(64)	1.568 (10)
C(61) - C(65)	1.581 (10)	C(63) - C(83)	1.497 (10)
C(63) - C(66)	1.507 (10)	C(64) - C(71)	1.506 (10)
C(64) - C(72)	1.511 (10)	C(65) - C(77)	1.506 (10)
C(65) - C(78)	1.508 (11)	C(66) - C(67)	1.383 (11)
C(66) - C(71)	1.402 (11)	C(67) - C(68)	1.413 (12)
C(68) - C(69)	1.404 (14)	C(69) - C(70)	1.391 (12)
C(70) - C(71)	1.401 (11)	C(72) - C(73)	1.365 (11)
C(72) - C(77)	1.386 (10)	C(73) - C(74)	1.378 (11)

C(76) - C(77)	1.375 (10)	C(78) - C(83)	1.368 (11)
C(78) - C(79)	1.384 (11)	C(79) - C(80)	1.387 (12)
C(80) - C(81)	1.366 (13)	C(81) - C(82)	1.370 (12)
C(82) - C(83)	1.372 (11)	C(84) - O(61)	1.136 (11)
C(85) - O(62)	1.121 (11)	C(86) - O(63)	1.164 (12)
B(1) - F(3)	1.284 (12)	B(1) - F(2)	1.303 (13)
B(1) - F(1)	1.307 (12)	B(1) - F(4)	1.329 (13)
B(31) - F(32)	1.329 (13)	B(31) - F(33)	1.33 (2)
B(31) - F(34)	1.333 (14)	B(31) - F(31)	1.350 (13)
B(61) - F(64)	1.31 (2)	B(61) - F(62)	1.31 (2)
B(61) - F(61)	1.320 (14)	B(61) - F(63)	1.34 (2)
C(26) - Mn(1) - C(25)	89.7 (5)	C(26) - Mn(1) - C(24)	88.6 (5)
C(25) - Mn(1) - C(24)	86.8 (5)	C(26) - Mn(1) - C(8)	88.5 (5)
C(25) - Mn(1) - C(8)	120.5 (5)	C(24) - Mn(1) - C(8)	152.6 (4)
C(26) - Mn(1) - C(9)	90.9 (5)	C(25) - Mn(1) - C(9)	157.6 (5)
C(24) - Mn(1) - C(9)	115.6 (4)	C(8) - Mn(1) - C(9)	37.2 (3)
C(26) - Mn(1) - C(7)	114.0 (5)	C(25) - Mn(1) - C(7)	92.3 (4)
C(24) - Mn(1) - C(7)	157.3 (4)	C(8) - Mn(1) - C(7)	37.4 (3)
C(9) - Mn(1) - C(7)	67.1 (4)	C(26) - Mn(1) - C(10)	118.7 (5)
C(25) - Mn(1) - C(10)	151.4 (4)	C(24) - Mn(1) - C(10)	91.0 (4)
C(8) - Mn(1) - C(10)	66.7 (4)	C(9) - Mn(1) - C(10)	36.7 (3)
C(7) - Mn(1) - C(10)	79.1 (4)	C(26) - Mn(1) - C(11)	156.0 (5)
C(25) - Mn(1) - C(11)	114.3 (4)	C(24) - Mn(1) - C(11)	93.1 (4)
C(8) - Mn(1) - C(11)	79.0 (3)	C(9) - Mn(1) - C(11)	66.8 (3)
C(7) - Mn(1) - C(11)	66.7 (3)	C(10) - Mn(1) - C(11)	37.4 (3)
C(26) - Mn(1) - C(6)	151.4 (5)	C(25) - Mn(1) - C(6)	90.3 (4)
C(24) - Mn(1) - C(6)	119.9 (4)	C(8) - Mn(1) - C(6)	67.0 (3)
C(9) - Mn(1) - C(6)	78.6 (3)	C(7) - Mn(1) - C(6)	37.4 (3)
C(10) - Mn(1) - C(6)	66.3 (3)	C(11) - Mn(1) - C(6)	36.2 (3)
C(2) - C(1) - C(5)	114.5 (8)	C(2) - C(1) - C(3)	111.9 (7)
C(5) - C(1) - C(3)	107.2 (7)	C(2) - C(1) - C(4)	111.0 (8)
C(5) - C(1) - C(4)	105.7 (6)	C(3) - C(1) - C(4)	106.0 (6)
C(6) - C(3) - C(23)	111.7 (7)	C(6) - C(3) - C(1)	104.7 (6)
C(23) - C(3) - C(1)	104.6 (7)	C(11) - C(4) - C(12)	113.2 (7)
C(11) - C(4) - C(1)	105.4 (7)	C(12) - C(4) - C(1)	104.9 (7)
C(17) - C(5) - C(18)	113.6 (8)	C(17) - C(5) - C(1)	106.0 (7)
C(18) - C(5) - C(1)	104.0 (7)	C(11) - C(6) - C(7)	119.6 (7)
C(11) - C(6) - C(3)	112.2 (6)	C(7) - C(6) - C(3)	128.1 (7)
C(11) - C(6) - Mn(1)	71.5 (4)	C(7) - C(6) - Mn(1)	69.3 (5)
C(3) - C(6) - Mn(1)	130.5 (5)	C(8) - C(7) - C(6)	119.8 (8)
C(8) - C(7) - Mn(1)	70.8 (5)	C(6) - C(7) - Mn(1)	73.2 (5)
C(9) - C(8) - C(7)	120.0 (8)	C(9) - C(8) - Mn(1)	71.6 (6)
C(7) - C(8) - Mn(1)	71.8 (5)	C(10) - C(9) - C(8)	120.8 (8)
C(10) - C(9) - Mn(1)	72.7 (6)	C(8) - C(9) - Mn(1)	71.2 (6)
C(9) - C(10) - C(11)	119.8 (8)	C(9) - C(10) - Mn(1)	70.6 (6)
C(11) - C(10) - Mn(1)	72.1 (5)	C(6) - C(11) - C(10)	119.8 (7)
C(6) - C(11) - C(4)	111.4 (6)	C(10) - C(11) - C(4)	128.8 (7)
C(6) - C(11) - Mn(1)	72.3 (4)	C(10) - C(11) - Mn(1)	70.5 (5)
C(4) - C(11) - Mn(1)	132.0 (6)	C(13) - C(12) - C(17)	119.2 (8)
C(13) - C(12) - C(4)	128.4 (9)	C(17) - C(12) - C(4)	112.4 (8)
C(12) - C(13) - C(14)	120.8 (9)	C(15) - C(14) - C(13)	120.2 (10)
C(14) - C(15) - C(16)	119.9 (10)	C(15) - C(16) - C(17)	119.7 (10)
C(12) - C(17) - C(16)	120.2 (9)	C(12) - C(17) - C(5)	110.6 (7)
C(16) - C(17) - C(5)	129.1 (9)	C(23) - C(18) - C(19)	120.4 (9)
C(23) - C(18) - C(5)	112.6 (8)	C(19) - C(18) - C(5)	127.0 (10)
C(18) - C(19) - C(20)	119.4 (10)	C(21) - C(20) - C(19)	118.8 (10)
C(20) - C(21) - C(22)	121.7 (11)	C(21) - C(22) - C(23)	119.3 (10)

