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Table SI
Atomic Coordinates (x10^4) and Isotropic Thermal Parameters (Å^2 x 10^4) for the Non-Hydrogen Atoms of Compound **4b**

Atom	*x/a*	*y/b*	*z/c*	*U*
I1	1715.6(12)	1329.7(7)	1792.8(12)	645(6)[a]
I2	-123(6)	1169(3)	4908(4)	913(23)[a]
Mn1	491.1(13)	1389.4(8)	3264.1(12)	428(6)[a]
P1	-213(2)	2454(1)	2911(2)	285(9)[a]
P2	-1329(2)	1272(1)	2448(2)	304(9)[a]
C1	1832(9)	1672(6)	3904(9)	697(66)[a]
C2	917(12)	521(4)	3373(10)	829(65)[a]
C3	-266(16)	1335(11)	4335(10)	466(71)[a]
C3b	988(28)	1450(16)	2080(10)	326(82)
O1	2589(6)	1851(5)	4276(7)	791(45)[a]
O2	1217(9)	1(4)	3455(9)	1102(51)[a]
O3	-775(21)	1377(11)	5005(13)	1267(126)[a]
O3b	1207(48)	1419(25)	1299(15)	1563(224)
N	-3436(8)	2832(4)	2313(6)	441(34)[a]
C4	-432(8)	3117(5)	3772(7)	309(36)[a]
C5	-347(10)	3004(6)	4746(8)	513(47)[a]
C6	-546(11)	3495(7)	5366(8)	632(54)[a]
C7	-841(11)	4122(7)	5033(10)	655(57)[a]
C8	-925(11)	4248(6)	4092(11)	681(57)[a]
C9	-731(10)	3743(6)	3431(9)	531(46)[a]
C10	352(8)	2915(5)	1930(7)	294(37)[a]
C11	1479(10)	3130(6)	2073(8)	585(49)[a]
C12	1963(11)	3497(6)	1368(10)	658(53)[a]
C13	1348(11)	3663(6)	555(9)	610(50)[a]
C14	198(11)	3448(6)	424(8)	545(47)[a]
C15	-292(10)	3073(5)	1119(8)	443(41)[a]
C16	-2493(9)	811(5)	2922(8)	378(39)[a]
C17	-3613(10)	960(5)	2667(8)	513(48)[a]
C18	-4541(11)	593(7)	2985(10)	661(55)[a]
C19	-4238(15)	46(7)	3566(10)	758(67)[a]
C20	-3151(14)	-108(7)	3827(10)	716(59)[a]
C21	-2278(11)	263(6)	3519(8)	557(47)[a]
C22	-1556(8)	1033(5)	1227(7)	364(38)[a]
C23	-2154(10)	1429(6)	521(8)	603(48)[a]
C24	-2409(13)	1183(7)	-402(10)	763(61)[a]
C25	-2042(12)	578(8)	-643(10)	716(61)[a]
C26	-1447(12)	183(7)	25(11)	783(64)[a]
C27	-1181(11)	412(6)	939(9)	649(53)[a]

Table SI (continued)

Atom	*x/a*	*y/b*	*z/c*	*U*
C28	-1634(8)	2155(4)	2496(7)	279(33)[a]
C29	-2586(10)	2501(5)	2436(7)	351(38)[a]
C30	-4261(9)	3075(6)	2986(9)	477(44)[a]
C31	-3767(12)	2959(9)	3986(10)	1035(76)[a]
C32	-4504(13)	3786(6)	2757(12)	1021(74)[a]
C33	-5370(12)	2685(7)	2765(12)	1032(75)[a]

[a] Equivalent isotropic *U* defined as one-third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor.

Table SII

Fractional Atomic Coordinates (x10^4) and Isotropic Thermal Parameters (x10^4) for the Hydrogen Atoms of Compound **4b**

Atom	*x/a*	*y/b*	*z/c*	*U*
H5	-166	2567	4984	829(79)
H6	-453	3419	6038	829(79)
H7	-995	4465	5475	829(79)
H8	-1132	4685	3871	829(79)
H9	-795	3828	2760	829(79)
H11	1911	3047	2669	829(79)
H12	2761	3623	1448	829(79)
H13	1680	3926	82	829(79)
H14	-248	3557	-156	829(79)
H15	-1080	2929	1025	829(79)
H17	-3765	1331	2251	829(79)
H18	-5323	716	2796	829(79)
H19	-4854	-207	3801	829(79)
H20	-2984	-492	4215	829(79)
H21	-1491	145	3702	829(79)
H23	-2408	1864	687	829(79)
H24	-2817	1456	-874	829(79)
H25	-2211	416	-1278	829(79)
H26	-1222	-256	-147	829(79)
H27	-707	146	1378	829(79)
H31a	-4291	3116	4428	829(79)
H31b	-3046	3190	4089	829(79)
H31c	-3641	2492	4079	829(79)
H32a	-5030	3974	3173	829(79)
H32b	-4836	3809	2114	829(79)
H32c	-3793	4030	2815	829(79)
H33a	-5946	2816	3176	829(79)
H33b	-5211	2221	2845	829(79)
H33c	-5646	2770	2117	829(79)

Table SIII

Anisotropic thermal parameters U_{ij} (x10^4 Å^2) for the non-hydrogen a of the compound **4b**. The anisotropic thermal parameters are in the for

$$\exp[-2\pi^2(U_{11}h^2a^{*2}+\ldots+2U_{12}hka^*b^*)]$$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I1	568(9)	639(10)	756(12)	-239(9)	222(8)	2(8)
I2	1451(53)	744(33)	512(26)	108(23)	-109(27)	-53(29)
Mn1	401(10)	349(10)	517(11)	53(9)	-71(8)	37(9)
P1	285(16)	294(15)	278(15)	8(13)	22(12)	-1(13)
P2	301(17)	283(15)	325(15)	-20(14)	17(13)	14(13)
C1	1239(153)	235(67)	648(100)	143(66)	260(99)	-81(87)
C2	910(118)	906(119)	640(95)	-21(95)	-130(84)	-436(97)
C3	437(113)	511(128)	434(123)	-180(125)	-56(102)	198(106)
O1	477(65)	939(84)	922(81)	430(67)	-159(53)	202(56)
O2	909(76)	710(71)	1639(108)	241(76)	-181(71)	448(65)
O3	1358(216)	760(132)	1638(276)	-330(132)	-161(157)	425(132)
N	353(56)	330(53)	642(67)	101(49)	48(51)	117(46)
C4	316(60)	242(59)	364(67)	-102(51)	-11(49)	-56(47)
C5	799(94)	418(73)	331(76)	-11(60)	99(65)	-7(64)
C6	972(109)	676(97)	239(67)	-171(70)	-1(66)	120(77)
C7	925(108)	580(95)	479(90)	-231(75)	162(79)	-82(80)
C8	848(106)	341(73)	868(113)	-77(79)	155(87)	-21(68)
C9	634(81)	405(79)	580(76)	-118(65)	204(62)	46(62)
C10	239(61)	320(61)	330(70)	42(49)	65(52)	-28(48)
C11	473(81)	803(93)	469(78)	167(70)	-12(62)	-99(70)
C12	501(80)	750(98)	739(97)	269(81)	146(77)	-143(70)
C13	644(91)	539(79)	683(88)	226(75)	271(73)	-139(76)
C14	643(89)	643(87)	330(68)	36(63)	-82(62)	59(67)
C15	481(72)	392(66)	468(75)	176(60)	110(61)	-27(56)
C16	381(72)	278(61)	487(70)	-49(57)	109(56)	-60(55)
C17	570(92)	311(65)	667(90)	-1(62)	110(72)	-104(61)
C18	536(88)	599(89)	865(105)	-144(83)	163(77)	-166(72)
C19	1021(137)	598(100)	707(106)	-157(82)	383(98)	-434(95)
C20	798(107)	600(92)	746(105)	45(76)	26(91)	-239(91)
C21	648(88)	413(73)	610(82)	52(68)	50(68)	-132(66)
C22	301(61)	335(65)	453(69)	22(55)	10(53)	-43(49)
C23	726(88)	624(82)	436(76)	-125(71)	-97(66)	110(72)
C24	963(114)	787(109)	522(90)	41(83)	-47(78)	102(88)
C25	760(102)	1007(123)	394(84)	-381(89)	134(75)	-247(91)
C26	1072(127)	502(89)	771(112)	-444(86)	50(98)	-121(84)
C27	966(106)	389(78)	572(86)	-128(69)	-59(75)	17(72)
C28	316(58)	177(52)	330(59)	18(46)	-62(48)	17(47)
C29	450(71)	219(56)	380(66)	0(52)	22(55)	-43(58)
C30	235(62)	558(79)	646(86)	-58(67)	90(60)	79(57)
C31	644(105)	1810(169)	679(110)	-187(114)	230(88)	28(109)
C32	1149(133)	530(97)	1443(148)	8(92)	463(112)	114(86)
C33	662(113)	1111(123)	1365(149)	-339(114)	331(103)	-25(94)

