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Supplementary Information

Univalent Transition Metal Complexes of Arenes Stabilized by a Bulky Terphenyl Ligand: Differences in the Stability of Cr(I), Mn(I) or Fe(I) complexes

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Crystallographic Data of [(μ-η^6:η^6-C_7H_8){MnAr*-3,5-Pr^i_2}$_2$] (**1**)

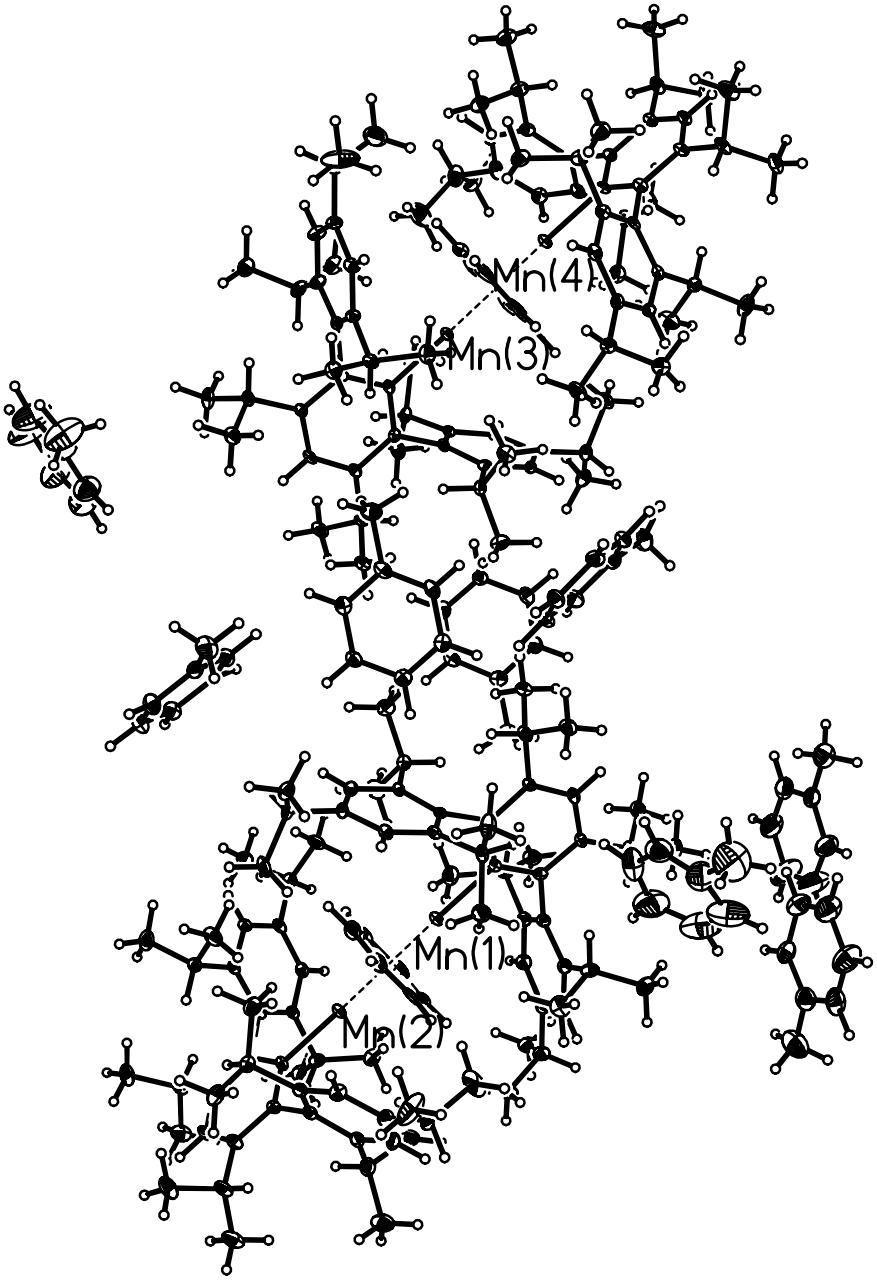

Table 1. Crystal data and structure refinement for [(μ-η^6:η^6-C_7H_8){MnAr*-3,5-Pr^i_2}$_2$] (**1**).

Identification code	jf1508affmi	
Empirical formula	$C_{119}H_{162}Mn_2$	
Formula weight	1687.32	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P n a 2(1)	
Unit cell dimensions	a = 23.2481(11) Å	α= 90°.
	b = 18.7415(9) Å	β= 90°.
	c = 46.380(2) Å	γ = 90°.
Volume	20208.1(17) Å^3	
Z	8	
Density (calculated)	1.109 Mg/m^3	
Absorption coefficient	0.297 mm^{-1}	
F(000)	7408	
Crystal size	0.44 x 0.34 x 0.23 mm^3	
Theta range for data collection	2.81 to 27.11°.	
Index ranges	-29<=h<=29, -24<=k<=24, -59<=l<=59	
Reflections collected	169346	
Independent reflections	44483 [R(int) = 0.0866]	
Completeness to theta = 27.11°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9348 and 0.8803	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	44483 / 13 / 2210	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0595, wR2 = 0.1374	
R indices (all data)	R1 = 0.0902, wR2 = 0.1501	
Absolute structure parameter	0.047(12)	
Largest diff. peak and hole	1.554 and -0.621 e.Å^{-3}	

Table 2. Bond lengths [Å] and angles [°] for [(μ-η^6:η^6-C_7H_8){MnAr*-3,5-Pr^i_2}$_2$] (**1**).

Mn(1)-C(1)	2.088(3)	C(10)-C(12)	1.521(5)
Mn(1)-C(95)	2.245(3)	C(10)-C(11)	1.534(5)
Mn(1)-C(94)	2.243(3)	C(10)-H(10)	1.0000
Mn(1)-C(96)	2.262(3)	C(11)-H(11A)	0.9800
Mn(1)-C(93)	2.258(3)	C(11)-H(11B)	0.9800
Mn(1)-C(91)	2.277(3)	C(11)-H(11C)	0.9800
Mn(1)-C(92)	2.275(3)	C(12)-H(12A)	0.9800
Mn(2)-C(43)	2.089(3)	C(12)-H(12B)	0.9800
Mn(2)-C(93)	2.249(3)	C(12)-H(12C)	0.9800
Mn(2)-C(94)	2.237(3)	C(13)-C(14)	1.397(5)
Mn(2)-C(92)	2.270(3)	C(13)-C(18)	1.430(5)
Mn(2)-C(95)	2.246(3)	C(14)-C(15)	1.404(5)
Mn(2)-C(91)	2.279(3)	C(14)-C(19)	1.536(5)
Mn(2)-C(96)	2.267(3)	C(15)-C(16)	1.382(5)
C(1)-C(6)	1.403(5)	C(15)-H(15)	0.9500
C(1)-C(2)	1.407(5)	C(16)-C(17)	1.390(5)
C(2)-C(3)	1.405(4)	C(16)-C(22)	1.538(5)
C(2)-C(13)	1.517(5)	C(17)-C(18)	1.391(5)
C(3)-C(4)	1.390(5)	C(17)-H(17)	0.9500
C(3)-C(7)	1.517(5)	C(18)-C(25)	1.515(5)
C(4)-C(5)	1.394(5)	C(19)-C(21)	1.507(5)
C(4)-H(4)	0.9500	C(19)-C(20)	1.511(5)
C(5)-C(6)	1.402(4)	C(19)-H(19)	1.0000
C(5)-C(10)	1.525(5)	C(20)-H(20A)	0.9800
C(6)-C(28)	1.512(4)	C(20)-H(20B)	0.9800
C(7)-C(8)	1.522(5)	C(20)-H(20C)	0.9800
C(7)-C(9)	1.536(5)	C(21)-H(21A)	0.9800
C(7)-H(7)	1.0000	C(21)-H(21B)	0.9800
C(8)-H(8A)	0.9800	C(21)-H(21C)	0.9800
C(8)-H(8B)	0.9800	C(22)-C(24)	1.496(6)
C(8)-H(8C)	0.9800	C(22)-C(23)	1.533(6)
C(9)-H(9A)	0.9800	C(22)-H(22)	1.0000
C(9)-H(9B)	0.9800	C(23)-H(23A)	0.9800
C(9)-H(9C)	0.9800	C(23)-H(23B)	0.9800

C(23)-H(23C)	0.9800	C(38)-H(38A)	0.9800
C(24)-H(24A)	0.9800	C(38)-H(38B)	0.9800
C(24)-H(24B)	0.9800	C(38)-H(38C)	0.9800
C(24)-H(24C)	0.9800	C(39)-H(39A)	0.9800
C(25)-C(27)	1.521(6)	C(39)-H(39B)	0.9800
C(25)-C(26)	1.542(6)	C(39)-H(39C)	0.9800
C(25)-H(25)	1.0000	C(40)-C(41)	1.510(5)
C(26)-H(26A)	0.9800	C(40)-C(42)	1.539(5)
C(26)-H(26B)	0.9800	C(40)-H(40)	1.0000
C(26)-H(26C)	0.9800	C(41)-H(41A)	0.9800
C(27)-H(27A)	0.9800	C(41)-H(41B)	0.9800
C(27)-H(27B)	0.9800	C(41)-H(41C)	0.9800
C(27)-H(27C)	0.9800	C(42)-H(42A)	0.9800
C(28)-C(33)	1.402(5)	C(42)-H(42B)	0.9800
C(28)-C(29)	1.416(5)	C(42)-H(42C)	0.9800
C(29)-C(30)	1.385(5)	C(43)-C(48)	1.396(5)
C(29)-C(34)	1.528(5)	C(43)-C(44)	1.426(5)
C(30)-C(31)	1.406(5)	C(44)-C(45)	1.396(5)
C(30)-H(30)	0.9500	C(44)-C(55)	1.508(5)
C(31)-C(32)	1.385(5)	C(45)-C(46)	1.382(5)
C(31)-C(37)	1.528(5)	C(45)-C(49)	1.514(5)
C(32)-C(33)	1.401(5)	C(46)-C(47)	1.383(5)
C(32)-H(32)	0.9500	C(46)-H(46)	0.9500
C(33)-C(40)	1.526(5)	C(47)-C(48)	1.412(4)
C(34)-C(35)	1.517(5)	C(47)-C(52)	1.539(5)
C(34)-C(36)	1.537(5)	C(48)-C(70)	1.514(5)
C(34)-H(34)	1.0000	C(49)-C(50)	1.524(6)
C(35)-H(35A)	0.9800	C(49)-C(51)	1.550(6)
C(35)-H(35B)	0.9800	C(49)-H(49)	1.0000
C(35)-H(35C)	0.9800	C(50)-H(50A)	0.9800
C(36)-H(36A)	0.9800	C(50)-H(50B)	0.9800
C(36)-H(36B)	0.9800	C(50)-H(50C)	0.9800
C(36)-H(36C)	0.9800	C(51)-H(51A)	0.9800
C(37)-C(38)	1.524(5)	C(51)-H(51B)	0.9800
C(37)-C(39)	1.524(5)	C(51)-H(51C)	0.9800
C(37)-H(37)	1.0000	C(52)-C(53)	1.522(5)

C(52)-C(54)	1.531(5)	C(66)-H(66C)	0.9800
C(52)-H(52)	1.0000	C(67)-C(69)	1.521(6)
C(53)-H(53A)	0.9800	C(67)-C(68)	1.537(6)
C(53)-H(53B)	0.9800	C(67)-H(67)	1.0000
C(53)-H(53C)	0.9800	C(68)-H(68A)	0.9800
C(54)-H(54A)	0.9800	C(68)-H(68B)	0.9800
C(54)-H(54B)	0.9800	C(68)-H(68C)	0.9800
C(54)-H(54C)	0.9800	C(69)-H(69A)	0.9800
C(55)-C(56)	1.399(5)	C(69)-H(69B)	0.9800
C(55)-C(60)	1.422(5)	C(69)-H(69C)	0.9800
C(56)-C(57)	1.400(5)	C(70)-C(71)	1.407(5)
C(56)-C(61)	1.526(5)	C(70)-C(75)	1.415(5)
C(57)-C(58)	1.388(5)	C(71)-C(72)	1.384(5)
C(57)-H(57)	0.9500	C(71)-C(76)	1.535(5)
C(58)-C(59)	1.381(5)	C(72)-C(73)	1.387(5)
C(58)-C(64)	1.534(5)	C(72)-H(72)	0.9500
C(59)-C(60)	1.379(5)	C(73)-C(74)	1.402(5)
C(59)-H(59)	0.9500	C(73)-C(79)	1.527(5)
C(60)-C(67)	1.534(5)	C(74)-C(75)	1.404(5)
C(61)-C(62)	1.519(5)	C(74)-H(74)	0.9500
C(61)-C(63)	1.536(5)	C(75)-C(82)	1.513(5)
C(61)-H(61)	1.0000	C(76)-C(77)	1.524(5)
C(62)-H(62A)	0.9800	C(76)-C(78)	1.540(5)
C(62)-H(62B)	0.9800	C(76)-H(76)	1.0000
C(62)-H(62C)	0.9800	C(77)-H(77A)	0.9800
C(63)-H(63A)	0.9800	C(77)-H(77B)	0.9800
C(63)-H(63B)	0.9800	C(77)-H(77C)	0.9800
C(63)-H(63C)	0.9800	C(78)-H(78A)	0.9800
C(64)-C(65)	1.496(7)	C(78)-H(78B)	0.9800
C(64)-C(66)	1.517(6)	C(78)-H(78C)	0.9800
C(64)-H(64)	1.0000	C(79)-C(81)	1.512(5)
C(65)-H(65A)	0.9800	C(79)-C(80)	1.542(5)
C(65)-H(65B)	0.9800	C(79)-H(79)	1.0000
C(65)-H(65C)	0.9800	C(80)-H(80A)	0.9800
C(66)-H(66A)	0.9800	C(80)-H(80B)	0.9800
C(66)-H(66B)	0.9800	C(80)-H(80C)	0.9800

