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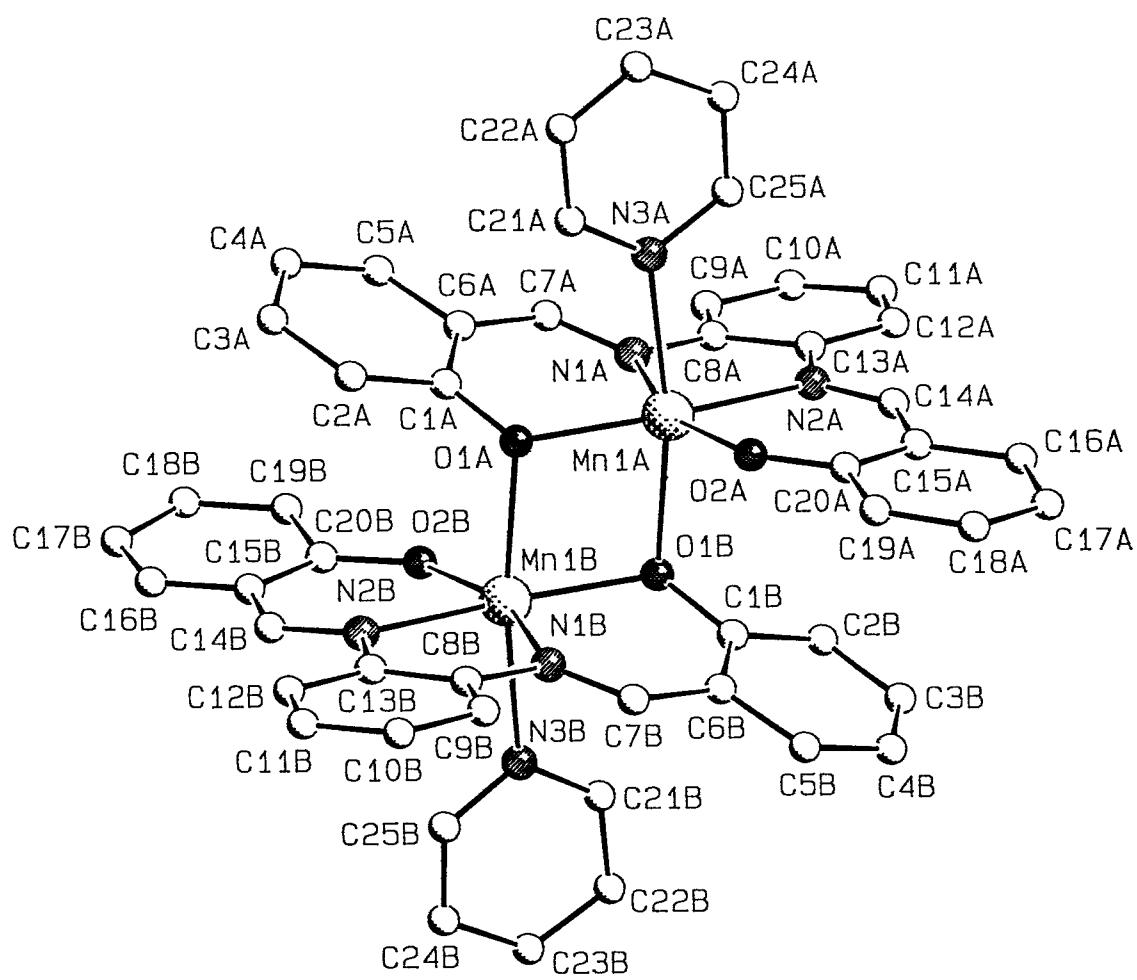
### Description of the structure of complex 14

Complex 14 consists of monomeric  $[\text{Mn}(\text{salophen})(\text{THF})]^+$  cations,  $\text{I}_3^-$  anions weakly interacting at a  $\text{Mn}\cdots\text{I1}$  distance of  $3.279(2)$  Å, and THF molecules of crystallization in a molar ratio of 1/1/1. The metal atom lies at  $0.079(2)$  Å from the planar  $\text{N}_2\text{O}_2$  core and achieves a square pyramidal coordination through the oxygen atom from a THF molecule (Figure S1).

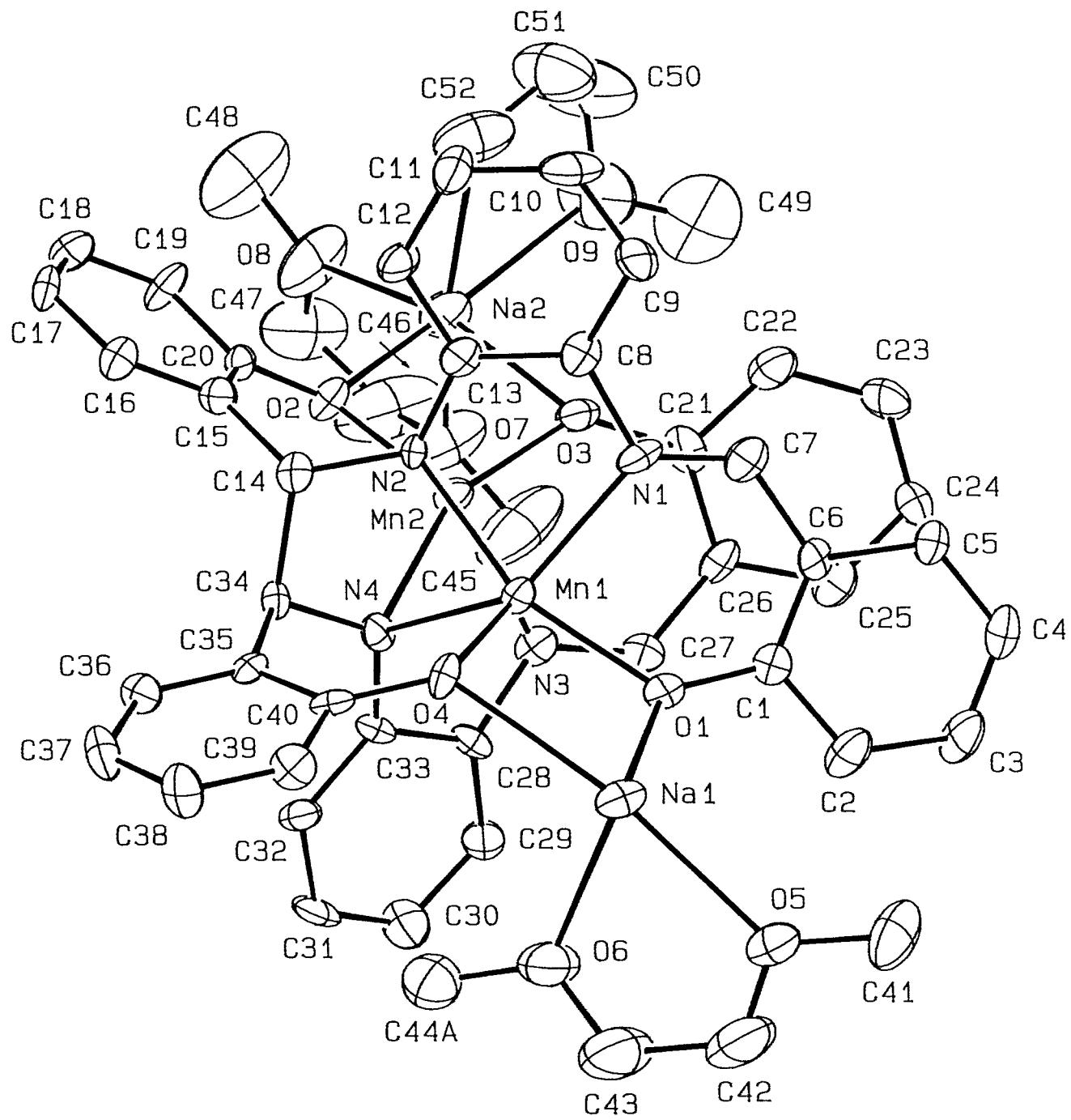
The  $\text{O3}-\text{Mn}\cdots\text{I1}$  angle is  $178.5(2)^\circ$ . Assuming the  $\text{Mn}\cdots\text{I}_3^-$  as a bonding interaction, the coordination polyhedron could be described as an asymmetrically elongated bipyramid. The salophen ligand assumes an umbrella conformation folded towards the  $\text{I}_3^-$  anion, the dihedral angles between the peripheral phenolic rings being  $15.3(4)^\circ$ . The  $\text{Mn}-\text{O}$  [mean value  $1.850(6)$  Å] and  $\text{Mn}-\text{N}$  [mean value  $1.972(6)$  Å] bond distances are remarkably shorter than those found in the previous complexes containing manganese(II), according to the increased oxidation state of the metal.

### X-ray crystallography for complex 16.

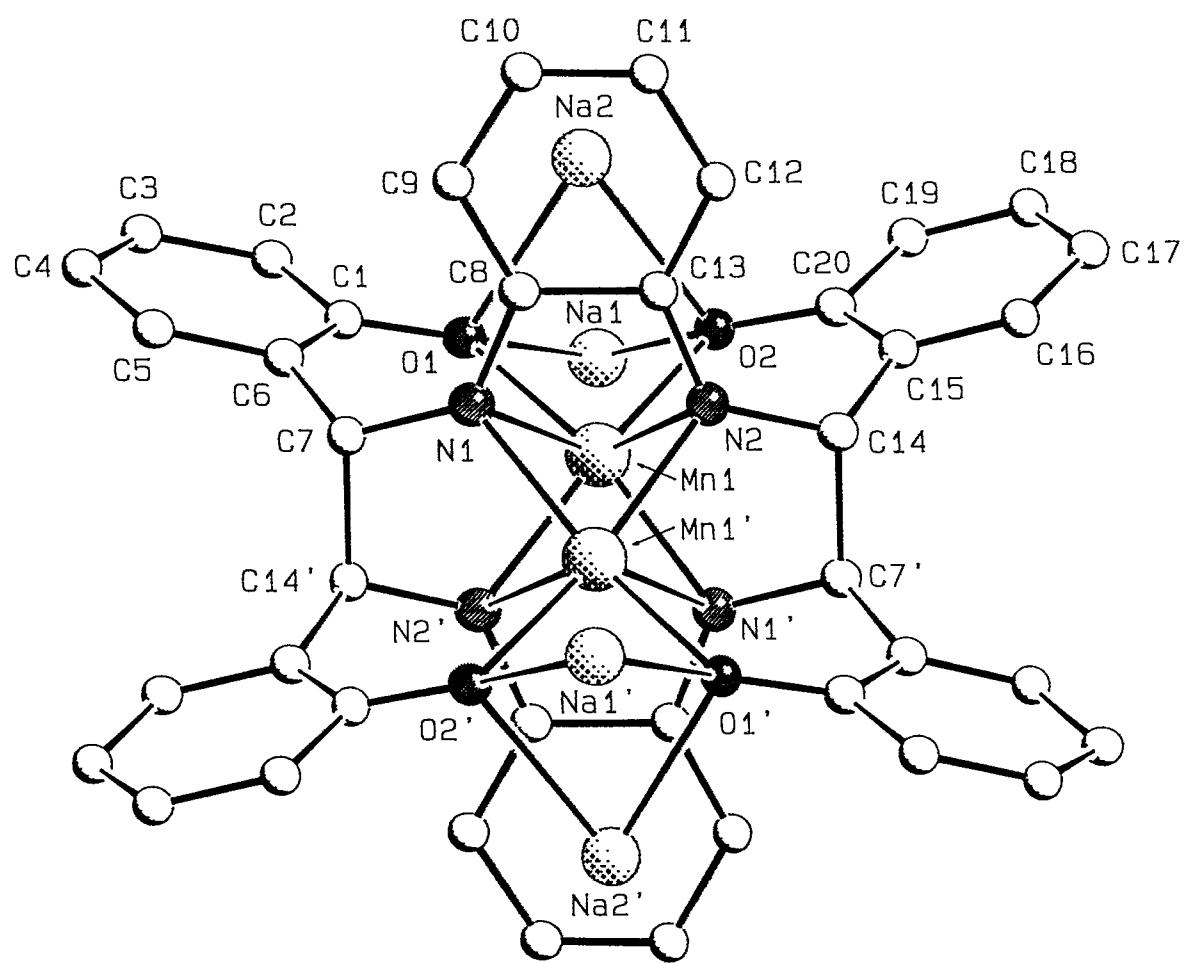
$\text{C}_{72}\text{H}_{92}\text{Mn}_2\text{N}_4\text{O}_6$ ,  $M = 1219.4$ , triclinic, space group  $P\bar{1}$ ,  $a = 12.668(2)$ ,  $b = 13.830(3)$ ,  $c = 10.469(1)$  Å,  $\alpha = 97.07(1)$ ,  $\beta = 113.74(1)$ ,  $\gamma = 80.87(1)^\circ$ ,  $V = 1654.1(5)$  Å $^3$ ,  $Z = 1$ ,  $D_{\text{calcd}} = 1.224$  g/cm $^3$ ,  $F(000) = 650$ ,  $\lambda(\text{Cu-K}\alpha) = 1.54178$  Å,  $\mu(\text{Cu-K}\alpha) = 35.22$  cm $^{-1}$ : crystal dimensions  $0.16 \times 0.24 \times 0.56$  mm. The structure was solved by the heavy atom method and anisotropically refined for all the non-H atoms. All the hydrogen atoms were located from a difference Fourier map and introduced as fixed contributors in the last stage of refinement ( $U_{\text{iso}} = 0.08$  Å $^2$ ). For 2621 unique observed reflections [ $I > 2\sigma(I)$ ] collected at  $T=295$  K on a Rigaku AFC6S diffractometer ( $5 < 2\theta < 140^\circ$ ) and corrected for absorption the final  $R$  is 0.055 ( $wR2 = 0.171$  for the 5146 reflections having  $I > 0$  used in the refinement). All calculations were carried out on a Quansan Personal Computer equipped with an Intel Pentium processor. Atomic coordinates, bond lengths and angles, and thermal parameters have been deposited with the Cambridge Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW (England).