C(22)-C(23)-C(3)	128.1(8)	O(1)-C(24)-Mn(1)	178.5(11)
O(2)-C(25)-Mn(1)	178.0(10)	O(3)-C(26)-Mn(1)	178.0(13)
C(56)-Mn(31)-C(55)	91.8(5)	C(56)-Mn(31)-C(54)	88.5(5)
C(55)-Mn(31)-C(54)	89.8(5)	C(56)-Mn(31)-C(37)	131.8(5)
C(55)-Mn(31)-C(37)	84.8(4)	C(54)-Mn(31)-C(37)	139.4(4)
C(56)-Mn(31)-C(38)	97.7(5)	C(55)-Mn(31)-C(38)	103.3(5)
C(54)-Mn(31)-C(38)	165.3(4)	C(37)-Mn(31)-C(38)	38.1(3)
C(56)-Mn(31)-C(39)	85.4(5)	C(55)-Mn(31)-C(39)	137.8(5)
C(54)-Mn(31)-C(39)	132.1(4)	C(37)-Mn(31)-C(39)	67.0(3)
C(38)-Mn(31)-C(39)	36.2(3)	C(56)-Mn(31)-C(40)	101.6(4)
C(55)-Mn(31)-C(40)	163.9(5)	C(54)-Mn(31)-C(40)	99.3(4)
C(37)-Mn(31)-C(40)	79.7(4)	C(38)-Mn(31)-C(40)	66.4(3)
C(39)-Mn(31)-C(40)	36.9(3)	C(56)-Mn(31)-C(36)	164.2(4)
C(55)-Mn(31)-C(36)	97.7(5)	C(54)-Mn(31)-C(36)	104.1(4)
C(37)-Mn(31)-C(36)	37.7(3)	C(38)-Mn(31)-C(36)	67.9(3)
C(39)-Mn(31)-C(36)	79.1(3)	C(40)-Mn(31)-C(36)	67.3(3)
C(56)-Mn(31)-C(41)	137.1(4)	C(55)-Mn(31)-C(41)	130.9(5)
C(54)-Mn(31)-C(41)	88.0(4)	C(37)-Mn(31)-C(41)	66.6(3)
C(38)-Mn(31)-C(41)	78.4(3)	C(39)-Mn(31)-C(41)	66.3(3)
C(40)-Mn(31)-C(41)	37.4(3)	C(36)-Mn(31)-C(41)	36.5(3)
C(32)-C(31)-C(35)	112.7(7)	C(32)-C(31)-C(34)	112.7(8)
C(35)-C(31)-C(34)	106.8(7)	C(32)-C(31)-C(33)	110.0(7)
C(35)-C(31)-C(33)	105.9(7)	C(34)-C(31)-C(33)	108.4(6)
C(53)-C(33)-C(36)	112.8(7)	C(53)-C(33)-C(31)	105.0(7)
C(36)-C(33)-C(31)	103.4(6)	C(42)-C(34)-C(41)	111.6(7)
C(42)-C(34)-C(31)	104.7(7)	C(41)-C(34)-C(31)	104.0(7)
C(47)-C(35)-C(48)	116.8(9)	C(47)-C(35)-C(31)	105.1(7)
C(48)-C(35)-C(31)	105.9(7)	C(41)-C(36)-C(37)	119.6(7)
C(41)-C(36)-C(33)	112.4(6)	C(37)-C(36)-C(33)	128.0(7)
C(41)-C(36)-Mn(31)	73.2(5)	C(37)-C(36)-Mn(31)	70.5(5)
C(33)-C(36)-Mn(31)	128.6(6)	C(36)-C(37)-C(38)	119.3(8)
C(36)-C(37)-Mn(31)	71.8(5)	C(38)-C(37)-Mn(31)	71.4(5)
C(39)-C(38)-C(37)	119.8(8)	C(39)-C(38)-Mn(31)	71.9(5)
C(37)-C(38)-Mn(31)	70.6(5)	C(38)-C(39)-C(40)	121.8(8)
C(38)-C(39)-Mn(31)	71.9(5)	C(40)-C(39)-Mn(31)	71.6(5)
C(39)-C(40)-C(41)	119.2(8)	C(39)-C(40)-Mn(31)	71.5(5)
C(41)-C(40)-Mn(31)	72.9(5)	C(36)-C(41)-C(40)	120.2(7)
C(36)-C(41)-C(34)	111.9(6)	C(40)-C(41)-C(34)	127.9(7)
C(36)-C(41)-Mn(31)	70.3(5)	C(40)-C(41)-Mn(31)	69.7(5)
C(34)-C(41)-Mn(31)	129.7(6)	C(43)-C(42)-C(47)	120.3(8)
C(43)-C(42)-C(34)	127.9(9)	C(47)-C(42)-C(34)	111.6(8)
C(42)-C(43)-C(44)	118.8(10)	C(45)-C(44)-C(43)	121.0(10)
C(46)-C(45)-C(44)	120.1(10)	C(45)-C(46)-C(47)	119.2(10)
C(42)-C(47)-C(46)	120.5(9)	C(42)-C(47)-C(35)	111.5(8)
C(46)-C(47)-C(35)	128.0(9)	C(53)-C(48)-C(49)	121.1(9)
C(53)-C(48)-C(35)	110.8(8)	C(49)-C(48)-C(35)	128.1(10)
C(50)-C(49)-C(48)	118.1(10)	C(51)-C(50)-C(49)	121.7(11)
C(50)-C(51)-C(52)	120.0(11)	C(51)-C(52)-C(53)	119.2(10)
C(48)-C(53)-C(52)	120.0(9)	C(48)-C(53)-C(33)	112.2(8)
C(52)-C(53)-C(33)	127.8(10)	O(31)-C(54)-Mn(31)	179.3(9)
O(32)-C(55)-Mn(31)	176.3(13)	O(33)-C(56)-Mn(31)	178.9(11)
C(86)-Mn(61)-C(85)	89.5(5)	C(86)-Mn(61)-C(84)	90.2(6)
C(85)-Mn(61)-C(84)	88.4(5)	C(86)-Mn(61)-C(69)	104.0(6)
C(85)-Mn(61)-C(69)	95.7(6)	C(84)-Mn(61)-C(69)	165.1(5)
C(86)-Mn(61)-C(68)	86.5(5)	C(85)-Mn(61)-C(68)	129.5(6)
C(84)-Mn(61)-C(68)	141.9(5)	C(69)-Mn(61)-C(68)	37.9(4)
C(86)-Mn(61)-C(70)	139.3(6)	C(85)-Mn(61)-C(70)	84.8(5)
C(84)-Mn(61)-C(70)	129.7(5)	C(69)-Mn(61)-C(70)	37.2(3)

C(85)-Mn(61)-C(67)	162.6(5)	C(84)-Mn(61)-C(67)	106.3(5)
C(69)-Mn(61)-C(67)	67.7(4)	C(68)-Mn(61)-C(67)	37.6(3)
C(70)-Mn(61)-C(67)	78.7(4)	C(86)-Mn(61)-C(71)	164.3(5)
C(85)-Mn(61)-C(71)	103.7(5)	C(84)-Mn(61)-C(71)	98.4(4)
C(69)-Mn(61)-C(71)	66.7(4)	C(68)-Mn(61)-C(71)	78.7(4)
C(70)-Mn(61)-C(71)	36.8(3)	C(67)-Mn(61)-C(71)	65.7(3)
C(86)-Mn(61)-C(66)	131.6(5)	C(85)-Mn(61)-C(66)	138.8(5)
C(84)-Mn(61)-C(66)	88.2(4)	C(69)-Mn(61)-C(66)	79.2(4)
C(68)-Mn(61)-C(66)	66.7(4)	C(70)-Mn(61)-C(66)	66.4(3)
C(67)-Mn(61)-C(66)	36.2(3)	C(71)-Mn(61)-C(66)	36.6(3)
C(62)-C(61)-C(63)	113.6(7)	C(62)-C(61)-C(64)	113.5(7)
C(63)-C(61)-C(64)	107.8(7)	C(62)-C(61)-C(65)	110.5(7)
C(63)-C(61)-C(65)	105.7(6)	C(64)-C(61)-C(65)	105.1(6)
C(83)-C(63)-C(66)	112.2(8)	C(83)-C(63)-C(61)	105.6(7)
C(66)-C(63)-C(61)	105.4(7)	C(71)-C(64)-C(72)	113.3(7)
C(71)-C(64)-C(61)	103.8(7)	C(72)-C(64)-C(61)	105.2(6)
C(77)-C(65)-C(78)	119.0(8)	C(77)-C(65)-C(61)	105.5(7)
C(78)-C(65)-C(61)	104.4(6)	C(67)-C(66)-C(71)	120.0(8)
C(67)-C(66)-C(63)	129.0(9)	C(71)-C(66)-C(63)	110.8(7)
C(67)-C(66)-Mn(61)	71.2(5)	C(71)-C(66)-Mn(61)	71.5(5)
C(63)-C(66)-Mn(61)	133.0(7)	C(66)-C(67)-C(68)	120.0(9)
C(66)-C(67)-Mn(61)	72.6(5)	C(68)-C(67)-Mn(61)	69.4(6)
C(69)-C(68)-C(67)	119.7(9)	C(69)-C(68)-Mn(61)	70.4(6)
C(67)-C(68)-Mn(61)	73.0(6)	C(70)-C(69)-C(68)	120.3(9)
C(70)-C(69)-Mn(61)	73.4(6)	C(68)-C(69)-Mn(61)	71.7(6)
C(69)-C(70)-C(71)	119.6(9)	C(69)-C(70)-Mn(61)	69.4(6)
C(71)-C(70)-Mn(61)	72.6(5)	C(70)-C(71)-C(66)	120.5(7)
C(70)-C(71)-C(64)	127.3(9)	C(66)-C(71)-C(64)	112.2(7)
C(70)-C(71)-Mn(61)	70.6(5)	C(66)-C(71)-Mn(61)	71.9(5)
C(64)-C(71)-Mn(61)	130.2(6)	C(73)-C(72)-C(77)	120.0(8)
C(73)-C(72)-C(64)	128.2(8)	C(77)-C(72)-C(64)	111.8(7)
C(72)-C(73)-C(74)	119.2(9)	C(75)-C(74)-C(73)	121.6(10)
C(74)-C(75)-C(76)	120.0(9)	C(77)-C(76)-C(75)	118.5(9)
C(76)-C(77)-C(72)	120.7(8)	C(76)-C(77)-C(65)	127.8(9)
C(72)-C(77)-C(65)	111.4(7)	C(83)-C(78)-C(79)	120.5(8)
C(83)-C(78)-C(65)	111.5(7)	C(79)-C(78)-C(65)	128.0(8)
C(78)-C(79)-C(80)	119.3(9)	C(81)-C(80)-C(79)	120.0(10)
C(80)-C(81)-C(82)	119.9(10)	C(81)-C(82)-C(83)	121.0(10)
C(78)-C(83)-C(82)	119.3(8)	C(78)-C(83)-C(63)	112.1(8)
C(82)-C(83)-C(63)	128.6(9)	O(61)-C(84)-Mn(61)	176.7(11)
O(62)-C(85)-Mn(61)	178.0(12)	O(63)-C(86)-Mn(61)	178(2)
F(3)-B(1)-F(2)	110.8(11)	F(3)-B(1)-F(1)	117.8(11)
F(2)-B(1)-F(1)	112.0(11)	F(3)-B(1)-F(4)	108.7(11)
F(2)-B(1)-F(4)	100.1(11)	F(1)-B(1)-F(4)	105.8(11)
F(32)-B(31)-F(33)	109.5(11)	F(32)-B(31)-F(34)	110.0(13)
F(33)-B(31)-F(34)	109.3(13)	F(32)-B(31)-F(31)	108.6(12)
F(33)-B(31)-F(31)	109.5(13)	F(34)-B(31)-F(31)	110.1(10)
F(64)-B(61)-F(62)	114.3(14)	F(64)-B(61)-F(61)	109.5(12)
F(62)-B(61)-F(61)	112.2(14)	F(64)-B(61)-F(63)	110(2)
F(62)-B(61)-F(63)	106.4(12)	F(61)-B(61)-F(63)	104.1(14)