C(81)-H(81A)	0.9800	Mn(4)-C(92G)	2.284(3)
C(81)-H(81B)	0.9800	Mn(4)-C(91G)	2.288(2)
C(81)-H(81C)	0.9800	C(101)-C(106)	1.412(5)
C(82)-C(83)	1.509(5)	C(101)-C(102)	1.424(5)
C(82)-C(84)	1.549(6)	C(102)-C(103)	1.410(4)
C(82)-H(82)	1.0000	C(102)-C(113)	1.510(4)
C(83)-H(83A)	0.9800	C(103)-C(104)	1.380(5)
C(83)-H(83B)	0.9800	C(103)-C(107)	1.506(5)
C(83)-H(83C)	0.9800	C(104)-C(105)	1.396(5)
C(84)-H(84A)	0.9800	C(104)-H(104)	0.9500
C(84)-H(84B)	0.9800	C(105)-C(106)	1.409(4)
C(84)-H(84C)	0.9800	C(105)-C(110)	1.518(5)
C(91)-C(92)	1.3900	C(106)-C(128)	1.515(4)
C(91)-C(96)	1.3900	C(107)-C(109)	1.528(5)
C(91)-H(91)	0.9500	C(107)-C(108)	1.539(5)
C(92)-C(93)	1.3900	C(107)-H(107)	1.0000
C(92)-H(92)	0.9500	C(108)-H(10A)	0.9800
C(93)-C(94)	1.3900	C(108)-H(10B)	0.9800
C(93)-H(93)	0.9500	C(108)-H(10C)	0.9800
C(94)-C(95)	1.3900	C(109)-H(10D)	0.9800
C(94)-H(94)	0.9500	C(109)-H(10E)	0.9800
C(95)-C(96)	1.3900	C(109)-H(10F)	0.9800
C(95)-H(95)	0.9500	C(110)-C(112)	1.520(5)
C(96)-H(96)	0.9500	C(110)-C(111)	1.542(5)
Mn(3)-C(101)	2.076(3)	C(110)-H(110)	1.0000
Mn(3)-C(94G)	2.246(2)	C(111)-H(11D)	0.9800
Mn(3)-C(93G)	2.249(3)	C(111)-H(11E)	0.9800
Mn(3)-C(95G)	2.254(3)	C(111)-H(11F)	0.9800
Mn(3)-C(92G)	2.261(3)	C(112)-H(11G)	0.9800
Mn(3)-C(96G)	2.265(3)	C(112)-H(11H)	0.9800
Mn(3)-C(91G)	2.268(2)	C(112)-H(11I)	0.9800
Mn(4)-C(143)	2.085(3)	C(113)-C(118)	1.410(4)
Mn(4)-C(94G)	2.244(2)	C(113)-C(114)	1.419(5)
Mn(4)-C(95G)	2.248(3)	C(114)-C(115)	1.383(5)
Mn(4)-C(93G)	2.263(3)	C(114)-C(119)	1.523(5)
Mn(4)-C(96G)	2.270(3)	C(115)-C(116)	1.391(5)

C(115)-H(115)	0.9500	C(129)-C(134)	1.519(5)
C(116)-C(117)	1.384(5)	C(130)-C(131)	1.390(5)
C(116)-C(122)	1.524(5)	C(130)-H(130)	0.9500
C(117)-C(118)	1.396(4)	C(131)-C(132)	1.396(5)
C(117)-H(117)	0.9500	C(131)-C(137)	1.512(5)
C(118)-C(125)	1.528(4)	C(132)-C(133)	1.396(5)
C(119)-C(121)	1.529(5)	C(132)-H(132)	0.9500
C(119)-C(120)	1.538(5)	C(133)-C(140)	1.506(5)
C(119)-H(119)	1.0000	C(134)-C(135)	1.519(6)
C(120)-H(12D)	0.9800	C(134)-C(136)	1.527(5)
C(120)-H(12E)	0.9800	C(134)-H(134)	1.0000
C(120)-H(12F)	0.9800	C(135)-H(13A)	0.9800
C(121)-H(12G)	0.9800	C(135)-H(13B)	0.9800
C(121)-H(12H)	0.9800	C(135)-H(13C)	0.9800
C(121)-H(12I)	0.9800	C(136)-H(13D)	0.9800
C(122)-C(124)	1.514(5)	C(136)-H(13E)	0.9800
C(122)-C(123)	1.540(5)	C(136)-H(13F)	0.9800
C(122)-H(122)	1.0000	C(137)-C(138)	1.498(6)
C(123)-H(12J)	0.9800	C(137)-C(139)	1.515(6)
C(123)-H(12K)	0.9800	C(137)-H(137)	1.0000
C(123)-H(12L)	0.9800	C(138)-H(13G)	0.9800
C(124)-H(12M)	0.9800	C(138)-H(13H)	0.9800
C(124)-H(12N)	0.9800	C(138)-H(13I)	0.9800
C(124)-H(12O)	0.9800	C(139)-H(13J)	0.9800
C(125)-C(126)	1.522(5)	C(139)-H(13K)	0.9800
C(125)-C(127)	1.539(5)	C(139)-H(13L)	0.9800
C(125)-H(125)	1.0000	C(140)-C(142)	1.533(5)
C(126)-H(12P)	0.9800	C(140)-C(141)	1.535(5)
C(126)-H(12Q)	0.9800	C(140)-H(140)	1.0000
C(126)-H(12R)	0.9800	C(141)-H(14A)	0.9800
C(127)-H(12S)	0.9800	C(141)-H(14B)	0.9800
C(127)-H(12T)	0.9800	C(141)-H(14C)	0.9800
C(127)-H(12U)	0.9800	C(142)-H(14D)	0.9800
C(128)-C(129)	1.399(5)	C(142)-H(14E)	0.9800
C(128)-C(133)	1.413(5)	C(142)-H(14F)	0.9800
C(129)-C(130)	1.399(5)	C(143)-C(144)	1.397(5)

C(143)-C(148)	1.431(5)	C(159)-C(160)	1.405(5)
C(144)-C(145)	1.419(5)	C(159)-H(159)	0.9500
C(144)-C(155)	1.523(5)	C(160)-C(167)	1.509(5)
C(145)-C(146)	1.381(5)	C(161)-C(162)	1.510(5)
C(145)-C(149)	1.525(5)	C(161)-C(163)	1.546(5)
C(146)-C(147)	1.404(5)	C(161)-H(161)	1.0000
C(146)-H(146)	0.9500	C(162)-H(16A)	0.9800
C(147)-C(148)	1.405(5)	C(162)-H(16B)	0.9800
C(147)-C(152)	1.505(5)	C(162)-H(16C)	0.9800
C(148)-C(170)	1.503(4)	C(163)-H(16D)	0.9800
C(149)-C(151)	1.533(5)	C(163)-H(16E)	0.9800
C(149)-C(150)	1.537(6)	C(163)-H(16F)	0.9800
C(149)-H(149)	1.0000	C(164)-C(166)	1.495(6)
C(150)-H(15A)	0.9800	C(164)-C(165)	1.521(7)
C(150)-H(15B)	0.9800	C(164)-H(164)	1.0000
C(150)-H(15C)	0.9800	C(165)-H(16G)	0.9800
C(151)-H(15D)	0.9800	C(165)-H(16H)	0.9800
C(151)-H(15E)	0.9800	C(165)-H(16I)	0.9800
C(151)-H(15F)	0.9800	C(166)-H(16J)	0.9800
C(152)-C(153)	1.532(5)	C(166)-H(16K)	0.9800
C(152)-C(154)	1.538(5)	C(166)-H(16L)	0.9800
C(152)-H(152)	1.0000	C(167)-C(168)	1.521(6)
C(153)-H(15G)	0.9800	C(167)-C(169)	1.539(5)
C(153)-H(15H)	0.9800	C(167)-H(167)	1.0000
C(153)-H(15I)	0.9800	C(168)-H(16M)	0.9800
C(154)-H(15J)	0.9800	C(168)-H(16N)	0.9800
C(154)-H(15K)	0.9800	C(168)-H(16O)	0.9800
C(154)-H(15L)	0.9800	C(169)-H(16P)	0.9800
C(155)-C(156)	1.404(5)	C(169)-H(16Q)	0.9800
C(155)-C(160)	1.407(5)	C(169)-H(16R)	0.9800
C(156)-C(157)	1.390(5)	C(170)-C(175)	1.409(5)
C(156)-C(161)	1.521(5)	C(170)-C(171)	1.414(5)
C(157)-C(158)	1.392(5)	C(171)-C(172)	1.383(5)
C(157)-H(157)	0.9500	C(171)-C(176)	1.537(4)
C(158)-C(159)	1.392(5)	C(172)-C(173)	1.378(5)
C(158)-C(164)	1.521(5)	C(172)-H(172)	0.9500

C(173)-C(174)	1.378(5)	C(92G)-H(92G)	0.9500
C(173)-C(179)	1.523(5)	C(93G)-C(94G)	1.3900
C(174)-C(175)	1.418(5)	C(93G)-H(93G)	0.9500
C(174)-H(174)	0.9500	C(94G)-C(95G)	1.3900
C(175)-C(182)	1.508(5)	C(94G)-H(94G)	0.9500
C(176)-C(177)	1.523(5)	C(95G)-C(96G)	1.3900
C(176)-C(178)	1.526(6)	C(95G)-H(95G)	0.9500
C(176)-H(176)	1.0000	C(96G)-H(96G)	0.9500
C(177)-H(17A)	0.9800	C(201)-C(206)	1.278(9)
C(177)-H(17B)	0.9800	C(201)-C(202)	1.409(10)
C(177)-H(17C)	0.9800	C(201)-C(207)	1.411(10)
C(178)-H(17D)	0.9800	C(202)-C(203)	1.317(12)
C(178)-H(17E)	0.9800	C(202)-H(202)	0.9500
C(178)-H(17F)	0.9800	C(203)-C(204)	1.454(12)
C(179)-C(180)	1.521(5)	C(203)-H(203)	0.9500
C(179)-C(181)	1.529(5)	C(204)-C(205)	1.281(9)
C(179)-H(179)	1.0000	C(204)-H(204)	0.9500
C(180)-H(18A)	0.9800	C(205)-C(206)	1.502(9)
C(180)-H(18B)	0.9800	C(205)-H(205)	0.9500
C(180)-H(18C)	0.9800	C(206)-H(206)	0.9500
C(181)-H(18D)	0.9800	C(207)-H(20D)	0.9800
C(181)-H(18E)	0.9800	C(207)-H(20E)	0.9800
C(181)-H(18F)	0.9800	C(207)-H(20F)	0.9800
C(182)-C(183)	1.506(5)	C(211)-C(212)	1.350(8)
C(182)-C(184)	1.540(5)	C(211)-C(216)	1.401(6)
C(182)-H(182)	1.0000	C(211)-H(211)	0.9500
C(183)-H(18G)	0.9800	C(212)-C(213)	1.432(8)
C(183)-H(18H)	0.9800	C(212)-H(212)	0.9500
C(183)-H(18I)	0.9800	C(213)-C(214)	1.330(8)
C(184)-H(18J)	0.9800	C(213)-H(213)	0.9500
C(184)-H(18K)	0.9800	C(214)-C(215)	1.478(8)
C(184)-H(18L)	0.9800	C(214)-H(214)	0.9500
C(91G)-C(92G)	1.3900	C(215)-C(216)	1.367(7)
C(91G)-C(96G)	1.3900	C(215)-H(215)	0.9500
C(91G)-H(91G)	0.9500	C(216)-C(217)	1.440(7)
C(92G)-C(93G)	1.3900	C(217)-H(21D)	0.9800

C(217)-H(21E)	0.9800	C(242)-H(242)	0.9500
C(217)-H(21F)	0.9800	C(243)-C(244)	1.371(5)
C(221)-C(222)	1.368(8)	C(243)-H(243)	0.9500
C(221)-C(226)	1.383(7)	C(244)-C(245)	1.380(5)
C(221)-H(221)	0.9500	C(244)-H(244)	0.9500
C(222)-C(223)	1.376(9)	C(245)-C(246)	1.368(5)
C(222)-H(222)	0.9500	C(245)-H(245)	0.9500
C(223)-C(224)	1.361(9)	C(246)-H(246)	0.9500
C(223)-H(223)	0.9500	C(247)-H(24D)	0.9800
C(224)-C(225)	1.367(7)	C(247)-H(24E)	0.9800
C(224)-H(224)	0.9500	C(247)-H(24F)	0.9800
C(225)-C(226)	1.375(6)	C(251)-C(252)	1.374(5)
C(225)-H(225)	0.9500	C(251)-C(256)	1.397(5)
C(226)-C(227)	1.498(6)	C(251)-C(257)	1.518(5)
C(227)-H(22A)	0.9800	C(252)-C(253)	1.390(5)
C(227)-H(22B)	0.9800	C(252)-H(252)	0.9500
C(227)-H(22C)	0.9800	C(253)-C(254)	1.386(5)
C(231)-C(232)	1.373(5)	C(253)-H(253)	0.9500
C(231)-C(236)	1.387(5)	C(254)-C(255)	1.377(5)
C(231)-C(237)	1.518(5)	C(254)-H(254)	0.9500
C(232)-C(233)	1.392(5)	C(255)-C(256)	1.394(5)
C(232)-H(232)	0.9500	C(255)-H(255)	0.9500
C(233)-C(234)	1.387(5)	C(256)-H(256)	0.9500
C(233)-H(233)	0.9500	C(257)-H(25A)	0.9800
C(234)-C(235)	1.374(5)	C(257)-H(25B)	0.9800
C(234)-H(234)	0.9500	C(257)-H(25C)	0.9800
C(235)-C(236)	1.395(5)	C(261)-C(266)	1.379(5)
C(235)-H(235)	0.9500	C(261)-C(262)	1.392(5)
C(236)-H(236)	0.9500	C(261)-C(267)	1.507(5)
C(237)-H(23D)	0.9800	C(262)-C(263)	1.377(5)
C(237)-H(23E)	0.9800	C(262)-H(262)	0.9500
C(237)-H(23F)	0.9800	C(263)-C(264)	1.374(5)
C(241)-C(246)	1.394(5)	C(263)-H(263)	0.9500
C(241)-C(242)	1.405(5)	C(264)-C(265)	1.378(5)
C(241)-C(247)	1.493(5)	C(264)-H(264)	0.9500
C(242)-C(243)	1.373(5)	C(265)-C(266)	1.387(5)