**Figure S1.** SCHAKAL view of complex 4.

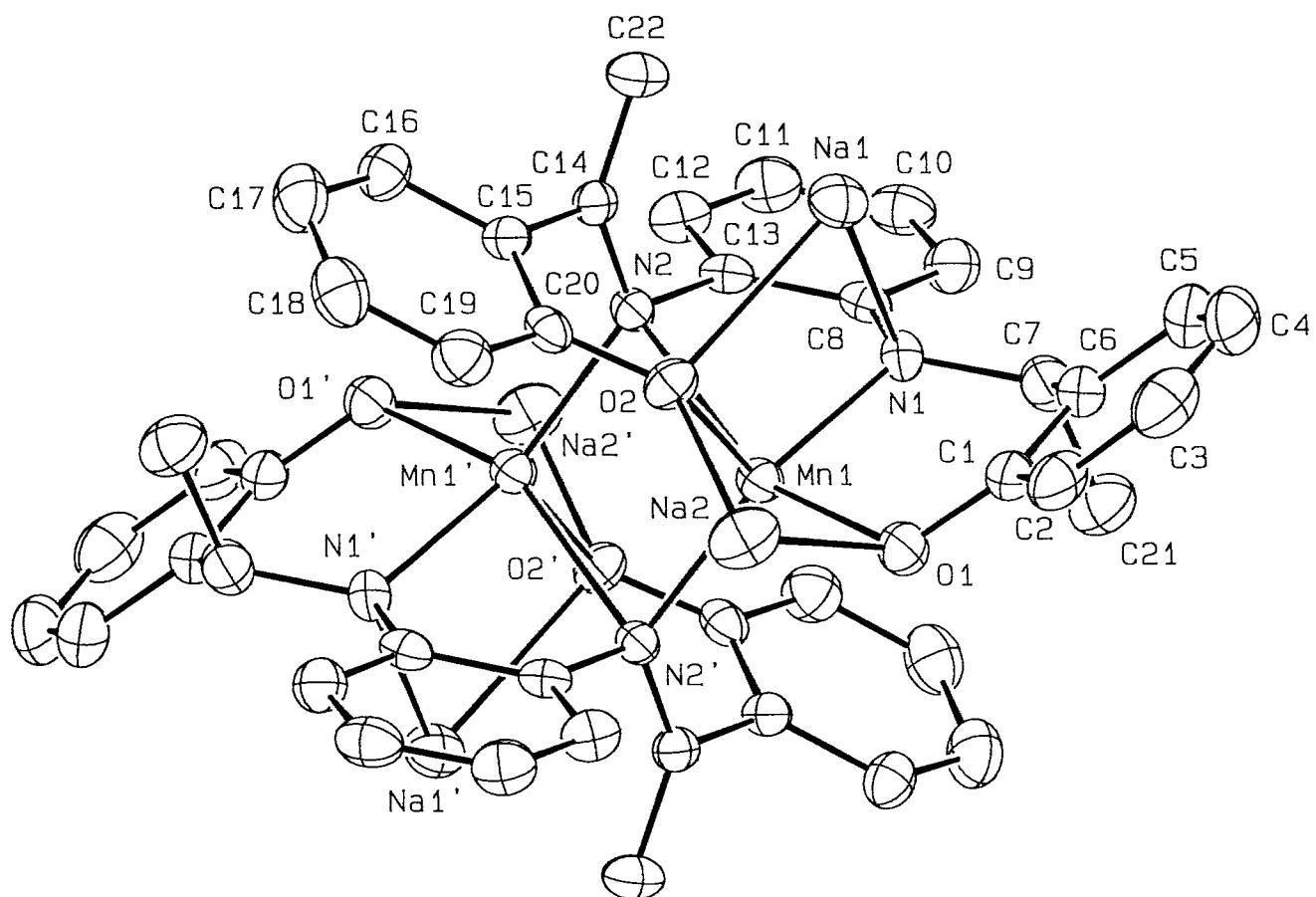
**Figure S2.** ORTEP view of complex **5** (30% probability ellipsoids). The B position of C44 is omitted for clarity.

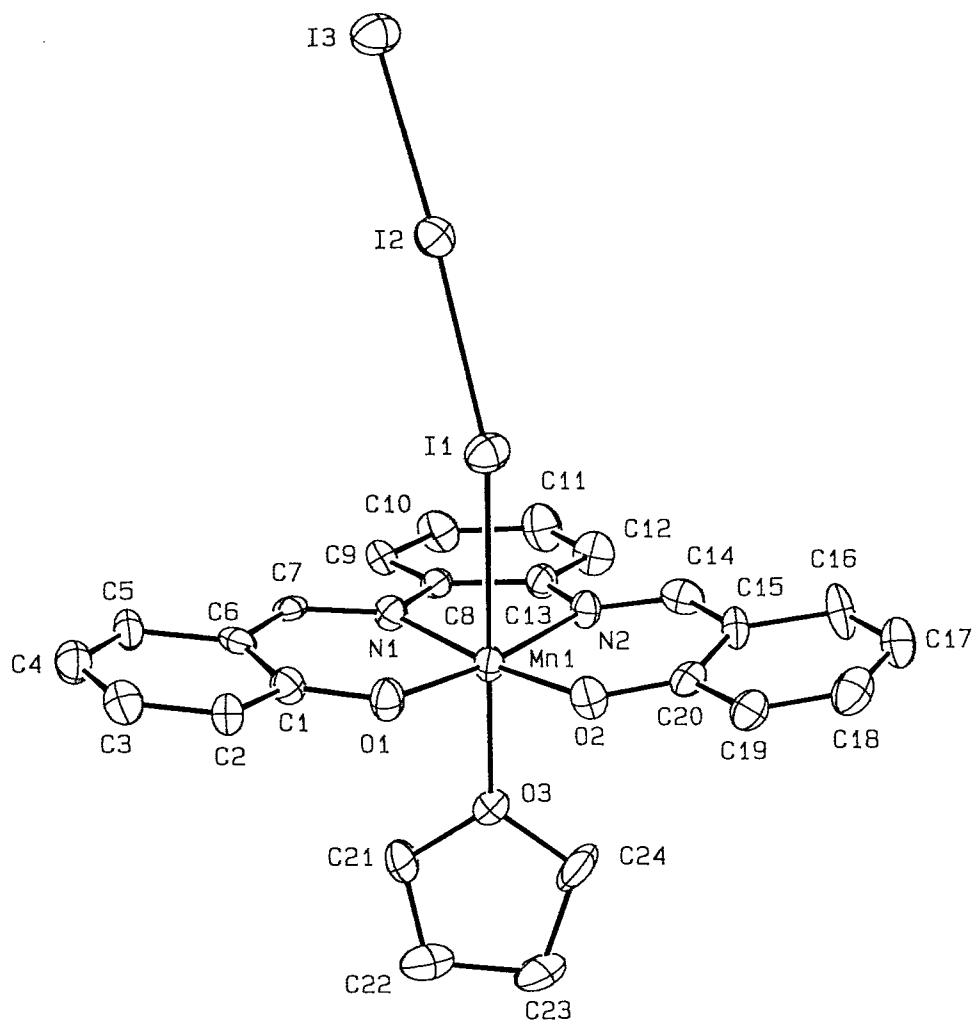


**Figure S3.** SCHAKAL view of complex **6**. DME molecules bonded to sodium are omitted for clarity. Prime denotes a transformation of  $1-x$ ,  $-y$ ,  $1-z$ .



**Figure S4.** ORTEP view of complex **9** (30% probability ellipsoids). DME molecules bonded to sodium are omitted for clarity. Prime denotes a transformation of  $1-x$ ,  $-y$ ,  $1-z$ .



**Figure S5.** ORTEP view of complex **14** (30% probability ellipsoids).

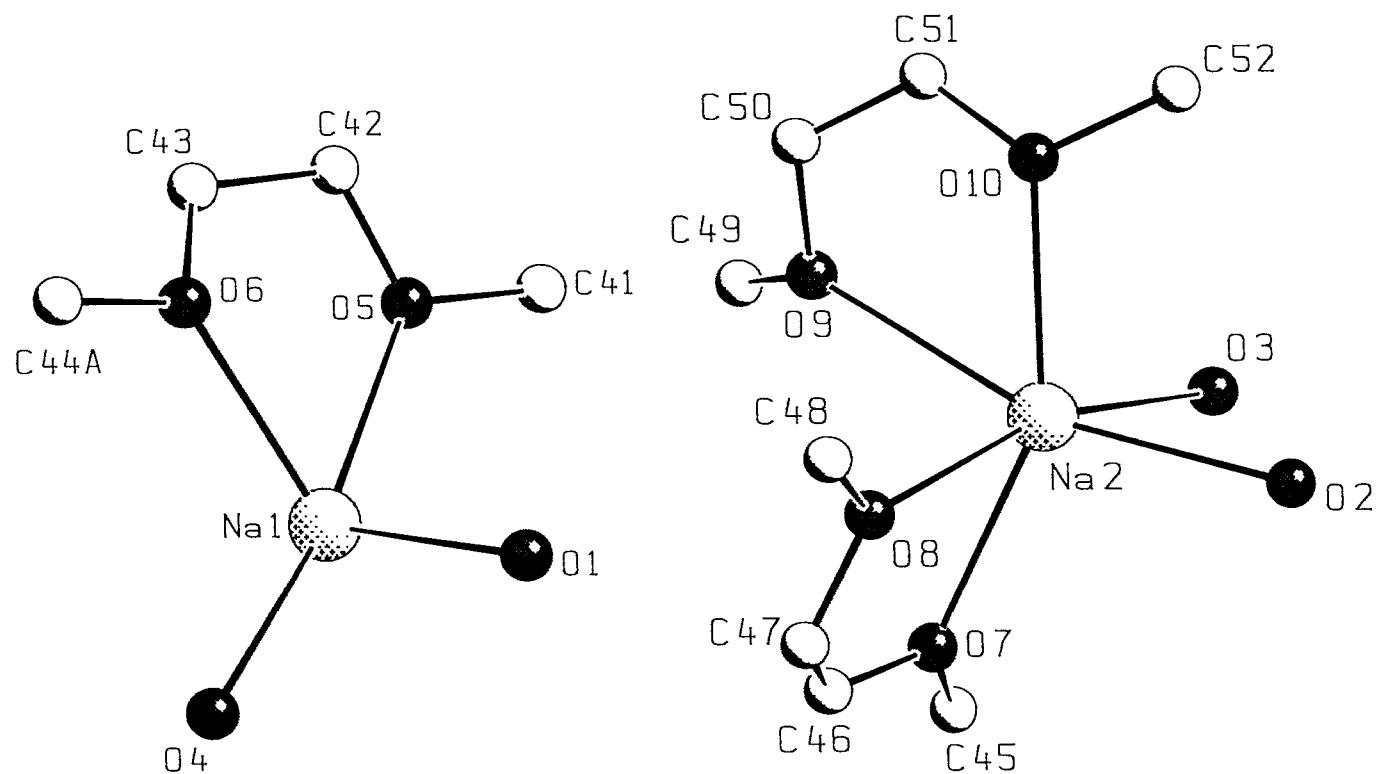
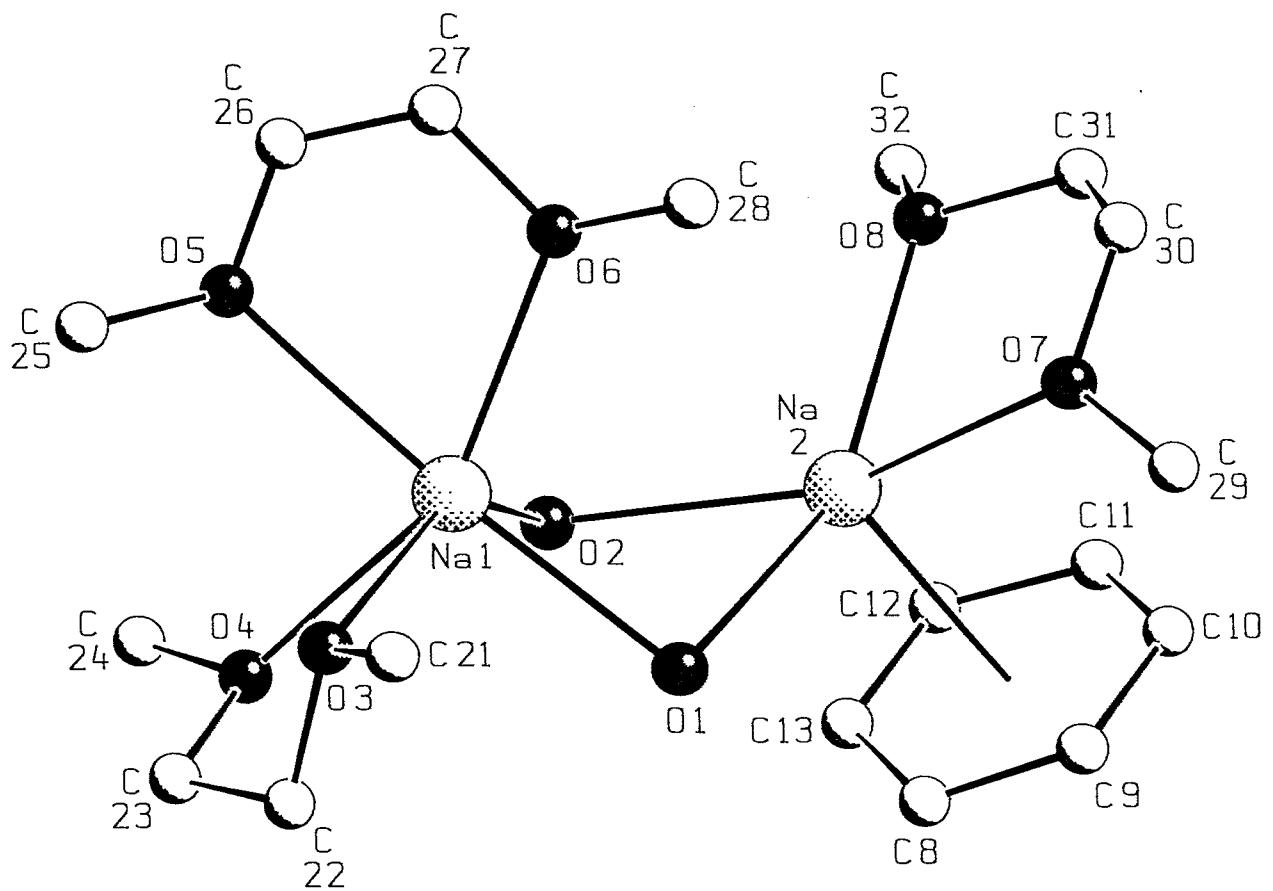
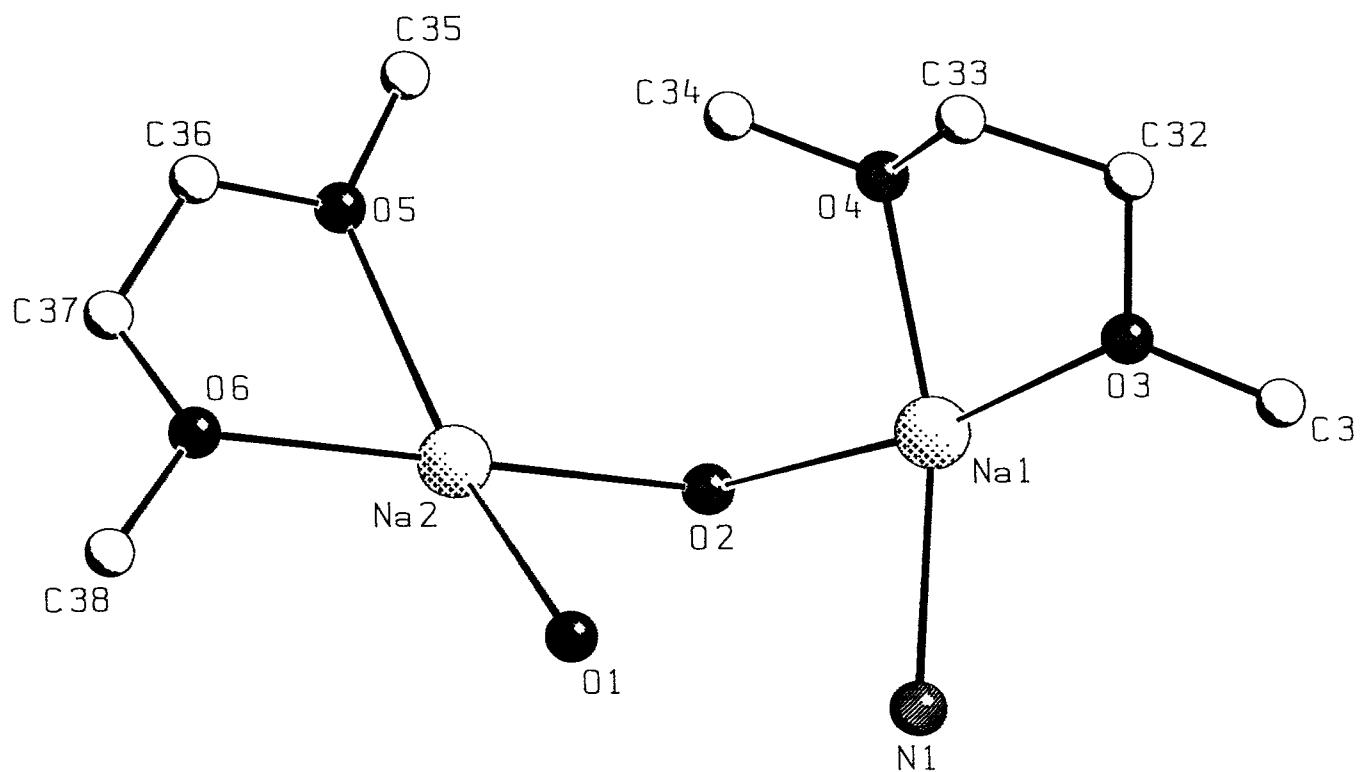
**Figure S6.** SCHAKAL drawing of coordination of sodium cations in complex 5.