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for [1]BF₄

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
Mn(1)	62(1)	44(1)	57(1)	-3(1)	-11(1)	-1(1)
C(1)	60(7)	71(8)	25(6)	10(6)	11(5)	-18(6)
C(2)	66(8)	87(9)	82(9)	-18(8)	14(7)	-8(7)
C(3)	43(6)	57(7)	56(7)	6(6)	6(5)	-9(5)
C(4)	45(6)	60(8)	55(7)	-13(6)	-1(5)	-1(5)
C(5)	89(9)	79(9)	31(7)	22(6)	-6(6)	-11(7)
C(6)	38(6)	46(6)	34(7)	7(5)	1(5)	4(5)
C(7)	54(6)	60(8)	38(7)	0(6)	9(5)	13(5)
C(8)	81(9)	67(8)	41(7)	7(7)	3(6)	8(7)
C(9)	82(9)	57(8)	66(9)	17(7)	-9(7)	-1(7)
C(10)	62(7)	47(7)	70(9)	-7(6)	-17(6)	0(6)
C(11)	60(6)	31(6)	39(6)	-2(5)	-3(5)	-14(5)
C(12)	54(6)	56(7)	46(7)	-21(6)	3(5)	-6(6)
C(13)	61(8)	78(9)	74(9)	-19(7)	-17(7)	-4(7)
C(14)	87(10)	58(8)	74(9)	-21(7)	-7(7)	-5(7)
C(15)	60(8)	113(12)	87(10)	-41(9)	-17(7)	8(9)
C(16)	79(9)	89(10)	54(8)	-2(7)	-14(7)	-11(8)
C(17)	65(8)	84(9)	30(7)	-1(6)	-5(6)	0(7)
C(18)	67(8)	41(7)	70(9)	20(6)	8(7)	-8(6)
C(19)	88(10)	73(10)	102(12)	35(9)	-15(8)	-3(8)
C(20)	72(9)	91(11)	143(15)	5(11)	-7(10)	24(9)
C(21)	90(10)	44(7)	150(14)	-21(9)	12(10)	17(8)
C(22)	58(7)	49(7)	80(9)	-4(7)	-3(6)	2(6)
C(23)	49(7)	54(7)	49(7)	11(6)	-1(6)	-6(6)
C(24)	49(7)	75(8)	78(9)	-22(8)	0(6)	-8(6)
O(1)	94(7)	139(9)	147(9)	-91(8)	14(6)	9(6)
C(25)	52(7)	73(9)	107(11)	-3(8)	-20(7)	3(7)
O(2)	76(6)	71(6)	155(9)	5(6)	-15(6)	-17(5)
C(26)	94(10)	60(9)	96(12)	-6(8)	-24(9)	3(7)
O(3)	125(8)	82(6)	113(8)	11(6)	-59(6)	11(6)
Mn(31)	60(1)	54(1)	48(1)	2(1)	-1(1)	-5(1)
C(31)	44(6)	53(7)	56(7)	-4(6)	-3(5)	-17(5)
C(32)	67(7)	91(9)	63(8)	-9(7)	-14(6)	-27(6)
C(33)	57(7)	65(7)	52(8)	-8(6)	-10(6)	18(5)
C(34)	62(7)	60(7)	40(7)	-2(6)	-14(5)	-9(6)
C(35)	32(6)	82(9)	90(10)	7(8)	4(6)	-9(6)
C(36)	64(7)	36(6)	44(7)	-12(5)	1(5)	-2(5)
C(37)	72(8)	54(7)	52(8)	13(6)	-4(6)	-1(6)
C(38)	60(7)	61(8)	55(8)	0(6)	2(6)	-13(6)
C(39)	55(7)	50(7)	68(8)	-1(6)	-3(5)	6(6)
C(40)	58(7)	46(7)	55(7)	2(6)	-11(6)	-10(5)
C(41)	45(6)	47(7)	35(6)	3(5)	-9(5)	-6(5)
C(42)	50(7)	54(7)	54(8)	-5(6)	-5(6)	-27(6)
C(43)	77(8)	59(8)	52(8)	11(7)	0(6)	-4(7)
C(44)	118(11)	50(8)	79(11)	-10(8)	2(9)	-18(7)
C(45)	123(11)	68(9)	32(7)	6(7)	5(8)	-27(8)
C(46)	83(8)	80(9)	53(8)	1(7)	6(7)	-27(7)