C(265)-H(265)	0.9500	C(273)-C(274)	1.404(9)
C(266)-H(266)	0.9500	C(273)-H(273)	0.9500
C(267)-H(26D)	0.9800	C(274)-C(275)	1.328(9)
C(267)-H(26E)	0.9800	C(274)-H(274)	0.9500
C(267)-H(26F)	0.9800	C(275)-C(276)	1.391(8)
C(271)-C(276)	1.336(8)	C(275)-H(275)	0.9500
C(271)-C(272)	1.418(9)	C(276)-H(276)	0.9500
C(271)-C(277)	1.504(8)	C(277)-H(27D)	0.9800
C(272)-C(273)	1.366(9)	C(277)-H(27E)	0.9800
C(272)-H(272)	0.9500	C(277)-H(27F)	0.9800

C(1)-Mn(1)-C(95)	142.05(11)	C(4)-C(5)-C(10)	119.2(3)
C(1)-Mn(1)-C(94)	140.27(11)	C(6)-C(5)-C(10)	123.2(3)
C(1)-Mn(1)-C(96)	143.83(12)	C(5)-C(6)-C(1)	121.8(3)
C(1)-Mn(1)-C(93)	140.23(12)	C(5)-C(6)-C(28)	121.3(3)
C(1)-Mn(1)-C(91)	143.77(11)	C(1)-C(6)-C(28)	116.9(3)
C(1)-Mn(1)-C(92)	141.96(12)	C(3)-C(7)-C(8)	111.8(3)
C(43)-Mn(2)-C(93)	141.55(12)	C(3)-C(7)-C(9)	111.6(3)
C(43)-Mn(2)-C(94)	138.68(11)	C(8)-C(7)-C(9)	108.7(3)
C(43)-Mn(2)-C(92)	144.94(12)	C(3)-C(7)-H(7)	108.2
C(43)-Mn(2)-C(95)	139.01(12)	C(8)-C(7)-H(7)	108.2
C(43)-Mn(2)-C(91)	145.29(11)	C(9)-C(7)-H(7)	108.2
C(43)-Mn(2)-C(96)	142.23(13)	C(7)-C(8)-H(8A)	109.5
C(6)-C(1)-C(2)	117.8(3)	C(7)-C(8)-H(8B)	109.5
C(6)-C(1)-Mn(1)	120.6(2)	H(8A)-C(8)-H(8B)	109.5
C(2)-C(1)-Mn(1)	121.5(2)	C(7)-C(8)-H(8C)	109.5
C(3)-C(2)-C(1)	122.3(3)	H(8A)-C(8)-H(8C)	109.5
C(3)-C(2)-C(13)	120.9(3)	H(8B)-C(8)-H(8C)	109.5
C(1)-C(2)-C(13)	116.9(3)	C(7)-C(9)-H(9A)	109.5
C(4)-C(3)-C(2)	117.0(3)	C(7)-C(9)-H(9B)	109.5
C(4)-C(3)-C(7)	119.7(3)	H(9A)-C(9)-H(9B)	109.5
C(2)-C(3)-C(7)	123.3(3)	C(7)-C(9)-H(9C)	109.5
C(3)-C(4)-C(5)	123.5(3)	H(9A)-C(9)-H(9C)	109.5
C(3)-C(4)-H(4)	118.2	H(9B)-C(9)-H(9C)	109.5
C(5)-C(4)-H(4)	118.2	C(12)-C(10)-C(5)	111.7(3)
C(4)-C(5)-C(6)	117.6(3)	C(12)-C(10)-C(11)	111.0(3)

C(5)-C(10)-C(11)	111.3(3)	C(20)-C(19)-C(14)	111.5(3)
C(12)-C(10)-H(10)	107.6	C(21)-C(19)-H(19)	107.0
C(5)-C(10)-H(10)	107.6	C(20)-C(19)-H(19)	107.0
C(11)-C(10)-H(10)	107.6	C(14)-C(19)-H(19)	107.0
C(10)-C(11)-H(11A)	109.5	C(19)-C(20)-H(20A)	109.5
C(10)-C(11)-H(11B)	109.5	C(19)-C(20)-H(20B)	109.5
H(11A)-C(11)-H(11B)	109.5	H(20A)-C(20)-H(20B)	109.5
C(10)-C(11)-H(11C)	109.5	C(19)-C(20)-H(20C)	109.5
H(11A)-C(11)-H(11C)	109.5	H(20A)-C(20)-H(20C)	109.5
H(11B)-C(11)-H(11C)	109.5	H(20B)-C(20)-H(20C)	109.5
C(10)-C(12)-H(12A)	109.5	C(19)-C(21)-H(21A)	109.5
C(10)-C(12)-H(12B)	109.5	C(19)-C(21)-H(21B)	109.5
H(12A)-C(12)-H(12B)	109.5	H(21A)-C(21)-H(21B)	109.5
C(10)-C(12)-H(12C)	109.5	C(19)-C(21)-H(21C)	109.5
H(12A)-C(12)-H(12C)	109.5	H(21A)-C(21)-H(21C)	109.5
H(12B)-C(12)-H(12C)	109.5	H(21B)-C(21)-H(21C)	109.5
C(14)-C(13)-C(18)	118.8(3)	C(24)-C(22)-C(23)	110.4(3)
C(14)-C(13)-C(2)	120.0(3)	C(24)-C(22)-C(16)	114.5(3)
C(18)-C(13)-C(2)	121.2(3)	C(23)-C(22)-C(16)	110.2(3)
C(13)-C(14)-C(15)	120.1(3)	C(24)-C(22)-H(22)	107.1
C(13)-C(14)-C(19)	121.9(3)	C(23)-C(22)-H(22)	107.1
C(15)-C(14)-C(19)	118.0(3)	C(16)-C(22)-H(22)	107.1
C(16)-C(15)-C(14)	121.6(3)	C(22)-C(23)-H(23A)	109.5
C(16)-C(15)-H(15)	119.2	C(22)-C(23)-H(23B)	109.5
C(14)-C(15)-H(15)	119.2	H(23A)-C(23)-H(23B)	109.5
C(15)-C(16)-C(17)	118.0(3)	C(22)-C(23)-H(23C)	109.5
C(15)-C(16)-C(22)	122.9(3)	H(23A)-C(23)-H(23C)	109.5
C(17)-C(16)-C(22)	119.1(3)	H(23B)-C(23)-H(23C)	109.5
C(16)-C(17)-C(18)	122.7(3)	C(22)-C(24)-H(24A)	109.5
C(16)-C(17)-H(17)	118.6	C(22)-C(24)-H(24B)	109.5
C(18)-C(17)-H(17)	118.6	H(24A)-C(24)-H(24B)	109.5
C(17)-C(18)-C(13)	118.7(3)	C(22)-C(24)-H(24C)	109.5
C(17)-C(18)-C(25)	119.8(3)	H(24A)-C(24)-H(24C)	109.5
C(13)-C(18)-C(25)	121.5(3)	H(24B)-C(24)-H(24C)	109.5
C(21)-C(19)-C(20)	111.0(3)	C(18)-C(25)-C(27)	111.8(3)
C(21)-C(19)-C(14)	112.8(3)	C(18)-C(25)-C(26)	111.5(3)

C(27)-C(25)-C(26)	111.0(3)	C(29)-C(34)-C(36)	110.9(3)
C(18)-C(25)-H(25)	107.4	C(35)-C(34)-H(34)	107.3
C(27)-C(25)-H(25)	107.4	C(29)-C(34)-H(34)	107.3
C(26)-C(25)-H(25)	107.4	C(36)-C(34)-H(34)	107.3
C(25)-C(26)-H(26A)	109.5	C(34)-C(35)-H(35A)	109.5
C(25)-C(26)-H(26B)	109.5	C(34)-C(35)-H(35B)	109.5
H(26A)-C(26)-H(26B)	109.5	H(35A)-C(35)-H(35B)	109.5
C(25)-C(26)-H(26C)	109.5	C(34)-C(35)-H(35C)	109.5
H(26A)-C(26)-H(26C)	109.5	H(35A)-C(35)-H(35C)	109.5
H(26B)-C(26)-H(26C)	109.5	H(35B)-C(35)-H(35C)	109.5
C(25)-C(27)-H(27A)	109.5	C(34)-C(36)-H(36A)	109.5
C(25)-C(27)-H(27B)	109.5	C(34)-C(36)-H(36B)	109.5
H(27A)-C(27)-H(27B)	109.5	H(36A)-C(36)-H(36B)	109.5
C(25)-C(27)-H(27C)	109.5	C(34)-C(36)-H(36C)	109.5
H(27A)-C(27)-H(27C)	109.5	H(36A)-C(36)-H(36C)	109.5
H(27B)-C(27)-H(27C)	109.5	H(36B)-C(36)-H(36C)	109.5
C(33)-C(28)-C(29)	119.6(3)	C(38)-C(37)-C(39)	110.8(3)
C(33)-C(28)-C(6)	121.2(3)	C(38)-C(37)-C(31)	110.8(3)
C(29)-C(28)-C(6)	119.2(3)	C(39)-C(37)-C(31)	112.4(3)
C(30)-C(29)-C(28)	119.3(3)	C(38)-C(37)-H(37)	107.5
C(30)-C(29)-C(34)	120.4(3)	C(39)-C(37)-H(37)	107.5
C(28)-C(29)-C(34)	120.3(3)	C(31)-C(37)-H(37)	107.5
C(29)-C(30)-C(31)	122.1(3)	C(37)-C(38)-H(38A)	109.5
C(29)-C(30)-H(30)	118.9	C(37)-C(38)-H(38B)	109.5
C(31)-C(30)-H(30)	118.9	H(38A)-C(38)-H(38B)	109.5
C(32)-C(31)-C(30)	117.3(3)	C(37)-C(38)-H(38C)	109.5
C(32)-C(31)-C(37)	121.2(3)	H(38A)-C(38)-H(38C)	109.5
C(30)-C(31)-C(37)	121.5(3)	H(38B)-C(38)-H(38C)	109.5
C(31)-C(32)-C(33)	122.7(3)	C(37)-C(39)-H(39A)	109.5
C(31)-C(32)-H(32)	118.6	C(37)-C(39)-H(39B)	109.5
C(33)-C(32)-H(32)	118.6	H(39A)-C(39)-H(39B)	109.5
C(32)-C(33)-C(28)	118.8(3)	C(37)-C(39)-H(39C)	109.5
C(32)-C(33)-C(40)	118.6(3)	H(39A)-C(39)-H(39C)	109.5
C(28)-C(33)-C(40)	122.5(3)	H(39B)-C(39)-H(39C)	109.5
C(35)-C(34)-C(29)	112.5(3)	C(41)-C(40)-C(33)	112.0(3)
C(35)-C(34)-C(36)	111.2(3)	C(41)-C(40)-C(42)	109.9(3)

C(33)-C(40)-C(42)	110.7(3)	C(50)-C(49)-C(51)	110.4(3)
C(41)-C(40)-H(40)	108.0	C(45)-C(49)-H(49)	107.8
C(33)-C(40)-H(40)	108.0	C(50)-C(49)-H(49)	107.8
C(42)-C(40)-H(40)	108.0	C(51)-C(49)-H(49)	107.8
C(40)-C(41)-H(41A)	109.5	C(49)-C(50)-H(50A)	109.5
C(40)-C(41)-H(41B)	109.5	C(49)-C(50)-H(50B)	109.5
H(41A)-C(41)-H(41B)	109.5	H(50A)-C(50)-H(50B)	109.5
C(40)-C(41)-H(41C)	109.5	C(49)-C(50)-H(50C)	109.5
H(41A)-C(41)-H(41C)	109.5	H(50A)-C(50)-H(50C)	109.5
H(41B)-C(41)-H(41C)	109.5	H(50B)-C(50)-H(50C)	109.5
C(40)-C(42)-H(42A)	109.5	C(49)-C(51)-H(51A)	109.5
C(40)-C(42)-H(42B)	109.5	C(49)-C(51)-H(51B)	109.5
H(42A)-C(42)-H(42B)	109.5	H(51A)-C(51)-H(51B)	109.5
C(40)-C(42)-H(42C)	109.5	C(49)-C(51)-H(51C)	109.5
H(42A)-C(42)-H(42C)	109.5	H(51A)-C(51)-H(51C)	109.5
H(42B)-C(42)-H(42C)	109.5	H(51B)-C(51)-H(51C)	109.5
C(48)-C(43)-C(44)	118.1(3)	C(53)-C(52)-C(54)	111.2(3)
C(48)-C(43)-Mn(2)	121.7(2)	C(53)-C(52)-C(47)	110.5(3)
C(44)-C(43)-Mn(2)	120.1(2)	C(54)-C(52)-C(47)	111.8(3)
C(45)-C(44)-C(43)	121.4(3)	C(53)-C(52)-H(52)	107.7
C(45)-C(44)-C(55)	122.7(3)	C(54)-C(52)-H(52)	107.7
C(43)-C(44)-C(55)	115.9(3)	C(47)-C(52)-H(52)	107.7
C(46)-C(45)-C(44)	117.8(3)	C(52)-C(53)-H(53A)	109.5
C(46)-C(45)-C(49)	119.7(3)	C(52)-C(53)-H(53B)	109.5
C(44)-C(45)-C(49)	122.5(3)	H(53A)-C(53)-H(53B)	109.5
C(45)-C(46)-C(47)	123.4(3)	C(52)-C(53)-H(53C)	109.5
C(45)-C(46)-H(46)	118.3	H(53A)-C(53)-H(53C)	109.5
C(47)-C(46)-H(46)	118.3	H(53B)-C(53)-H(53C)	109.5
C(46)-C(47)-C(48)	118.2(3)	C(52)-C(54)-H(54A)	109.5
C(46)-C(47)-C(52)	119.5(3)	C(52)-C(54)-H(54B)	109.5
C(48)-C(47)-C(52)	122.3(3)	H(54A)-C(54)-H(54B)	109.5
C(43)-C(48)-C(47)	121.0(3)	C(52)-C(54)-H(54C)	109.5
C(43)-C(48)-C(70)	117.6(3)	H(54A)-C(54)-H(54C)	109.5
C(47)-C(48)-C(70)	121.4(3)	H(54B)-C(54)-H(54C)	109.5
C(45)-C(49)-C(50)	111.4(3)	C(56)-C(55)-C(60)	118.6(3)
C(45)-C(49)-C(51)	111.4(3)	C(56)-C(55)-C(44)	121.5(3)

