Table 1. Positional ($x10^4$) and equivalent thermal parameters ($x10^3$) of the non-H atoms for $(NH_4)_4[Mn(II)(C_6H_5O_7)_2]$ (**1**). E.s.d.s are given in parentheses. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mn	5000	5000	5000	20(1)
O(1)	3680(2)	6340(1)	4405(2)	31(1)
O(3)	5029(2)	5167(1)	2595(2)	21(1)
O(5)	7198(2)	5829(1)	5277(2)	27(1)
C(1)	3192(3)	6879(2)	3181(3)	25(1)
O(2)	1962(2)	7426(2)	2826(2)	51(1)
C(2)	4132(3)	6883(2)	2112(3)	25(1)
C(3)	5579(2)	6151(1)	2484(2)	19(1)
C(4)	6969(2)	6413(1)	4113(2)	20(1)
O(4)	7756(2)	7174(1)	4219(2)	32(1)
C(5)	6185(3)	6211(2)	1128(2)	24(1)
C(6)	7607(2)	5530(2)	1270(2)	22(1)
O(6)	8719(2)	5375(1)	2614(2)	31(1)
O(7)	7626(2)	5171(1)	9(2)	33(1)
N(1)	1126(3)	6192(2)	5403(2)	28(1)
N(2)	9514(3)	6310(2)	8357(3)	38(1)

Table 2. Anisotropic thermal parameters ($x10^3$) of the non-H atoms for **1**.
E.s.d.s are given in parentheses.

	U11	U22	U33	U23	U13	U12
Mn	21(1)	19(1)	20(1)	5(1)	9(1)	2(1)
O(1)	40(1)	28(1)	34(1)	11(1)	23(1)	14(1)
O(3)	23(1)	19(1)	18(1)	0(1)	6(1)	-2(1)
O(5)	25(1)	32(1)	19(1)	3(1)	3(1)	-6(1)
C(1)	27(1)	22(1)	30(1)	6(1)	14(1)	6(1)
O(2)	50(1)	57(1)	62(1)	34(1)	39(1)	36(1)
C(2)	25(1)	26(1)	25(1)	8(1)	12(1)	8(1)
C(3)	20(1)	19(1)	18(1)	3(1)	7(1)	2(1)
C(4)	20(1)	20(1)	23(1)	-1(1)	11(1)	1(1)
O(4)	33(1)	24(1)	39(1)	-4(1)	15(1)	-9(1)
C(5)	25(1)	30(1)	17(1)	5(1)	10(1)	5(1)
C(6)	21(1)	24(1)	21(1)	-1(1)	9(1)	-3(1)
O(6)	28(1)	38(1)	23(1)	1(1)	5(1)	7(1)
O(7)	28(1)	45(1)	25(1)	-10(1)	10(1)	2(1)
N(1)	25(1)	31(1)	28(1)	-2(1)	9(1)	-3(1)
N(2)	35(1)	46(1)	32(1)	-7(1)	13(1)	6(1)

Table 3. Positional ($x10^4$) and isotropic thermal parameters ($x10^3$) of the hydrogen atoms for **1**. E.s.d.s are given in parentheses.

	x	y	z	U(eq)
HO3	4143(41)	5026(22)	1744(39)	47(9)
H(2A)	3337(33)	6776(19)	1049(32)	32(7)
H(2B)	4570(37)	7501(23)	2126(36)	46(8)
H(5A)	5218(30)	6086(18)	126(29)	22(6)
H(5B)	6622(34)	6900(21)	1101(32)	38(7)
HN1A	1994(46)	6250(26)	5023(41)	65(10)
HN1B	1281(38)	5612(24)	6043(38)	49(8)
HN1C	161(55)	6153(31)	4642(54)	86(13)
HN1D	1261(41)	6730(26)	6074(41)	58(9)
HN2A	8669(50)	6168(29)	7177(52)	79(12)
HN2B	8965(63)	6460(38)	8824(62)	111(18)
HN2C	10223(64)	5749(41)	8761(60)	122(19)
HN2D	10283(77)	6908(48)	8292(71)	159(23)

Table 4. Hydrogen Bond Distances (Å) and Angles (deg) for **1**.