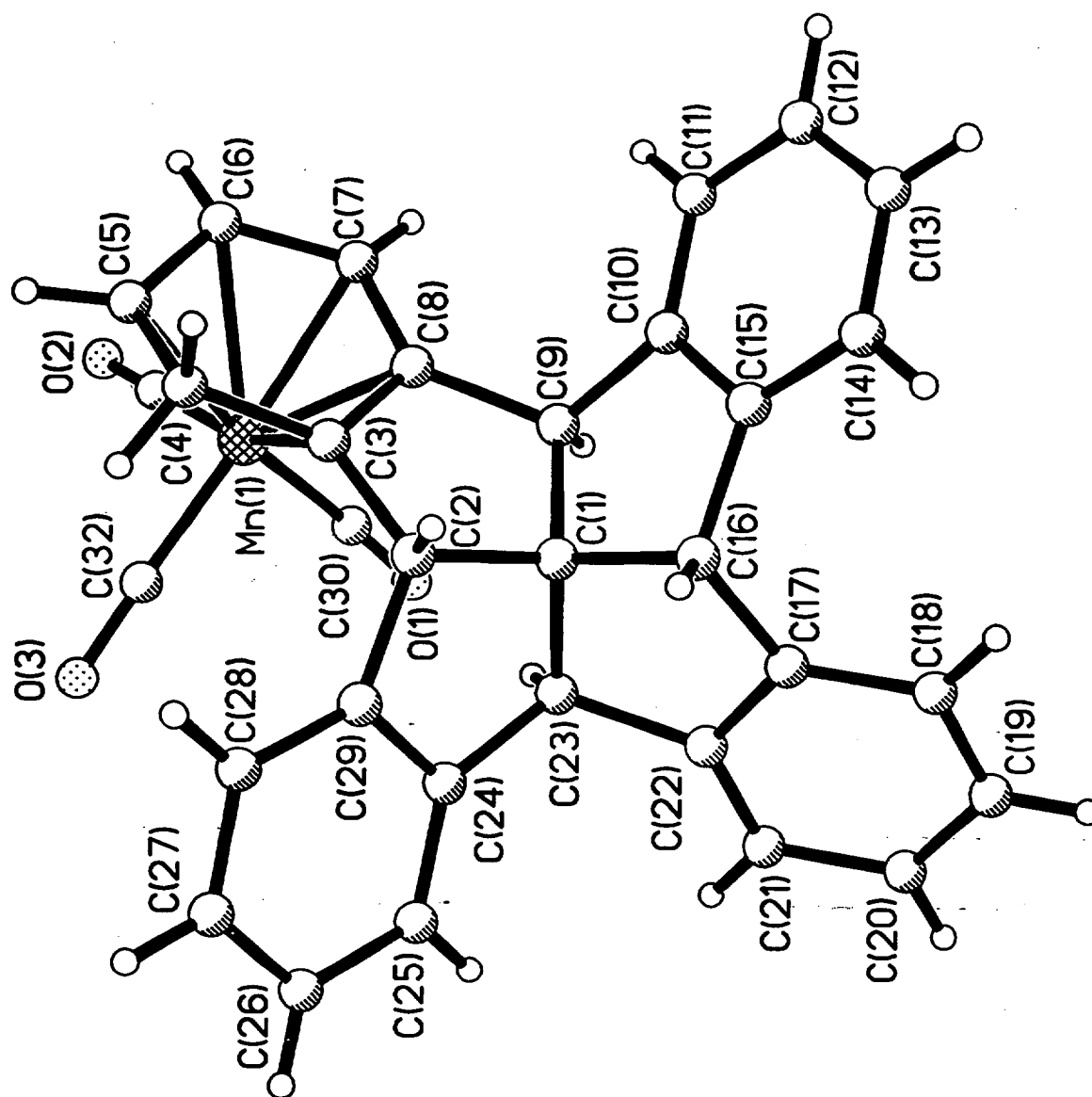
C(12)	O(10)	O(8)	N(8)	S(6)	-2(6)	-20(6)
C(48)	41(7)	82(10)	71(9)	-2(8)	-11(6)	0(6)
C(49)	56(8)	97(11)	91(11)	-6(9)	-5(7)	5(7)
C(50)	78(10)	89(11)	137(15)	-43(12)	-13(9)	34(8)
C(51)	94(11)	75(10)	123(14)	-11(10)	-27(10)	20(9)
C(52)	62(8)	93(11)	86(11)	-10(9)	9(7)	5(7)
C(53)	53(7)	74(9)	55(8)	-19(7)	-20(6)	6(7)
C(54)	96(10)	68(9)	55(8)	4(7)	20(7)	-5(7)
O(31)	127(8)	96(8)	91(7)	-22(6)	-17(6)	-38(6)
C(55)	148(13)	68(10)	49(9)	-7(8)	1(8)	-4(9)
O(32)	186(10)	84(8)	97(8)	24(6)	-29(7)	23(7)
C(56)	66(8)	89(10)	70(9)	18(8)	2(7)	-6(7)
O(33)	87(6)	135(8)	69(6)	6(6)	23(5)	14(6)
Mn(61)	62(1)	85(1)	55(1)	-6(1)	-3(1)	13(1)
C(61)	68(7)	54(7)	30(6)	9(6)	6(5)	2(5)
C(62)	60(8)	72(8)	77(9)	11(7)	-12(6)	-14(6)
C(63)	63(7)	53(7)	50(7)	-8(6)	-18(6)	1(5)
C(64)	53(6)	67(7)	44(7)	1(6)	13(5)	-4(6)
C(65)	52(7)	59(7)	52(7)	10(6)	6(5)	7(5)
C(66)	56(7)	94(10)	29(6)	-6(6)	0(5)	14(7)
C(67)	87(9)	93(10)	49(8)	-3(7)	1(7)	28(8)
C(68)	87(9)	133(13)	53(9)	29(9)	2(7)	40(10)
C(69)	89(10)	98(12)	91(12)	26(10)	28(9)	21(9)
C(70)	81(8)	73(9)	50(8)	-4(8)	11(7)	6(7)
C(71)	70(7)	69(8)	35(7)	5(7)	10(5)	10(7)
C(72)	66(7)	45(7)	41(7)	-4(5)	5(5)	0(6)
C(73)	76(9)	73(9)	57(8)	-8(7)	14(6)	2(7)
C(74)	79(9)	78(9)	62(8)	3(7)	-6(7)	-11(8)
C(75)	50(7)	84(9)	76(9)	11(8)	-11(7)	-18(7)
C(76)	64(7)	59(8)	67(8)	1(7)	1(6)	5(7)
C(77)	56(7)	62(8)	47(7)	7(6)	-9(5)	-13(6)
C(78)	47(6)	53(7)	64(8)	8(6)	-1(6)	7(5)
C(79)	66(8)	39(7)	82(9)	-12(7)	0(7)	8(6)
C(80)	92(10)	33(7)	106(12)	9(8)	15(8)	18(7)
C(81)	92(10)	68(8)	67(9)	-12(7)	15(8)	13(8)
C(82)	80(8)	65(8)	52(8)	-5(7)	8(7)	11(7)
C(83)	58(7)	58(7)	51(7)	2(6)	7(6)	12(6)
C(84)	84(9)	91(11)	48(9)	-9(8)	18(7)	21(8)
O(61)	170(10)	127(9)	85(7)	21(7)	17(7)	-25(8)
C(85)	76(9)	129(14)	80(11)	1(10)	17(8)	32(9)
O(62)	127(8)	131(9)	126(9)	-54(8)	41(7)	16(7)
C(86)	72(9)	134(13)	117(13)	5(11)	29(9)	10(10)
O(63)	86(8)	338(19)	128(9)	-38(11)	-32(7)	-25(11)
B(1)	65(9)	70(10)	45(9)	2(8)	-1(7)	8(8)
F(1)	120(6)	89(5)	197(9)	30(6)	-68(7)	19(5)
F(2)	207(11)	341(18)	122(9)	117(11)	-18(8)	-93(11)
F(3)	147(8)	84(6)	286(13)	34(7)	-100(8)	-49(6)
F(4)	214(12)	209(12)	276(16)	-106(12)	-65(12)	95(10)
B(31)	119(15)	75(12)	121(16)	27(13)	-18(12)	-78(12)
F(31)	243(11)	65(5)	133(7)	13(6)	3(7)	-10(6)
F(32)	201(9)	66(5)	196(10)	-2(6)	-96(8)	-15(6)
F(33)	236(13)	274(16)	156(11)	75(11)	45(9)	52(11)
F(34)	121(7)	145(8)	235(12)	2(8)	-71(8)	-19(6)
B(61)	85(13)	118(18)	134(19)	-4(16)	18(14)	33(14)
F(61)	128(8)	302(15)	140(9)	-63(10)	-29(7)	79(9)
F(62)	203(11)	116(8)	235(13)	67(8)	-103(9)	-19(7)
F(63)	161(10)	241(13)	258(15)	123(11)	82(10)	28(9)
F(64)	294(15)	177(11)	234(14)	-73(10)	-184(13)	50(10)

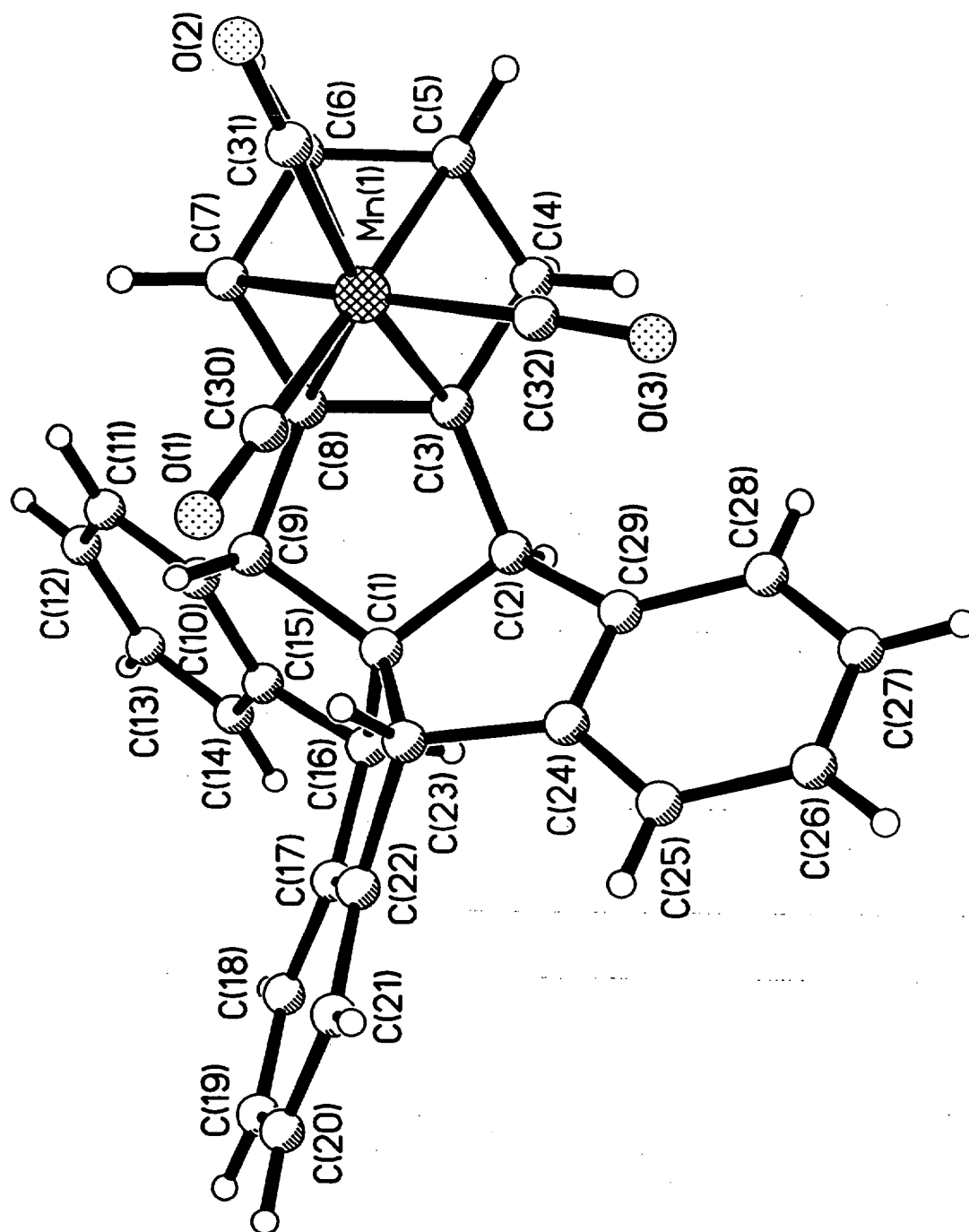
Table 5. Hydrogen coordinates ($\times 10^{-3}$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{1}]\text{BF}_4$