Figure S7. SCHAKAL drawing of coordination of sodium cations in complex 6.



**Figure S8.** SCHAKAL drawing of coordination of sodium cations in complex **9**.



**Figure S9.** SCHAKAL view of complex 16. Prime denotes a transformation of -x, -y, -z.

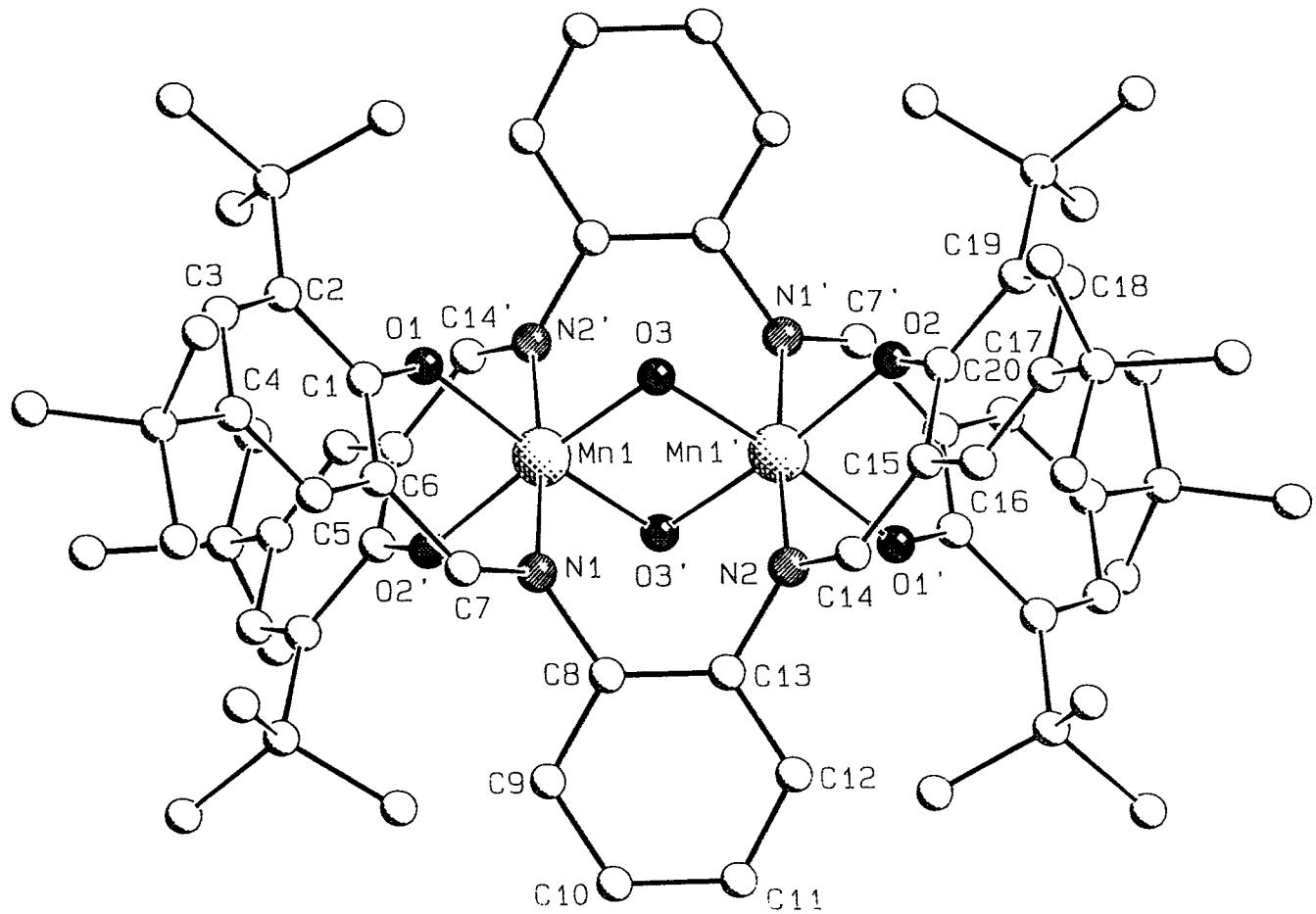


Table S1. Experimental Data for the X-ray Diffraction Studies on Crystalline Complexes **4**, **5**, **6**, **9**, **14**, and **16**.

compound	<b>4</b>	<b>5</b>	<b>6</b>	<b>9</b>	<b>14</b>	<b>16</b>
formula	C <sub>50</sub> H <sub>38</sub> Mn <sub>2</sub> N <sub>6</sub> O <sub>4</sub>	C <sub>52</sub> H <sub>58</sub> Mn <sub>2</sub> N <sub>4</sub> Na <sub>2</sub> O <sub>10</sub>	C <sub>64</sub> H <sub>88</sub> Mn <sub>2</sub> N <sub>4</sub> Na <sub>4</sub> O <sub>16</sub>	C <sub>60</sub> H <sub>76</sub> Mn <sub>2</sub> N <sub>4</sub> Na <sub>4</sub> O <sub>12</sub>	C <sub>24</sub> H <sub>22</sub> I <sub>3</sub> MnN <sub>2</sub> O <sub>3</sub> • C <sub>4</sub> H <sub>8</sub> O	C <sub>72</sub> H <sub>92</sub> Mn <sub>2</sub> N <sub>4</sub> O <sub>6</sub>
cryst habit	prism	irregular prism	irregular prism	prism	irregular prism	elongated prism
cryst colour	dark red	black	yellow	pale brown	black	red
fw	896.8	1054.9	1371.3	1247.1	894.2	1219.4
cryst syst	orthorhombic	triclinic	monoclinic	monoclinic	monoclinic	triclinic
space group	P <sub>2</sub> <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P $\bar{1}$	P <sub>2</sub> <sub>1</sub> /n	P <sub>2</sub> <sub>1</sub> /n	P <sub>2</sub> <sub>1</sub> /n	P $\bar{1}$
cell parameters <sup>a</sup>						
a, Å	24.632(4)	14.241(3)	12.678(3)	13.303(3)	9.886(8)	12.668(2)
b, Å	16.821(3)	16.080(4)	18.314(3)	17.456(4)	19.377(3)	13.830(3)
c, Å	10.098(3)	12.426(2)	14.807(2)	14.039(3)	15.883(4)	10.469(1)
α, deg	90	101.91(2)	90	90	90	97.07(1)
β, deg	90	111.42(2)	92.83(2)	104.56(2)	94.47(3)	113.74(1)
γ, deg	90	88.71(2)	90	90	90	80.87(1)
V, Å <sup>3</sup>	4184.0(16)	2587.6(10)	3433.8(11)	3155.4(12)	3033(3)	1654.1(5)
Z	4	2	2	2	4	1

Table S1. Experimental Data for the X-ray Diffraction Studies on Crystalline Complexes **4**, **5**, **6**, **9**, **14**, and **16**. (cont.)

compound	<b>4</b>	<b>5</b>	<b>6</b>	<b>9</b>	<b>14</b>	<b>16</b>
d <sub>calc</sub> , Mg m <sup>-3</sup>	1.424	1.354	1.326	1.313	1.958	1.224
cryst dimens, mm	0.21x0.28x0.53	0.16x0.19x0.33	0.21x0.33x0.42	0.16x0.23x0.34	0.21x0.29x0.48	0.16x0.24x0.56
linear abs coeff, cm <sup>-1</sup>	6.31	46.41	4.40	4.68	34.74	35.22
diffractometer	Philips PW1100	Rigaku AFC6S	Rigaku AFC6S	Enraf-Nonius CAD4	Rigaku AFC6S	Rigaku AFC6S
diffraction geometry	equatorial	equatorial	equatorial	equatorial	equatorial	equatorial
scan type	$\omega/2\theta$	$\omega/2\theta$	$\omega/2\theta$	$\omega/2\theta$	$\omega/2\theta$	$\omega/2\theta$
scan speed deg min <sup>-1</sup>	3-12	1-4	2-8	3-12	2-8	2-8
scan width, deg	1.20 + 0.35 tgθ	1.25 + 0.30 tgθ	1.23 + 0.35 tgθ	1.20 + 0.35 tgθ	1.73 + 0.35 tgθ	1.63 + 0.30 tgθ
radiation	b	c	b	b	b	c
data collcn range of 2θ, deg	6-50	6-140	5-50	6-50	6-50	5-140
reflcns measd	h,k,l	h, ±k, ±l	h,k,±l	±h,k, l	h,k,±l	h, ±k, ±l
unique measured data	7274	9751	6092	5531	5372	6244
unique "observed" data (NO)	3336	7403	5006	4423	4299	5146
criterion for obsn	F <sup>2</sup> > -2σ(F <sup>2</sup> )	F <sup>2</sup> > 0				
unique obs data [I>2σ(I)]	1819	2728	2818	2016	2416	2621

Table S1. Experimental Data for the X-ray Diffraction Studies on Crystalline Complexes **4**, **5**, **6**, **9**, **14** and **16**. (cont.)

compound	<b>4</b>	<b>5</b>	<b>6</b>	<b>9</b>	<b>14</b>	<b>16</b>
no. of params refined (NV)	559	630	406	370	343	379
overdetermin ratio (NO/NV)	5.9	11.8	12.3	11.9	12.5	13.6
transm factors	0.885-1.000	0.820-1.000	0.828-1.000	0.934-1.000	0.691-1.000	0.675-1.000
R = $\sum  \Delta F  / \sum  F_o ^d$	0.046	0.074	0.045	0.044	0.045	0.055
wR2 = $[\sum w  \Delta F^2 ^2 / \sum w  F_o^2 ^2]^{1/2}$ e	0.137	0.222	0.131	0.108	0.129	0.171
GOF = $[\sum w  \Delta F^2 ^2 / (\text{NO-NV})]^{1/2}$	1.353	0.979	0.989	0.804	1.027	0.974
largest shift/esd, final cycle	0.02	0.01	0.001	<0.001	0.01	0.006
largest peak, e Å <sup>-3</sup>	0.63	0.76	0.31	0.25	0.78	0.40

<sup>a</sup> unit cell parameters were obtained by least-squares analysis of the setting angles of 25 carefully centered reflections chosen from diverse regions of reciprocal space collected at 295 K.

<sup>b</sup> Graphite monochromated Mo Kα ( $\lambda = 0.71069 \text{ \AA}$ )

<sup>c</sup> Graphite monochromated Cu Kα ( $\lambda = 1.54178 \text{ \AA}$ )

<sup>d</sup> calculated on the unique observed data [ $I > 2\sigma(I)$ ]

<sup>e</sup> calculated on the unique “observed” data

Table S2. Fractional atomic coordinates (x104) for complex 4.