O3-H	0.874
H...O7(1-X,1-Y,-Z)	1.751
O3-H...O7	175.9
O3...O7	2.624
N1-HN1A	0.960
HN1A....O1(X,Y,Z)	1.788
N1-HN1A...O1	177.2
N1....O1	2.747
N1-HN1B	0.961
HN1B....O6(1-X,1-Y,1-Z)	1.825
N1-HN1B...O6	168.7
N1....O6 2.774	
N1-HN1C	0.856
HN1C....O6(-1+X,Y,Z)	2.074
N1-HN1C...O6	144.2
N1....O6	2.813
N1-HN1D	0.935
HN1D....O2(X,1.5-Y,0.5+Z)	1.869
N1-HN1D...O2	164.0
N1....O2	2.779
N2-HN2A	1.056
HN2A....O5(X,Y,Z)	1.764
N2-HN2A...O5	174.5
N2....O5	2.816
N2-HN2B	0.789
HN2B....O4(X,1.5-Y,0.5+Z)	2.246
N2-HN2B...O4	137.1
N2....O4	2.874
N2-HN2C	0.964
HN2C....O7(2-X,1-Y,1-Z)	2.169
N2-HN2C...O7	162.6
N2....O7	3.102
N2-HN2D	1.076
HN2D....O2(1+X,1.5-Y,0.5+Z)	1.919
N2-HN2D...O2	157.9
N2....O2	2.944

Table 5. Positional (x 10^4) and equivalent thermal parameters (x 10^3) of the non-H atoms for $(NH_4)_5[Mn(III)(C_6H_4O_7)_2]\cdot 2H_2O$ (**2**). E.s.d.s are given in parentheses. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mn	0	0	0	19(1)
O(1)	73(2)	-2081(2)	994(2)	31(1)
O(3)	-1900(2)	-1422(1)	-2099(2)	21(1)
O(5)	-1639(2)	-433(2)	1340(2)	29(1)
C(1)	-1116(2)	-3502(2)	517(3)	25(1)
O(2)	-998(2)	-4596(2)	1211(2)	41(1)
C(2)	-2775(2)	-3927(2)	-1000(3)	24(1)
C(3)	-3122(2)	-2578(2)	-1353(2)	20(1)
C(4)	-2952(2)	-1812(2)	632(3)	24(1)
O(4)	-3929(2)	-2525(2)	1538(2)	38(1)
C(5)	-4879(2)	-3253(2)	-2824(3)	27(1)
C(6)	-5476(2)	-2093(2)	-3257(3)	30(1)
O(6)	-6488(3)	-2377(3)	-4931(3)	63(1)
O(7)	-5061(2)	-1030(2)	-1933(3)	56(1)
N(1)	2958(3)	-2310(2)	983(3)	36(1)
N(2)	2288(3)	-326(3)	5109(3)	38(1)
N(3)	0	5000	5000	84(2)
OW	1196(3)	2634(3)	4954(3)	57(1)

Table 6. Anisotropic thermal parameters (x 10^3) of the non-H atoms for **2**.
E.s.d.s are given in parentheses.

	U11	U22	U33	U23	U13	U12
Mn	15(1)	17(1)	18(1)	1(1)	4(1)	5(1)
O(1)	22(1)	24(1)	36(1)	4(1)	0(1)	10(1)
O(3)	20(1)	19(1)	19(1)	4(1)	5(1)	6(1)
O(5)	22(1)	27(1)	28(1)	-4(1)	9(1)	5(1)
C(1)	28(1)	25(1)	23(1)	5(1)	7(1)	15(1)
O(2)	46(1)	28(1)	40(1)	7(1)	-2(1)	21(1)
C(2)	22(1)	17(1)	29(1)	5(1)	5(1)	8(1)
C(3)	17(1)	17(1)	22(1)	3(1)	5(1)	6(1)
C(4)	19(1)	25(1)	25(1)	5(1)	7(1)	10(1)
O(4)	31(1)	37(1)	36(1)	3(1)	19(1)	6(1)
C(5)	20(1)	23(1)	29(1)	1(1)	0(1)	8(1)
C(6)	22(1)	32(1)	35(1)	10(1)	8(1)	14(1)
O(6)	83(1)	90(2)	36(1)	7(1)	-1(1)	69(1)
O(7)	60(1)	42(1)	60(1)	-6(1)	-4(1)	34(1)
N(1)	31(1)	34(1)	42(1)	2(1)	9(1)	17(1)
N(2)	52(1)	47(1)	28(1)	10(1)	13(1)	34(1)
N(3)	78(4)	73(3)	48(2)	23(2)	-13(2)	14(3)
OW	78(1)	62(1)	47(1)	8(1)	34(1)	40(1)