Table SIV

Bond distances (Å) and angles (deg) with e.s.d.'s in parentheses for compound **4b**.

I1	- Mn1	2.617(3)
I2	- Mn1	2.525(6)
Mn1	- P1	2.338(3)
Mn1	- P2	2.339(3)
Mn1	- C1	1.829(11)
Mn1	- C2	1.824(9)
Mn1	- C3	1.816(16)
Mn1	- C3B	1.818(19)
P1	- C4	1.841(10)
P1	- C10	1.835(10)
P1	- C28	1.811(10)
P2	- C16	1.816(11)
P2	- C22	1.791(11)
P2	- C28	1.819(9)
C1	- O1	1.051(13)
C2	- O2	1.110(12)
C3	- O3	1.160(26)
C3B	- O3B	1.156(32)
N	- C29	1.194(14)
N	- C30	1.489(15)
C4	- C5	1.391(15)
C4	- C9	1.387(15)
C5	- C6	1.355(17)
C6	- C7	1.383(19)
C7	- C8	1.349(20)
C8	- C9	1.413(18)
C10	- C11	1.380(15)
C10	- C15	1.355(14)
C11	- C12	1.397(18)
C12	- C13	1.345(18)
C13	- C14	1.404(18)
C14	- C15	1.397(16)
C16	- C17	1.357(16)
C16	- C21	1.400(15)
C17	- C18	1.411(18)
C18	- C19	1.404(20)
C19	- C20	1.323(23)
C20	- C21	1.362(20)
C22	- C23	1.416(15)
C22	- C27	1.397(16)
C23	- C24	1.405(18)
C24	- C25	1.347(22)
C25	- C26	1.378(20)

Table SIV (continued)

C26	- C27	1.384(19)
C28	- C29	1.305(15)
C30	- C31	1.500(18)
C30	- C32	1.492(17)
C30	- C33	1.521(17)

I2	-Mn1	-C3B	173.4(5)
I2	-Mn1	-C2	81.3(4)
I2	-Mn1	-C1	83.9(4)
I2	-Mn1	-P2	97.1(2)
I2	-Mn1	-P1	103.8(2)
I1	-Mn1	-C3	172.7(5)
I1	-Mn1	-C2	82.0(4)
I1	-Mn1	-C1	84.8(4)
I1	-Mn1	-P2	97.6(1)
I1	-Mn1	-P1	94.4(1)
C2	-Mn1	-C3B	92.2(11)
C2	-Mn1	-C3	91.0(8)
C1	-Mn1	-C3B	96.4(8)
C1	-Mn1	-C3	93.3(7)
C1	-Mn1	-C2	92.5(5)
P2	-Mn1	-C3B	84.0(7)
P2	-Mn1	-C3	85.7(6)
P2	-Mn1	-C2	100.0(4)
P2	-Mn1	-C1	167.5(4)
P1	-Mn1	-C3B	82.7(9)
P1	-Mn1	-C3	92.8(7)
P1	-Mn1	-C2	171.3(3)
P1	-Mn1	-C1	95.1(4)
P1	-Mn1	-P2	72.6(1)
Mn1	-P1	-C28	93.3(3)
Mn1	-P1	-C10	119.1(3)
Mn1	-P1	-C4	126.3(3)
C10	-P1	-C28	107.3(4)
C4	-P1	-C28	106.5(4)
C4	-P1	-C10	102.0(4)
Mn1	-P2	-C28	93.1(3)
Mn1	-P2	-C22	124.0(4)
Mn1	-P2	-C16	122.8(4)
C22	-P2	-C28	106.7(5)
C16	-P2	-C28	109.6(4)
C16	-P2	-C22	99.3(5)
Mn1	-C1	-O1	178.0(10)
Mn1	-C2	-O2	177.3(8)
Mn1	-C3	-O3	172.1(15)
Mn1	-C3B	-O3B	171.0(16)
C29	-N	-C30	131.3(10)
P1	-C4	-C9	118.5(8)

Table SIV (continued)

P1	-C4	-C5	122.2(8)
C5	-C4	-C9	119.3(10)
C4	-C5	-C6	121.2(10)
C5	-C6	-C7	119.9(12)
C6	-C7	-C8	120.3(12)
C7	-C8	-C9	120.9(13)
C4	-C9	-C8	118.3(10)
P1	-C10	-C15	123.5(8)
P1	-C10	-C11	116.3(8)
C11	-C10	-C15	120.2(10)
C10	-C11	-C12	119.7(10)
C11	-C12	-C13	121.6(12)
C12	-C13	-C14	118.0(12)
C13	-C14	-C15	120.9(11)
C10	-C15	-C14	119.5(10)
P2	-C16	-C21	121.7(8)
P2	-C16	-C17	121.1(9)
C17	-C16	-C21	117.1(10)
C16	-C17	-C18	122.8(11)
C17	-C18	-C19	115.9(12)
C18	-C19	-C20	122.3(14)
C19	-C20	-C21	120.2(15)
C16	-C21	-C20	121.6(11)
P2	-C22	-C27	119.8(8)
P2	-C22	-C23	123.4(8)
C23	-C22	-C27	116.7(10)
C22	-C23	-C24	120.6(11)
C23	-C24	-C25	120.6(13)
C24	-C25	-C26	120.2(14)
C25	-C26	-C27	120.5(13)
C22	-C27	-C26	121.3(11)
P1	-C28	-P2	99.3(4)
P2	-C28	-C29	133.5(8)
P1	-C28	-C29	126.1(8)
N	-C29	-C28	175.0(12)
N	-C30	-C33	106.1(9)
N	-C30	-C32	107.4(10)
N	-C30	-C31	109.5(10)
C32	-C30	-C33	108.1(10)
C31	-C30	-C33	111.5(11)
C31	-C30	-C32	113.9(12)

Table SV

Atomic Coordinates ($x10^4$) and Isotropic Thermal Parameters ($Å^2x10^4$) for the Non-Hydrogen Atoms of Compound **6**