C(60)-C(55)-C(44)	119.8(3)	C(66)-C(64)-C(58)	113.3(4)
C(55)-C(56)-C(57)	119.6(3)	C(65)-C(64)-H(64)	106.9
C(55)-C(56)-C(61)	121.5(3)	C(66)-C(64)-H(64)	106.9
C(57)-C(56)-C(61)	118.9(3)	C(58)-C(64)-H(64)	106.9
C(58)-C(57)-C(56)	122.3(3)	C(64)-C(65)-H(65A)	109.5
C(58)-C(57)-H(57)	118.9	C(64)-C(65)-H(65B)	109.5
C(56)-C(57)-H(57)	118.9	H(65A)-C(65)-H(65B)	109.5
C(59)-C(58)-C(57)	117.1(3)	C(64)-C(65)-H(65C)	109.5
C(59)-C(58)-C(64)	119.7(3)	H(65A)-C(65)-H(65C)	109.5
C(57)-C(58)-C(64)	123.3(3)	H(65B)-C(65)-H(65C)	109.5
C(60)-C(59)-C(58)	123.4(4)	C(64)-C(66)-H(66A)	109.5
C(60)-C(59)-H(59)	118.3	C(64)-C(66)-H(66B)	109.5
C(58)-C(59)-H(59)	118.3	H(66A)-C(66)-H(66B)	109.5
C(59)-C(60)-C(55)	119.1(3)	C(64)-C(66)-H(66C)	109.5
C(59)-C(60)-C(67)	120.6(3)	H(66A)-C(66)-H(66C)	109.5
C(55)-C(60)-C(67)	120.3(3)	H(66B)-C(66)-H(66C)	109.5
C(62)-C(61)-C(56)	113.4(3)	C(69)-C(67)-C(60)	111.1(4)
C(62)-C(61)-C(63)	110.2(3)	C(69)-C(67)-C(68)	110.9(4)
C(56)-C(61)-C(63)	111.1(3)	C(60)-C(67)-C(68)	111.0(3)
C(62)-C(61)-H(61)	107.3	C(69)-C(67)-H(67)	107.9
C(56)-C(61)-H(61)	107.3	C(60)-C(67)-H(67)	107.9
C(63)-C(61)-H(61)	107.3	C(68)-C(67)-H(67)	107.9
C(61)-C(62)-H(62A)	109.5	C(67)-C(68)-H(68A)	109.5
C(61)-C(62)-H(62B)	109.5	C(67)-C(68)-H(68B)	109.5
H(62A)-C(62)-H(62B)	109.5	H(68A)-C(68)-H(68B)	109.5
C(61)-C(62)-H(62C)	109.5	C(67)-C(68)-H(68C)	109.5
H(62A)-C(62)-H(62C)	109.5	H(68A)-C(68)-H(68C)	109.5
H(62B)-C(62)-H(62C)	109.5	H(68B)-C(68)-H(68C)	109.5
C(61)-C(63)-H(63A)	109.5	C(67)-C(69)-H(69A)	109.5
C(61)-C(63)-H(63B)	109.5	C(67)-C(69)-H(69B)	109.5
H(63A)-C(63)-H(63B)	109.5	H(69A)-C(69)-H(69B)	109.5
C(61)-C(63)-H(63C)	109.5	C(67)-C(69)-H(69C)	109.5
H(63A)-C(63)-H(63C)	109.5	H(69A)-C(69)-H(69C)	109.5
H(63B)-C(63)-H(63C)	109.5	H(69B)-C(69)-H(69C)	109.5
C(65)-C(64)-C(66)	111.7(5)	C(71)-C(70)-C(75)	119.3(3)
C(65)-C(64)-C(58)	110.7(4)	C(71)-C(70)-C(48)	121.7(3)

C(75)-C(70)-C(48)	118.9(3)	C(73)-C(79)-C(80)	110.3(3)
C(72)-C(71)-C(70)	119.6(3)	C(81)-C(79)-H(79)	107.9
C(72)-C(71)-C(76)	119.4(3)	C(73)-C(79)-H(79)	107.9
C(70)-C(71)-C(76)	120.9(3)	C(80)-C(79)-H(79)	107.9
C(71)-C(72)-C(73)	122.7(3)	C(79)-C(80)-H(80A)	109.5
C(71)-C(72)-H(72)	118.7	C(79)-C(80)-H(80B)	109.5
C(73)-C(72)-H(72)	118.7	H(80A)-C(80)-H(80B)	109.5
C(72)-C(73)-C(74)	117.6(3)	C(79)-C(80)-H(80C)	109.5
C(72)-C(73)-C(79)	122.6(3)	H(80A)-C(80)-H(80C)	109.5
C(74)-C(73)-C(79)	119.8(3)	H(80B)-C(80)-H(80C)	109.5
C(73)-C(74)-C(75)	121.8(3)	C(79)-C(81)-H(81A)	109.5
C(73)-C(74)-H(74)	119.1	C(79)-C(81)-H(81B)	109.5
C(75)-C(74)-H(74)	119.1	H(81A)-C(81)-H(81B)	109.5
C(74)-C(75)-C(70)	119.0(3)	C(79)-C(81)-H(81C)	109.5
C(74)-C(75)-C(82)	119.4(3)	H(81A)-C(81)-H(81C)	109.5
C(70)-C(75)-C(82)	121.6(3)	H(81B)-C(81)-H(81C)	109.5
C(77)-C(76)-C(71)	112.0(3)	C(83)-C(82)-C(75)	112.1(3)
C(77)-C(76)-C(78)	110.0(3)	C(83)-C(82)-C(84)	109.9(4)
C(71)-C(76)-C(78)	110.8(3)	C(75)-C(82)-C(84)	111.0(3)
C(77)-C(76)-H(76)	108.0	C(83)-C(82)-H(82)	107.9
C(71)-C(76)-H(76)	108.0	C(75)-C(82)-H(82)	107.9
C(78)-C(76)-H(76)	108.0	C(84)-C(82)-H(82)	107.9
C(76)-C(77)-H(77A)	109.5	C(82)-C(83)-H(83A)	109.5
C(76)-C(77)-H(77B)	109.5	C(82)-C(83)-H(83B)	109.5
H(77A)-C(77)-H(77B)	109.5	H(83A)-C(83)-H(83B)	109.5
C(76)-C(77)-H(77C)	109.5	C(82)-C(83)-H(83C)	109.5
H(77A)-C(77)-H(77C)	109.5	H(83A)-C(83)-H(83C)	109.5
H(77B)-C(77)-H(77C)	109.5	H(83B)-C(83)-H(83C)	109.5
C(76)-C(78)-H(78A)	109.5	C(82)-C(84)-H(84A)	109.5
C(76)-C(78)-H(78B)	109.5	C(82)-C(84)-H(84B)	109.5
H(78A)-C(78)-H(78B)	109.5	H(84A)-C(84)-H(84B)	109.5
C(76)-C(78)-H(78C)	109.5	C(82)-C(84)-H(84C)	109.5
H(78A)-C(78)-H(78C)	109.5	H(84A)-C(84)-H(84C)	109.5
H(78B)-C(78)-H(78C)	109.5	H(84B)-C(84)-H(84C)	109.5
C(81)-C(79)-C(73)	112.5(3)	C(92)-C(91)-C(96)	120.0
C(81)-C(79)-C(80)	110.1(3)	Mn(2)-C(91)-Mn(1)	102.81(9)

C(92)-C(91)-H(91)	120.0	C(101)-Mn(3)-C(95G)	141.23(12)
C(96)-C(91)-H(91)	120.0	C(101)-Mn(3)-C(92G)	142.73(12)
Mn(2)-C(91)-H(91)	128.7	C(101)-Mn(3)-C(96G)	142.49(11)
Mn(1)-C(91)-H(91)	128.5	C(101)-Mn(3)-C(91G)	143.26(11)
C(93)-C(92)-C(91)	120.0	C(143)-Mn(4)-C(94G)	140.10(11)
Mn(2)-C(92)-Mn(1)	103.16(10)	C(143)-Mn(4)-C(95G)	143.06(13)
C(93)-C(92)-H(92)	120.0	C(143)-Mn(4)-C(93G)	139.18(12)
C(91)-C(92)-H(92)	120.0	C(143)-Mn(4)-C(96G)	145.15(12)
Mn(2)-C(92)-H(92)	128.4	C(143)-Mn(4)-C(92G)	141.12(12)
Mn(1)-C(92)-H(92)	128.4	C(143)-Mn(4)-C(91G)	144.10(11)
C(92)-C(93)-C(94)	120.0	C(106)-C(101)-C(102)	117.1(3)
Mn(2)-C(93)-Mn(1)	104.39(11)	C(106)-C(101)-Mn(3)	121.3(2)
C(92)-C(93)-H(93)	120.0	C(102)-C(101)-Mn(3)	121.5(2)
C(94)-C(93)-H(93)	120.0	C(103)-C(102)-C(101)	121.7(3)
Mn(2)-C(93)-H(93)	127.7	C(103)-C(102)-C(113)	122.0(3)
Mn(1)-C(93)-H(93)	127.9	C(101)-C(102)-C(113)	116.2(3)
C(95)-C(94)-C(93)	120.0	C(104)-C(103)-C(102)	117.8(3)
Mn(1)-C(94)-Mn(2)	105.29(9)	C(104)-C(103)-C(107)	120.4(3)
C(95)-C(94)-H(94)	120.0	C(102)-C(103)-C(107)	121.8(3)
C(93)-C(94)-H(94)	120.0	C(103)-C(104)-C(105)	123.8(3)
Mn(1)-C(94)-H(94)	127.4	C(103)-C(104)-H(104)	118.1
Mn(2)-C(94)-H(94)	127.3	C(105)-C(104)-H(104)	118.1
C(94)-C(95)-C(96)	120.0	C(104)-C(105)-C(106)	117.1(3)
Mn(1)-C(95)-Mn(2)	104.91(10)	C(104)-C(105)-C(110)	119.2(3)
C(94)-C(95)-H(95)	120.0	C(106)-C(105)-C(110)	123.6(3)
C(96)-C(95)-H(95)	120.0	C(105)-C(106)-C(101)	122.4(3)
Mn(1)-C(95)-H(95)	127.5	C(105)-C(106)-C(128)	121.3(3)
Mn(2)-C(95)-H(95)	127.6	C(101)-C(106)-C(128)	116.3(3)
C(95)-C(96)-C(91)	120.0	C(103)-C(107)-C(109)	111.2(3)
Mn(1)-C(96)-Mn(2)	103.66(11)	C(103)-C(107)-C(108)	111.5(3)
C(95)-C(96)-H(96)	120.0	C(109)-C(107)-C(108)	110.5(3)
C(91)-C(96)-H(96)	120.0	C(103)-C(107)-H(107)	107.8
Mn(1)-C(96)-H(96)	128.0	C(109)-C(107)-H(107)	107.8
Mn(2)-C(96)-H(96)	128.3	C(108)-C(107)-H(107)	107.8
C(101)-Mn(3)-C(94G)	140.72(11)	C(107)-C(108)-H(10A)	109.5
C(101)-Mn(3)-C(93G)	141.47(11)	C(107)-C(108)-H(10B)	109.5