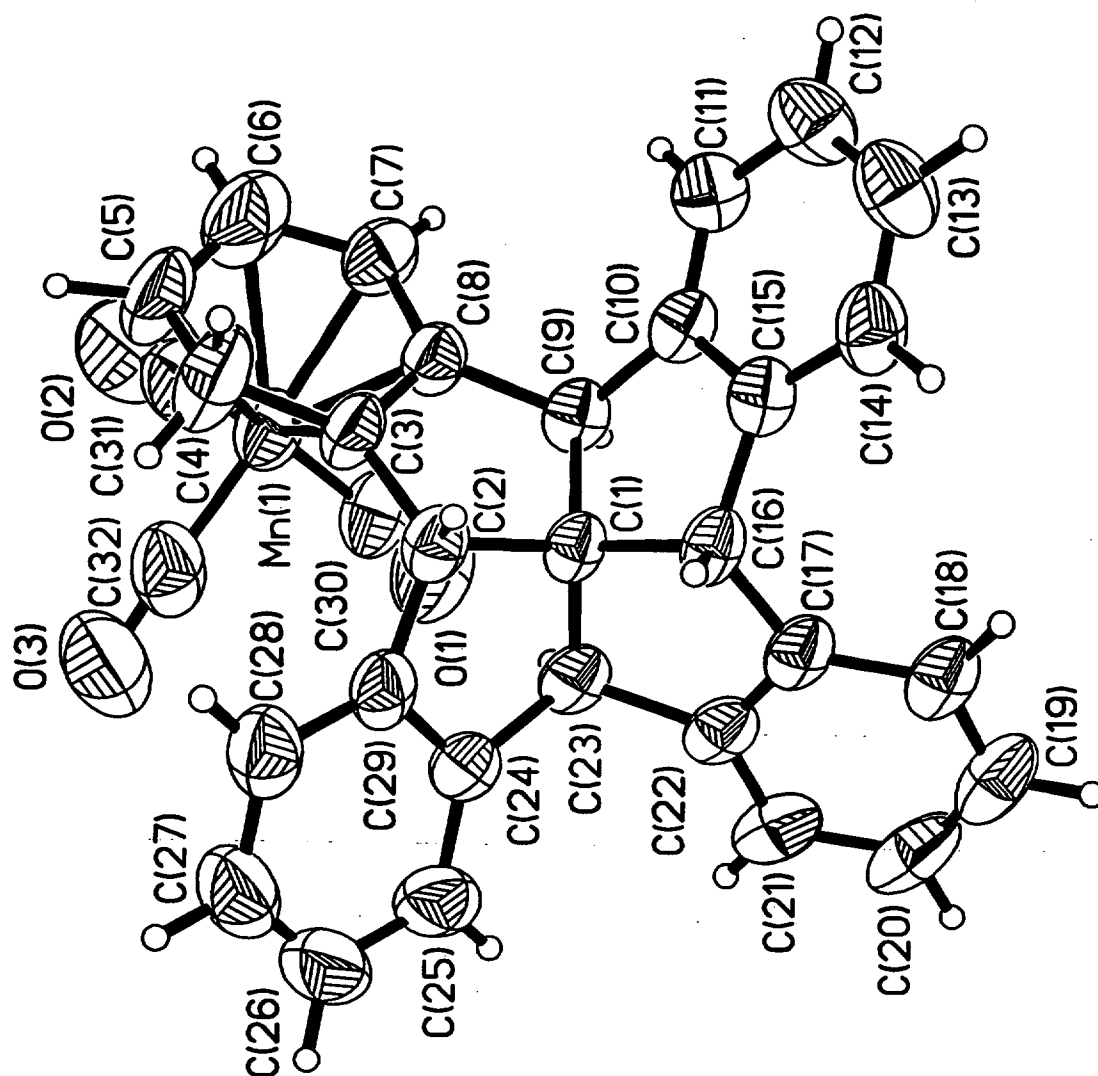
	x	y	z	U(eq)
H(2A)	2973 (3)	8401 (11)	2651 (5)	118
H(2B)	3261 (3)	8605 (11)	3198 (5)	118
H(2C)	3185 (3)	7140 (11)	2955 (5)	118
H(3A)	3323 (3)	6922 (8)	1901 (3)	62
H(4A)	3506 (3)	10348 (9)	2511 (3)	64
H(5A)	4019 (3)	7367 (9)	3162 (4)	79
H(7A)	3491 (3)	7487 (9)	721 (4)	61
H(8A)	3564 (4)	9403 (11)	121 (4)	76
H(9A)	3676 (3)	11575 (11)	512 (5)	82
H(10A)	3721 (3)	11869 (9)	1495 (4)	72
H(13A)	4296 (3)	11984 (11)	2312 (5)	85
H(14A)	5010 (4)	12152 (11)	2669 (5)	87
H(15A)	5316 (4)	10373 (14)	3161 (5)	104
H(16A)	4928 (3)	8348 (12)	3244 (5)	89
H(19A)	4811 (4)	5934 (12)	2788 (5)	105
H(20A)	5036 (4)	4464 (14)	2066 (7)	122
H(21A)	4597 (4)	4237 (11)	1280 (6)	114
H(22A)	3951 (3)	5467 (10)	1180 (5)	75
H(32A)	4978 (3)	1280 (11)	6727 (4)	110
H(32B)	5267 (3)	2200 (11)	6327 (4)	110
H(32C)	5395 (3)	669 (11)	6417 (4)	110
H(33A)	4774 (3)	-972 (9)	6326 (4)	70
H(34A)	4440 (3)	2578 (9)	6100 (4)	65
H(35A)	5420 (3)	1203 (9)	5380 (4)	82
H(37A)	3932 (3)	-2377 (9)	6079 (4)	71
H(38A)	3158 (3)	-1754 (10)	6021 (4)	70
H(39A)	2959 (3)	511 (10)	5925 (4)	69
H(40A)	3500 (3)	2238 (9)	5870 (4)	63
H(43A)	3995 (4)	3783 (10)	5151 (5)	75
H(44A)	4188 (4)	4530 (11)	4254 (5)	99
H(45A)	4795 (4)	3626 (12)	3791 (4)	90
H(46A)	5227 (4)	1999 (12)	4225 (4)	87
H(49A)	5479 (3)	-534 (13)	4392 (5)	98
H(50A)	5389 (4)	-2814 (15)	4200 (6)	121
H(51A)	4992 (5)	-4194 (13)	4794 (6)	117
H(52A)	4660 (4)	-3299 (12)	5596 (5)	96
H(62A)	7778 (3)	2840 (11)	5185 (4)	105
H(62B)	7682 (3)	1551 (11)	4814 (4)	105
H(62C)	7297 (3)	2579 (11)	4949 (4)	105
H(63A)	7246 (3)	2134 (8)	3909 (4)	67
H(64A)	7489 (2)	5080 (9)	4756 (4)	66
H(65A)	8377 (3)	2532 (9)	4471 (4)	65
H(67A)	6891 (4)	3415 (12)	2894 (4)	92
H(68A)	6646 (4)	5610 (14)	2604 (4)	109
H(69A)	6826 (4)	7542 (12)	3162 (6)	111
H(70A)	7257 (3)	7289 (10)	3990 (5)	82
H(73A)	8007 (3)	7452 (10)	4589 (4)	82
H(74A)	8745 (4)	8083 (11)	4532 (5)	87

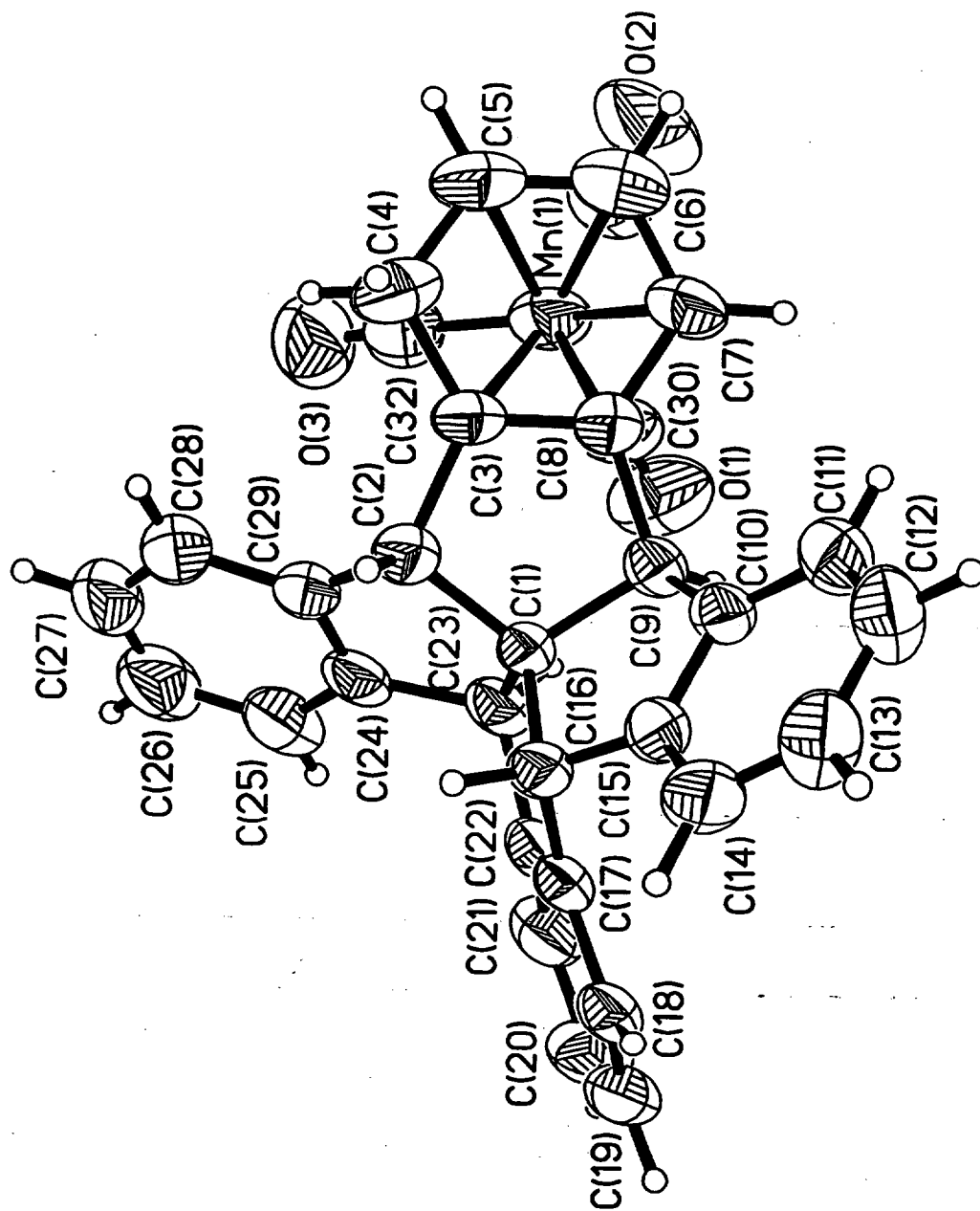
H(76A)	9091 (3)	4289 (11)	4123 (5)	76
H(79A)	8896 (3)	2226 (10)	3440 (5)	75
H(80A)	8787 (4)	1058 (10)	2598 (5)	92
H(81A)	8076 (4)	671 (11)	2273 (5)	91
H(82A)	7474 (4)	1348 (11)	2803 (4)	79