Atom	Molecule A			Molecule B		
	x/a	y/b	z/c	x/a	y/b	z/c
Mn1	-1961 (1)	-2949 (2)	-1399 (2)	-2989 (1)	-2054 (2)	-3040 (2)
O1	-2807 (4)	-2891 (9)	-1354 (10)	-2138 (4)	-2081 (9)	-3055 (9)
O2	-1647 (6)	-3769 (8)	-2709 (12)	-3319 (5)	-1270 (8)	-1764 (12)
N1	-1982 (8)	-2031 (12)	175 (12)	-2926 (7)	-2958 (11)	-4659 (13)
N2	-1111 (7)	-2584 (13)	-1039 (18)	-3830 (7)	-2435 (10)	-3410 (16)
N3	-1945 (9)	-3940 (9)	285 (14)	-3028 (9)	-1050 (9)	-4708 (13)
C1	-3095 (10)	-2765 (12)	-280 (20)	-1821 (8)	-2162 (13)	-4149 (22)
C2	-3623 (9)	-3133 (14)	-190 (21)	-1312 (10)	-1795 (12)	-4193 (17)
C3	-3956 (7)	-2996 (18)	905 (28)	-976 (9)	-1919 (17)	-5309 (27)
C4	-3766 (12)	-2532 (17)	1984 (20)	-1136 (13)	-2402 (19)	-6329 (27)
C5	-3258 (11)	-2197 (15)	1885 (21)	-1634 (12)	-2718 (15)	-6303 (22)
C6	-2908 (10)	-2339 (13)	806 (22)	-2002 (10)	-2649 (14)	-5214 (22)
C7	-2395 (11)	-1963 (14)	991 (19)	-2513 (9)	-3021 (13)	-5410 (18)
C8	-1493 (11)	-1649 (14)	507 (20)	-3420 (10)	-3339 (14)	-4951 (21)
C9	-1428 (11)	-1017 (14)	1373 (22)	-3431 (11)	-4000 (15)	-5861 (21)
C10	-925 (13)	-714 (14)	1673 (20)	-3935 (14)	-4300 (18)	-6178 (24)
C11	-464 (12)	-1046 (17)	1147 (26)	-4406 (14)	-4034 (21)	-5635 (32)
C12	-498 (11)	-1649 (18)	256 (22)	-4379 (10)	-3419 (16)	-4720 (23)
C13	-1014 (10)	-1951 (14)	-86 (21)	-3884 (9)	-3060 (16)	-4363 (19)
C14	-716 (9)	-2843 (18)	-1706 (25)	-4280 (9)	-2121 (17)	-2894 (23)
C15	-706 (10)	-3454 (15)	-2758 (23)	-4288 (10)	-1543 (13)	-1911 (25)
C16	-188 (10)	-3651 (18)	-3339 (25)	-4794 (11)	-1355 (19)	-1443 (28)
C17	-159 (11)	-4168 (18)	-4401 (23)	-4875 (11)	-834 (22)	-433 (29)
C18	-613 (14)	-4556 (14)	-4808 (22)	-4429 (14)	-495 (16)	185 (22)
C19	-1103 (9)	-4414 (14)	-4239 (23)	-3898 (10)	-642 (14)	-259 (23)
C20	-1158 (9)	-3852 (13)	-3182 (20)	-3821 (11)	-1150 (13)	-1374 (18)
C21	-2369 (11)	-4342 (16)	683 (20)	-2591 (8)	-610 (14)	-5091 (23)
C22	-2358 (11)	-4952 (17)	1605 (26)	-2602 (9)	-19 (16)	-6035 (24)
C23	-1888 (14)	-5133 (15)	2173 (23)	-3109 (12)	127 (13)	-6598 (20)
C24	-1426 (12)	-4709 (15)	1822 (25)	-3560 (11)	-302 (17)	-6276 (24)
C25	-1465 (10)	-4104 (15)	882 (23)	-3490 (11)	-875 (15)	-5337 (23)

Table S3. Fractional atomic coordinates (x104) for complex 5.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
Mn1	1428.8(12)	1359.4(9)	2144.6(13)	C19	2021(8)	5368(6)	3739(9)
Mn2	2600.0(12)	2763.7(9)	3802.2(13)	C20	1985(8)	4491(6)	3385(9)
Na1	1082(3)	-562(2)	452(3)	C21	3326(7)	2111(6)	6063(8)
Na2	3432(3)	4240(2)	6207(4)	C22	3043(8)	2049(6)	7021(9)
O1	1901(5)	189(4)	2415(5)	C23	3441(10)	1412(7)	7667(9)
O2	2638(5)	4032(4)	4095(6)	C24	4081(9)	864(7)	7397(9)
O3	2968(5)	2746(4)	5521(5)	C25	4327(8)	893(6)	6459(9)
O4	706(4)	971(3)	371(5)	C26	3942(7)	1482(5)	5724(8)
O5	1721(7)	-1996(5)	431(8)	C27	4143(7)	1391(6)	4660(8)
O6	2273(8)	-746(6)	-416(9)	C28	4079(7)	1716(6)	2884(8)
O7	5206(7)	4136(6)	6587(10)	C29	4976(8)	1397(6)	2818(9)
O8	4349(9)	5624(6)	6819(11)	C30	5220(8)	1370(7)	1848(10)
O9	3816(9)	4326(9)	8450(9)	C31	4566(8)	1682(7)	916(9)
O10	2009(7)	4636(5)	6766(8)	C32	3652(8)	2009(6)	922(8)
N1	801(5)	1340(4)	3523(7)	C33	3361(7)	2018(5)	1876(7)
N2	1020(5)	2631(4)	2609(6)	C34	1786(7)	2753(5)	1154(8)
N3	3811(6)	1865(5)	3877(6)	C35	1250(6)	2272(5)	-97(8)
N4	2481(6)	2267(4)	2016(6)	C36	1165(7)	2665(6)	-977(9)
C1	2079(7)	-137(6)	3372(8)	C37	673(8)	2316(7)	-2179(10)
C2	2669(9)	-858(6)	3458(9)	C38	242(8)	1491(7)	-2498(8)
C3	2862(9)	-1279(7)	4366(10)	C39	320(8)	1072(6)	-1620(9)
C4	2507(9)	-990(7)	5237(10)	C40	770(7)	1426(6)	-407(8)
C5	1938(7)	-286(6)	5211(8)	C41	1590(10)	-2630(8)	1029(14)
C6	1731(7)	148(5)	4273(9)	C42	2402(14)	-2171(9)	-59(16)
C7	1113(8)	890(6)	4311(9)	C43	2459(16)	-1576(11)	-748(20)
C8	164(7)	2034(6)	3625(9)	C44A	2501(21)	-155(17)	-977(24)
C9	-561(8)	2044(6)	4153(9)	C44B	3082(32)	-126(26)	0(37)
C10	-1173(9)	2717(8)	4136(11)	C45	5666(12)	3398(11)	6567(20)
C11	-1121(8)	3351(7)	3556(10)	C46	5718(15)	4832(13)	7047(23)
C12	-412(8)	3332(6)	3034(10)	C47	5331(18)	5633(12)	7013(19)
C13	271(7)	2687(6)	3072(8)	C48	4012(13)	6398(11)	6975(19)
C14	1035(7)	3149(6)	1795(8)	C49	4364(16)	3861(13)	9218(17)
C15	1233(8)	4118(6)	2287(9)	C50	3056(19)	4775(15)	8726(13)
C16	649(8)	4657(6)	1598(9)	C51	2133(15)	4661(13)	7892(17)
C17	743(9)	5519(6)	1959(10)	C52	1083(11)	4283(8)	5931(14)
C18	1436(10)	5872(6)	3058(11)				

The site occupation factors for the A and B positions of C44 are 0.6 and 0.4 respectively.

Table S4. Fractional atomic coordinates (x104) for complex 6.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
Mn1	4399.8 (5)	230.0 (3)	4291.2 (4)	C11	7978 (4)	941 (3)	3278 (4)
Na1	2774 (1)	727 (1)	2709 (1)	C12	7433 (3)	295 (3)	3447 (3)
Na2	5451 (2)	1226 (1)	2802 (1)	C13	6647 (3)	279 (2)	4067 (2)
O1	3927 (2)	1293 (2)	3764 (2)	C14	5878 (3)	-987 (2)	3866 (3)
O2	4420 (2)	91 (2)	2870 (2)	C15	5589 (3)	-956 (2)	2850 (3)
O3	1180 (3)	1089 (2)	3549 (3)	C16	6019 (4)	-1479 (2)	2316 (3)
O4	2183 (3)	-215 (2)	3633 (2)	C17	5778 (5)	-1540 (3)	1387 (3)
O5	1492 (5)	294 (3)	1506 (3)	C18	5109 (5)	-1049 (3)	983 (3)
O6	2886 (4)	1387 (3)	1304 (3)	C19	4646 (4)	-525 (3)	1492 (3)
O7	5767 (4)	2497 (2)	2329 (3)	C20	4873 (4)	-449 (2)	2430 (3)
O8	6157 (3)	1284 (2)	1329 (2)	C21	803 (5)	1806 (4)	3645 (6)
N1	5617 (2)	863 (2)	5136 (2)	C22	1320 (5)	701 (6)	4390 (5)
N2	6036 (2)	-290 (2)	4323 (2)	C23	1354 (5)	-83 (5)	4188 (4)
C1	3972 (3)	1930 (2)	4196 (3)	C24	2251 (5)	-964 (4)	3379 (5)
C2	3453 (4)	2534 (2)	3800 (3)	C25	484 (6)	95 (5)	1664 (5)
C3	3487 (4)	3215 (2)	4188 (3)	C26	1682 (8)	555 (8)	713 (6)
C4	4045 (4)	3319 (2)	4999 (3)	C27	2294 (10)	1094 (5)	589 (5)
C5	4549 (3)	2726 (2)	5404 (3)	C28	3227 (10)	2030 (5)	1214 (5)
C6	4527 (3)	2033 (2)	5042 (3)	C29	5824 (5)	3115 (4)	2849 (5)
C7	5033 (3)	1411 (2)	5597 (3)	C30	6165 (7)	2575 (4)	1483 (5)
C8	6394 (3)	960 (2)	4546 (3)	C31	6651 (8)	1962 (5)	1149 (5)
C9	6931 (4)	1590 (2)	4324 (3)	C32	6763 (5)	705 (4)	1024 (4)
C10	7735 (4)	1574 (3)	3694 (4)				

Table S5. Fractional atomic coordinates (x104) for complex 9.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
Mn1	280.6 (6)	806.4 (5)	4737.9 (6)	C11	831 (5)	-1557 (3)	2474 (4)
Na1	-899 (2)	1251 (1)	2663 (2)	C12	121 (4)	-1309 (3)	2982 (4)
Na2	-814 (2)	2329 (1)	5330 (2)	C13	128 (4)	-557 (3)	3304 (4)
O1	739 (3)	1970 (2)	4887 (2)	C14	-1579 (4)	-118 (3)	3268 (4)
O2	-1246 (2)	1260 (2)	4403 (2)	C15	-2325 (4)	173 (3)	3806 (4)
O3	-812 (3)	1369 (2)	992 (3)	C16	-3283 (4)	-185 (3)	3697 (4)
O4	-1989 (3)	2206 (2)	1963 (4)	C17	-4015 (4)	99 (4)	4155 (5)
O5	-2342 (4)	3164 (3)	5266 (4)	C18	-3785 (5)	750 (4)	4736 (5)
O6	-357 (4)	3440 (2)	6293 (4)	C19	-2841 (5)	1112 (3)	4851 (4)
N1	806 (3)	722 (2)	3460 (3)	C20	-2105 (4)	850 (3)	4365 (3)
N2	-601 (3)	-306 (2)	3854 (3)	C21	2637 (4)	1185 (4)	3927 (4)
C1	812 (4)	2385 (3)	4124 (4)	C22	-1869 (4)	-160 (3)	2273 (4)
C2	524 (4)	3177 (4)	4101 (5)	C31	-616 (5)	726 (4)	468 (4)
C3	558 (5)	3626 (4)	3307 (6)	C32	-1657 (6)	1797 (4)	463 (5)
C4	872 (5)	3347 (5)	2524 (6)	C33	-1786 (5)	2475 (4)	1079 (6)
C5	1180 (5)	2577 (4)	2539 (5)	C34	-2230 (5)	2797 (4)	2540 (6)
C6	1156 (4)	2097 (3)	3323 (4)	C35	-3374 (7)	3137 (4)	4688 (6)
C7	1545 (4)	1276 (3)	3281 (4)	C36	-2099 (8)	3853 (5)	5735 (8)
C8	875 (4)	-17 (3)	3131 (4)	C37	-1161 (9)	3848 (5)	6491 (7)
C9	1569 (4)	-290 (4)	2604 (4)	C38	608 (7)	3545 (5)	6926 (7)
C10	1541 (5)	-1041 (4)	2294 (4)				

Table S6. Fractional atomic coordinates (x104) for complex 14.

Atom	x/a	y/b	z/c
Mn1	1281.5 (15)	1436.1 (8)	3597.4 (10)
I1	2727.8 (8)	1408.5 (5)	5526.4 (5)
I2	2611.3 (8)	1045.7 (4)	7353.2 (5)
I3	2519.0 (9)	637.4 (5)	9076.3 (6)
O1	2508 (7)	739 (4)	3398 (5)
O2	2541 (7)	2113 (4)	3433 (5)
O3	363 (8)	1458 (4)	2287 (5)
O4	4194 (16)	1733 (11)	1006 (11)
N1	-115 (8)	778 (4)	3888 (5)
N2	-91 (8)	2106 (4)	3937 (5)
C1	2403 (10)	70 (6)	3495 (7)
C2	3517 (11)	-340 (6)	3351 (7)
C3	3483 (12)	-1040 (7)	3439 (8)
C4	2324 (12)	-1364 (6)	3670 (8)
C5	1213 (11)	-993 (6)	3845 (7)
C6	1244 (10)	-260 (6)	3764 (6)
C7	27 (9)	101 (5)	3930 (5)
C8	-1388 (9)	1094 (5)	4026 (6)
C9	-2595 (11)	735 (5)	4124 (7)
C10	-3766 (10)	1122 (7)	4241 (8)
C11	-3715 (11)	1830 (7)	4287 (8)
C12	-2537 (11)	2178 (6)	4180 (8)
C13	-1357 (10)	1813 (6)	4055 (6)
C14	160 (10)	2761 (6)	4075 (7)
C15	1394 (11)	3109 (6)	3929 (7)
C16	1446 (12)	3825 (6)	4083 (9)
C17	2550 (13)	4210 (6)	3924 (8)
C18	3636 (13)	3892 (8)	3609 (8)
C19	3644 (11)	3190 (7)	3443 (7)
C20	2504 (10)	2786 (6)	3595 (6)
C21	79 (16)	858 (7)	1793 (9)
C22	-100 (17)	1030 (9)	923 (9)
C23	88 (18)	1799 (9)	865 (9)
C24	215 (15)	2052 (7)	1769 (9)
C25	5162 (30)	2145 (8)	1395 (16)
C26	6123 (17)	1653 (16)	1802 (18)
C27	5293 (32)	1048 (12)	1971 (18)
C28	4139 (25)	1092 (14)	1360 (16)

Table S7. Fractional atomic coordinates ( $\times 10^4$ ) for complex 16.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
Mn1	-352.9 (7)	-908.0 (6)	-320.3 (8)	C16	3413 (5)	1557 (4)	-912 (5)
O1	454 (3)	-2211 (2)	45 (3)	C17	4452 (5)	1773 (4)	24 (5)
O2	1827 (3)	1401 (2)	1290 (3)	C18	4579 (5)	1919 (4)	1432 (6)
O3	982 (3)	-357 (2)	558 (3)	C19	3711 (4)	1833 (4)	1896 (5)
N1	-226 (4)	-1028 (3)	-2212 (4)	C20	2642 (4)	1551 (4)	912 (5)
N2	541 (4)	891 (3)	-1525 (4)	C21	1699 (6)	-3981 (4)	1402 (6)
C1	853 (4)	-2882 (4)	-689 (5)	C22	2458 (6)	-3236 (5)	2378 (6)
C2	1449 (5)	-3794 (4)	-123 (5)	C23	559 (7)	-3887 (5)	1597 (7)
C3	1840 (5)	-4483 (4)	-955 (6)	C24	2335 (9)	-5004 (5)	1779 (8)
C4	1699 (6)	-4345 (4)	-2340 (6)	C25	2204 (7)	-5153 (5)	-3136 (7)
C5	1153 (5)	-3472 (4)	-2849 (5)	C26	1944 (11)	-4925 (7)	-4576 (9)
C6	720 (5)	-2733 (4)	-2063 (5)	C27	3474 (12)	-5282 (8)	-2419 (13)
C7	187 (4)	-1837 (4)	-2722 (5)	C28	1819 (11)	-6118 (6)	-3147 (11)
C8	-757 (4)	-258 (4)	-3155 (5)	C29	5516 (5)	1815 (5)	-320 (6)
C9	-1631 (5)	-447 (4)	-4444 (5)	C30	5224 (7)	1638 (8)	-1860 (8)
C10	-2140 (5)	271 (4)	-5415 (5)	C31	6469 (7)	1101 (7)	422 (10)
C11	-1753 (5)	1185 (4)	-5062 (6)	C32	5905 (7)	2826 (6)	119 (9)
C12	-882 (5)	1388 (4)	-3774 (5)	C33	3960 (5)	1964 (5)	3474 (6)
C13	-389 (4)	676 (4)	-2815 (5)	C34	2983 (6)	2644 (4)	3745 (6)
C14	1459 (4)	1152 (4)	-1605 (5)	C35	4046 (7)	947 (5)	3959 (6)
C15	2475 (5)	1434 (4)	-532 (5)	C36	5078 (7)	2396 (7)	4329 (7)

Table S8. Fractional atomic coordinates ( $\times 10^4$ ) for hydrogen atoms for complex 4.