H(10A)-C(108)-H(10B)	109.5	C(116)-C(115)-H(115)	118.9
C(107)-C(108)-H(10C)	109.5	C(117)-C(116)-C(115)	117.9(3)
H(10A)-C(108)-H(10C)	109.5	C(117)-C(116)-C(122)	121.3(3)
H(10B)-C(108)-H(10C)	109.5	C(115)-C(116)-C(122)	120.8(3)
C(107)-C(109)-H(10D)	109.5	C(116)-C(117)-C(118)	122.2(3)
C(107)-C(109)-H(10E)	109.5	C(116)-C(117)-H(117)	118.9
H(10D)-C(109)-H(10E)	109.5	C(118)-C(117)-H(117)	118.9
C(107)-C(109)-H(10F)	109.5	C(117)-C(118)-C(113)	119.2(3)
H(10D)-C(109)-H(10F)	109.5	C(117)-C(118)-C(125)	119.4(3)
H(10E)-C(109)-H(10F)	109.5	C(113)-C(118)-C(125)	121.3(3)
C(105)-C(110)-C(112)	112.9(3)	C(114)-C(119)-C(121)	112.3(3)
C(105)-C(110)-C(111)	111.9(3)	C(114)-C(119)-C(120)	111.4(3)
C(112)-C(110)-C(111)	109.3(3)	C(121)-C(119)-C(120)	110.6(3)
C(105)-C(110)-H(110)	107.5	C(114)-C(119)-H(119)	107.4
C(112)-C(110)-H(110)	107.5	C(121)-C(119)-H(119)	107.4
C(111)-C(110)-H(110)	107.5	C(120)-C(119)-H(119)	107.4
C(110)-C(111)-H(11D)	109.5	C(119)-C(120)-H(12D)	109.5
C(110)-C(111)-H(11E)	109.5	C(119)-C(120)-H(12E)	109.5
H(11D)-C(111)-H(11E)	109.5	H(12D)-C(120)-H(12E)	109.5
C(110)-C(111)-H(11F)	109.5	C(119)-C(120)-H(12F)	109.5
H(11D)-C(111)-H(11F)	109.5	H(12D)-C(120)-H(12F)	109.5
H(11E)-C(111)-H(11F)	109.5	H(12E)-C(120)-H(12F)	109.5
C(110)-C(112)-H(11G)	109.5	C(119)-C(121)-H(12G)	109.5
C(110)-C(112)-H(11H)	109.5	C(119)-C(121)-H(12H)	109.5
H(11G)-C(112)-H(11H)	109.5	H(12G)-C(121)-H(12H)	109.5
C(110)-C(112)-H(11I)	109.5	C(119)-C(121)-H(12I)	109.5
H(11G)-C(112)-H(11I)	109.5	H(12G)-C(121)-H(12I)	109.5
H(11H)-C(112)-H(11I)	109.5	H(12H)-C(121)-H(12I)	109.5
C(118)-C(113)-C(114)	118.9(3)	C(124)-C(122)-C(116)	112.3(3)
C(118)-C(113)-C(102)	119.6(3)	C(124)-C(122)-C(123)	111.1(3)
C(114)-C(113)-C(102)	121.4(3)	C(116)-C(122)-C(123)	110.6(3)
C(115)-C(114)-C(113)	119.4(3)	C(124)-C(122)-H(122)	107.6
C(115)-C(114)-C(119)	119.4(3)	C(116)-C(122)-H(122)	107.6
C(113)-C(114)-C(119)	121.2(3)	C(123)-C(122)-H(122)	107.6
C(114)-C(115)-C(116)	122.2(3)	C(122)-C(123)-H(12J)	109.5
C(114)-C(115)-H(115)	118.9	C(122)-C(123)-H(12K)	109.5

H(12J)-C(123)-H(12K)	109.5	C(129)-C(130)-H(130)	118.6
C(122)-C(123)-H(12L)	109.5	C(130)-C(131)-C(132)	117.4(3)
H(12J)-C(123)-H(12L)	109.5	C(130)-C(131)-C(137)	119.1(3)
H(12K)-C(123)-H(12L)	109.5	C(132)-C(131)-C(137)	123.5(3)
C(122)-C(124)-H(12M)	109.5	C(131)-C(132)-C(133)	122.2(3)
C(122)-C(124)-H(12N)	109.5	C(131)-C(132)-H(132)	118.9
H(12M)-C(124)-H(12N)	109.5	C(133)-C(132)-H(132)	118.9
C(122)-C(124)-H(12O)	109.5	C(132)-C(133)-C(128)	118.8(3)
H(12M)-C(124)-H(12O)	109.5	C(132)-C(133)-C(140)	119.5(3)
H(12N)-C(124)-H(12O)	109.5	C(128)-C(133)-C(140)	121.7(3)
C(126)-C(125)-C(118)	111.7(3)	C(129)-C(134)-C(135)	111.6(3)
C(126)-C(125)-C(127)	111.0(3)	C(129)-C(134)-C(136)	111.3(3)
C(118)-C(125)-C(127)	110.8(3)	C(135)-C(134)-C(136)	109.7(3)
C(126)-C(125)-H(125)	107.7	C(129)-C(134)-H(134)	108.0
C(118)-C(125)-H(125)	107.7	C(135)-C(134)-H(134)	108.0
C(127)-C(125)-H(125)	107.7	C(136)-C(134)-H(134)	108.0
C(125)-C(126)-H(12P)	109.5	C(134)-C(135)-H(13A)	109.5
C(125)-C(126)-H(12Q)	109.5	C(134)-C(135)-H(13B)	109.5
H(12P)-C(126)-H(12Q)	109.5	H(13A)-C(135)-H(13B)	109.5
C(125)-C(126)-H(12R)	109.5	C(134)-C(135)-H(13C)	109.5
H(12P)-C(126)-H(12R)	109.5	H(13A)-C(135)-H(13C)	109.5
H(12Q)-C(126)-H(12R)	109.5	H(13B)-C(135)-H(13C)	109.5
C(125)-C(127)-H(12S)	109.5	C(134)-C(136)-H(13D)	109.5
C(125)-C(127)-H(12T)	109.5	C(134)-C(136)-H(13E)	109.5
H(12S)-C(127)-H(12T)	109.5	H(13D)-C(136)-H(13E)	109.5
C(125)-C(127)-H(12U)	109.5	C(134)-C(136)-H(13F)	109.5
H(12S)-C(127)-H(12U)	109.5	H(13D)-C(136)-H(13F)	109.5
H(12T)-C(127)-H(12U)	109.5	H(13E)-C(136)-H(13F)	109.5
C(129)-C(128)-C(133)	120.1(3)	C(138)-C(137)-C(131)	115.4(4)
C(129)-C(128)-C(106)	121.0(3)	C(138)-C(137)-C(139)	112.0(4)
C(133)-C(128)-C(106)	118.8(3)	C(131)-C(137)-C(139)	109.2(3)
C(130)-C(129)-C(128)	118.6(3)	C(138)-C(137)-H(137)	106.6
C(130)-C(129)-C(134)	119.6(3)	C(131)-C(137)-H(137)	106.6
C(128)-C(129)-C(134)	121.8(3)	C(139)-C(137)-H(137)	106.6
C(131)-C(130)-C(129)	122.8(3)	C(137)-C(138)-H(13G)	109.5
C(131)-C(130)-H(130)	118.6	C(137)-C(138)-H(13H)	109.5

H(13G)-C(138)-H(13H)	109.5	C(144)-C(145)-C(149)	122.8(3)
C(137)-C(138)-H(13I)	109.5	C(145)-C(146)-C(147)	123.9(3)
H(13G)-C(138)-H(13I)	109.5	C(145)-C(146)-H(146)	118.0
H(13H)-C(138)-H(13I)	109.5	C(147)-C(146)-H(146)	118.0
C(137)-C(139)-H(13J)	109.5	C(148)-C(147)-C(146)	117.4(3)
C(137)-C(139)-H(13K)	109.5	C(148)-C(147)-C(152)	123.4(3)
H(13J)-C(139)-H(13K)	109.5	C(146)-C(147)-C(152)	119.1(3)
C(137)-C(139)-H(13L)	109.5	C(147)-C(148)-C(143)	121.3(3)
H(13J)-C(139)-H(13L)	109.5	C(147)-C(148)-C(170)	121.5(3)
H(13K)-C(139)-H(13L)	109.5	C(143)-C(148)-C(170)	117.2(3)
C(133)-C(140)-C(142)	112.4(3)	C(145)-C(149)-C(151)	111.7(3)
C(133)-C(140)-C(141)	111.2(3)	C(145)-C(149)-C(150)	111.7(3)
C(142)-C(140)-C(141)	109.4(3)	C(151)-C(149)-C(150)	109.9(3)
C(133)-C(140)-H(140)	107.9	C(145)-C(149)-H(149)	107.8
C(142)-C(140)-H(140)	107.9	C(151)-C(149)-H(149)	107.8
C(141)-C(140)-H(140)	107.9	C(150)-C(149)-H(149)	107.8
C(140)-C(141)-H(14A)	109.5	C(149)-C(150)-H(15A)	109.5
C(140)-C(141)-H(14B)	109.5	C(149)-C(150)-H(15B)	109.5
H(14A)-C(141)-H(14B)	109.5	H(15A)-C(150)-H(15B)	109.5
C(140)-C(141)-H(14C)	109.5	C(149)-C(150)-H(15C)	109.5
H(14A)-C(141)-H(14C)	109.5	H(15A)-C(150)-H(15C)	109.5
H(14B)-C(141)-H(14C)	109.5	H(15B)-C(150)-H(15C)	109.5
C(140)-C(142)-H(14D)	109.5	C(149)-C(151)-H(15D)	109.5
C(140)-C(142)-H(14E)	109.5	C(149)-C(151)-H(15E)	109.5
H(14D)-C(142)-H(14E)	109.5	H(15D)-C(151)-H(15E)	109.5
C(140)-C(142)-H(14F)	109.5	C(149)-C(151)-H(15F)	109.5
H(14D)-C(142)-H(14F)	109.5	H(15D)-C(151)-H(15F)	109.5
H(14E)-C(142)-H(14F)	109.5	H(15E)-C(151)-H(15F)	109.5
C(144)-C(143)-C(148)	117.9(3)	C(147)-C(152)-C(153)	112.6(3)
C(144)-C(143)-Mn(4)	121.4(2)	C(147)-C(152)-C(154)	112.0(3)
C(148)-C(143)-Mn(4)	120.7(2)	C(153)-C(152)-C(154)	109.6(3)
C(143)-C(144)-C(145)	122.2(3)	C(147)-C(152)-H(152)	107.5
C(143)-C(144)-C(155)	116.3(3)	C(153)-C(152)-H(152)	107.5
C(145)-C(144)-C(155)	121.5(3)	C(154)-C(152)-H(152)	107.5
C(146)-C(145)-C(144)	117.2(3)	C(152)-C(153)-H(15G)	109.5
C(146)-C(145)-C(149)	120.0(3)	C(152)-C(153)-H(15H)	109.5

H(15G)-C(153)-H(15H)	109.5	H(16A)-C(162)-H(16B)	109.5
C(152)-C(153)-H(15I)	109.5	C(161)-C(162)-H(16C)	109.5
H(15G)-C(153)-H(15I)	109.5	H(16A)-C(162)-H(16C)	109.5
H(15H)-C(153)-H(15I)	109.5	H(16B)-C(162)-H(16C)	109.5
C(152)-C(154)-H(15J)	109.5	C(161)-C(163)-H(16D)	109.5
C(152)-C(154)-H(15K)	109.5	C(161)-C(163)-H(16E)	109.5
H(15J)-C(154)-H(15K)	109.5	H(16D)-C(163)-H(16E)	109.5
C(152)-C(154)-H(15L)	109.5	C(161)-C(163)-H(16F)	109.5
H(15J)-C(154)-H(15L)	109.5	H(16D)-C(163)-H(16F)	109.5
H(15K)-C(154)-H(15L)	109.5	H(16E)-C(163)-H(16F)	109.5
C(156)-C(155)-C(160)	120.4(3)	C(166)-C(164)-C(158)	114.9(4)
C(156)-C(155)-C(144)	119.4(3)	C(166)-C(164)-C(165)	113.5(4)
C(160)-C(155)-C(144)	120.2(3)	C(158)-C(164)-C(165)	111.0(4)
C(157)-C(156)-C(155)	118.9(3)	C(166)-C(164)-H(164)	105.5
C(157)-C(156)-C(161)	118.6(3)	C(158)-C(164)-H(164)	105.5
C(155)-C(156)-C(161)	122.4(3)	C(165)-C(164)-H(164)	105.5
C(156)-C(157)-C(158)	122.6(4)	C(164)-C(165)-H(16G)	109.5
C(156)-C(157)-H(157)	118.7	C(164)-C(165)-H(16H)	109.5
C(158)-C(157)-H(157)	118.7	H(16G)-C(165)-H(16H)	109.5
C(157)-C(158)-C(159)	117.2(3)	C(164)-C(165)-H(16I)	109.5
C(157)-C(158)-C(164)	119.9(4)	H(16G)-C(165)-H(16I)	109.5
C(159)-C(158)-C(164)	122.9(4)	H(16H)-C(165)-H(16I)	109.5
C(158)-C(159)-C(160)	122.8(4)	C(164)-C(166)-H(16J)	109.5
C(158)-C(159)-H(159)	118.6	C(164)-C(166)-H(16K)	109.5
C(160)-C(159)-H(159)	118.6	H(16J)-C(166)-H(16K)	109.5
C(159)-C(160)-C(155)	118.0(3)	C(164)-C(166)-H(16L)	109.5
C(159)-C(160)-C(167)	120.1(3)	H(16J)-C(166)-H(16L)	109.5
C(155)-C(160)-C(167)	121.9(3)	H(16K)-C(166)-H(16L)	109.5
C(162)-C(161)-C(156)	111.9(3)	C(160)-C(167)-C(168)	112.4(3)
C(162)-C(161)-C(163)	110.2(3)	C(160)-C(167)-C(169)	111.4(3)
C(156)-C(161)-C(163)	112.3(3)	C(168)-C(167)-C(169)	109.1(3)
C(162)-C(161)-H(161)	107.4	C(160)-C(167)-H(167)	107.9
C(156)-C(161)-H(161)	107.4	C(168)-C(167)-H(167)	107.9
C(163)-C(161)-H(161)	107.4	C(169)-C(167)-H(167)	107.9
C(161)-C(162)-H(16A)	109.5	C(167)-C(168)-H(16M)	109.5
C(161)-C(162)-H(16B)	109.5	C(167)-C(168)-H(16N)	109.5