Table 7. Positional ($x10^4$) and isotropic thermal parameters ($x10^3$) of the hydrogen atoms for **2**. E.s.d.s are given in parentheses.

	x	y	z	U(eq)
H(2A)	-2808(27)	-4388(25)	-2250(33)	27(5)
H(2B)	-3621(31)	-4697(28)	-655(34)	32(6)
H(5A)	-4893(29)	-3715(27)	-4005(36)	34(6)
H(5B)	-5661(32)	-4092(30)	-2363(36)	38(6)
HN1A	2375(36)	-3230(36)	247(42)	46(7)
HN1B	3747(48)	-1657(44)	623(53)	73(11)
HN1C	2195(45)	-2079(38)	843(48)	64(9)
HN1D	3378(39)	-2333(34)	2180(50)	55(8)
HN2A	2823(42)	-927(39)	5243(48)	68(9)
HN2B	2299(39)	255(38)	4078(51)	63(9)
HN2C	2787(46)	360(44)	6102(57)	74(11)
HN2D	1242(48)	-1012(41)	5015(47)	66(10)
HN3A	-287(77)	5062(69)	3977(90)	43(16)
HN3B	930(66)	5516(64)	4986(83)	29(16)
HWA	1428(41)	2361(39)	4175(51)	61(10)
HWB	639(95)	3165(97)	4630(112)	233(38)

Table 8. Hydrogen Bonds (Å) and Angles (deg) for **2**.

N1-HN1A	0.868
HN1A...O2(-X,-1-Y,-Z)	1.975
N1-HN1A...O2	174.6
N1...O2	2.840
N1-HN1B	0.835
HN1B...O7(1+X,Y,Z)	2.370
N1-HN1B...O7	146.3
N1...O7	3.099
N1-HN1C	0.851
HN1C...O1(X,Y,Z)	2.070
N1-HN1C...O1	161.9
N1...O1	2.891
N1-HN1D	0.858
HN1D...O6(1+X,Y,Z)	2.065
N1-HN1D...O6	156.3
N1...O6	2.872
N2-HN2A	0.950
HN2A...O6(1+X,Y,1+Z)	1.867
N2-HN2A...O6	168.5
N2...O6	2.804
N2-HN2B	0.951
HN2B...O3(-X,-Y,-Z)	1.934
N2-HN2B...O3	167.3
N2...O3	2.869
N2-HN2C	0.830
HN2C...O4(-X,-Y,1-Z)	2.302
N2-HN2C...O4	168.0
N2...O4	3.119
N2-HN2D	0.879
HN2D...OW(-X,-Y,1-Z)	2.105
N2-HN2D...OW	175.2
N2...OW	2.981
N3-HN3A	0.733
HN3A...O2(X,1+Y,Z)	2.028
N3-HN3A...O2	175.2
N3...O2	2.760
N3-HN3B	0.787
HN3B...O6(1+X,1+Y,1+Z)	2.231

N3-HN3B...O6	163.2
N3...O6	3.083
OW-HWA	0.750
HWA...O3(-X,-Y,-Z)	2.016
OW-HWA...O3	174.7
OW...O3	2.764
OW-HWB	0.910
HWB...N3(X,Y,Z)	2.217
OW-HWB...N3	157.0
OW...N3	3.076