Atom	*x/a*	*y/b*	*z/c*	*U*
Mn(1A)	4041.1(13)	3809.8(8)	7296.9(5)	546(6)[a]
I(1A)	3366.7(9)	2889.8(5)	7701.6(3)	735(4)[a]
I(1A')	4979(8)	4524(6)	6839(3)	1150(47)[a]
P(1A)	3527.4(22)	4580.4(13)	7680.1(8)	452(9)[a]
P(2A)	2305.4(22)	4112.4(13)	7088.7(7)	456(10)[a]
O(1A)	4449(8)	2865(5)	6774(3)	946(45)[a]
O(2A)	6221(9)	3710(7)	7661(4)	1580(71)[a]
O(3A)	4753(31)	4704(15)	6777(10)	3587(272)[a]
N(1A)	431(7)	5122(4)	7277(2)	516(33)[a]
N(2A)	2264(7)	5694(4)	7974(2)	515(34)[a]
C(1A)	4257(11)	3185(7)	6962(4)	771(59)[a]
C(2A)	5365(11)	3731(7)	7528(3)	825(58)[a]
C(3A)	4601(15)	4341(7)	6985(4)	641(72)[a]
C(4A)	2241(8)	4710(4)	7424(2)	379(33)[a]
C(5A)	1433(8)	5105(5)	7482(2)	395(35)[a]
C(6A)	1429(9)	5616(5)	7763(3)	470(39)[a]
C(7A)	372(9)	5908(5)	7687(3)	501(40)[a]
C(8A)	-202(9)	5598(5)	7401(3)	497(41)[a]
C(9A)	-1246(9)	5757(6)	7274(3)	670(49)[a]
C(10A)	-1690(11)	6269(7)	7441(4)	882(63)[a]
C(11A)	-1110(11)	6584(7)	7720(3)	808(59)[a]
C(12A)	-98(10)	6408(6)	7856(3)	669(49)[a]
C(13A)	2281(9)	6154(6)	8249(3)	613(47)[a]
C(14A)	2881(10)	6676(6)	8220(3)	746(54)[a]
C(15A)	2948(14)	7110(8)	8496(5)	1224(86)[a]
C(16A)	2405(14)	7014(9)	8801(5)	1193(88)[a]
C(17A)	1821(13)	6476(10)	8823(4)	1075(82)[a]
C(18A)	1760(10)	6055(7)	8552(4)	813(59)[a]
C(19A)	3374(9)	4355(5)	8147(2)	438(37)[a]
C(20A)	4266(9)	4077(6)	8353(3)	661(49)[a]
C(21A)	4179(12)	3877(7)	8704(4)	810(59)[a]
C(22A)	3242(14)	3930(7)	8851(3)	966(69)[a]
C(23A)	2356(11)	4167(6)	8650(3)	746(54)[a]
C(24A)	2409(9)	4379(5)	8299(3)	547(43)[a]
C(25A)	4303(9)	5296(5)	7719(3)	539(43)[a]
C(26A)	4246(12)	5695(6)	7438(4)	818(59)[a]

C(27A)	4882(13)	6229(7)	7464(5)	879(69)[a]
C(28A)	5530(14)	6358(7)	7751(6)	1070(86)[a]

Table SV (continued)

Atom	*x/a*	*y/b*	*z/c*	*U*
C(29A)	5586(12)	5962(8)	8037(5)	1157(81)[a]
C(30A)	4950(12)	5443(7)	8023(4)	963(65)[a]
C(31A)	2133(8)	4459(5)	6641(3)	520(41)[a]
C(32A)	1924(9)	5080(6)	6584(3)	629(47)[a]
C(33A)	1868(10)	5324(7)	6235(3)	773(57)[a]
C(34A)	1939(12)	4953(8)	5938(3)	934(69)[a]
C(35A)	2141(12)	4340(8)	5984(4)	960(72)[a]
C(36A)	2275(11)	4083(6)	6339(3)	783(56)[a]
C(37A)	1097(9)	3637(5)	7116(4)	607(47)[a]
C(38A)	584(10)	3351(6)	6808(3)	746(52)[a]
C(39A)	-335(13)	2980(6)	6854(5)	1015(76)[a]
C(40A)	-714(12)	2928(8)	7186(6)	1073(80)[a]
C(41A)	-181(12)	3209(7)	7475(5)	961(70)[a]
C(42A)	704(10)	3564(6)	7444(3)	739(54)[a]
Mn(1B)	-407.5(13)	2482.5(8)	4849.9(4)	510(6)[a]
I(1B)	-316.6(35)	3298.5(15)	5419.6(7)	702(9)[a]
I(1B')	-730.0(21)	1633.2(13)	4288.2(7)	652(10)[a]
P(1B)	1023.0(23)	2930.3(14)	4592.9(8)	497(10)[a]
P(2B)	1143.3(22)	1975.1(13)	5080.0(8)	481(10)[a]
O(1B)	-1867(7)	1786(5)	5263(3)	854(40)[a]
O(2B)	-1999(7)	3315(5)	4474(3)	923(42)[a]
O(3B)	-859(42)	1522(16)	4300(11)	4238(389)
O(3B')	-105(48)	3429(20)	5417(11)	491(177)
N(1B)	3715(7)	1801(4)	4883(3)	642(38)[a]
N(2B)	3235(9)	3104(6)	4322(3)	968(55)[a]
C(1B)	-1335(9)	2060(6)	5102(3)	668(50)[a]
C(2B)	-1413(10)	2999(7)	4615(4)	768(58)[a]
C(3B)	-701(16)	1947(7)	4482(4)	647(55)
C(3B')	-249(30)	3034(13)	5214(7)	699(110)
C(4B)	2007(8)	2399(5)	4801(3)	465(37)[a]
C(5B)	3013(9)	2265(5)	4722(3)	544(43)[a]
C(6B)	3630(9)	2585(5)	4475(3)	531(42)[a]
C(7B)	4648(9)	2275(5)	4458(3)	560(43)[a]
C(8B)	4688(9)	1800(5)	4709(3)	620(47)[a]
C(9B)	5529(10)	1401(6)	4758(3)	722(52)[a]
C(10B)	6386(10)	1495(7)	4554(4)	787(58)[a]
C(11B)	6367(9)	1961(7)	4315(4)	774(57)[a]
C(12B)	5521(10)	2369(6)	4248(3)	757(54)[a]
C(13B)	3851(18)	3495(10)	4089(7)	721(80)

C(14B)	3674(18)	3431(10)	3713(7)	1882(167)
C(15B)	4263(18)	3784(10)	3489(7)	3221(346)
C(16B)	5028(18)	4201(10)	3641(7)	1916(180)

Table SV (continued)

Atom	*x/a*	*y/b*	*z/c*	*U*
C(17B)	5204(18)	4265(10)	4016(7)	1959(185)
C(18B)	4616(18)	3912(10)	4240(7)	1405(128)
C(13C)	3652(22)	3376(12)	4018(6)	620(136)
C(14C)	3938(22)	3994(12)	4063(6)	873(135)
C(15C)	4260(22)	4329(12)	3772(6)	1370(205)
C(16C)	4296(22)	4045(12)	3436(6)	1163(175)
C(17C)	4010(22)	3427(12)	3391(6)	868(126)
C(18C)	3688(22)	3093(12)	3682(6)	563(96)
C(19B)	1374(10)	3723(5)	4716(3)	613(46)[a]
C(20B)	2346(11)	3885(7)	4897(3)	791(59)[a]
C(21B)	2564(13)	4505(8)	4976(4)	929(67)[a]
C(22B)	1794(16)	4952(7)	4869(5)	967(76)[a]
C(23B)	860(14)	4790(7)	4708(4)	874(69)[a]
C(24B)	619(11)	4176(6)	4631(3)	692(51)[a]
C(25B)	1019(9)	2908(6)	4099(3)	581(43)[a]
C(26B)	1217(13)	2370(7)	3921(4)	985(70)[a]
C(27B)	1206(15)	2335(8)	3547(4)	1189(86)[a]
C(28B)	931(13)	2831(8)	3342(4)	979(72)[a]
C(29B)	727(14)	3369(9)	3501(4)	1193(85)[a]
C(30B)	756(12)	3402(7)	3887(3)	927(65)[a]
C(31B)	1616(9)	2076(5)	5567(3)	577(44)[a]
C(32B)	926(11)	1931(7)	5818(3)	808(59)[a]
C(33B)	1242(14)	1957(7)	6179(4)	976(72)[a]
C(34B)	2231(15)	2187(8)	6297(4)	1103(80)[a]
C(35B)	2902(12)	2375(7)	6042(4)	980(69)[a]
C(36B)	2592(10)	2312(6)	5674(3)	750(54)[a]
C(37B)	1334(8)	1143(5)	5007(3)	504(40)[a]
C(38B)	1256(12)	715(6)	5274(4)	906(64)[a]
C(39B)	1347(13)	92(7)	5203(5)	1045(76)[a]
C(40B)	1546(12)	-110(7)	4876(5)	936(71)[a]
C(41B)	1635(13)	310(8)	4609(4)	1034(75)[a]
C(42B)	1515(12)	936(6)	4667(4)	876(64)[a]
O(4A)	8975(8)	369(5)	1699(3)	1068(30)
C(43A)	7970(14)	659(8)	1761(5)	1278(58)
C(44A)	7491(18)	918(11)	1423(7)	1727(82)
C(45A)	8094(21)	590(12)	1134(7)	1914(99)
C(46A)	9095(14)	276(8)	1311(5)	1200(56)
O(4B)	7667(15)	1573(9)	8206(6)	2276(77)
C(43B)	7972(20)	1910(14)	7897(7)	1825(98)
C(44B)	7500(28)	2478(18)	7969(10)	2616(151)
C(45B)	6984(28)	2575(18)	8317(11)	2756(155)