Identification code	cad09
Empirical formula	$C_{33}H_{23}Cl_2MnO_3$
Formula weight	593.35
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 10.4080(5)$ Å $\alpha = 94.5070(10)^\circ$ $b = 10.9907(6)$ Å $\beta = 97.899(2)^\circ$ $c = 12.2715(6)$ Å $\gamma = 102.0910(10)^\circ$
Volume, Z	$1351.21(12)$ Å ³ , 2
Density (calculated)	1.458 Mg/m ³
Absorption coefficient	0.720 mm ⁻¹
F(000)	608
Crystal size	$0.16 \times 0.18 \times 0.20$ mm
θ range for data collection	1.69 to 23.60°
Limiting indices	$-10 \leq h \leq 11$, $-11 \leq k \leq 12$, $-13 \leq l \leq 13$
Reflections collected	5921
Independent reflections	3719 ($R_{int} = 0.0389$)
Absorption correction	Empirical (SADABS)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3719 / 139 / 352
Goodness-of-fit on F^2	1.020
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0740$, $wR2 = 0.1645$
R indices (all data)	$R1 = 0.1406$, $wR2 = 0.1996$
Largest diff. peak and hole	0.576 and -0.277 eÅ ⁻³









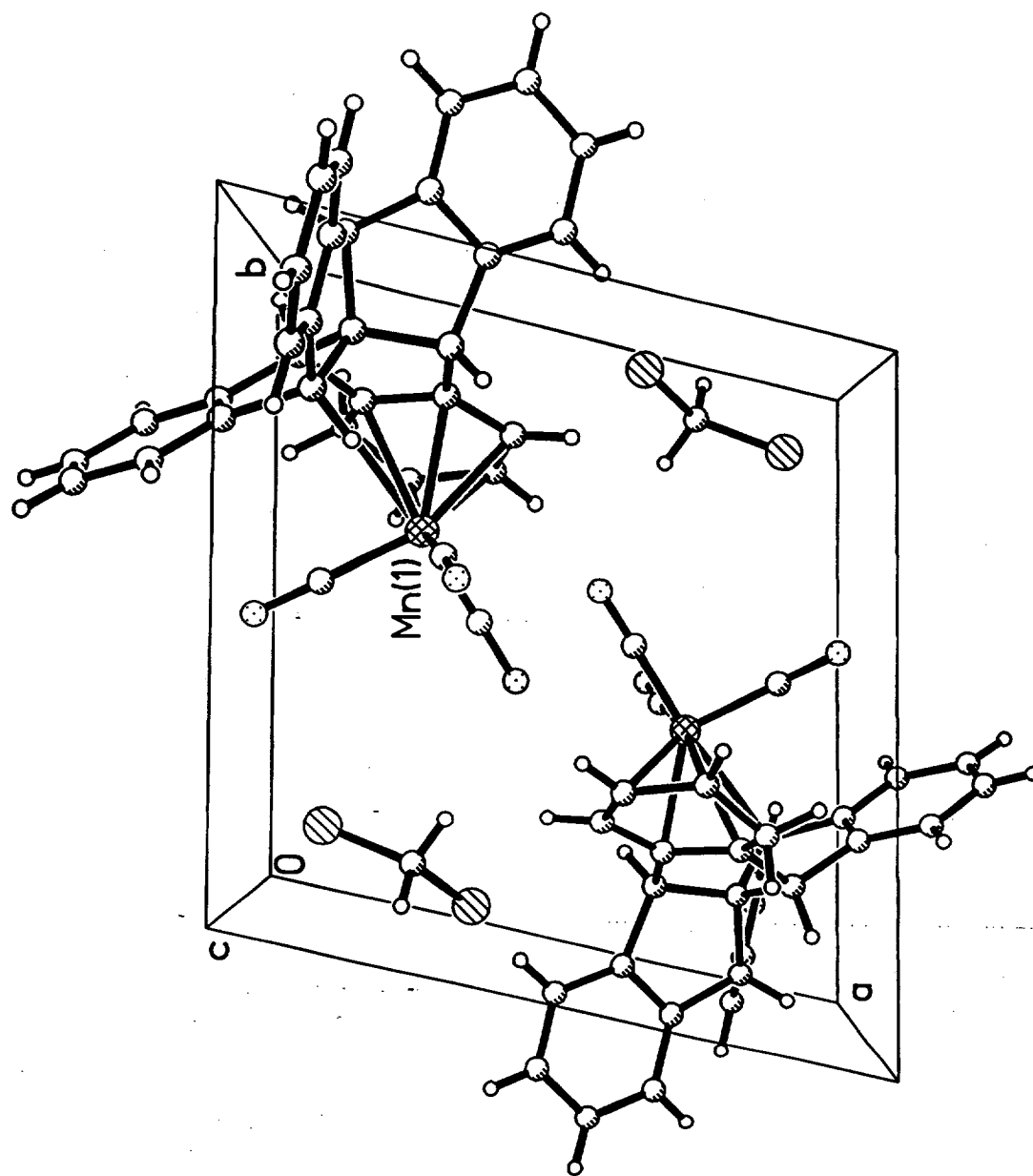


Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 5. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mn(1)	2862(1)	6026(1)	6890(1)	66(1)
C(1)	1874(5)	8520(5)	8722(4)	41(1)
C(2)	988(6)	8100(6)	7569(5)	49(1)
C(3)	1916(6)	7685(6)	6853(5)	52(2)
C(4)	1560(8)	7325(8)	5655(5)	88(2)
C(5)	2575(8)	6752(7)	5269(6)	81(2)
C(6)	3928(9)	7177(8)	5738(7)	92(2)
C(7)	4261(7)	7731(6)	6830(6)	63(2)
C(8)	3227(6)	8022(5)	7363(5)	49(2)
C(9)	3325(5)	8656(5)	8518(5)	44(1)
C(10)	3873(6)	10047(5)	8624(5)	44(1)
C(11)	5033(6)	10698(6)	8353(5)	56(2)
C(12)	5331(7)	11974(6)	8478(6)	68(2)
C(13)	4462(7)	12616(6)	8898(6)	68(2)
C(14)	3307(7)	11987(6)	9180(5)	60(2)
C(15)	3012(6)	10699(5)	9040(5)	46(1)
C(16)	1783(6)	9817(5)	9256(5)	46(1)
C(17)	1669(6)	9610(6)	10429(5)	48(2)
C(18)	1818(6)	10497(6)	11338(5)	55(2)
C(19)	1665(7)	10110(8)	12347(6)	72(2)
C(20)	1348(7)	8850(9)	12478(6)	80(2)
C(21)	1201(6)	7946(7)	11584(6)	66(2)
C(22)	1365(5)	8350(6)	10569(5)	50(2)
C(23)	1352(6)	7562(5)	9489(5)	48(1)
C(24)	-5(6)	6875(5)	8878(6)	51(2)
C(25)	-990(7)	6052(6)	9256(7)	70(2)
C(26)	-2169(8)	5529(7)	8537(8)	89(3)
C(27)	-2312(7)	5811(8)	7463(8)	89(3)
C(28)	-1344(7)	6619(7)	7077(6)	70(2)
C(29)	-167(6)	7158(6)	7798(5)	53(2)
C(30)	3241(8)	5712(7)	8274(7)	71(2)
O(1)	3468(6)	5438(5)	9146(5)	101(2)
C(31)	3746(8)	4897(7)	6481(7)	87(2)
O(2)	4324(7)	4174(6)	6216(6)	139(3)
C(32)	1299(8)	4959(7)	6693(7)	81(2)
O(3)	290(6)	4260(6)	6601(5)	115(2)
C(33)	2727(11)	1175(10)	6122(8)	123(3)
Cl(1)	3620(4)	675(4)	5229(3)	171(2)
Cl(2)	1288(4)	1394(6)	5577(4)	217(2)

Table 3. Bond lengths [Å] and angles [°] for 5.