H(16M)-C(168)-H(16N)	109.5	H(17A)-C(177)-H(17B)	109.5
C(167)-C(168)-H(16O)	109.5	C(176)-C(177)-H(17C)	109.5
H(16M)-C(168)-H(16O)	109.5	H(17A)-C(177)-H(17C)	109.5
H(16N)-C(168)-H(16O)	109.5	H(17B)-C(177)-H(17C)	109.5
C(167)-C(169)-H(16P)	109.5	C(176)-C(178)-H(17D)	109.5
C(167)-C(169)-H(16Q)	109.5	C(176)-C(178)-H(17E)	109.5
H(16P)-C(169)-H(16Q)	109.5	H(17D)-C(178)-H(17E)	109.5
C(167)-C(169)-H(16R)	109.5	C(176)-C(178)-H(17F)	109.5
H(16P)-C(169)-H(16R)	109.5	H(17D)-C(178)-H(17F)	109.5
H(16Q)-C(169)-H(16R)	109.5	H(17E)-C(178)-H(17F)	109.5
C(175)-C(170)-C(171)	119.2(3)	C(180)-C(179)-C(173)	110.6(3)
C(175)-C(170)-C(148)	121.3(3)	C(180)-C(179)-C(181)	109.7(3)
C(171)-C(170)-C(148)	119.4(3)	C(173)-C(179)-C(181)	112.1(3)
C(172)-C(171)-C(170)	119.3(3)	C(180)-C(179)-H(179)	108.1
C(172)-C(171)-C(176)	119.3(3)	C(173)-C(179)-H(179)	108.1
C(170)-C(171)-C(176)	121.4(3)	C(181)-C(179)-H(179)	108.1
C(173)-C(172)-C(171)	122.9(3)	C(179)-C(180)-H(18A)	109.5
C(173)-C(172)-H(172)	118.6	C(179)-C(180)-H(18B)	109.5
C(171)-C(172)-H(172)	118.6	H(18A)-C(180)-H(18B)	109.5
C(174)-C(173)-C(172)	117.8(3)	C(179)-C(180)-H(18C)	109.5
C(174)-C(173)-C(179)	121.4(3)	H(18A)-C(180)-H(18C)	109.5
C(172)-C(173)-C(179)	120.8(3)	H(18B)-C(180)-H(18C)	109.5
C(173)-C(174)-C(175)	122.3(3)	C(179)-C(181)-H(18D)	109.5
C(173)-C(174)-H(174)	118.8	C(179)-C(181)-H(18E)	109.5
C(175)-C(174)-H(174)	118.8	H(18D)-C(181)-H(18E)	109.5
C(170)-C(175)-C(174)	118.3(3)	C(179)-C(181)-H(18F)	109.5
C(170)-C(175)-C(182)	122.3(3)	H(18D)-C(181)-H(18F)	109.5
C(174)-C(175)-C(182)	119.4(3)	H(18E)-C(181)-H(18F)	109.5
C(177)-C(176)-C(178)	111.8(4)	C(183)-C(182)-C(175)	113.0(3)
C(177)-C(176)-C(171)	111.2(3)	C(183)-C(182)-C(184)	110.2(3)
C(178)-C(176)-C(171)	111.1(3)	C(175)-C(182)-C(184)	111.7(3)
C(177)-C(176)-H(176)	107.5	C(183)-C(182)-H(182)	107.2
C(178)-C(176)-H(176)	107.5	C(175)-C(182)-H(182)	107.2
C(171)-C(176)-H(176)	107.5	C(184)-C(182)-H(182)	107.2
C(176)-C(177)-H(17A)	109.5	C(182)-C(183)-H(18G)	109.5
C(176)-C(177)-H(17B)	109.5	C(182)-C(183)-H(18H)	109.5

H(18G)-C(183)-H(18H)	109.5	C(94G)-C(93G)-H(93G)	120.0
C(182)-C(183)-H(18I)	109.5	C(92G)-C(93G)-H(93G)	120.0
H(18G)-C(183)-H(18I)	109.5	Mn(3)-C(93G)-H(93G)	127.8
H(18H)-C(183)-H(18I)	109.5	Mn(4)-C(93G)-H(93G)	127.7
C(182)-C(184)-H(18J)	109.5	C(93G)-C(94G)-C(95G)	120.0
C(182)-C(184)-H(18K)	109.5	C(93G)-C(94G)-Mn(4)	72.75(10)
H(18J)-C(184)-H(18K)	109.5	C(95G)-C(94G)-Mn(4)	72.12(10)
C(182)-C(184)-H(18L)	109.5	C(93G)-C(94G)-Mn(3)	72.13(10)
H(18J)-C(184)-H(18L)	109.5	C(95G)-C(94G)-Mn(3)	72.31(9)
H(18K)-C(184)-H(18L)	109.5	Mn(4)-C(94G)-Mn(3)	105.23(9)
C(92G)-C(91G)-C(96G)	120.0	C(93G)-C(94G)-H(94G)	120.0
C(92G)-C(91G)-Mn(3)	71.83(9)	C(95G)-C(94G)-H(94G)	120.0
C(96G)-C(91G)-Mn(3)	72.00(10)	Mn(4)-C(94G)-H(94G)	127.1
C(92G)-C(91G)-Mn(4)	72.16(10)	Mn(3)-C(94G)-H(94G)	127.6
C(96G)-C(91G)-Mn(4)	71.54(10)	C(96G)-C(95G)-C(94G)	120.0
Mn(3)-C(91G)-Mn(4)	103.09(9)	C(96G)-C(95G)-Mn(4)	72.93(9)
C(92G)-C(91G)-H(91G)	120.0	C(94G)-C(95G)-Mn(4)	71.83(9)
C(96G)-C(91G)-H(91G)	120.0	C(96G)-C(95G)-Mn(3)	72.53(9)
Mn(3)-C(91G)-H(91G)	128.4	C(94G)-C(95G)-Mn(3)	71.70(9)
Mn(4)-C(91G)-H(91G)	128.5	Mn(4)-C(95G)-Mn(3)	104.85(11)
C(93G)-C(92G)-C(91G)	120.0	C(96G)-C(95G)-H(95G)	120.0
C(93G)-C(92G)-Mn(3)	71.61(9)	C(94G)-C(95G)-H(95G)	120.0
C(91G)-C(92G)-Mn(3)	72.43(9)	Mn(4)-C(95G)-H(95G)	127.2
C(93G)-C(92G)-Mn(4)	71.35(9)	Mn(3)-C(95G)-H(95G)	127.9
C(91G)-C(92G)-Mn(4)	72.44(9)	C(95G)-C(96G)-C(91G)	120.0
Mn(3)-C(92G)-Mn(4)	103.44(10)	C(95G)-C(96G)-Mn(3)	71.64(9)
C(93G)-C(92G)-H(92G)	120.0	C(91G)-C(96G)-Mn(3)	72.28(9)
C(91G)-C(92G)-H(92G)	120.0	C(95G)-C(96G)-Mn(4)	71.23(9)
Mn(3)-C(92G)-H(92G)	128.1	C(91G)-C(96G)-Mn(4)	72.95(10)
Mn(4)-C(92G)-H(92G)	128.4	Mn(3)-C(96G)-Mn(4)	103.77(10)
C(94G)-C(93G)-C(92G)	120.0	C(95G)-C(96G)-H(96G)	120.0
C(94G)-C(93G)-Mn(3)	71.85(9)	C(91G)-C(96G)-H(96G)	120.0
C(92G)-C(93G)-Mn(3)	72.49(9)	Mn(3)-C(96G)-H(96G)	128.3
C(94G)-C(93G)-Mn(4)	71.33(10)	Mn(4)-C(96G)-H(96G)	128.0
C(92G)-C(93G)-Mn(4)	73.05(9)	C(206)-C(201)-C(202)	123.1(8)
Mn(3)-C(93G)-Mn(4)	104.51(10)	C(206)-C(201)-C(207)	123.3(8)

C(202)-C(201)-C(207)	112.1(8)	C(214)-C(215)-H(215)	119.9
C(203)-C(202)-C(201)	113.8(10)	C(215)-C(216)-C(211)	118.1(5)
C(203)-C(202)-H(202)	123.1	C(215)-C(216)-C(217)	120.3(5)
C(201)-C(202)-H(202)	123.1	C(211)-C(216)-C(217)	121.6(5)
C(202)-C(203)-C(204)	126.5(9)	C(216)-C(217)-H(21D)	109.5
C(202)-C(203)-H(203)	116.7	C(216)-C(217)-H(21E)	109.5
C(204)-C(203)-H(203)	116.7	H(21D)-C(217)-H(21E)	109.5
C(205)-C(204)-C(203)	116.5(8)	C(216)-C(217)-H(21F)	109.5
C(205)-C(204)-H(204)	121.7	H(21D)-C(217)-H(21F)	109.5
C(203)-C(204)-H(204)	121.7	H(21E)-C(217)-H(21F)	109.5
C(204)-C(205)-C(206)	118.1(7)	C(222)-C(221)-C(226)	119.9(6)
C(204)-C(205)-H(205)	121.0	C(222)-C(221)-H(221)	120.1
C(206)-C(205)-H(205)	121.0	C(226)-C(221)-H(221)	120.1
C(201)-C(206)-C(205)	120.3(6)	C(221)-C(222)-C(223)	121.4(7)
C(201)-C(206)-H(206)	119.8	C(221)-C(222)-H(222)	119.3
C(205)-C(206)-H(206)	119.8	C(223)-C(222)-H(222)	119.3
C(201)-C(207)-H(20D)	109.5	C(224)-C(223)-C(222)	118.5(6)
C(201)-C(207)-H(20E)	109.5	C(224)-C(223)-H(223)	120.8
H(20D)-C(207)-H(20E)	109.5	C(222)-C(223)-H(223)	120.8
C(201)-C(207)-H(20F)	109.5	C(223)-C(224)-C(225)	120.8(6)
H(20D)-C(207)-H(20F)	109.5	C(223)-C(224)-H(224)	119.6
H(20E)-C(207)-H(20F)	109.5	C(225)-C(224)-H(224)	119.6
C(212)-C(211)-C(216)	123.1(5)	C(224)-C(225)-C(226)	121.0(5)
C(212)-C(211)-H(211)	118.5	C(224)-C(225)-H(225)	119.5
C(216)-C(211)-H(211)	118.5	C(226)-C(225)-H(225)	119.5
C(211)-C(212)-C(213)	118.5(6)	C(225)-C(226)-C(221)	118.4(5)
C(211)-C(212)-H(212)	120.8	C(225)-C(226)-C(227)	120.8(4)
C(213)-C(212)-H(212)	120.8	C(221)-C(226)-C(227)	120.7(5)
C(214)-C(213)-C(212)	121.6(6)	C(226)-C(227)-H(22A)	109.5
C(214)-C(213)-H(213)	119.2	C(226)-C(227)-H(22B)	109.5
C(212)-C(213)-H(213)	119.2	H(22A)-C(227)-H(22B)	109.5
C(213)-C(214)-C(215)	118.3(5)	C(226)-C(227)-H(22C)	109.5
C(213)-C(214)-H(214)	120.8	H(22A)-C(227)-H(22C)	109.5
C(215)-C(214)-H(214)	120.8	H(22B)-C(227)-H(22C)	109.5
C(216)-C(215)-C(214)	120.3(5)	C(232)-C(231)-C(236)	118.6(3)
C(216)-C(215)-H(215)	119.9	C(232)-C(231)-C(237)	121.1(4)

C(236)-C(231)-C(237)	120.3(4)	C(244)-C(245)-H(245)	120.0
C(231)-C(232)-C(233)	121.5(3)	C(245)-C(246)-C(241)	122.1(4)
C(231)-C(232)-H(232)	119.2	C(245)-C(246)-H(246)	118.9
C(233)-C(232)-H(232)	119.2	C(241)-C(246)-H(246)	118.9
C(234)-C(233)-C(232)	119.0(4)	C(241)-C(247)-H(24D)	109.5
C(234)-C(233)-H(233)	120.5	C(241)-C(247)-H(24E)	109.5
C(232)-C(233)-H(233)	120.5	H(24D)-C(247)-H(24E)	109.5
C(235)-C(234)-C(233)	120.5(4)	C(241)-C(247)-H(24F)	109.5
C(235)-C(234)-H(234)	119.7	H(24D)-C(247)-H(24F)	109.5
C(233)-C(234)-H(234)	119.7	H(24E)-C(247)-H(24F)	109.5
C(234)-C(235)-C(236)	119.5(4)	C(252)-C(251)-C(256)	118.2(4)
C(234)-C(235)-H(235)	120.3	C(252)-C(251)-C(257)	121.5(3)
C(236)-C(235)-H(235)	120.3	C(256)-C(251)-C(257)	120.3(4)
C(231)-C(236)-C(235)	120.9(4)	C(251)-C(252)-C(253)	121.5(3)
C(231)-C(236)-H(236)	119.6	C(251)-C(252)-H(252)	119.3
C(235)-C(236)-H(236)	119.6	C(253)-C(252)-H(252)	119.3
C(231)-C(237)-H(23D)	109.5	C(254)-C(253)-C(252)	120.1(4)
C(231)-C(237)-H(23E)	109.5	C(254)-C(253)-H(253)	119.9
H(23D)-C(237)-H(23E)	109.5	C(252)-C(253)-H(253)	119.9
C(231)-C(237)-H(23F)	109.5	C(255)-C(254)-C(253)	119.1(4)
H(23D)-C(237)-H(23F)	109.5	C(255)-C(254)-H(254)	120.4
H(23E)-C(237)-H(23F)	109.5	C(253)-C(254)-H(254)	120.4
C(246)-C(241)-C(242)	116.4(4)	C(254)-C(255)-C(256)	120.5(4)
C(246)-C(241)-C(247)	121.5(4)	C(254)-C(255)-H(255)	119.7
C(242)-C(241)-C(247)	122.1(3)	C(256)-C(255)-H(255)	119.7
C(243)-C(242)-C(241)	121.5(4)	C(255)-C(256)-C(251)	120.5(4)
C(243)-C(242)-H(242)	119.3	C(255)-C(256)-H(256)	119.7
C(241)-C(242)-H(242)	119.3	C(251)-C(256)-H(256)	119.7
C(244)-C(243)-C(242)	120.4(4)	C(251)-C(257)-H(25A)	109.5
C(244)-C(243)-H(243)	119.8	C(251)-C(257)-H(25B)	109.5
C(242)-C(243)-H(243)	119.8	H(25A)-C(257)-H(25B)	109.5
C(243)-C(244)-C(245)	119.7(4)	C(251)-C(257)-H(25C)	109.5
C(243)-C(244)-H(244)	120.2	H(25A)-C(257)-H(25C)	109.5
C(245)-C(244)-H(244)	120.2	H(25B)-C(257)-H(25C)	109.5
C(246)-C(245)-C(244)	120.0(4)	C(266)-C(261)-C(262)	117.2(4)
C(246)-C(245)-H(245)	120.0	C(266)-C(261)-C(267)	119.9(4)