C(46B)	7403(24)	2051(17)	8496(8)	2250(124)
O(4C)	4248(10)	1026(6)	5454(3)	1413(42)

Table SV (continued)

Atom	*x/a*	*y/b*	*z/c*	*U*
C(43C)	4141(21)	373(13)	5458(7)	2006(98)
C(44C)	5121(34)	181(20)	5761(12)	3172(186)
C(45C)	5543(20)	734(14)	5932(7)	1896(96)
C(46C)	5011(18)	1269(11)	5761(6)	1702(79)
O(4D)	5309(28)	1879(18)	592(10)	3618(169)
C(43D)	4948(29)	1273(20)	729(10)	2593(163)
C(44D)	5477(22)	902(13)	401(8)	2036(107)
C(45D)	5949(30)	1309(22)	165(10)	2656(165)
C(46D)	6031(30)	1966(19)	321(11)	2434(159)
O(4E)	309(22)	-235(14)	6503(9)	2981(122)
C(43E)	923(49)	86(22)	6252(13)	3277(223)
C(44E)	2008(44)	-112(24)	6402(16)	3308(228)
C(45E)	1993(44)	-402(24)	6734(16)	3645(243)
C(46E)	1012(42)	-541(19)	6834(12)	3308(197)

[a] Equivalent isotropic *U* defined as one-third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor.

Table SVI

Fractional Atomic Coordinates ($x10^4$) and Isotropic Thermal Parameters ($x10^4$) for the Hydrogen Atoms of Compound **6**

Atom	*x/a*	*y/b*	*z/c*	*U*
H1A	203	4851	7080	1012(86)
H9A	-1641	5521	7086	1012(86)
H10A	-2400	6402	7355	1012(86)
H11A	-1435	6937	7820	1012(86)
H12A	281	6615	8059	1012(86)
H14A	3251	6745	8010	1012(86)
H15A	3365	7477	8477	1012(86)
H16A	2452	7312	8993	1012(86)
H17A	1450	6407	9034	1012(86)
H18A	1342	5688	8571	1012(86)
H20A	4933	4047	8248	1012(86)
H21A	4797	3704	8842	1012(86)
H22A	3193	3787	9093	1012(86)
H23A	1689	4196	8756	1012(86)
H24A	1791	4552	8162	1012(86)
H26A	3778	5604	7224	1012(86)
H27A	4839	6507	7262	1012(86)
H28A	5954	6726	7763	1012(86)
H29A	6054	6053	8252	1012(86)
H30A	4993	5165	8225	1012(86)
H32A	1843	5339	6789	1012(86)
H33A	1729	5756	6201	1012(86)
H34A	1881	5126	5699	1012(86)
H35A	2222	4081	5778	1012(86)
H36A	2414	3651	6374	1012(86)
H38A	856	3396	6577	1012(86)
H39A	-689	2779	6645	1012(86)
H40A	-1339	2682	7208	1012(86)
H41A	-453	3164	7706	1012(86)
H42A	1058	3766	7654	1012(86)
H1B	3553	1528	5074	1020(93)
H9B	5531	1065	4926	1020(93)
H10B	6997	1227	4583	1020(93)
H11B	6979	2019	4183	1020(93)
H12B	5510	2691	4070	1020(93)
H20B	2872	3573	4965	1020(93)
H21B	3247	4619	5099	1020(93)
H22B	1951	5376	4923	1020(93)
H23B	334	5101	4639	1020(93)
H24B	-64	4062	4509	1020(93)
H26B	1404	2010	4063	1020(93)
H27B	1363	1956	3430	1020(93)
H28B	901	2812	3083	1020(93)

Table SVI (Continued)

Fractional Atomic Coordinates ($x10^4$) and Isotropic Thermal Parameters ($x10^4$) for the Hydrogen Atoms of Compound **6**

Atom	*x/a*	*y/b*	*z/c*	*U*
H29B	540	3729	3359	1020(93)
H30B	599	3781	4004	1020(93)
H32B	226	1773	5739	1020(93)
H33B	769	1836	6355	1020(93)
H34B	2458	2224	6551	1020(93)
H35B	3602	2532	6121	1020(93)
H36B	3065	2433	5498	1020(93)
H38B	1126	854	5511	1020(93)
H39B	1283	-202	5393	1020(93)
H40B	1612	-542	4829	1020(93)
H41B	1765	171	4372	1020(93)
H42B	1579	1230	4477	1020(93)

Table SVII

Anisotropic thermal parameters U_{ij} (x10^4 Å^2) for the non-hydrogen atoms of the compound **6**. The anisotropic thermal parameters are in the form:

$$\exp[-2\pi^2(U_{11}h^2a^{*2}+\ldots+2U_{12}hka^*b^*)]$$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mn1A	509(10)	572(11)	553(11)	-71(9)	36(8)	114(9)
I1A	920(9)	463(6)	811(8)	-9(6)	34(6)	-39(6)
I1A'	801(54)	1860(113)	830(65)	-14(63)	290(44)	12(62)
P1A	438(17)	452(16)	465(17)	6(14)	37(13)	-4(14)
P2A	511(17)	457(17)	397(16)	-40(13)	31(13)	15(14)
O1A	1147(82)	898(76)	793(71)	-148(59)	95(59)	570(65)
O2A	600(71)	2149(148)	1970(133)	-130(114)	19(80)	437(86)
O3A	3372(422)	3174(458)	4508(513)	-791(356)	1829(359)	-769(337)
N1A	521(58)	676(63)	332(50)	-68(46)	-51(43)	113(49)
N2A	493(59)	540(58)	519(57)	-167(47)	79(48)	-11(46)
C1A	674(93)	772(104)	832(106)	-70(83)	-98(77)	101(77)
C2A	699(94)	1364(130)	386(69)	-70(78)	-71(64)	292(92)
C3A	1091(171)	504(84)	254(96)	125(71)	-300(93)	91(93)
C4A	429(61)	460(60)	230(50)	-63(44)	-46(43)	9(49)
C5A	468(65)	478(61)	217(52)	-20(46)	-70(47)	21(51)
C6A	445(67)	460(65)	511(70)	87(55)	84(56)	50(54)
C7A	616(74)	542(68)	359(62)	106(55)	124(55)	124(60)
C8A	523(75)	523(68)	453(69)	185(56)	90(57)	153(57)
C9A	471(75)	947(100)	581(78)	-17(72)	0(61)	91(69)
C10A	566(86)	1065(118)	1029(117)	74(99)	144(82)	476(85)
C11A	858(105)	1004(110)	587(85)	32(81)	197(76)	491(91)
C12A	727(90)	705(83)	586(77)	33(64)	115(65)	318(70)
C13A	492(71)	859(96)	477(74)	-167(70)	2(57)	108(67)
C14A	810(96)	679(89)	743(91)	-158(77)	44(72)	-16(78)
C15A	1108(140)	1099(136)	1497(163)	-593(132)	288(124)	-110(109)
C16A	963(132)	1341(166)	1177(154)	-829(137)	-369(112)	291(117)
C17A	909(120)	1605(183)	736(107)	-432(118)	200(88)	272(119)
C18A	733(93)	976(113)	760(99)	-181(87)	228(78)	28(81)
C19A	613(73)	436(62)	248(53)	15(46)	-31(50)	-33(54)
C20A	556(77)	670(84)	742(93)	82(72)	-8(67)	65(64)
C21A	874(107)	923(108)	579(89)	242(80)	-198(77)	-17(86)
C22A	1217(132)	1305(141)	323(73)	166(82)	-170(85)	-378(113)
C23A	838(97)	986(106)	417(75)	15(72)	70(70)	-84(81)
C24A	599(76)	722(80)	313(63)	85(56)	3(54)	-65(62)