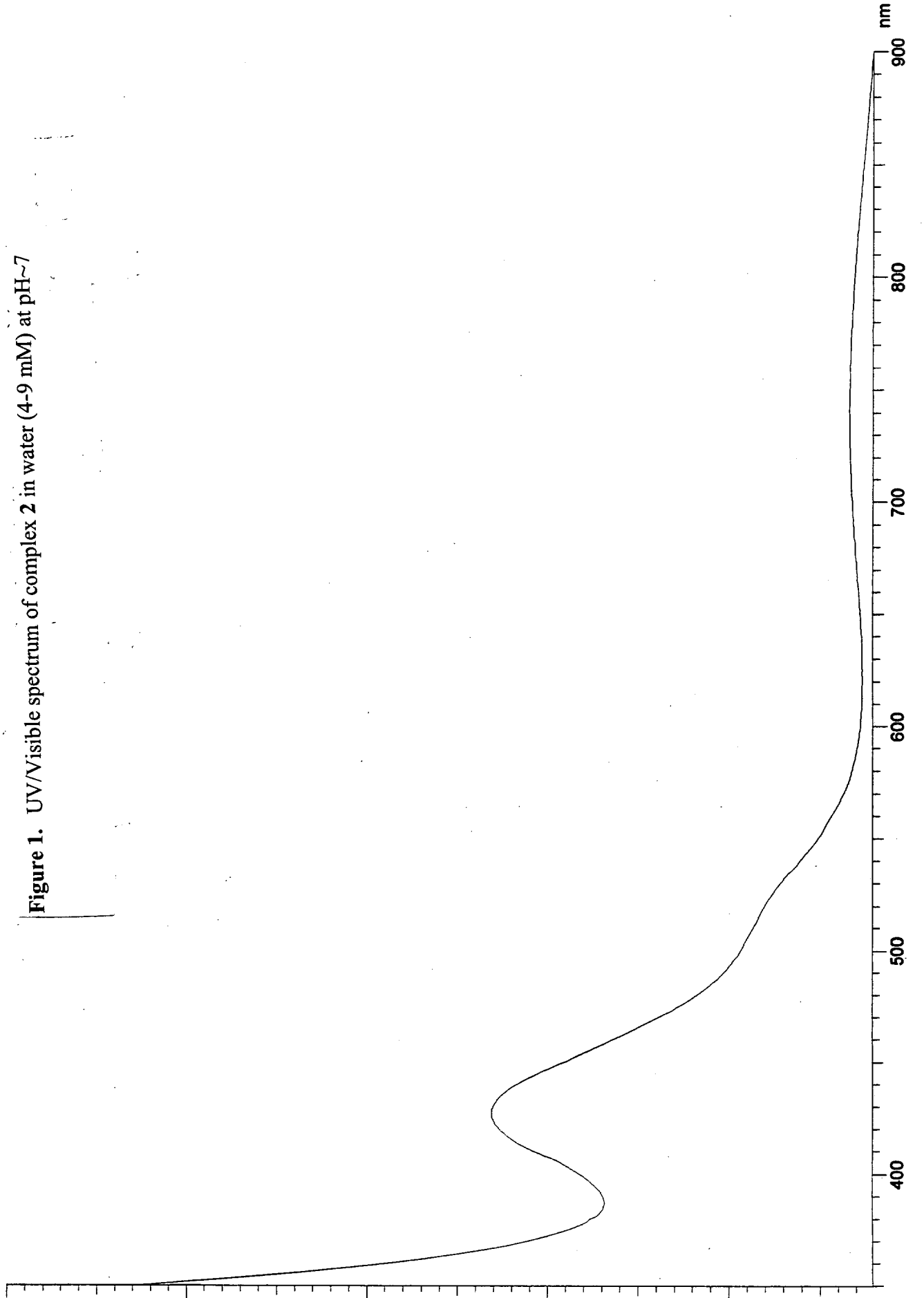

Figure 1. UV/Visible spectrum of complex **2** in water (4-9 mM) at pH~7