Atom	Molecule A			Molecule B		
	x/a	y/b	z/c	x/a	y/b	z/c
H2	-3755	-3417	-826	-1208	-1436	-3522
H3	-4294	-3213	981	-636	-1629	-5288
H4	-3975	-2445	2723	-879	-2524	-6979
H5	-3144	-1881	2593	-1734	-3040	-7020
H7	-2350	-1598	1708	-2541	-3311	-6164
H9	-1716	-765	1731	-3093	-4177	-6220
H10	-883	-302	2232	-3923	-4738	-6769
H11	-102	-869	1388	-4729	-4256	-5922
H12	-196	-1877	-185	-4684	-3265	-4327
H14	-376	-2626	-1517	-4609	-2253	-3216
H16	122	-3389	-3020	-5097	-1568	-1789
H17	174	-4261	-4788	-5207	-704	-45
H18	-569	-4930	-5499	-4445	-133	915
H19	-1397	-4694	-4554	-3598	-406	142
H21	-2694	-4221	218	-2254	-726	-4721
H22	-2676	-5215	1783	-2299	251	-6304
H23	-1870	-5544	2768	-3145	523	-7235
H24	-1092	-4803	2207	-3896	-214	-6674
H25	-1181	-3796	694	-3805	-1165	-5074

Table S9. Fractional atomic coordinates ( $\times 10^4$ ) for hydrogen atoms for complex 5.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
H2	2947	-1046	2888	H411	1081	-2484	1341
H3	3238	-1758	4383	H412	2221	-2683	1650
H4	2635	-1267	5865	H413	1401	-3174	467
H5	1693	-94	5818	H421	2273	-2737	-542
H7	931	1053	4967	H422	3074	-2153	571
H9	-620	1597	4503	H431	3118	-1582	-814
H10	-1633	2736	4518	H432	1969	-1785	-1560
H11	-1567	3783	3520	H451	5175	2922	6176
H12	-391	3762	2650	H452	6039	3331	7374
H14	360	3076	1175	H453	6131	3382	6169
H16	171	4415	852	H461	6233	4795	6691
H17	340	5861	1472	H462	6071	4815	7866
H18	1497	6460	3325	H471	5708	6005	7745
H19	2474	5622	4487	H472	5446	5825	6376
H22	2591	2420	7215	H481	3293	6350	6838
H23	3257	1379	8300	H482	4104	6709	6449
H24	4353	464	7856	H483	4356	6701	7784
H25	4777	510	6283	H491	4865	3576	8926
H27	4549	953	4518	H492	3943	3456	9295
H29	5426	1193	3453	H493	4723	4236	9968
H30	5815	1137	1812	H501	3039	4581	9418
H31	4749	1677	268	H502	3267	5355	8955
H32	3236	2214	278	H511	1755	5101	8147
H34	2192	3225	1129	H512	1844	4118	7921
H36	1456	3215	-768	H521	1069	4280	5151
H37	638	2620	-2753	H522	553	4605	6067
H38	-89	1229	-3291	H523	996	3703	5995
H39	64	511	-1845				

Table S10. Fractional atomic coordinates ( $\times 10^4$ ) for hydrogen atoms for complex 6.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
H2	3076	2485	3285	H242	1504	-1200	3074
H3	3136	3625	3857	H243	2416	-1287	3904
H4	4149	3782	5250	H251	396	-81	2240
H5	4973	2849	5920	H252	123	-81	1291
H7	5507	1665	6067	H253	30	573	1695
H9	6829	1973	4637	H261	1033	643	479
H10	8117	1955	3573	H262	1940	162	300
H11	8485	966	2870	H271	1934	1508	317
H12	7494	-123	3169	H272	2718	1048	-1
H14	6516	-1290	3916	H281	3584	2181	1712
H16	6547	-1771	2601	H282	2635	2343	1136
H17	6148	-1922	1190	H283	3529	2213	738
H18	4838	-1071	337	H291	5532	3069	3455
H19	4159	-139	1212	H292	5456	3499	2613
H211	865	2037	3007	H293	6508	3287	2924
H212	1369	2096	3987	H301	6587	3039	1355
H213	145	1744	3967	H302	5464	2537	1011
H221	696	838	4832	H311	7328	1881	1592
H222	2024	941	4737	H312	6808	2019	481
H231	632	-317	3861	H321	6445	262	1232
H232	1413	-360	4798	H322	7441	644	1313
H241	2915	-1006	3006	H323	6923	778	328

Table S11. Fractional atomic coordinates ( $\times 10^4$ ) for hydrogen atoms for complex 9.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
H2	516	3371	4881	H312	-398	901	-197
H3	380	4160	3397	H313	-1387	371	218
H4	1075	3636	1950	H321	-1878	2007	-181
H5	1408	2319	1975	H322	-2388	1409	480
H7	1627	1294	2574	H331	-1117	2897	1220
H9	2209	48	2554	H332	-2247	2780	654
H10	2019	-1208	1992	H341	-2871	3094	2421
H11	757	-2074	2260	H342	-1658	3087	2600
H12	-443	-1673	3069	H343	-2025	2749	3318
H16	-3444	-623	3260	H351	-3605	2630	4289
H17	-4613	27	4035	H352	-3453	3567	4112
H18	-4323	1008	5031	H353	-4007	3241	5091
H19	-2671	1525	5336	H361	-1892	4209	5208
H211	3013	710	3838	H362	-2760	4098	5948
H212	3167	1542	3756	H371	-1381	3533	7105
H213	2533	1316	4548	H372	-910	4371	6837
H221	-2575	-16	1885	H381	1212	3218	6735
H222	-1412	-520	1837	H382	546	3319	7682
H311	14	389	937	H383	838	4061	7001

Table S12. Fractional atomic coordinates ( $\times 10^4$ ) for hydrogen atoms for complex 14.

Atom	x/a	y/b	z/c
H2	4278	-150	3169
H3	4263	-1299	3366
H4	2296	-1858	3688
H5	455	-1208	4031
H7	-714	-159	4069
H9	-2638	268	4115
H10	-4585	897	4294
H11	-4495	2080	4382
H12	-2538	2650	4224
H14	-519	3033	4290
H16	695	4040	4286
H17	2591	4676	4033
H18	4390	4149	3487
H19	4405	2978	3236
H211	-657	607	1983
H212	902	549	1863
H221	-1063	919	702
H222	480	791	562
H231	931	1901	617
H232	-648	2024	541
H241	922	2378	1864
H242	-662	2295	1877
H251	4789	2440	1811
H252	5590	2425	988
H261	6588	1836	2305
H262	6785	1502	1415
H271	5752	633	2005
H272	4906	1128	2553
H281	4329	728	918
H282	3309	975	1573

Table S13. Fractional atomic coordinates ( $\times 10^4$ ) for hydrogen atoms for complex 16.

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
H3	2419	-5105	-574	H272	3770	-4687	-2439
H5	786	-3314	-3956	H273	3797	-5810	-2899
H7	192	-1980	-3663	H281	2025	-6288	-2213
H9	-2000	-1150	-4718	H282	2163	-6619	-3630
H10	-2800	-37	-6322	H283	977	-6076	-3635
H11	-1994	1685	-5806	H301	4598	2121	-2347
H12	-392	2071	-3391	H302	4975	993	-2174
H14	1400	951	-2714	H303	5885	1680	-2063
H16	3201	1450	-1999	H311	6666	1215	1416
H18	5408	2000	2297	H312	7140	1162	234
H221	2615	-3337	3332	H313	6258	450	131
H222	2060	-2579	2173	H321	5266	3304	-374
H223	3175	-3292	2253	H322	6554	2872	-102
H231	79	-4358	977	H323	6107	2960	1108
H232	145	-3232	1368	H341	3171	2719	4743
H233	696	-3979	2542	H342	2269	2381	3277
H241	1876	-5483	1175	H343	2932	3281	3423
H242	2497	-5092	2734	H351	4187	986	4937
H243	3067	-5063	1661	H352	4651	511	3795
H261	2182	-4322	-4596	H353	3312	674	3441
H262	1096	-4895	-5112	H361	5186	2483	5301
H263	2300	-5448	-5024	H362	5019	3048	4011
H271	3689	-5432	-1477	H363	5721	1999	4226

Table S14. Anisotropic thermal parameters  $U_{(i,j)}$  ( $\times 10^4 \text{ \AA}^2$ ) for complex 4.  
 $U_{(i,j)}$  are in the form  $\exp[-2\pi^2(U_{11}h^2a^{\star 2}+\dots+2U_{12}hka^{\star}b^{\star}+\dots)]$

## Molecule A

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
Mn1	454 (22)	426 (25)	407 (19)	-15 (18)	47 (16)	33 (25)
O1	314 (87)	569 (113)	300 (81)	-28 (88)	-35 (58)	117 (92)
O2	602 (114)	309 (96)	548 (99)	-34 (72)	81 (82)	95 (81)
N1	612 (129)	468 (113)	204 (92)	93 (113)	-73 (109)	168 (142)
N2	303 (125)	803 (181)	605 (143)	245 (121)	32 (106)	-64 (120)
N3	601 (154)	382 (120)	399 (115)	9 (92)	359 (131)	-72 (133)
C1	704 (167)	291 (158)	258 (131)	-83 (103)	-8 (129)	-7 (139)
C2	413 (154)	717 (214)	942 (200)	411 (157)	48 (148)	17 (157)
C3	173 (127)	1087 (250)	1088 (221)	666 (200)	291 (140)	-45 (168)
C4	1036 (241)	1266 (274)	316 (149)	49 (156)	-33 (165)	345 (198)
C5	773 (172)	662 (191)	785 (191)	210 (153)	-35 (157)	133 (170)
C6	682 (192)	616 (194)	446 (161)	-36 (131)	472 (152)	56 (144)
C7	861 (188)	388 (158)	412 (159)	68 (136)	-8 (143)	-1 (170)
C8	676 (197)	357 (175)	395 (161)	-118 (122)	-157 (139)	-218 (145)
C9	979 (224)	665 (202)	613 (178)	-330 (146)	-277 (157)	-77 (166)
C10	1270 (263)	324 (161)	369 (162)	52 (114)	-28 (159)	-138 (174)
C11	1260 (258)	672 (213)	864 (229)	-104 (165)	105 (191)	-688 (191)
C12	715 (190)	1226 (280)	654 (179)	-205 (167)	348 (151)	-345 (180)
C13	680 (177)	377 (166)	470 (154)	-156 (132)	117 (142)	25 (162)
C14	507 (183)	606 (231)	854 (201)	150 (168)	-262 (142)	-246 (193)
C15	398 (190)	662 (212)	838 (200)	-115 (151)	91 (140)	-113 (158)
C16	565 (208)	1142 (291)	961 (209)	-289 (172)	-206 (163)	181 (189)
C17	613 (223)	1187 (275)	802 (211)	-436 (181)	192 (154)	186 (188)
C18	709 (250)	772 (245)	699 (196)	-198 (151)	-143 (178)	-13 (176)
C19	293 (177)	752 (203)	795 (195)	-134 (150)	-9 (136)	124 (145)
C20	449 (179)	345 (164)	336 (146)	8 (106)	5 (125)	41 (143)
C21	943 (239)	605 (193)	229 (150)	118 (133)	84 (133)	7 (169)
C22	783 (228)	755 (234)	639 (206)	25 (163)	-5 (166)	-105 (176)
C23	1137 (306)	644 (202)	701 (205)	266 (150)	377 (197)	-160 (213)
C24	846 (234)	450 (193)	804 (204)	260 (143)	-350 (165)	355 (169)
C25	329 (166)	673 (211)	700 (197)	113 (151)	26 (131)	37 (144)

## Molecule B

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
Mn1	426 (21)	410 (25)	392 (19)	-10 (18)	21 (16)	-3 (23)
O1	432 (93)	458 (98)	286 (74)	-15 (86)	40 (62)	67 (89)
O2	322 (91)	578 (112)	501 (92)	-292 (76)	183 (75)	2 (77)
N1	372 (117)	233 (100)	433 (101)	85 (111)	43 (93)	45 (115)
N2	534 (132)	267 (112)	520 (117)	89 (89)	3 (105)	-101 (100)
N3	511 (143)	321 (112)	374 (113)	-17 (82)	-202 (116)	-2 (121)
C1	280 (140)	222 (142)	699 (190)	192 (134)	80 (125)	18 (122)
C2	730 (183)	634 (198)	307 (136)	36 (106)	172 (127)	148 (150)
C3	688 (179)	807 (232)	840 (206)	315 (170)	331 (166)	195 (169)
C4	1170 (281)	1034 (315)	870 (238)	-40 (201)	287 (239)	518 (231)
C5	940 (212)	636 (227)	501 (171)	96 (142)	-26 (165)	267 (178)
C6	426 (154)	715 (192)	392 (149)	-136 (124)	37 (146)	266 (152)
C7	416 (156)	395 (147)	546 (154)	-142 (136)	-19 (122)	136 (153)
C8	619 (194)	328 (171)	459 (168)	41 (125)	120 (140)	16 (134)
C9	1076 (229)	380 (174)	425 (166)	29 (133)	104 (142)	90 (150)

Table S14. Anisotropic thermal parameters  $U_{(i,j)}$  ( $\times 10^4 \text{ \AA}^2$ ) for complex 4  
(cont.).