Mn(1) - C(30)	1.768 (9)	Mn(1) - C(32)	1.768 (9)
Mn(1) - C(31)	1.774 (8)	Mn(1) - C(7)	2.132 (7)
Mn(1) - C(8)	2.165 (6)	Mn(1) - C(5)	2.206 (8)
Mn(1) - C(6)	2.226 (8)	<u>Mn(1) - C(3)</u>	2.247 (6)
Mn(1) - C(4)	2.598 (8)	C(1) - C(23)	1.532 (8)
C(1) - C(9)	1.543 (7)	C(1) - C(16)	1.549 (7)
C(1) - C(2)	1.557 (8)	C(2) - C(29)	1.487 (8)
C(2) - C(3)	1.507 (8)	C(3) - C(8)	1.382 (8)
C(3) - C(4)	1.466 (8)	C(4) - C(5)	1.451 (10)
C(5) - C(6)	1.411 (10)	C(6) - C(7)	1.394 (9)
C(7) - C(8)	1.412 (8)	C(8) - C(9)	1.511 (8)
C(9) - C(10)	1.504 (8)	C(10) - C(11)	1.366 (8)
C(10) - C(15)	1.383 (7)	C(11) - C(12)	1.363 (8)
C(12) - C(13)	1.386 (9)	C(13) - C(14)	1.359 (9)
C(14) - C(15)	1.376 (8)	C(15) - C(16)	1.504 (8)
C(16) - C(17)	1.491 (8)	C(17) - C(22)	1.384 (8)
C(17) - C(18)	1.392 (8)	C(18) - C(19)	1.360 (9)
C(19) - C(20)	1.382 (10)	C(20) - C(21)	1.390 (10)
C(21) - C(22)	1.376 (8)	C(22) - C(23)	1.522 (8)
C(23) - C(24)	1.516 (8)	C(24) - C(25)	1.376 (8)
C(24) - C(29)	1.381 (8)	C(25) - C(26)	1.394 (10)
C(26) - C(27)	1.373 (11)	C(27) - C(28)	1.361 (10)
C(28) - C(29)	1.397 (9)	C(30) - O(1)	1.141 (8)
C(31) - O(2)	1.145 (8)	C(32) - O(3)	1.149 (8)
C(33) - Cl(2)	1.628 (10)	C(33) - Cl(1)	1.663 (10)
C(30) - Mn(1) - C(32)	92.3 (4)	C(30) - Mn(1) - C(31)	88.7 (4)
C(32) - Mn(1) - C(31)	94.9 (3)	C(30) - Mn(1) - C(7)	102.8 (3)
C(32) - Mn(1) - C(7)	157.8 (3)	C(31) - Mn(1) - C(7)	101.5 (3)
C(30) - Mn(1) - C(8)	92.6 (3)	C(32) - Mn(1) - C(8)	126.1 (3)
C(31) - Mn(1) - C(8)	138.9 (3)	C(7) - Mn(1) - C(8)	38.4 (2)
C(30) - Mn(1) - C(5)	170.1 (3)	C(32) - Mn(1) - C(5)	95.8 (4)
C(31) - Mn(1) - C(5)	96.3 (3)	C(7) - Mn(1) - C(5)	67.9 (3)
C(8) - Mn(1) - C(5)	78.0 (3)	C(30) - Mn(1) - C(6)	135.6 (3)
C(32) - Mn(1) - C(6)	131.9 (4)	C(31) - Mn(1) - C(6)	84.6 (3)
C(7) - Mn(1) - C(6)	37.2 (3)	C(8) - Mn(1) - C(6)	66.3 (3)
C(5) - Mn(1) - C(6)	37.1 (3)	C(30) - Mn(1) - C(3)	109.6 (3)
C(32) - Mn(1) - C(3)	92.3 (3)	C(31) - Mn(1) - C(3)	160.1 (3)
C(7) - Mn(1) - C(3)	67.5 (2)	C(8) - Mn(1) - C(3)	36.4 (2)
C(5) - Mn(1) - C(3)	64.5 (2)	C(6) - Mn(1) - C(3)	76.9 (3)
C(30) - Mn(1) - C(4)	142.6 (3)	C(32) - Mn(1) - C(4)	83.1 (3)
C(31) - Mn(1) - C(4)	128.6 (3)	C(7) - Mn(1) - C(4)	75.0 (3)
C(8) - Mn(1) - C(4)	62.1 (2)	C(5) - Mn(1) - C(4)	33.9 (2)
C(6) - Mn(1) - C(4)	61.6 (3)	C(3) - Mn(1) - C(4)	34.3 (2)
C(23) - C(1) - C(9)	118.0 (5)	C(23) - C(1) - C(16)	106.7 (4)
C(9) - C(1) - C(16)	106.1 (4)	C(23) - C(1) - C(2)	106.3 (5)
C(9) - C(1) - C(2)	106.1 (4)	C(16) - C(1) - C(2)	114.1 (5)
C(29) - C(2) - C(3)	118.9 (5)	C(29) - C(2) - C(1)	104.3 (5)
C(3) - C(2) - C(1)	103.9 (5)	C(8) - C(3) - C(4)	121.5 (6)
C(8) - C(3) - C(2)	112.1 (5)	C(4) - C(3) - C(2)	123.8 (6)
C(8) - C(3) - Mn(1)	68.5 (4)	C(4) - C(3) - Mn(1)	86.1 (4)
C(2) - C(3) - Mn(1)	130.4 (4)	C(5) - C(4) - C(3)	109.1 (6)
C(5) - C(4) - Mn(1)	58.1 (4)	C(3) - C(4) - Mn(1)	59.6 (4)
C(6) - C(5) - C(4)	121.1 (7)	C(6) - C(5) - Mn(1)	72.2 (5)

C(7) - C(6) - Mn(1)	67.7 (4)	C(5) - C(6) - Mn(1)	70.7 (5)
C(6) - C(7) - C(8)	117.7 (7)	C(6) - C(7) - Mn(1)	75.0 (5)
C(8) - C(7) - Mn(1)	72.1 (4)	C(3) - C(8) - C(7)	121.3 (6)
C(3) - C(8) - C(9)	110.4 (5)	C(7) - C(8) - C(9)	128.2 (6)
C(3) - C(8) - Mn(1)	75.0 (4)	C(7) - C(8) - Mn(1)	69.6 (4)
C(9) - C(8) - Mn(1)	126.2 (4)	C(10) - C(9) - C(8)	113.4 (5)
C(10) - C(9) - C(1)	104.4 (4)	C(8) - C(9) - C(1)	105.3 (5)
C(11) - C(10) - C(15)	119.2 (6)	C(11) - C(10) - C(9)	129.4 (5)
C(15) - C(10) - C(9)	111.4 (5)	C(12) - C(11) - C(10)	120.4 (6)
C(11) - C(12) - C(13)	119.8 (6)	C(14) - C(13) - C(12)	120.7 (6)
C(13) - C(14) - C(15)	118.9 (6)	C(14) - C(15) - C(10)	121.0 (6)
C(14) - C(15) - C(16)	128.0 (6)	C(10) - C(15) - C(16)	111.0 (5)
C(17) - C(16) - C(15)	117.7 (5)	C(17) - C(16) - C(1)	103.5 (5)
C(15) - C(16) - C(1)	104.5 (4)	C(22) - C(17) - C(18)	119.4 (6)
C(22) - C(17) - C(16)	112.1 (5)	C(18) - C(17) - C(16)	128.5 (6)
C(19) - C(18) - C(17)	119.4 (7)	C(18) - C(19) - C(20)	120.9 (7)
C(19) - C(20) - C(21)	120.8 (7)	C(22) - C(21) - C(20)	117.7 (7)
C(21) - C(22) - C(17)	121.8 (6)	C(21) - C(22) - C(23)	127.9 (6)
C(17) - C(22) - C(23)	110.1 (5)	C(24) - C(23) - C(22)	116.2 (5)
C(24) - C(23) - C(1)	104.5 (5)	C(22) - C(23) - C(1)	104.2 (5)
C(25) - C(24) - C(29)	120.7 (6)	C(25) - C(24) - C(23)	129.0 (7)
C(29) - C(24) - C(23)	110.3 (5)	C(24) - C(25) - C(26)	118.8 (8)
C(27) - C(26) - C(25)	119.8 (7)	C(28) - C(27) - C(26)	122.0 (7)
C(27) - C(28) - C(29)	118.4 (7)	C(24) - C(29) - C(28)	120.2 (6)
C(24) - C(29) - C(2)	112.2 (5)	C(28) - C(29) - C(2)	127.5 (6)
O(1) - C(30) - Mn(1)	176.1 (7)	O(2) - C(31) - Mn(1)	179.5 (7)
O(3) - C(32) - Mn(1)	177.7 (8)	Cl(2) - C(33) - Cl(1)	115.4 (6)

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 5.