C(262)-C(261)-C(267)	122.9(4)	C(276)-C(271)-C(277)	121.3(6)
C(263)-C(262)-C(261)	121.4(4)	C(272)-C(271)-C(277)	119.4(6)
C(263)-C(262)-H(262)	119.3	C(273)-C(272)-C(271)	119.2(6)
C(261)-C(262)-H(262)	119.3	C(273)-C(272)-H(272)	120.4
C(264)-C(263)-C(262)	120.7(4)	C(271)-C(272)-H(272)	120.4
C(264)-C(263)-H(263)	119.6	C(272)-C(273)-C(274)	120.2(6)
C(262)-C(263)-H(263)	119.6	C(272)-C(273)-H(273)	119.9
C(263)-C(264)-C(265)	118.7(4)	C(274)-C(273)-H(273)	119.9
C(263)-C(264)-H(264)	120.7	C(275)-C(274)-C(273)	119.2(6)
C(265)-C(264)-H(264)	120.7	C(275)-C(274)-H(274)	120.4
C(264)-C(265)-C(266)	120.5(4)	C(273)-C(274)-H(274)	120.4
C(264)-C(265)-H(265)	119.7	C(274)-C(275)-C(276)	121.4(7)
C(266)-C(265)-H(265)	119.7	C(274)-C(275)-H(275)	119.3
C(261)-C(266)-C(265)	121.4(4)	C(276)-C(275)-H(275)	119.3
C(261)-C(266)-H(266)	119.3	C(271)-C(276)-C(275)	120.6(6)
C(265)-C(266)-H(266)	119.3	C(271)-C(276)-H(276)	119.7
C(261)-C(267)-H(26D)	109.5	C(275)-C(276)-H(276)	119.7
C(261)-C(267)-H(26E)	109.5	C(271)-C(277)-H(27D)	109.5
H(26D)-C(267)-H(26E)	109.5	C(271)-C(277)-H(27E)	109.5
C(261)-C(267)-H(26F)	109.5	H(27D)-C(277)-H(27E)	109.5
H(26D)-C(267)-H(26F)	109.5	C(271)-C(277)-H(27F)	109.5
H(26E)-C(267)-H(26F)	109.5	H(27D)-C(277)-H(27F)	109.5
C(276)-C(271)-C(272)	119.3(6)	H(27E)-C(277)-H(27F)	109.5

Symmetry transformations used to generate equivalent atoms:

Crystallographic Data of [(η^6-C_6H_6)FeAr*-3,5-Pr^i_2] (**2**)

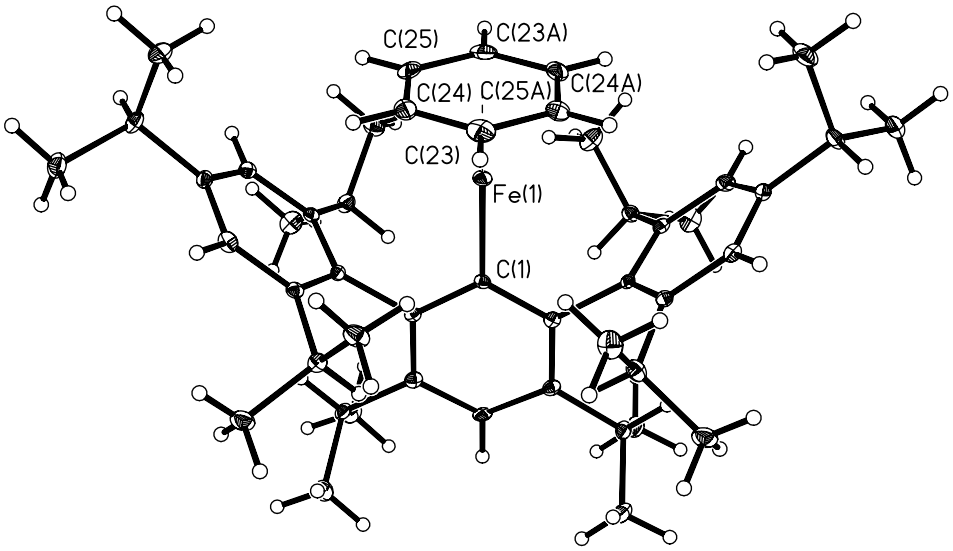

Table 3. Crystal data and structure refinement for [(μ-η^6:η^6-C_6H_6)FeAr*-3,5-Pr^i_2] (**2**).

Identification code	pbcn	
Empirical formula	$C_{48}H_{67}Fe$	
Formula weight	699.87	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c n	
Unit cell dimensions	a = 22.0866(14) Å	α= 90°.
	b = 10.9907(7) Å	β= 90°.
	c = 17.4459(11) Å	γ = 90°.
Volume	4234.9(5) $Å^3$	
Z	4	
Density (calculated)	1.098 Mg/m^3	
Absorption coefficient	0.386 mm^{-1}	
F(000)	1524	
Crystal size	0.19 x 0.18 x 0.17 mm^3	
Theta range for data collection	1.84 to 25.25°.	
Index ranges	-26<=h<=26, -13<=k<=13, -20<=l<=20	
Reflections collected	43524	
Independent reflections	3842 [R(int) = 0.1351]	
Completeness to theta = 25.25°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.936 and 0.913	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3842 / 0 / 231	
Goodness-of-fit on F^2	0.998	
Final R indices [I>2sigma(I)]	R1 = 0.0428, wR2 = 0.0953	
R indices (all data)	R1 = 0.0961, wR2 = 0.1227	
Largest diff. peak and hole	0.334 and -0.369 $e.Å^{-3}$	

Table 4. Bond lengths [Å] and angles [°] for [(μ-η^6:η^6-C_6H_6)FeAr*-3,5-Pr^i_2] (**2**).

C(1)-C(2)#1	1.413(3)	C(15)-H(15C)	0.9600
C(1)-C(2)	1.413(3)	C(16)-H(16A)	0.9600
C(1)-Fe(1)	2.029(4)	C(16)-H(16B)	0.9600
C(2)-C(3)	1.401(4)	C(16)-H(16C)	0.9600
C(2)-C(8)	1.512(4)	C(17)-C(19)	1.525(4)
C(3)-C(4)	1.391(3)	C(17)-C(18)	1.527(4)
C(3)-C(5)	1.522(4)	C(17)-H(17)	0.9800
C(4)-C(3)#1	1.391(3)	C(18)-H(18A)	0.9600
C(4)-H(4)	0.9300	C(18)-H(18B)	0.9600
C(5)-C(7)	1.528(4)	C(18)-H(18C)	0.9600
C(5)-C(6)	1.534(4)	C(19)-H(19A)	0.9600
C(5)-H(5)	0.9800	C(19)-H(19B)	0.9600
C(6)-H(6A)	0.9600	C(19)-H(19C)	0.9600
C(6)-H(6B)	0.9600	C(20)-C(22)	1.532(4)
C(6)-H(6C)	0.9600	C(20)-C(21)	1.532(4)
C(7)-H(7A)	0.9600	C(20)-H(20)	0.9800
C(7)-H(7B)	0.9600	C(21)-H(21A)	0.9600
C(7)-H(7C)	0.9600	C(21)-H(21B)	0.9600
C(8)-C(13)	1.410(4)	C(21)-H(21C)	0.9600
C(8)-C(9)	1.410(4)	C(22)-H(22A)	0.9600
C(9)-C(10)	1.394(4)	C(22)-H(22B)	0.9600
C(9)-C(14)	1.525(4)	C(22)-H(22C)	0.9600
C(10)-C(11)	1.390(4)	C(23)-C(25)#1	1.406(5)
C(10)-H(10)	0.9300	C(23)-C(24)	1.412(4)
C(11)-C(12)	1.394(4)	C(23)-Fe(1)	2.163(3)
C(11)-C(17)	1.518(4)	C(23)-H(23)	0.9300
C(12)-C(13)	1.391(4)	C(24)-C(25)	1.407(5)
C(12)-H(12)	0.9300	C(24)-Fe(1)	2.166(3)
C(13)-C(20)	1.524(4)	C(24)-H(24)	0.9300
C(14)-C(15)	1.528(4)	C(25)-C(23)#1	1.406(5)
C(14)-C(16)	1.535(4)	C(25)-Fe(1)	2.163(3)
C(14)-H(14)	0.9800	C(25)-H(25)	0.9300
C(15)-H(15A)	0.9600	Fe(1)-C(23)#1	2.163(3)
C(15)-H(15B)	0.9600	Fe(1)-C(25)#1	2.163(3)

Fe(1)-C(24)#1	2.166(3)

C(2)#1-C(1)-C(2)	117.9(3)	C(10)-C(9)-C(8)	119.2(3)
C(2)#1-C(1)-Fe(1)	121.05(17)	C(10)-C(9)-C(14)	119.3(2)
C(2)-C(1)-Fe(1)	121.05(17)	C(8)-C(9)-C(14)	121.4(2)
C(3)-C(2)-C(1)	121.5(3)	C(11)-C(10)-C(9)	122.5(3)
C(3)-C(2)-C(8)	122.1(3)	C(11)-C(10)-H(10)	118.8
C(1)-C(2)-C(8)	116.4(2)	C(9)-C(10)-H(10)	118.8
C(4)-C(3)-C(2)	117.9(3)	C(10)-C(11)-C(12)	117.3(3)
C(4)-C(3)-C(5)	119.8(3)	C(10)-C(11)-C(17)	122.8(3)
C(2)-C(3)-C(5)	122.3(3)	C(12)-C(11)-C(17)	119.9(3)
C(3)#1-C(4)-C(3)	123.2(4)	C(13)-C(12)-C(11)	122.3(3)
C(3)#1-C(4)-H(4)	118.4	C(13)-C(12)-H(12)	118.8
C(3)-C(4)-H(4)	118.4	C(11)-C(12)-H(12)	118.8
C(3)-C(5)-C(7)	111.5(2)	C(12)-C(13)-C(8)	119.4(3)
C(3)-C(5)-C(6)	111.4(2)	C(12)-C(13)-C(20)	118.7(2)
C(7)-C(5)-C(6)	110.1(2)	C(8)-C(13)-C(20)	121.8(2)
C(3)-C(5)-H(5)	107.9	C(9)-C(14)-C(15)	111.7(2)
C(7)-C(5)-H(5)	107.9	C(9)-C(14)-C(16)	111.7(2)
C(6)-C(5)-H(5)	107.9	C(15)-C(14)-C(16)	110.5(2)
C(5)-C(6)-H(6A)	109.5	C(9)-C(14)-H(14)	107.6
C(5)-C(6)-H(6B)	109.5	C(15)-C(14)-H(14)	107.6
H(6A)-C(6)-H(6B)	109.5	C(16)-C(14)-H(14)	107.6
C(5)-C(6)-H(6C)	109.5	C(14)-C(15)-H(15A)	109.5
H(6A)-C(6)-H(6C)	109.5	C(14)-C(15)-H(15B)	109.5
H(6B)-C(6)-H(6C)	109.5	H(15A)-C(15)-H(15B)	109.5
C(5)-C(7)-H(7A)	109.5	C(14)-C(15)-H(15C)	109.5
C(5)-C(7)-H(7B)	109.5	H(15A)-C(15)-H(15C)	109.5
H(7A)-C(7)-H(7B)	109.5	H(15B)-C(15)-H(15C)	109.5
C(5)-C(7)-H(7C)	109.5	C(14)-C(16)-H(16A)	109.5
H(7A)-C(7)-H(7C)	109.5	C(14)-C(16)-H(16B)	109.5
H(7B)-C(7)-H(7C)	109.5	H(16A)-C(16)-H(16B)	109.5
C(13)-C(8)-C(9)	119.0(2)	C(14)-C(16)-H(16C)	109.5
C(13)-C(8)-C(2)	120.7(2)	H(16A)-C(16)-H(16C)	109.5
C(9)-C(8)-C(2)	120.1(2)	H(16B)-C(16)-H(16C)	109.5