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
C10	1240 (299)	902 (255)	605 (192)	-25 (167)	-158 (201)	-392 (226)
C11	1229 (302)	1374 (338)	1451 (321)	-555 (248)	104 (238)	-464 (250)
C12	658 (178)	908 (228)	1000 (197)	-285 (159)	-141 (146)	-495 (159)
C13	383 (145)	644 (203)	474 (151)	60 (140)	-17 (119)	-261 (161)
C14	457 (162)	489 (201)	919 (187)	25 (169)	-63 (133)	-91 (184)
C15	550 (211)	228 (159)	891 (196)	15 (139)	-169 (162)	-101 (139)
C16	503 (206)	1090 (300)	1318 (257)	-484 (197)	173 (181)	-192 (201)
C17	425 (205)	1711 (360)	1032 (250)	-77 (216)	206 (168)	-62 (211)
C18	655 (242)	1089 (299)	858 (213)	-302 (177)	75 (175)	552 (189)
C19	725 (220)	638 (185)	581 (165)	248 (141)	41 (153)	92 (147)
C20	966 (234)	243 (157)	148 (134)	14 (101)	-18 (136)	292 (161)
C21	220 (139)	500 (179)	837 (202)	-55 (150)	30 (132)	-182 (132)
C22	377 (169)	576 (198)	777 (204)	-29 (158)	243 (140)	-23 (139)
C23	818 (224)	434 (171)	640 (164)	145 (118)	329 (172)	102 (171)
C24	621 (205)	993 (280)	641 (204)	164 (163)	-65 (156)	-119 (191)
C25	805 (218)	561 (189)	331 (160)	-7 (136)	139 (144)	-55 (153)

Table S15. Anisotropic and isotropic thermal parameters  $U_{(i,j)}$  ( $\times 10^4 \text{ \AA}^2$ ) for complex 5.  $U_{(i,j)}$  are in the form  $\exp[-2\pi^2(U_{11}h^2a^{\star 2}+\dots+2U_{12}hka^{\star}b^{\star}+\dots)]$

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
Mn1	396 (10)	244 (9)	398 (10)	85 (7)	155 (8)	38 (8)
Mn2	306 (10)	312 (9)	313 (10)	53 (7)	67 (8)	73 (7)
Na1	471 (26)	392 (23)	600 (28)	11 (20)	210 (22)	71 (19)
Na2	523 (27)	438 (24)	537 (27)	-3 (19)	89 (22)	-13 (20)
O1	409 (42)	369 (38)	429 (42)	99 (32)	184 (34)	98 (32)
O2	452 (44)	303 (37)	518 (46)	119 (33)	94 (36)	97 (33)
O3	549 (46)	394 (39)	411 (42)	56 (33)	228 (36)	179 (35)
O4	358 (40)	224 (32)	483 (42)	163 (31)	58 (33)	-23 (29)
O5	1063 (77)	647 (60)	1251 (82)	369 (55)	768 (67)	428 (55)
O6	1427 (95)	564 (61)	1673 (99)	131 (63)	1221 (84)	76 (63)
O7	652 (67)	569 (63)	1753 (104)	-116 (64)	347 (66)	-94 (55)
O8	863 (82)	392 (56)	2130 (121)	124 (64)	464 (82)	-186 (57)
O9	1070 (97)	1779 (123)	794 (84)	359 (79)	102 (72)	371 (86)
O10	889 (71)	632 (55)	651 (61)	126 (47)	305 (55)	23 (50)
N1	274 (47)	239 (42)	590 (58)	14 (39)	160 (42)	57 (36)
N2	389 (49)	186 (37)	362 (47)	123 (33)	192 (39)	23 (35)
N3	369 (49)	364 (45)	255 (45)	11 (37)	-24 (38)	46 (38)
N4	381 (50)	255 (41)	330 (45)	31 (34)	139 (38)	-93 (36)
C1	309 (58)	358 (55)	336 (60)	66 (46)	41 (47)	-23 (45)
C2	682 (84)	313 (59)	558 (76)	32 (53)	79 (63)	68 (56)
C3	696 (86)	504 (72)	448 (72)	208 (60)	-36 (63)	219 (63)
C4	645 (83)	445 (67)	560 (78)	288 (60)	116 (64)	64 (60)
C5	370 (61)	358 (55)	406 (60)	176 (48)	74 (48)	39 (47)
C6	326 (59)	237 (49)	512 (66)	87 (45)	174 (50)	-121 (43)
C7	436 (68)	282 (54)	495 (68)	19 (49)	72 (54)	-54 (49)
C8	278 (59)	332 (55)	495 (65)	87 (49)	65 (50)	-72 (46)
C9	587 (79)	444 (64)	670 (79)	140 (56)	399 (66)	-52 (58)
C10	591 (88)	718 (89)	882 (101)	-3 (76)	477 (78)	184 (72)
C11	521 (76)	426 (65)	714 (82)	276 (60)	211 (64)	107 (56)
C12	565 (75)	273 (55)	924 (92)	165 (57)	477 (71)	54 (52)
C13	355 (62)	285 (52)	377 (59)	9 (44)	73 (48)	-41 (46)
C14	179 (51)	414 (58)	321 (55)	128 (45)	-11 (42)	26 (44)
C15	486 (69)	327 (56)	493 (68)	93 (51)	270 (57)	24 (52)
C16	487 (70)	338 (58)	527 (71)	126 (52)	167 (57)	36 (51)
C17	908 (97)	333 (61)	607 (80)	309 (58)	386 (73)	215 (63)
C18	920 (103)	272 (60)	757 (93)	48 (61)	466 (82)	104 (63)
C19	653 (81)	192 (52)	667 (80)	79 (52)	130 (63)	99 (53)
C20	428 (66)	256 (52)	532 (69)	149 (49)	293 (56)	28 (48)
C21	421 (66)	512 (66)	110 (47)	17 (44)	-68 (43)	-123 (53)
C22	624 (81)	388 (62)	510 (76)	15 (54)	143 (62)	98 (57)
C23	1011 (108)	560 (76)	423 (72)	-8 (58)	414 (73)	47 (73)
C24	852 (95)	538 (71)	426 (71)	225 (58)	344 (68)	152 (66)
C25	410 (69)	519 (69)	513 (74)	185 (58)	21 (58)	117 (55)
C26	364 (60)	192 (47)	364 (59)	1 (43)	-51 (48)	-29 (43)
C27	307 (58)	427 (59)	385 (60)	63 (48)	120 (48)	0 (47)
C28	282 (56)	398 (56)	250 (52)	-4 (43)	139 (44)	-99 (45)
C29	448 (70)	522 (67)	599 (75)	226 (57)	293 (60)	154 (55)
C30	462 (74)	690 (81)	549 (79)	214 (65)	160 (62)	47 (61)
C31	530 (76)	611 (73)	510 (71)	32 (57)	423 (63)	41 (60)
C32	429 (65)	363 (57)	457 (65)	39 (48)	221 (53)	126 (49)
C33	244 (54)	344 (51)	239 (52)	-34 (41)	125 (43)	-55 (42)
C34	265 (53)	318 (51)	309 (54)	153 (42)	81 (43)	15 (42)
C35	123 (47)	270 (49)	368 (59)	73 (43)	50 (42)	71 (39)
C36	324 (60)	525 (66)	329 (61)	133 (52)	66 (49)	90 (50)

Table S15. Anisotropic and isotropic thermal parameters  $U_{(i,j)}$   
 $(\times 10^4 \text{ \AA}^2)$  for complex 5 (cont.).

C37	554 (79)	697 (82)	580 (79)	358 (67)	233 (64)	-14 (65)
C38	578 (78)	569 (72)	247 (59)	99 (52)	-24 (52)	-125 (60)
C39	473 (70)	516 (67)	322 (62)	21 (52)	19 (52)	-10 (55)
C40	278 (57)	344 (56)	328 (59)	-40 (46)	100 (46)	121 (46)
C41	804 (105)	556 (82)	1526 (143)	442 (90)	336 (98)	-23 (75)
C42	1393 (164)	611 (99)	1556 (165)	131 (100)	775 (136)	349 (103)
C43	2131 (221)	656 (113)	2739 (253)	297 (140)	1931 (207)	215 (128)
C45	658 (115)	745 (118)	3061 (261)	377 (140)	469 (140)	101 (95)
C46	1091 (158)	820 (139)	3448 (311)	-439 (170)	1252 (182)	-351 (124)
C47	1481 (196)	795 (131)	2306 (229)	-392 (134)	1213 (181)	-557 (135)
C48	950 (141)	794 (129)	2502 (240)	-13 (139)	123 (140)	-274 (109)
C49	1589 (195)	1478 (183)	1135 (166)	37 (133)	-107 (139)	-183 (149)
C50	1553 (213)	2641 (264)	287 (94)	-269 (122)	60 (112)	531 (194)
C51	1310 (172)	1893 (193)	807 (136)	246 (138)	433 (130)	574 (147)
C52	731 (107)	694 (98)	1365 (142)	-243 (90)	364 (102)	-59 (82)

Atom	$U_{iso}$	Atom	$U_{iso}$
C44A	1026 (84)	C44B	1082 (134)

Table S16. Anisotropic thermal parameters  $U_{(i,j)}$  ( $\times 10^4 \text{ \AA}^2$ ) for complex 6.  
 $U_{(i,j)}$  are in the form  $\exp[-2\pi^2(U_{11}h^2a^{\star 2}+\dots+2U_{12}hka^{\star}b^{\star}+\dots)]$

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
Mn1	372 (3)	318 (3)	305 (3)	5 (3)	-1 (2)	2 (3)
Na1	535 (11)	546 (12)	462 (11)	6 (9)	-119 (8)	30 (9)
Na2	718 (13)	583 (13)	472 (11)	77 (9)	111 (9)	-11 (10)
O1	586 (19)	315 (17)	378 (16)	-36 (13)	-70 (14)	75 (14)
O2	604 (19)	440 (18)	356 (16)	-79 (14)	-54 (14)	165 (16)
O3	770 (28)	1007 (34)	1075 (36)	-327 (29)	-59 (25)	309 (25)
O4	738 (25)	745 (28)	771 (26)	147 (22)	-16 (20)	-36 (23)
O5	1457 (49)	1486 (49)	797 (35)	81 (34)	-439 (33)	-507 (39)
O6	1156 (35)	936 (34)	709 (29)	261 (26)	-222 (25)	-108 (29)
O7	1548 (43)	801 (31)	816 (31)	118 (26)	529 (29)	-11 (30)
O8	953 (30)	982 (34)	585 (25)	-11 (23)	241 (22)	-25 (27)
N1	348 (19)	300 (19)	323 (19)	-5 (15)	23 (15)	-18 (15)
N2	384 (18)	348 (19)	316 (18)	-46 (16)	39 (14)	-54 (17)
C1	397 (23)	278 (23)	413 (25)	30 (19)	50 (19)	10 (19)
C2	558 (29)	431 (28)	437 (27)	21 (22)	28 (22)	76 (23)
C3	624 (31)	351 (27)	566 (32)	99 (23)	98 (25)	124 (23)
C4	734 (35)	346 (27)	613 (33)	-63 (24)	75 (27)	14 (25)
C5	519 (28)	328 (26)	490 (27)	-75 (21)	-7 (22)	-11 (21)
C6	380 (23)	277 (22)	362 (24)	14 (18)	35 (19)	-15 (18)
C7	408 (25)	322 (24)	380 (24)	-6 (19)	-41 (19)	-55 (20)
C8	313 (22)	387 (25)	354 (23)	1 (19)	-64 (19)	-8 (19)
C9	441 (26)	409 (26)	574 (29)	-7 (23)	6 (23)	-147 (22)
C10	479 (30)	548 (32)	716 (36)	42 (27)	126 (26)	-199 (25)
C11	530 (31)	686 (38)	712 (36)	86 (30)	256 (27)	-132 (28)
C12	402 (24)	538 (29)	495 (26)	20 (24)	93 (20)	-16 (24)
C13	305 (21)	415 (24)	352 (22)	49 (20)	-18 (17)	-8 (21)
C14	388 (24)	359 (25)	364 (24)	0 (19)	7 (19)	-1 (20)
C15	441 (25)	325 (24)	351 (24)	-20 (19)	10 (20)	20 (20)
C16	657 (33)	484 (29)	404 (28)	-6 (22)	86 (23)	122 (25)
C17	991 (43)	603 (35)	484 (31)	-99 (26)	66 (29)	310 (32)
C18	1106 (46)	651 (35)	386 (28)	-140 (26)	-18 (30)	246 (35)
C19	893 (39)	746 (38)	361 (28)	-61 (26)	-102 (26)	248 (31)
C20	507 (27)	462 (28)	342 (25)	-79 (21)	45 (21)	-27 (22)
C21	748 (48)	1091 (64)	2235 (96)	-560 (63)	286 (53)	-36 (44)
C22	806 (49)	1825 (90)	726 (49)	-321 (56)	212 (38)	116 (55)
C23	566 (36)	1534 (70)	671 (39)	192 (44)	74 (30)	-218 (42)
C24	975 (48)	717 (45)	1099 (53)	139 (39)	-370 (39)	-180 (37)
C25	938 (53)	1801 (86)	885 (52)	-209 (51)	-302 (42)	-55 (56)
C26	1543 (84)	2701 (149)	589 (54)	-414 (73)	-269 (53)	-385 (86)
C27	2474 (122)	1305 (75)	599 (49)	202 (48)	-209 (64)	-666 (76)
C28	2856 (131)	1470 (86)	881 (60)	275 (59)	-282 (67)	-796 (94)
C29	931 (51)	851 (51)	1494 (71)	-15 (49)	384 (48)	-98 (42)
C30	1562 (74)	1061 (61)	1000 (58)	168 (49)	550 (52)	-170 (55)
C31	1994 (91)	1086 (63)	1001 (60)	343 (52)	802 (60)	205 (67)
C32	931 (49)	1248 (61)	844 (48)	-118 (44)	249 (39)	-4 (46)

Table S17. Anisotropic thermal parameters  $U_{(i,j)}$  ( $\times 10^4 \text{ \AA}^2$ ) for complex 9.  
 $U_{(i,j)}$  are in the form  $\exp[-2\pi^2(U_{11}h^2a^{\star 2}+\dots+2U_{12}hka^{\star}b^{\star}+\dots)]$