Table SVII (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C25A	466(69)	511(70)	647(79)	4(63)	95(60)	-33(55)
C26A	1083(115)	607(86)	786(100)	56(78)	207(82)	-141(80)
C27A	1026(130)	677(101)	946(121)	29(91)	156(98)	-312(94)
C28A	972(133)	617(105)	1725(191)	-143(118)	644(131)	-301(93)
C29A	980(124)	1031(133)	1393(156)	-75(120)	-210(108)	-457(106)
C30A	1065(118)	805(102)	952(112)	178(87)	-220(93)	-441(92)
C31A	502(69)	600(76)	454(68)	21(59)	23(53)	65(57)
C32A	690(84)	674(85)	519(75)	81(65)	44(61)	85(67)
C33A	874(101)	906(106)	534(84)	250(79)	48(71)	140(81)
C34A	1141(127)	1276(140)	350(78)	281(89)	-96(75)	136(108)
C35A	1067(122)	1257(145)	584(98)	-152(98)	227(83)	-31(108)
C36A	1022(107)	694(88)	649(91)	-36(75)	160(76)	124(77)
C37A	546(75)	378(64)	901(96)	-62(64)	90(70)	-2(55)
C38A	785(92)	666(85)	741(89)	-118(73)	-148(72)	-112(76)
C39A	1111(133)	482(89)	1409(159)	-197(97)	-81(116)	-184(88)
C40A	655(104)	1080(128)	1503(171)	48(128)	205(110)	-343(93)
C41A	803(110)	854(107)	1250(139)	141(99)	221(98)	-271(88)
C42A	699(88)	869(100)	663(88)	-31(73)	129(70)	-257(75)
Mn1B	438(9)	571(11)	527(10)	23(9)	81(8)	28(8)
I1B	844(20)	624(14)	669(14)	-114(9)	229(10)	26(14)
I1B'	503(16)	747(19)	705(18)	-130(14)	62(12)	16(12)
P1B	503(18)	518(17)	468(17)	83(15)	45(13)	15(15)
P2B	466(17)	502(18)	485(17)	89(14)	99(13)	-24(14)
O1B	660(61)	987(74)	929(71)	12(58)	153(52)	-243(54)
O2B	636(61)	899(71)	1185(81)	372(63)	-146(55)	192(54)
N1B	504(59)	689(67)	739(69)	61(55)	93(51)	29(51)
N2B	961(90)	1170(107)	838(85)	-57(78)	412(71)	-203(80)
C1B	413(71)	768(89)	818(94)	100(77)	41(65)	-98(66)
C2B	546(85)	799(101)	977(108)	38(86)	158(76)	13(75)
C4B	362(61)	551(68)	483(63)	27(54)	54(49)	-71(51)
C5B	531(73)	553(74)	555(72)	-22(58)	82(58)	-78(58)
C6B	528(72)	563(72)	502(69)	170(60)	53(55)	41(60)
C7B	468(70)	611(77)	613(75)	-11(61)	112(58)	-54(57)
C8B	463(72)	507(73)	903(95)	-36(69)	132(66)	-47(58)
C9B	726(92)	755(91)	667(83)	87(70)	-11(71)	106(75)
C10B	456(79)	980(112)	908(104)	68(88)	-20(73)	112(72)
C11B	286(68)	1071(113)	988(106)	-2(92)	182(67)	63(72)
C12B	563(79)	916(102)	825(95)	11(79)	229(70)	-160(75)
C19B	649(82)	562(75)	661(81)	162(65)	225(66)	-3(67)
C20B	834(101)	914(113)	615(85)	116(79)	27(73)	-159(84)
C21B	1154(129)	867(114)	742(101)	-205(89)	-25(88)	-417(104)

Table SVII (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C22B	1440(160)	530(92)	1003(129)	28(87)	470(117)	-64(107)
C23B	1063(127)	756(112)	857(113)	41(86)	355(97)	0(92)
C24B	880(96)	484(77)	744(89)	79(66)	236(72)	-18(69)
C25B	617(75)	619(77)	519(71)	111(68)	119(57)	30(64)
C26B	1593(155)	771(103)	570(91)	64(79)	9(90)	227(100)
C27B	1935(188)	913(128)	733(115)	-180(98)	200(114)	154(123)
C28B	1400(146)	975(125)	572(94)	-45(98)	153(90)	171(113)
C29B	1538(163)	1262(156)	755(117)	505(112)	0(106)	317(130)
C30B	1509(143)	779(102)	506(82)	40(76)	174(84)	213(97)
C31B	675(81)	574(73)	514(71)	21(61)	216(63)	5(64)
C32B	768(94)	1093(119)	599(89)	58(80)	239(73)	-139(82)
C33B	1268(141)	1184(135)	508(90)	-9(87)	245(89)	-206(111)
C34B	1411(155)	1418(156)	495(89)	-203(98)	174(98)	-70(128)
C35B	886(110)	1344(142)	699(102)	-88(96)	20(85)	-272(99)
C36B	778(93)	1062(111)	409(73)	-47(70)	61(64)	-351(82)
C37B	491(67)	541(71)	489(67)	104(58)	87(53)	-71(54)
C38B	1354(132)	519(85)	884(105)	120(77)	305(91)	-159(84)
C39B	1405(147)	743(117)	976(125)	252(98)	71(108)	-202(101)
C40B	1121(129)	584(93)	1122(137)	146(100)	213(108)	-9(83)
C41B	1476(152)	1076(136)	532(92)	-273(95)	17(91)	-31(114)
C42B	1316(130)	478(81)	874(112)	73(77)	313(94)	0(80)

Table SVIII

Bond distances (Å) and angles (deg) with e.s.d.'s in parentheses for compound **6**

Mn1A - I1A	2.687(2)
Mn1A - I1A'	2.661(12)
Mn1A - P1A	2.329(4)
Mn1A - P2A	2.329(3)
Mn1A - C1A	1.877(15)
Mn1A - C2A	1.798(13)
Mn1A - C3A	1.824(16)
P1A - C4A	1.810(9)
P1A - C19A	1.829(10)
P1A - C25A	1.831(11)
P2A - C4A	1.805(10)
P2A - C31A	1.815(11)
P2A - C37A	1.845(12)
O1A - C1A	1.030(18)
O2A - C2A	1.136(17)
O3A - C3A	1.132(38)
N1A - C5A	1.401(12)
N1A - C8A	1.410(14)
N2A - C6A	1.253(13)
N2A - C13A	1.429(15)
C4A - C5A	1.361(14)
C5A - C6A	1.522(14)
C6A - C7A	1.471(15)
C7A - C8A	1.392(15)
C7A - C12A	1.413(17)
C8A - C9A	1.389(15)
C9A - C10A	1.416(20)
C10A - C11A	1.384(20)
C11A - C12A	1.372(18)
C13A - C14A	1.370(19)
C13A - C18A	1.373(19)
C14A - C15A	1.387(23)
C15A - C16A	1.394(28)
C16A - C17A	1.386(28)
C17A - C18A	1.355(23)
C19A - C20A	1.424(15)
C19A - C24A	1.387(16)
C20A - C21A	1.387(19)
C21A - C22A	1.349(23)
C22A - C23A	1.372(20)
C23A - C24A	1.391(16)
C25A - C26A	1.351(18)
C25A - C30A	1.358(18)
C26A - C27A	1.405(21)