C(11)-C(17)-C(19)	112.9(2)	C(25)#1-C(23)-C(24)	120.1(3)
C(11)-C(17)-C(18)	110.3(2)	C(25)#1-C(23)-Fe(1)	71.06(17)
C(19)-C(17)-C(18)	110.4(3)	C(24)-C(23)-Fe(1)	71.06(19)
C(11)-C(17)-H(17)	107.6	C(25)#1-C(23)-H(23)	119.9
C(19)-C(17)-H(17)	107.6	C(24)-C(23)-H(23)	119.9
C(18)-C(17)-H(17)	107.6	Fe(1)-C(23)-H(23)	130.6
C(17)-C(18)-H(18A)	109.5	C(25)-C(24)-C(23)	119.9(3)
C(17)-C(18)-H(18B)	109.5	C(25)-C(24)-Fe(1)	70.95(17)
H(18A)-C(18)-H(18B)	109.5	C(23)-C(24)-Fe(1)	70.86(19)
C(17)-C(18)-H(18C)	109.5	C(25)-C(24)-H(24)	120.1
H(18A)-C(18)-H(18C)	109.5	C(23)-C(24)-H(24)	120.1
H(18B)-C(18)-H(18C)	109.5	Fe(1)-C(24)-H(24)	130.8
C(17)-C(19)-H(19A)	109.5	C(23)#1-C(25)-C(24)	120.0(3)
C(17)-C(19)-H(19B)	109.5	C(23)#1-C(25)-Fe(1)	71.02(17)
H(19A)-C(19)-H(19B)	109.5	C(24)-C(25)-Fe(1)	71.11(17)
C(17)-C(19)-H(19C)	109.5	C(23)#1-C(25)-H(25)	120.0
H(19A)-C(19)-H(19C)	109.5	C(24)-C(25)-H(25)	120.0
H(19B)-C(19)-H(19C)	109.5	Fe(1)-C(25)-H(25)	130.5
C(13)-C(20)-C(22)	110.1(2)	C(1)-Fe(1)-C(23)#1	139.43(9)
C(13)-C(20)-C(21)	112.5(2)	C(1)-Fe(1)-C(23)	139.43(9)
C(22)-C(20)-C(21)	110.1(2)	C(23)#1-Fe(1)-C(23)	81.13(18)
C(13)-C(20)-H(20)	108.0	C(1)-Fe(1)-C(25)#1	139.35(8)
C(22)-C(20)-H(20)	108.0	C(23)#1-Fe(1)-C(25)#1	68.67(13)
C(21)-C(20)-H(20)	108.0	C(23)-Fe(1)-C(25)#1	37.92(12)
C(20)-C(21)-H(21A)	109.5	C(1)-Fe(1)-C(25)	139.35(8)
C(20)-C(21)-H(21B)	109.5	C(23)#1-Fe(1)-C(25)	37.92(12)
H(21A)-C(21)-H(21B)	109.5	C(23)-Fe(1)-C(25)	68.67(13)
C(20)-C(21)-H(21C)	109.5	C(25)#1-Fe(1)-C(25)	81.31(16)
H(21A)-C(21)-H(21C)	109.5	C(1)-Fe(1)-C(24)#1	139.40(9)
H(21B)-C(21)-H(21C)	109.5	C(23)#1-Fe(1)-C(24)#1	38.09(11)
C(20)-C(22)-H(22A)	109.5	C(23)-Fe(1)-C(24)#1	68.50(11)
C(20)-C(22)-H(22B)	109.5	C(25)#1-Fe(1)-C(24)#1	37.94(12)
H(22A)-C(22)-H(22B)	109.5	C(25)-Fe(1)-C(24)#1	68.69(12)
C(20)-C(22)-H(22C)	109.5	C(1)-Fe(1)-C(24)	139.40(9)
H(22A)-C(22)-H(22C)	109.5	C(23)#1-Fe(1)-C(24)	68.50(11)
H(22B)-C(22)-H(22C)	109.5	C(23)-Fe(1)-C(24)	38.09(11)

C(25)#1-Fe(1)-C(24)	68.69(12)	C(24)#1-Fe(1)-C(24)	81.20(17)
C(25)-Fe(1)-C(24)	37.94(12)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2

Magnetic susceptibilities of complexes **1** and **2**

Magnetic measurements. The samples for the magnetic studies were sealed under vacuum in 3 or 4 mm quartz tubing. The magnetic susceptibilities have been measured on a Quantum Design MPMSXL7 superconducting quantum interference magnetometer. For each measurement the sample was zero-field cooled to 2 K and the susceptibility has been measured on warming to 320 K in an applied field of 0.01 T. Extra time was used to ensure that the sample was at thermal equilibrium with the temperature sensor. The observed molar magnetic susceptibilities have been corrected for the diamagnetic contribution of the constituents by subtracting –0.000956 emu/mol of [(μ-η^6:η^6-C_7H_8){MnAr*-3,5-Pr^i_2}$_2$] (**1**) and –0.000499 emu/mol of [(μ-η^6:η^6-C_6H_6)FeAr*-3,5-Pr^i_2] (**2**), corrections that have been obtained from tables of Pascal's constants.

Results and Discussion

Magnetic properties of [(μ-η^6:η^6-C_7H_8){MnAr*-3,5-Pr^i_2}$_2$] (**1**): In **1**, each manganese is present in a highly distorted environment as manganese(I) with a nominal $3d^6$ $t_2^4e^2$ electronic ground state, a nominal $^5T_2$ spectroscopic ground state, and $S = 2$. The manganese(I) in the absence of any Mn–Mn magnetic exchange would be expected to have a μ_{eff} of ca. 5.2 μ_B per manganese ion, a moment that is increased somewhat above the 4.90 μ_B spin-only value due to an orbital contribution to the moment.

The molar magnetic susceptibility, χ_M', of **1**, and its inverse, are shown in Figure 1; the inverse susceptibility is linear between 150 and 320 K and yields a Weiss temperature of –14.6 K, a Curie constant of 3.34 mol Mn/emu K, and a corresponding μ_{eff} of 5.17 μ_B per manganese(I) ion. A bit surprisingly, the μ_{eff} of **1** increases virtually linearly from 4.78 to 5.05 μ_B between 2 and 320 K whilst χ_M' × T increases almost linearly from 2.87 to 3.19 emu K/mol Mn between 2 and 320 K. This increase presumably is a result of a combination of a small intramolecular Mn–Mn antiferromagnetic exchange coupling, an orbital contribution to the moment, and a positive zero-field splitting. Indeed, a Mn(I)–Mn(I) antiferromagnetic exchange coupling constant, J, of –2 cm^{-1} rather well reproduces the linear increase in μ_{eff} observed between ca. 100 and 320 K.

Magnetic properties of [(μ-η^6:η^6-C_6H_6)FeAr*-3,5-Pr^i_2] (**2**)**.** In **2** the iron is present in a highly distorted environment as iron(I) with a nominal $3d^7$ $t_2^5e^2$ electronic ground

state, a nominal $^4T_1$ spectroscopic ground state, and $S = 3/2$. Thus the iron(I) might be expected to approximate a spin-only compound with an effective magnetic moment, μ_{eff}, of 3.87 μ_B, a moment that could be substantially increased by an orbital contribution as is often observed[A] in analogous cobalt(II) complexes.

The molar magnetic susceptibility, χ_M', of **2** and its inverse are shown in Figure 2; the inverse susceptibility is linear between 200 and 320 K and yields a Weiss temperature of –84 K, a Curie constant of 2.74 mol/emu K, and a corresponding μ_{eff} of 4.68 μ_B. Perhaps more informative is a plot of χ_M' × T, see Figure 3, which indicates that χ_M' × T increases virtually linearly between 20 and 320 K; below 20 K χ_M' × T decreases sharply as a result of the extensive zero-field splitting arising from the very low-symmetry of the iron(I) coordination environment. The linear increase in χ_M' × T observed above ca. 20 K is expected[A] of iron(I) in a highly distorted environment in which the degeneracy of the $^4T_1$ states has been fully removed. A comparison of the χ_M' × T values observed for **2** above 20 K with the values shown in Figure 3.4 of reference A indicates that ν may be of the order of 20, where $\nu = \Delta / |\lambda|$ is the ratio of the crystal field splitting and the magnitude of the iron(I) spin-orbit coupling constant.

Reference

(A) Kahn, O. *Molecular Magnetism*: VCH Publishers: New York, 1993.

Figure 1**.** The molar magnetic susceptibility, χ_M', of **1** obtained in a 0.01 T applied field. The points are the observed susceptibility and the line corresponds to the susceptibility expected for an effective magnetic moment of 5.17 μ_B. Inset: The inverse molar magnetic susceptibility of **1** and the Curie-Weiss law fit obtained between 150 and 320 K.

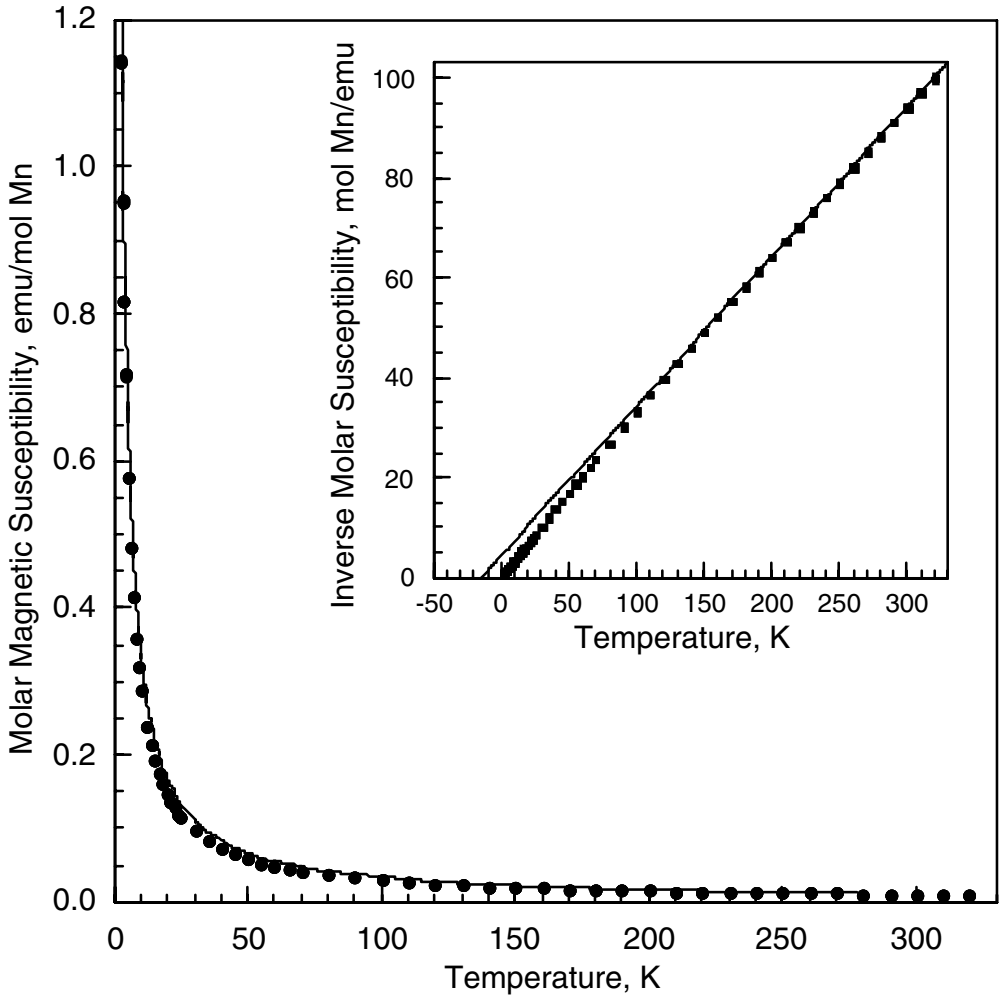

Figure 2**.** The molar magnetic susceptibility, χ_M', of **2** obtained in a 0.01 T applied field. The points are the observed susceptibility and the line corresponds to the susceptibility expected for the effective spin—only magnetic moment of 3.87 μ_B. Inset: The inverse molar magnetic susceptibility of **2** and the Curie-Weiss law fit obtained between 200 and 320 K.

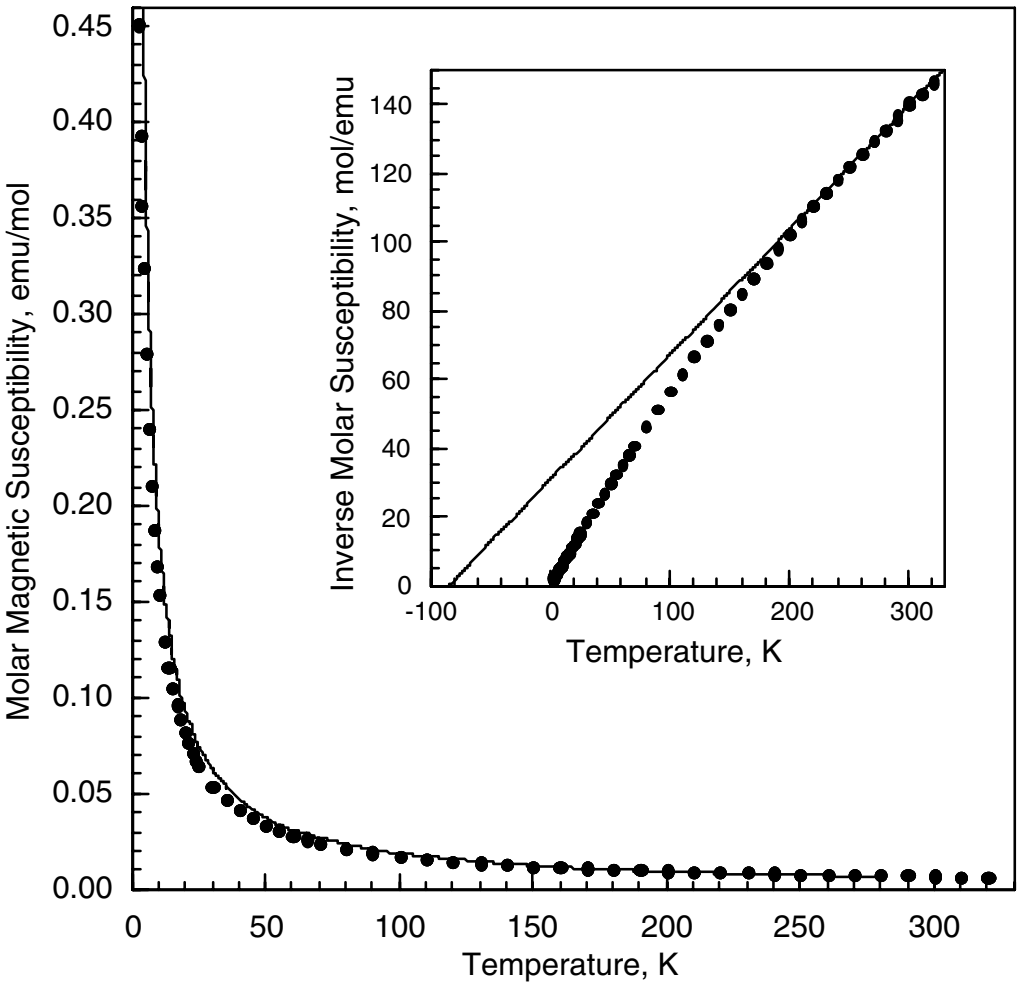

Figure 3. The temperature dependence of χ_M' × T of **2** obtained in a 0.01 T applied field.