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
Mn1	447 (5)	395 (5)	356 (4)	19 (5)	75 (4)	-28 (5)
Na1	595 (15)	526 (14)	510 (14)	83 (12)	69 (11)	70 (12)
Na2	715 (16)	522 (15)	796 (18)	-209 (13)	121 (14)	35 (13)
O1	652 (26)	415 (23)	483 (24)	-35 (20)	165 (21)	-115 (19)
O2	369 (22)	423 (22)	531 (23)	-53 (19)	79 (19)	12 (18)
O3	860 (34)	772 (32)	498 (26)	69 (25)	78 (24)	137 (27)
O4	778 (32)	611 (30)	875 (36)	84 (29)	128 (28)	198 (25)
O5	918 (40)	873 (39)	1153 (43)	-135 (34)	33 (33)	341 (33)
O6	819 (38)	741 (35)	1224 (44)	-437 (31)	239 (34)	-112 (30)
N1	431 (27)	406 (27)	430 (26)	43 (25)	151 (21)	-56 (24)
N2	415 (26)	357 (25)	314 (24)	-2 (21)	104 (21)	-39 (22)
C1	471 (37)	492 (41)	470 (38)	70 (33)	63 (30)	-113 (31)
C2	635 (43)	431 (39)	765 (47)	124 (37)	-19 (35)	-125 (34)
C3	638 (49)	508 (44)	1044 (62)	86 (47)	39 (46)	-20 (36)
C4	787 (55)	827 (60)	857 (59)	385 (50)	115 (45)	-219 (46)
C5	625 (44)	704 (49)	741 (50)	90 (42)	211 (37)	-179 (38)
C6	482 (38)	531 (40)	452 (38)	29 (34)	115 (31)	-102 (31)
C7	531 (41)	609 (42)	505 (38)	82 (33)	155 (33)	-3 (34)
C8	415 (35)	482 (36)	280 (32)	23 (28)	42 (26)	82 (30)
C9	448 (38)	649 (45)	533 (40)	-29 (35)	160 (31)	-1 (34)
C10	580 (43)	728 (50)	452 (38)	-94 (34)	98 (31)	144 (36)
C11	636 (45)	587 (44)	582 (43)	-129 (35)	132 (36)	77 (37)
C12	525 (40)	465 (38)	528 (38)	-44 (32)	64 (32)	48 (32)
C13	436 (35)	469 (37)	283 (31)	-43 (27)	23 (26)	33 (29)
C14	440 (35)	282 (31)	379 (34)	38 (27)	47 (28)	-54 (26)
C15	413 (35)	438 (35)	349 (32)	-13 (28)	52 (27)	-16 (29)
C16	471 (38)	438 (37)	617 (41)	36 (31)	111 (32)	-16 (32)
C17	494 (43)	815 (52)	833 (51)	121 (43)	268 (38)	11 (38)
C18	674 (47)	740 (47)	756 (45)	71 (44)	368 (37)	92 (42)
C19	636 (43)	617 (43)	573 (40)	-58 (33)	159 (36)	-2 (36)
C20	394 (33)	508 (36)	340 (30)	110 (31)	99 (26)	88 (33)
C21	500 (40)	835 (48)	785 (46)	-83 (39)	102 (35)	4 (36)
C22	590 (38)	495 (37)	380 (35)	5 (30)	-15 (28)	42 (31)
C31	1100 (60)	1027 (59)	619 (46)	74 (46)	345 (41)	104 (49)
C32	1023 (61)	943 (59)	603 (47)	218 (46)	-145 (42)	170 (50)
C33	949 (57)	749 (55)	951 (62)	351 (50)	-56 (47)	141 (45)
C34	821 (57)	984 (60)	1322 (69)	-274 (58)	94 (49)	280 (48)
C35	1113 (70)	1198 (69)	1119 (66)	82 (56)	99 (56)	409 (58)
C36	1359 (86)	992 (73)	1531 (92)	-207 (68)	556 (72)	335 (66)
C37	1376 (87)	940 (66)	1505 (89)	-730 (62)	149 (71)	340 (62)
C38	1202 (79)	1311 (81)	1586 (87)	-553 (67)	171 (68)	-131 (65)

Table S18. Anisotropic thermal parameters  $U_{(i,j)}$  ( $\times 10^4 \text{ \AA}^2$ ) for complex 14.  
 $U_{(i,j)}$  are in the form  $\exp[-2\pi^2(U_{11}h^2a^{\star 2}+\dots+2U_{12}hka^{\star}b^{\star}+\dots)]$

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
Mn1	362 (8)	283 (9)	443 (10)	15 (8)	104 (7)	2 (8)
I1	537 (5)	647 (6)	514 (5)	68 (4)	12 (4)	-99 (4)
I2	444 (4)	510 (5)	521 (5)	-50 (4)	11 (3)	-42 (4)
I3	642 (6)	756 (7)	547 (5)	38 (5)	43 (4)	-159 (5)
O1	447 (45)	344 (49)	650 (56)	3 (41)	171 (39)	-51 (37)
O2	363 (42)	435 (55)	631 (55)	-60 (42)	159 (38)	-33 (36)
O3	705 (53)	402 (50)	398 (47)	78 (38)	37 (39)	-10 (41)
O4	1409 (134)	1699 (188)	1930 (174)	504 (148)	-586 (117)	-331 (119)
N1	299 (45)	321 (57)	411 (54)	23 (40)	61 (38)	80 (38)
N2	310 (46)	287 (55)	473 (56)	15 (43)	49 (40)	53 (38)
C1	363 (61)	370 (74)	459 (70)	-38 (53)	67 (51)	-74 (51)
C2	412 (64)	291 (69)	556 (75)	-8 (57)	19 (55)	-12 (53)
C3	460 (69)	463 (83)	606 (80)	-45 (68)	-71 (58)	41 (65)
C4	597 (77)	387 (82)	595 (85)	-2 (63)	-9 (65)	43 (64)
C5	528 (70)	248 (64)	530 (73)	-32 (56)	31 (56)	3 (57)
C6	411 (62)	428 (70)	217 (54)	-72 (49)	12 (45)	50 (53)
C7	350 (55)	354 (67)	182 (54)	44 (45)	-31 (43)	-49 (47)
C8	323 (53)	304 (63)	290 (54)	32 (48)	40 (42)	18 (49)
C9	512 (68)	293 (65)	382 (62)	-71 (52)	50 (51)	-1 (53)
C10	343 (61)	525 (83)	586 (77)	-75 (65)	139 (54)	33 (57)
C11	421 (69)	492 (90)	755 (91)	-66 (71)	82 (61)	104 (63)
C12	343 (62)	528 (83)	622 (81)	18 (64)	63 (56)	41 (55)
C13	406 (60)	306 (69)	408 (63)	4 (52)	130 (49)	20 (52)
C14	389 (65)	569 (90)	406 (70)	-44 (61)	21 (52)	72 (59)
C15	491 (67)	216 (64)	560 (74)	-25 (54)	9 (56)	18 (53)
C16	447 (70)	267 (71)	977 (106)	-183 (66)	-36 (69)	58 (54)
C17	578 (80)	377 (81)	801 (102)	-64 (67)	-13 (72)	-87 (64)
C18	583 (84)	554 (96)	704 (93)	159 (78)	-140 (71)	-102 (75)
C19	422 (66)	460 (84)	541 (76)	91 (64)	0 (55)	12 (61)
C20	303 (57)	392 (74)	362 (62)	92 (51)	-87 (46)	-18 (50)
C21	1440 (142)	319 (84)	523 (87)	-104 (64)	-92 (87)	-229 (81)
C22	1355 (142)	871 (126)	427 (83)	124 (86)	136 (85)	110 (113)
C23	1555 (155)	806 (124)	449 (87)	278 (87)	47 (91)	249 (116)
C24	1113 (119)	531 (97)	641 (97)	359 (77)	-120 (83)	-146 (82)
C25	2679 (336)	193 (100)	1980 (270)	116 (118)	427 (239)	-194 (144)
C26	747 (140)	2650 (393)	1920 (269)	409 (261)	-196 (150)	-332 (185)
C27	2264 (343)	2086 (340)	1670 (269)	767 (242)	-710 (253)	-10 (263)
C28	2227 (293)	2320 (332)	1375 (218)	642 (213)	-205 (195)	-1747 (265)

Table S19. Anisotropic thermal parameters  $U_{(i,j)}$  ( $\times 10^4 \text{ \AA}^2$ ) for complex 16.  
 $U_{(i,j)}$  are in the form  $\exp[-2\pi^2(U_{11}h^2a^*{}^2 + \dots + 2U_{12}hka^*b^* + \dots)]$

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
Mn1	383 (5)	475 (5)	299 (4)	32 (3)	191 (4)	-23 (4)
O1	581 (23)	402 (21)	392 (19)	44 (16)	273 (18)	3 (17)
O2	397 (20)	615 (24)	405 (19)	-38 (17)	221 (17)	-172 (18)
O3	359 (19)	510 (22)	329 (18)	60 (16)	172 (16)	-8 (17)
N1	435 (25)	447 (26)	313 (21)	8 (19)	191 (20)	-9 (20)
N2	384 (24)	426 (25)	355 (22)	33 (19)	196 (20)	-48 (19)
C1	432 (29)	383 (29)	443 (28)	50 (23)	251 (25)	-13 (24)
C2	573 (34)	484 (33)	413 (29)	10 (24)	263 (27)	-29 (27)
C3	750 (43)	472 (34)	601 (37)	124 (29)	389 (35)	121 (31)
C4	874 (47)	543 (37)	509 (34)	53 (29)	435 (35)	117 (34)
C5	662 (38)	544 (36)	369 (29)	67 (26)	239 (28)	82 (30)
C6	532 (33)	438 (31)	402 (27)	38 (24)	260 (26)	-6 (26)
C7	403 (28)	514 (33)	344 (26)	5 (24)	217 (23)	-56 (25)
C8	437 (29)	459 (31)	305 (25)	19 (23)	214 (23)	-23 (25)
C9	512 (34)	542 (36)	333 (27)	11 (26)	136 (26)	-52 (28)
C10	504 (34)	633 (40)	313 (26)	32 (26)	98 (25)	-38 (29)
C11	593 (37)	633 (40)	400 (30)	120 (27)	211 (29)	13 (31)
C12	522 (35)	589 (37)	402 (30)	134 (27)	237 (28)	-49 (29)
C13	311 (26)	606 (36)	286 (24)	-25 (24)	159 (21)	-30 (25)
C14	440 (30)	435 (31)	371 (27)	-41 (22)	208 (25)	-31 (25)
C15	450 (30)	489 (32)	366 (26)	48 (23)	200 (25)	-63 (25)
C16	543 (34)	550 (35)	463 (30)	-11 (26)	303 (28)	-124 (28)
C17	414 (30)	589 (37)	442 (29)	47 (26)	213 (26)	-113 (26)
C18	488 (34)	676 (41)	449 (31)	14 (28)	172 (28)	-126 (30)
C19	417 (30)	472 (32)	371 (27)	31 (23)	165 (24)	-43 (25)
C20	372 (28)	417 (30)	421 (27)	11 (23)	215 (24)	-37 (23)
C21	780 (45)	638 (41)	492 (34)	125 (30)	322 (34)	3 (35)
C22	745 (48)	945 (53)	458 (35)	104 (34)	205 (35)	27 (40)
C23	1089 (58)	774 (48)	672 (42)	52 (36)	555 (43)	-198 (42)
C24	1932 (96)	770 (54)	689 (48)	331 (41)	650 (58)	400 (56)
C25	1057 (59)	657 (46)	694 (44)	167 (36)	542 (45)	337 (43)
C26	3218 (157)	1192 (73)	976 (65)	355 (56)	1414 (89)	1220 (87)
C27	1889 (118)	1346 (89)	1763 (109)	-240 (78)	1241 (100)	348 (84)
C28	2387 (125)	693 (57)	1556 (86)	-119 (55)	1477 (92)	219 (65)
C29	489 (36)	850 (49)	561 (37)	68 (34)	240 (30)	-171 (34)
C30	887 (58)	2247 (103)	829 (54)	-199 (60)	642 (50)	-668 (64)
C31	844 (58)	1348 (76)	1642 (88)	537 (66)	856 (64)	228 (54)
C32	852 (57)	1211 (69)	1177 (68)	66 (54)	572 (54)	-337 (51)
C33	538 (37)	802 (45)	407 (30)	-36 (29)	208 (29)	-95 (32)
C34	829 (46)	662 (41)	563 (37)	-108 (31)	424 (36)	-93 (35)
C35	992 (57)	1053 (58)	461 (36)	221 (37)	366 (38)	239 (46)
C36	699 (49)	2050 (93)	486 (40)	-250 (49)	236 (38)	-539 (56)

Table S20. Bond distances (Å) and angles (°) for complex 4.

	Molecule A	Molecule B	
Mn1A - O1B	2.262(12)	2.254(13)	
Mn1 - O1	2.087(10)	2.097(10)	
Mn1 - O2	2.062(13)	2.015(13)	
Mn1 - N1	2.217(17)	2.238(16)	
Mn1 - N2	2.212(18)	2.200(17)	
Mn1 - N3	2.382(15)	2.387(15)	
O1 - C1	1.31(2)	1.36(2)	
O2 - C20	1.30(3)	1.31(3)	
N1 - C7	1.31(3)	1.27(3)	
N1 - C8	1.41(3)	1.41(3)	
N2 - C13	1.46(3)	1.43(3)	
N2 - C14	1.26(3)	1.33(3)	
N3 - C21	1.31(3)	1.36(3)	
N3 - C25	1.36(3)	1.34(3)	
C1 - C2	1.44(3)	1.40(3)	
C1 - C6	1.39(3)	1.42(3)	
C2 - C3	1.40(3)	1.41(3)	
C3 - C4	1.42(4)	1.37(4)	
C4 - C5	1.38(4)	1.34(4)	
C5 - C6	1.41(3)	1.43(3)	
C6 - C7	1.42(4)	1.42(3)	
C8 - C9	1.39(3)	1.44(3)	
C8 - C13	1.42(4)	1.37(3)	
C9 - C10	1.37(4)	1.38(4)	
C10 - C11	1.37(4)	1.36(5)	
C11 - C12	1.36(4)	1.39(4)	
C12 - C13	1.41(4)	1.41(3)	
C14 - C15	1.48(4)	1.39(4)	
C15 - C16	1.44(4)	1.37(4)	
C15 - C20	1.37(3)	1.43(4)	
C16 - C17	1.38(4)	1.36(4)	
C17 - C18	1.36(4)	1.39(4)	
C18 - C19	1.36(4)	1.41(4)	
C19 - C20	1.43(3)	1.43(3)	
C21 - C22	1.39(4)	1.38(4)	
C22 - C23	1.33(4)	1.39(4)	
C23 - C24	1.39(4)	1.36(4)	
C24 - C25	1.40(4)	1.36(4)	
N3A - Mn1A- O1B	169.3(6)	169.3(5)	
N2A - Mn1A- O1B	97.2(6)	97.7(5)	
N1A - Mn1A- O1B	94.3(5)	96.5(6)	
O2A - Mn1A- O1B	91.7(4)	90.3(5)	
O1A - Mn1A- O1B	78.1(4)	78.1(4)	
Mn1A- O1A - Mn1B	102.2(4)	Mn1A- O1B - Mn1B	101.6(4)
C1A - O1A - Mn1B	114.5(11)	C1B - O1B - Mn1A	115.2(11)
N2 - Mn1 - N3	93.5(7)	92.8(6)	
N1 - Mn1 - N3	88.6(5)	88.2(5)	
N1 - Mn1 - N2	73.2(7)	75.1(6)	
O2 - Mn1 - N3	89.1(5)	88.4(5)	
O2 - Mn1 - N2	86.3(6)	85.4(6)	
O2 - Mn1 - N1	159.2(6)	160.0(6)	
O1 - Mn1 - N3	91.9(5)	92.9(5)	
O1 - Mn1 - N2	158.2(7)	159.0(6)	
O1 - Mn1 - N1	85.9(5)	84.9(5)	

Table S20. Bond distances (Å) and angles (°) for complex 4 (cont.).