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
Mn(1)	76(1)	61(1)	64(1)	-13(1)	19(1)	21(1)
C(1)	36(3)	54(3)	37(3)	-3(3)	3(2)	19(2)
C(2)	49(3)	56(4)	44(3)	-3(3)	6(3)	20(3)
C(3)	57(4)	63(4)	39(3)	-7(3)	12(3)	21(3)
C(4)	92(5)	127(6)	45(4)	-15(4)	5(3)	38(5)
C(5)	96(5)	96(5)	55(4)	-22(3)	22(4)	33(4)
C(6)	90(5)	111(6)	82(5)	-17(4)	33(4)	37(5)
C(7)	62(4)	69(4)	67(4)	-5(3)	25(3)	26(3)
C(8)	48(3)	55(3)	45(3)	-3(3)	8(3)	15(3)
C(9)	40(3)	50(3)	48(4)	1(3)	6(3)	25(3)
C(10)	41(3)	55(3)	40(4)	3(3)	4(3)	24(3)
C(11)	49(4)	58(4)	64(4)	5(3)	8(3)	21(3)
C(12)	46(4)	61(4)	93(6)	5(4)	3(4)	11(3)
C(13)	61(5)	47(4)	92(6)	1(4)	-3(4)	15(3)
C(14)	62(4)	51(4)	68(5)	-11(3)	7(4)	24(3)
C(15)	41(3)	53(3)	46(4)	-2(3)	1(3)	20(3)
C(16)	43(3)	56(3)	41(3)	-5(3)	3(3)	25(3)
C(17)	35(3)	67(4)	47(3)	-5(3)	7(3)	25(3)
C(18)	41(4)	80(4)	52(4)	-6(3)	4(3)	35(3)
C(19)	61(5)	116(5)	48(4)	-9(4)	7(4)	45(4)
C(20)	81(5)	132(6)	41(4)	14(4)	25(4)	43(5)
C(21)	57(4)	94(5)	57(4)	19(3)	20(4)	30(4)
C(22)	34(4)	76(4)	45(3)	5(3)	8(3)	22(3)
C(23)	44(3)	55(3)	52(3)	3(3)	13(3)	26(3)
C(24)	46(4)	48(4)	66(4)	-5(3)	21(3)	19(3)
C(25)	64(4)	64(4)	89(5)	2(4)	34(4)	15(3)
C(26)	62(5)	79(5)	118(6)	-20(5)	36(5)	-3(4)
C(27)	49(5)	94(6)	109(6)	-39(5)	11(4)	3(4)
C(28)	55(4)	79(5)	70(5)	-20(4)	3(3)	19(3)
C(29)	48(4)	56(4)	55(4)	-12(3)	9(3)	20(3)
C(30)	89(5)	60(4)	69(4)	-10(3)	15(4)	30(4)
O(1)	147(5)	83(4)	85(4)	3(3)	9(4)	58(4)
C(31)	76(5)	72(4)	112(6)	-24(4)	31(5)	14(4)
O(2)	111(5)	104(5)	210(7)	-46(5)	72(5)	37(4)
C(32)	76(5)	72(4)	90(6)	-26(4)	9(4)	23(3)
O(3)	79(4)	106(4)	142(5)	-35(4)	8(4)	6(3)
C(33)	167(9)	119(8)	88(8)	24(6)	8(6)	49(8)
Cl(1)	160(3)	218(4)	146(3)	12(3)	43(3)	57(3)
Cl(2)	160(4)	344(7)	195(4)	69(4)	53(3)	131(4)

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

	x	y	z	U(eq)
H(2A)	682 (6)	8816 (6)	7284 (5)	59
H(4A)	704 (8)	6737 (8)	5493 (5)	105
H(4B)	1494 (8)	8058 (8)	5279 (5)	105
H(5A)	2338 (8)	6160 (7)	4595 (6)	98
H(6A)	4603 (9)	6864 (8)	5384 (7)	110
H(7A)	5175 (7)	7883 (6)	7224 (6)	76
H(9A)	3831 (5)	8261 (5)	9065 (5)	53
H(11A)	5623 (6)	10268 (6)	8080 (5)	67
H(12A)	6117 (7)	12413 (6)	8283 (6)	82
H(13A)	4670 (7)	13487 (6)	8987 (6)	82
H(14A)	2726 (7)	12419 (6)	9463 (5)	72
H(16A)	984 (6)	10056 (5)	8900 (5)	55
H(18A)	2019 (6)	11347 (6)	11255 (5)	66
H(19A)	1776 (7)	10701 (8)	12958 (6)	86
H(20A)	1232 (7)	8604 (9)	13172 (6)	96
H(21A)	999 (6)	7097 (7)	11670 (6)	79
H(23A)	1942 (6)	6980 (5)	9604 (5)	57
H(25A)	-871 (7)	5847 (6)	9979 (7)	84
H(26A)	-2858 (8)	4991 (7)	8784 (8)	107
H(27A)	-3093 (7)	5438 (8)	6985 (8)	107
H(28A)	-1463 (7)	6808 (7)	6349 (6)	84
H(33A)	2584 (11)	571 (10)	6652 (8)	147
H(33B)	3243 (11)	1957 (10)	6526 (8)	147

More planes for 5.

Least-squares plane number 1 (XO = orthogonal, x = Crystal coordinates)
The flap of the envelope

$$0.5051 \text{ XO} + 0.8048 \text{ YO} + -0.3117 \text{ ZO} = 5.0656$$

$$3.671 \text{ x} + 9.087 \text{ y} + -3.825 \text{ z} = 5.0656$$

Deviation	Weight	
-1.1745	1.0000	MN1
0.0283	1.0000	C1
-0.2377	1.0000	C2
0.4095	1.0000	H2A
+ 0.0000	1.0000	C3
+ 0.0000	1.0000	C4
-0.7863	1.0000	H4A
0.7861	1.0000	H4B
+ 0.0000	1.0000	C5
-0.3666	1.0000	H5A
0.7033	1.0000	C6
0.8020	1.0000	H6A
0.9118	1.0000	C7
1.2343	1.0000	H7A
0.5929	1.0000	C8
0.7629	1.0000	C9
2.1872	1.0000	C10
3.3087	1.0000	C11
4.5298	1.0000	C12
4.6337	1.0000	C13
3.5296	1.0000	C14
2.3048	1.0000	C15
0.9693	1.0000	C16
0.2909	1.0000	C17
0.8038	1.0000	C18
0.0101	1.0000	C19
-1.3015	1.0000	C20
-1.8355	1.0000	C21
-1.0195	1.0000	C22
-1.3274	1.0000	C23
-2.2158	1.0000	C24
-3.4705	1.0000	C25
-4.1029	1.0000	C26
-3.4883	1.0000	C27
-2.2506	1.0000	C28
-1.6047	1.0000	C29
-1.8503	1.0000	C30
-2.3490	1.0000	O1
-1.7197	1.0000	C31
-2.0625	1.0000	O2
-2.6424	1.0000	C32
-3.6129	1.0000	O3
-5.3386	1.0000	C33
-5.1239	1.0000	CL1
-5.4596	1.0000	CL2

Mean deviation from plane = 0.0000 Angstroms

Least-squares plane number 2 (XO = orthogonal, x = Crystal coordinates)
The rest of the ring (aromatic part)

$$0.0859 \text{ XO} + 0.8786 \text{ YO} + -0.4698 \text{ ZO} = 3.6474$$

$$-0.485 \text{ x} + 10.032 \text{ y} + -5.765 \text{ z} = 3.6474$$

Deviation	Weight	
-1.7129	1.0000	MN1
-0.2197	1.0000	C1
0.0667	1.0000	C2
0.9640	1.0000	H2A
+ 0.0186	1.0000	C3
0.3646	1.0000	C4
-0.0898	1.0000	H4A
1.3205	1.0000	H4B
+ -0.0365	1.0000	C5
-0.2296	1.0000	H5A
+ 0.0539	1.0000	C6

	-0.0888	1.0000	H6A
+	-0.0355	1.0000	C7
	-0.1548	1.0000	H7A
+	-0.0005	1.0000	C8
	-0.0356	1.0000	C9
	1.2717	1.0000	C10
	2.0255	1.0000	C11
	3.2188	1.0000	C12
	3.6634	1.0000	C13
	2.9248	1.0000	C14
	1.7281	1.0000	C15
	0.7784	1.0000	C16
	-0.1000	1.0000	C17
	0.2587	1.0000	C18
	-0.7040	1.0000	C19
	-2.0283	1.0000	C20
	-2.4131	1.0000	C21
	-1.4300	1.0000	C22
	-1.5975	1.0000	C23
	-1.8686	1.0000	C24
	-2.8650	1.0000	C25
	-2.9171	1.0000	C26
	-2.0084	1.0000	C27
	-1.0216	1.0000	C28
	-0.9539	1.0000	C29
	-2.8447	1.0000	C30
	-3.6328	1.0000	O1
	-2.6529	1.0000	C31
	-3.2528	1.0000	O2
	-2.5939	1.0000	C32
	-3.1937	1.0000	O3
	-6.1303	1.0000	C33
	-6.1607	1.0000	CL1
	-5.5269	1.0000	CL2

Mean deviation from plane = 0.0290 Angstroms

Angles to previous planes:

1: 26.2