Table VIII (continued)

C27A - C28A	1.301(25)
C28A - C29A	1.363(27)
C29A - C30A	1.378(22)
C31A - C32A	1.386(17)
C31A - C36A	1.411(17)
C32A - C33A	1.393(17)
C33A - C34A	1.375(20)
C34A - C35A	1.364(25)
C35A - C36A	1.427(20)
C37A - C38A	1.398(18)
C37A - C42A	1.369(19)
C38A - C39A	1.431(21)
C39A - C40A	1.369(29)
C40A - C41A	1.349(25)
C41A - C42A	1.366(20)
Mn1B - I1B	2.752(3)
Mn1B - I1B'	2.782(3)
Mn1B - P1B	2.328(4)
Mn1B - P2B	2.321(3)
Mn1B - C1B	1.814(13)
Mn1B - C2B	1.840(14)
Mn1B - C3B	1.803(15)
Mn1B - C3B'	1.800(27)
P1B - C4B	1.805(10)
P1B - C19B	1.822(12)
P1B - C25B	1.831(11)
P2B - C4B	1.822(11)
P2B - C31B	1.855(11)
P2B - C37B	1.847(11)
O1B - C1B	1.112(16)
O2B - C2B	1.099(16)
O3B - C3B	1.148(39)
O3B' - C3B'	1.144(50)
N1B - C5B	1.430(14)
N1B - C8B	1.438(15)
N2B - C6B	1.335(17)
N2B - C13B	1.485(28)
N2B - C13C	1.419(27)
C4B - C5B	1.355(15)
C5B - C6B	1.436(16)
C6B - C7B	1.451(16)
C7B - C8B	1.387(17)
C7B - C12B	1.422(17)
C8B - C9B	1.363(17)
C9B - C10B	1.390(19)
C10B - C11B	1.342(21)
C11B - C12B	1.386(18)
C13B - C14B	1.395(36)

Table SVIII (continued)

C13B - C18B	1.395(32)
C14B - C15B	1.395(35)
C15B - C16B	1.395(32)
C16B - C17B	1.395(36)
C17B - C18B	1.395(35)
C13C - C14C	1.395(36)
C13C - C18C	1.395(32)
C14C - C15C	1.395(34)
C15C - C16C	1.395(32)
C16C - C17C	1.395(36)
C17C - C18C	1.395(34)
C19B - C20B	1.377(18)
C19B - C24B	1.379(17)
C20B - C21B	1.401(22)
C21B - C22B	1.397(24)
C22B - C23B	1.308(25)
C23B - C24B	1.392(20)
C25B - C26B	1.377(19)
C25B - C30B	1.353(18)
C26B - C27B	1.388(21)
C27B - C28B	1.342(24)
C28B - C29B	1.344(26)
C29B - C30B	1.429(20)
C31B - C32B	1.372(18)
C31B - C36B	1.349(17)
C32B - C33B	1.360(19)
C33B - C34B	1.367(25)
C34B - C35B	1.388(23)
C35B - C36B	1.389(18)
C37B - C38B	1.369(18)
C37B - C42B	1.377(19)
C38B - C39B	1.386(21)
C39B - C40B	1.337(25)
C40B - C41B	1.359(23)
C41B - C42B	1.388(22)
O4A - C43A	1.448(21)
O4A - C46A	1.478(21)
C43A - C44A	1.449(29)
C44A - C45A	1.546(37)
C45A - C46A	1.517(31)
O4B - C43B	1.446(36)
O4B - C46B	1.555(40)
C43B - C44B	1.405(48)
C44B - C45B	1.517(56)
C45B - C46B	1.395(51)
O4C - C43C	1.425(31)
O4C - C46C	1.508(25)
C43C - C44C	1.632(48)

Table SVIII (continued)

C44C - C45C	1.433(51)
C45C - C46C	1.454(37)
O4D - C43D	1.498(58)
O4D - C46D	1.431(56)
C43D - C44D	1.655(51)
C44D - C45D	1.415(52)
C45D - C46D	1.541(61)
O4E - C43E	1.445(63)
O4E - C46E	1.583(54)
C43E - C44E	1.480(78)
C44E - C45E	1.384(81)
C45E - C46E	1.354(78)

C2A -Mn1A-C3A	88.1(7)
C1A -Mn1A-C3A	86.9(6)
C1A -Mn1A-C2A	93.4(6)
P2A -Mn1A-C3A	91.0(6)
P2A -Mn1A-C2A	166.3(4)
P2A -Mn1A-C1A	100.2(4)
P1A -Mn1A-C3A	94.7(5)
P1A -Mn1A-C2A	94.4(4)
P1A -Mn1A-C1A	172.1(5)
P1A -Mn1A-P2A	72.1(1)
I1A'-Mn1A-C2A	85.0(5)
I1A'-Mn1A-C1A	84.1(5)
I1A'-Mn1A-P2A	94.7(2)
I1A'-Mn1A-P1A	97.9(3)
I1A -Mn1A-C3A	171.1(5)
I1A -Mn1A-C2A	89.5(4)
I1A -Mn1A-C1A	84.7(5)
I1A -Mn1A-P2A	93.4(1)
I1A -Mn1A-P1A	94.1(1)
I1A -Mn1A-I1A'	167.1(3)
Mn1A-P1A -C25A	118.7(4)
Mn1A-P1A -C19A	116.6(3)
Mn1A-P1A -C4A	94.5(3)
C19A-P1A -C25A	105.0(5)
C4A -P1A -C25A	110.3(5)
C4A -P1A -C19A	111.5(4)
Mn1A-P2A -C37A	124.7(4)
Mn1A-P2A -C31A	116.2(4)
Mn1A-P2A -C4A	94.6(3)
C31A-P2A -C37A	105.0(5)
C4A -P2A -C37A	105.7(5)
C4A -P2A -C31A	108.8(5)
C5A -N1A -C8A	110.3(8)
C6A -N2A -C13A	119.4(9)
Mn1A-C1A -O1A	174.0(14)

Table SVIII (continued)

Mn1A-C2A -O2A	175.7(12)
Mn1A-C3A -O3A	167.1(21)
P1A -C4A -P2A	98.6(4)
P2A -C4A -C5A	130.4(8)
P1A -C4A -C5A	130.7(8)
N1A -C5A -C4A	124.8(9)
C4A -C5A -C6A	128.4(9)
N1A -C5A -C6A	106.7(8)
N2A -C6A -C5A	117.7(9)
C5A -C6A -C7A	104.3(8)
N2A -C6A -C7A	137.8(10)
C6A -C7A -C12A	130.9(10)
C6A -C7A -C8A	108.9(9)
C8A -C7A -C12A	120.2(10)
N1A -C8A -C7A	109.7(9)
C7A -C8A -C9A	122.5(10)
N1A -C8A -C9A	127.8(10)
C8A -C9A -C10A	116.3(11)
C9A -C10A-C11A	121.1(13)
C10A-C11A-C12A	122.3(13)
C7A -C12A-C11A	117.5(11)
N2A -C13A-C18A	120.2(11)
N2A -C13A-C14A	119.3(11)
C14A-C13A-C18A	120.3(12)
C13A-C14A-C15A	119.8(13)
C14A-C15A-C16A	119.9(17)
C15A-C16A-C17A	118.7(17)
C16A-C17A-C18A	121.0(17)
C13A-C18A-C17A	120.4(13)
P1A -C19A-C24A	123.7(8)
P1A -C19A-C20A	118.1(8)
C20A-C19A-C24A	117.9(10)
C19A-C20A-C21A	120.3(11)
C20A-C21A-C22A	120.4(13)
C21A-C22A-C23A	120.3(15)
C22A-C23A-C24A	121.3(11)
C19A-C24A-C23A	119.7(10)
P1A -C25A-C30A	122.2(10)
P1A -C25A-C26A	119.8(9)
C26A-C25A-C30A	118.0(12)
C25A-C26A-C27A	119.4(12)
C26A-C27A-C28A	122.4(15)
C27A-C28A-C29A	118.7(19)
C28A-C29A-C30A	120.1(16)
C25A-C30A-C29A	121.3(14)
P2A -C31A-C36A	118.2(9)
P2A -C31A-C32A	123.2(9)
C32A-C31A-C36A	118.5(11)

Table SVIII (continued)

C31A-C32A-C33A	120.3(11)
C32A-C33A-C34A	121.3(11)
C33A-C34A-C35A	119.9(15)
C34A-C35A-C36A	120.0(14)
C31A-C36A-C35A	119.7(12)
P2A -C37A-C42A	119.0(9)
P2A -C37A-C38A	121,1(9)
C38A-C37A-C42A	119.9(12)
C37A-C38A-C39A	117.6(12)
C38A-C39A-C40A	120.7(15)
C39A-C40A-C41A	119.2(19)
C40A-C41A-C42A	122.0(14)
C37A-C42A-C41A	120.5(12)
C3B -Mn1B-C3B'	174.5(10)
C2B -Mn1B-C3B'	88.2(11)
C2B -Mn1B-C3B	87.5(7)
C1B -Mn1B-C3B'	88.7(11)
C1B -Mn1B-C3B	88.4(7)
C1B -Mn1B-C2B	96.2(6)
P2B -Mn1B-C3B'	90.9(10)
P2B -Mn1B-C3B	94.1(6)
P2B -Mn1B-C2B	166.4(4)
P2B -Mn1B-C1B	97.3(4)
P1B -Mn1B-C3B'	89.9(10)
P1B -Mn1B-C3B	93.8(6)
P1B -Mn1B-C2B	94.1(4)
P1B -Mn1B-C1B	169.6(4)
P1B -Mn1B-P2B	72.4(1)
I1B'-Mn1B-C3B'	178.0(9)
I1B'-Mn1B-C2B	90.5(5)
I1B'-Mn1B-C1B	89.9(4)
I1B'-Mn1B-P2B	90.8(1)
I1B'-Mn1B-P1B	91.7(1)
I1B -Mn1B-C3B	170.6(5)
I1B -Mn1B-C2B	86.8(5)
I1B -Mn1B-C1B	84.8(4)
I1B -Mn1B-P2B	93.2(1)
I1B -Mn1B-P1B	94.1(1)
I1B -Mn1B-I1B'	173.7(1)
Mn1B-P1B -C25B	118.3(4)
Mn1B-P1B -C19B	118.0(4)
Mn1B-P1B -C4B	94.6(3)
C19B-P1B -C25B	104.5(6)
C4B -P1B -C25B	110.1(5)
C4B -P1B -C19B	111.0(5)
Mn1B-P2B -C37B	121.8(4)
Mn1B-P2B -C31B	118.3(4)
Mn1B-P2B -C4B	94.3(3)

Table SVIII (continued)

C31B-P2B -C37B	103.1(5)
C4B -P2B -C37B	108.5(5)
C4B -P2B -C31B	110.0(5)
C5B -N1B -C8B	109.1(9)
C13B-N2B -C13C	16.8(13)
C6B -N2B -C13C	122.7(14)
C6B -N2B -C13B	122.7(14)
Mn1B-C1B -O1B	177.0(11)
Mn1B-C2B -O2B	178.7(13)
Mn1B-C3B -O3B	166.6(22)
Mn1B-C3B'-O3B'	172.0(30)
P1B -C4B -P2B	98.4(5)
P2B -C4B -C5B	129.4(8)
P1B -C4B -C5B	130.9(8)
N1B -C5B -C4B	127.4(10)
C4B -C5B -C6B	127.4(10)
N1B -C5B -C6B	105.0(9)
N2B -C6B -C5B	118.6(11)
C5B -C6B -C7B	109.7(9)
N2B -C6B -C7B	131.5(11)
C6B -C7B -C12B	133.5(10)
C6B -C7B -C8B	106.7(10)
C8B -C7B -C12B	119.8(11)
N1B -C8B -C7B	109.1(10)
C7B -C8B -C9B	122.4(11)
N1B -C8B -C9B	128.5(11)
C8B -C9B -C10B	117.7(12)
C9B -C10B-C11B	120.5(13)
C10B-C11B-C12B	124.3(13)
C7B -C12B-C11B	115.3(11)
N2B -C13B-C18B	120.9(19)
N2B -C13B-C14B	119.1(20)
C14B-C13B-C18B	120.0(22)
C13B-C14B-C15B	120.0(23)
C14B-C15B-C16B	120.0(21)
C15B-C16B-C17B	120.0(22)
C16B-C17B-C18B	120.0(23)
C13B-C18B-C17B	120.0(21)
N2B -C13C-C18C	125.0(19)
N2B -C13C-C14C	114.6(20)
C14C-C13C-C18C	120.0(22)
C13C-C14C-C15C	120.0(23)
C14C-C15C-C16C	120.0(20)
C15C-C16C-C17C	120.0(22)
C16C-C17C-C18C	120.0(23)
C15B-C17C-C18C	104.7(28)
C13C-C18C-C17C	120.0(20)
P1B -C19B-C24B	118.3(9)

Table SVIII (continued)

P1B -C19B-C20B	122.9(10)
C20B-C19B-C24B	118.8(12)
C19B-C20B-C21B	119.5(13)
C20B-C21B-C22B	119.5(15)
C21B-C22B-C23B	120.3(17)
C22B-C23B-C24B	121.1(15)
C19B-C24B-C23B	120.5(12)
P1B -C25B-C30B	122.5(9)
P1B -C25B-C26B	121.5(9)
C26B-C25B-C30B	115.9(13)
C25B-C26B-C27B	123.0(13)
C26B-C27B-C28B	119.8(15)
C27B-C28B-C29B	119.9(17)
C28B-C29B-C30B	119.8(15)
C25B-C30B-C29B	121.6(12)
P2B -C31B-C36B	121.5(9)
P2B -C31B-C32B	118.2(9)
C32B-C31B-C36B	120.2(12)
C31B-C32B-C33B	121.3(12)
C32B-C33B-C34B	119.5(14)
C33B-C34B-C35B	118.9(16)
C34B-C35B-C36B	120.8(13)
C31B-C36B-C35B	118.8(12)
P2B -C37B-C42B	119.3(9)
P2B -C37B-C38B	122.5(9)
C38B-C37B-C42B	118.1(11)
C37B-C38B-C39B	120.9(13)
C38B-C39B-C40B	121.2(15)
C39B-C40B-C41B	118.6(16)
C40B-C41B-C42B	121.8(15)
C37B-C42B-C41B	119.5(13)
C43A-O4A -C46A	112.9(12)
O4A -C43A-C44A	108.9(15)
C43A-C44A-C45A	103.4(19)
C44A-C45A-C46A	110.4(20)
O4A -C46A-C45A	101.5(15)
C43B-O4B -C46B	107.7(21)
O4B -C43B-C44B	98.2(25)
C43B-C44B-C45B	120.6(31)
C44B-C45B-C46B	96.8(30)
O4B -C46B-C45B	108.1(28)
C43C-O4C -C46C	113.1(17)
O4C -C43C-C44C	101.4(22)
C43C-C44C-C45C	108.0(29)
C44C-C45C-C46C	110.2(28)
O4C -C46C-C45C	106.1(18)
C43D-O4D -C46D	126.2(33)
O4D -C43D-C44D	91.1(28)

Table SVIII (continued)

C43D-C44D-C45D	112.1(27)
C44D-C45D-C46D	111.2(35)
O4D -C46D-C45D	96.8(31)
C43E-O4E -C46E	114.2(32)
O4E -C43E-C44E	98.5(43)
C43E-C44E-C45E	111.8(47)
C44E-C45E-C46E	116.1(50)
O4E -C46E-C45E	98.3(40)

Table SIX - Experimental Data for the X-ray Diffraction Studies

Compound	**4b**	**6**
formula	$C_{33}H_{29}IMnNO_3P_2$	$C_{42}H_{30}IMnN_2O_3P_2 \cdot 2.5C_4H_8O$
mol wt	731.39	1034.77
cryst system	monoclinic	monoclinic
space group	$P2_1/n$	$P2_1/c$
radiation (λ Å)	graphite-monochromated (Mo-Kα, 0.71073)	
a, Å	11.629(3)	12.540(3)
b, Å	20.177(5)	21.717(5)
c, Å	14.134(4)	37.098(7)
β, deg	94.68(2)	95.81(2)
V, Å^3	3305(1)	10051(4)
Z	4	8
D_{calcd}, g cm^{-3}	1.470	1.368
F(000)	1464	4224
cryst size, mm	0.18x0.22x0.25	0.20x0.25x0.30
μ(Mo-Kα), cm^{-1}	14.62	9.88
diffractometer	Philips PW 1100	Philips PW 1100
scan type	θ/2θ	θ/2θ
scan speed, deg/min	3-12	3-12
θ range, deg	3-27	3-30
std reflctn	one measd after 100 reflctns	
reflectns measd	±*h*,*k*,*l*	±*h*,*k*,*l*
unique total data	7186	29394
unique obsd data [$I > 2\sigma(I)$]	2265	8317
R^a	0.0567	0.0766
$R_W{}^b$	0.0664	0.0832

^{a} $R = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. ^{b} $R_W = [\Sigma w(|F_o|-|F_c|)^2/\Sigma w(F_o)^2]^{1/2}$

Description of the synthetic procedures for the new compounds and additional spectroscopic data.

The synthesis of complexes type **1** and **2** has been described in: Ruiz, J.; Riera, V.; Vivanco, M.; García-Granda, S.; García-Fernández, A. *Organometallics* **1992**, *11*, 4077.

***fac*-[Mn(CO)$_3$(CN^{t}Bu){(PPh$_2$)$_2$CI}]** (**3b**). A solution of **2b** (0.30 g, 0.49 mmol) in 20 mL of CH_2Cl_2 was added dropwise to an stirred solution of iodine (0.19 g, 0.74 mmol) in 5 mL of CH_2Cl_2. The resulting mixture was vigorously stirred with an excess of KOH (1 g, 18 mmol) for 1 h. The solution was then filtered off and the solvent was evaporated to dryness affording a yellow solid corresponding to **3b**. Yield: 0.33 g, 90 %. Anal. Calcd for $C_{33}H_{29}IMnNO_3P_2$: C, 54.19; H, 4.00; N, 1.91. Found: C, 53.95; H, 3.99; N, 1.94. FTIR (CH_2Cl_2) ν(CO) 2016 (vs), 1951 (s), 1936 (s) cm^{-1}, ν(CN) 2172 (m) cm^{-1}; ^{1}H NMR (CD_2Cl_2) δ 0.73 (s, C(CH$_3$)$_3$); ^{13}C NMR (CD_2Cl_2) δ -35.3 (t, $^1J_{C\text{-}P}$ = 49 Hz, P$_2$CI); ^{31}P {^{1}H} NMR (CD_2Cl_2) δ 12.1 (s).

Complex ***fac*-[Mn(CO)$_3$(CNPh){(PPh$_2$)$_2$CI}]** (**3a**) was prepared in a similar way starting from **2a** (0.10 g, 0.16 mmol). In this case the reaction mixture must be maintained at 0 °C to avoid significant transformation of **3a** into **4a**. Yield: 0.10 g, 85 %. Anal. Calcd for $C_{35}H_{25}IMnNO_3P_2$: C, 55.95; H, 3.35; N, 1.86. Found: C, 55.73; H, 3.58; N, 1.75. FTIR (CH_2Cl_2) ν(CO) 2017 (vs), 1961 (s), 1943 (s) cm^{-1}, ν(CN) 2148 (m) cm^{-1}; ^{31}P {^{1}H} NMR (CD_2Cl_2) δ 11.8 (s).

***fac*-[Mn(CO)$_3$I{(PPh$_2$)$_2$CCNPh}]** (**4a**). A solution of *fac*-[Mn(CO)$_3$(CNPh){(PPh$_2$)$_2$CH}] (**2a**) (0.30 g, 0.48 mmol) in 25 mL of CH_2Cl_2 was added dropwise to 0.18 g of iodine (0.72 mmol) at room temperature with continuous stirring. Once the addition was finished, an excess of KOH (1 g, 18 mmol) was added to the solution, and the resulting mixture was stirred for 1 h. The solution was filtered off and let to stay at room temperature for 2 h. The solvent was then removed under reduced pressure affording an orange solid, which was purified by recrystallization from a mixture

of toluene/hexane at -15 °C. Yield: 0.25 g, 70 %. Anal. Calcd for $C_{35}H_{25}IMnNO_3P_2$: C, 55.95; H, 3.35; N, 1.86. Found: C, 56.02; H, 3.40; N, 1.92

***fac*-[Mn(CO)$_3$I{(PPh$_2$)$_2$CCN^{t}Bu}] (4b).** A suspension of **3b** (0.40 g, 0.54 mmol) in 25 mL of toluene was refluxed for 10 min. After this time, an orange solution was formed which was concentrated under vacuum to about 7 mL and cooled to -15 °C to obtain orange needles of **4b**. Yield: 0.36 g, 90 %. Anal. Calcd for $C_{33}H_{29}IMnNO_3P_2$: C, 54.19; H, 4.00; N, 1.91. Found: C, 54.03; H, 3.86; N, 1.72. Suitable crystals for X-ray analysis were obtained from a dichloromethane solution layered with hexane.

{(PPh$_2$)$_2$CCNPh} (5a). A solution of 0.2 g of **4a** (0.27 mmol) in 25 mL of toluene was irradiated with visible-uv light at 10 °C for 3 h. The solvent was then removed under vacuum and the remaining solid chromatographed through an alumina column (activity III) prepared in hexane. Elution with toluene/hexane (1/2) gave a very pale yellow fraction, from which, after removing the solvent to dryness, a pale yellow oil corresponding to **5a** was obtained (spectroscopically pure by ^{31}P and ^{13}C N.M.R.). Aprox. yield: 48 mg, 37 %.

{(PPh$_2$)$_2$CCN^{t}Bu} (5b). This was prepared similarly to **5a** starting from **4b** (0.30 g, 0.41 mmol). The product was isolated as a white microcystalline solid from an hexane solution at -20 °C. Yield: 63 mg, 33 %. Melting Point: 118 °C. Anal. Calcd for $C_{30}H_{29}NP_2$: C, 77.40; H, 6.38; N, 3.01. Found: C, 77.27; H, 6.20; N, 3.02.

***fac*-[Mn(CO)$_3$I{(PPh$_2$)$_2$CC(NH)(CNPh)(C$_6$H$_4$)}] (6).** To a solution of **4a** (0.30 g, 0.40 mmol) in 20 mL of CH_2Cl_2 was added phenylisocyanide (50 mg, 0.48 mmol). After stirring at room temperature for 12 h, the color of the solution changed from orange to dark red. The solvent was evaporated to dryness and the residue washed with hexane (3 x 10 mL) to provide a dark red solid. Yield: 0.31 g, 90 %. Anal. Calcd for $C_{42}H_{30}IMnN_2O_3P_2$: C, 59.04; H, 3.54; N, 3.28. Found: C, 58.83; H, 3.62; N, 3.15. Suitable crystals for X-ray analysis where obtained from a saturated solution of **6** in a mixture of THF/toluene/hexane.