Molecule A			Molecule B			
O1	-	Mn1	-	O2	114.8(5)	115.0(5)
Mn1	-	O1	-	C1	124.4(11)	125.6(11)
Mn1	-	O2	-	C20	130.8(13)	132.2(13)
Mn1	-	N1	-	C8	118.0(13)	113.7(13)
Mn1	-	N1	-	C7	121.9(15)	123.2(14)
C7	-	N1	-	C8	118.3(16)	121.9(17)
Mn1	-	N2	-	C14	123.1(17)	126.9(15)
Mn1	-	N2	-	C13	117.9(13)	114.5(13)
C13	-	N2	-	C14	118.6(20)	118.4(18)
Mn1	-	N3	-	C25	118.3(14)	121.7(14)
Mn1	-	N3	-	C21	124.6(15)	123.6(13)
C21	-	N3	-	C25	117.0(18)	114.7(18)
O1	-	C1	-	C6	124(2)	119.4(18)
O1	-	C1	-	C2	118.0(18)	119.8(18)
C2	-	C1	-	C6	118.1(20)	120.7(18)
C1	-	C2	-	C3	121(2)	119(2)
C2	-	C3	-	C4	120.3(20)	121(2)
C3	-	C4	-	C5	118.0(19)	119(2)
C4	-	C5	-	C6	123(2)	124(2)
C1	-	C6	-	C5	120(2)	115(2)
C5	-	C6	-	C7	111.4(20)	114.8(20)
C1	-	C6	-	C7	129(2)	129.5(20)
N1	-	C7	-	C6	124.4(19)	126.1(19)
N1	-	C8	-	C13	116.7(20)	118.3(20)
N1	-	C8	-	C9	127(2)	120(2)
C9	-	C8	-	C13	116(2)	122(2)
C8	-	C9	-	C10	122(2)	117(2)
C9	-	C10	-	C11	121(2)	124(3)
C10	-	C11	-	C12	121(3)	118(3)
C11	-	C12	-	C13	119(2)	122(2)
C8	-	C13	-	C12	121(2)	118(2)
N2	-	C13	-	C12	125.0(20)	124.6(20)
N2	-	C13	-	C8	113.9(20)	117.7(20)
N2	-	C14	-	C15	130(2)	125(2)
C14	-	C15	-	C20	124(2)	126(2)
C14	-	C15	-	C16	118(2)	115(2)
C16	-	C15	-	C20	119(2)	120(2)
C15	-	C16	-	C17	120(2)	123(2)
C16	-	C17	-	C18	120(2)	119(3)
C17	-	C18	-	C19	121(2)	122(2)
C18	-	C19	-	C20	121(2)	119(2)
C15	-	C20	-	C19	119(2)	118(2)
O2	-	C20	-	C19	115.5(19)	117(2)
O2	-	C20	-	C15	125.8(20)	124.8(19)
N3	-	C21	-	C22	125(2)	125.0(19)
C21	-	C22	-	C23	118(3)	115(2)
C22	-	C23	-	C24	119(2)	123(2)
C23	-	C24	-	C25	120(2)	116(2)
N3	-	C25	-	C24	121(2)	126(2)

Table S21. Bond distances (Å) and angles (°) for complex 5.

Mn1	- O1	2.036 (7)	C1	- C2	1.415 (14)
Mn1	- O4	2.027 (6)	C1	- C6	1.376 (16)
Mn1	- N1	2.208 (10)	C2	- C3	1.374 (17)
Mn1	- N2	2.135 (7)	C3	- C4	1.351 (20)
Mn1	- N4	2.184 (9)	C4	- C5	1.376 (15)
Mn2	- O2	1.995 (7)	C5	- C6	1.417 (15)
Mn2	- O3	2.011 (7)	C6	- C7	1.470 (14)
Mn2	- N2	2.182 (6)	C8	- C9	1.409 (18)
Mn2	- N3	2.213 (8)	C8	- C13	1.407 (16)
Mn2	- N4	2.143 (8)	C9	- C10	1.373 (16)
Na1	- O1	2.353 (6)	C10	- C11	1.382 (20)
Na1	- O4	2.525 (6)	C11	- C12	1.382 (19)
Na1	- O5	2.458 (9)	C12	- C13	1.402 (14)
Na1	- O6	2.304 (14)	C14	- C15	1.543 (13)
Na2	- O2	2.401 (8)	C14	- C34	1.602 (15)
Na2	- O3	2.398 (7)	C15	- C16	1.389 (14)
Na2	- O7	2.403 (11)	C15	- C20	1.411 (12)
Na2	- O8	2.438 (11)	C16	- C17	1.359 (13)
Na2	- O9	2.611 (13)	C17	- C18	1.372 (14)
Na2	- O10	2.405 (12)	C18	- C19	1.343 (15)
O1	- C1	1.336 (13)	C19	- C20	1.384 (13)
O2	- C20	1.351 (12)	C21	- C22	1.411 (17)
O3	- C21	1.329 (12)	C21	- C26	1.423 (14)
O4	- C40	1.355 (13)	C22	- C23	1.413 (16)
O5	- C41	1.431 (20)	C23	- C24	1.336 (18)
O5	- C42	1.32 (2)	C24	- C25	1.343 (19)
O6	- C43	1.363 (20)	C25	- C26	1.414 (14)
O6	- C44A	1.40 (4)	C26	- C27	1.430 (16)
O6	- C44B	1.41 (4)	C28	- C29	1.390 (16)
O7	- C45	1.343 (20)	C28	- C33	1.464 (12)
O7	- C46	1.26 (2)	C29	- C30	1.363 (19)
O8	- C47	1.33 (3)	C30	- C31	1.375 (15)
O8	- C48	1.33 (2)	C31	- C32	1.395 (16)
O9	- C49	1.34 (2)	C32	- C33	1.389 (16)
O9	- C50	1.39 (3)	C34	- C35	1.504 (11)
O10	- C51	1.34 (2)	C35	- C36	1.340 (16)
O10	- C52	1.389 (15)	C35	- C40	1.449 (13)
N1	- C7	1.281 (14)	C36	- C37	1.394 (14)
N1	- C8	1.437 (12)	C37	- C38	1.391 (16)
N2	- C13	1.378 (14)	C38	- C39	1.367 (17)
N2	- C14	1.443 (14)	C39	- C40	1.401 (13)
N3	- C27	1.306 (13)	C42	- C43	1.43 (3)
N3	- C28	1.394 (14)	C46	- C47	1.39 (3)
N4	- C33	1.367 (14)	C50	- C51	1.33 (3)
N4	- C34	1.508 (11)			
N2	- Mn1 - N4	69.8 (3)	Mn2	- N3 - C27	124.5 (7)
N1	- Mn1 - N4	131.5 (3)	C27	- N3 - C28	120.2 (9)
N1	- Mn1 - N2	74.8 (3)	Mn1	- N4 - Mn2	80.8 (3)
O4	- Mn1 - N4	94.8 (3)	Mn2	- N4 - C34	112.7 (5)
O4	- Mn1 - N2	106.6 (3)	Mn2	- N4 - C33	115.6 (5)
O4	- Mn1 - N1	126.9 (3)	Mn1	- N4 - C34	102.3 (6)
O1	- Mn1 - N4	118.8 (3)	Mn1	- N4 - C33	121.4 (5)
O1	- Mn1 - N2	156.2 (3)	C33	- N4 - C34	118.0 (8)
O1	- Mn1 - N1	84.5 (3)	O1	- C1 - C6	126.5 (9)
O1	- Mn1 - O4	95.1 (2)	O1	- C1 - C2	116.8 (9)
N3	- Mn2 - N4	73.0 (3)	C2	- C1 - C6	116.6 (9)
N2	- Mn2 - N4	69.6 (3)	C1	- C2 - C3	122.5 (10)
N2	- Mn2 - N3	129.5 (3)	C2	- C3 - C4	119.7 (11)

Table S21. Bond distances (Å) and angles (°) for complex 5 (cont.).

O3	-	Mn2	-	N4	155.4 (3)	C3	-	C4	-	C5	120.5 (11)
O3	-	Mn2	-	N3	84.8 (3)	C4	-	C5	-	C6	120.0 (10)
O3	-	Mn2	-	N2	120.3 (3)	C1	-	C6	-	C5	120.6 (9)
O2	-	Mn2	-	N4	109.0 (3)	C5	-	C6	-	C7	116.4 (9)
O2	-	Mn2	-	N3	131.1 (3)	C1	-	C6	-	C7	123.0 (9)
O2	-	Mn2	-	N2	93.0 (3)	N1	-	C7	-	C6	126.1 (9)
O2	-	Mn2	-	O3	93.4 (3)	N1	-	C8	-	C13	114.1 (9)
O5	-	Na1	-	O6	69.1 (4)	N1	-	C8	-	C9	123.7 (9)
O4	-	Na1	-	O6	100.3 (3)	C9	-	C8	-	C13	122.0 (10)
O4	-	Na1	-	O5	169.1 (3)	C8	-	C9	-	C10	118.8 (10)
O1	-	Na1	-	O6	107.2 (4)	C9	-	C10	-	C11	120.8 (12)
O1	-	Na1	-	O5	104.6 (3)	C10	-	C11	-	C12	119.8 (11)
O1	-	Na1	-	O4	75.8 (2)	C11	-	C12	-	C13	122.2 (10)
O9	-	Na2	-	O10	67.0 (4)	C8	-	C13	-	C12	116.2 (10)
O8	-	Na2	-	O10	99.5 (4)	N2	-	C13	-	C12	126.2 (9)
O8	-	Na2	-	O9	86.5 (4)	N2	-	C13	-	C8	117.6 (9)
O7	-	Na2	-	O10	153.8 (4)	N2	-	C14	-	C34	108.2 (7)
O7	-	Na2	-	O9	89.1 (4)	N2	-	C14	-	C15	117.0 (8)
O7	-	Na2	-	O8	67.0 (4)	C15	-	C14	-	C34	113.0 (8)
O3	-	Na2	-	O10	96.9 (3)	C14	-	C15	-	C20	124.0 (9)
O3	-	Na2	-	O9	97.8 (3)	C14	-	C15	-	C16	118.1 (9)
O3	-	Na2	-	O8	163.4 (4)	C16	-	C15	-	C20	117.9 (9)
O3	-	Na2	-	O7	97.0 (3)	C15	-	C16	-	C17	122.9 (10)
O2	-	Na2	-	O10	100.0 (3)	C16	-	C17	-	C18	118.6 (10)
O2	-	Na2	-	O9	164.6 (4)	C17	-	C18	-	C19	119.9 (10)
O2	-	Na2	-	O8	104.4 (3)	C18	-	C19	-	C20	123.4 (10)
O2	-	Na2	-	O7	105.0 (4)	C15	-	C20	-	C19	117.0 (9)
O2	-	Na2	-	O3	74.8 (3)	O2	-	C20	-	C19	119.9 (9)
Mn1	-	O1	-	Na1	96.9 (3)	O2	-	C20	-	C15	123.1 (9)
Na1	-	O1	-	C1	124.7 (6)	O3	-	C21	-	C26	124.8 (8)
Mn1	-	O1	-	C1	129.0 (6)	O3	-	C21	-	C22	116.9 (9)
Mn2	-	O2	-	Na2	95.0 (3)	C22	-	C21	-	C26	118.3 (9)
Na2	-	O2	-	C20	132.5 (6)	C21	-	C22	-	C23	119.4 (10)
Mn2	-	O2	-	C20	125.1 (6)	C22	-	C23	-	C24	121.8 (10)
Mn2	-	O3	-	Na2	94.7 (3)	C23	-	C24	-	C25	119.6 (11)
Na2	-	O3	-	C21	129.0 (6)	C24	-	C25	-	C26	123.3 (10)
Mn2	-	O3	-	C21	128.1 (6)	C21	-	C26	-	C25	117.3 (9)
Mn1	-	O4	-	Na1	92.0 (2)	C25	-	C26	-	C27	119.0 (9)
Na1	-	O4	-	C40	129.3 (5)	C21	-	C26	-	C27	123.6 (8)
Mn1	-	O4	-	C40	122.6 (5)	N3	-	C27	-	C26	126.0 (9)
Na1	-	O5	-	C42	115.8 (8)	N3	-	C28	-	C33	113.8 (8)
Na1	-	O5	-	C41	129.7 (8)	N3	-	C28	-	C29	126.5 (9)
C41	-	O5	-	C42	113.6 (11)	C29	-	C28	-	C33	119.4 (9)
Na1	-	O6	-	C44B	117.8 (18)	C28	-	C29	-	C30	122.0 (10)
Na1	-	O6	-	C44A	123.7 (14)	C29	-	C30	-	C31	118.9 (11)
Na1	-	O6	-	C43	113.9 (11)	C30	-	C31	-	C32	122.1 (10)
C43	-	O6	-	C44B	118 (2)	C31	-	C32	-	C33	120.6 (9)
C43	-	O6	-	C44A	118.0 (17)	C28	-	C33	-	C32	116.9 (9)
Na2	-	O7	-	C46	114.3 (12)	N4	-	C33	-	C32	129.1 (8)
Na2	-	O7	-	C45	123.8 (10)	N4	-	C33	-	C28	114.0 (8)
C45	-	O7	-	C46	120.3 (16)	N4	-	C34	-	C14	103.2 (7)
Na2	-	O8	-	C48	129.6 (12)	C14	-	C34	-	C35	113.5 (8)
Na2	-	O8	-	C47	117.5 (11)	N4	-	C34	-	C35	117.3 (7)
C47	-	O8	-	C48	112.9 (15)	C34	-	C35	-	C40	123.9 (8)
Na2	-	O9	-	C50	107.2 (9)	C34	-	C35	-	C36	118.1 (8)
Na2	-	O9	-	C49	133.1 (11)	C36	-	C35	-	C40	117.9 (8)
C49	-	O9	-	C50	116.5 (14)	C35	-	C36	-	C37	125.2 (10)

Table S21. Bond distances (Å) and angles (°) for complex 5 (cont.).

Na2 - O10 - C52	114.4 (8)	C36 - C37 - C38	117.8 (10)
Na2 - O10 - C51	116.6 (11)	C37 - C38 - C39	118.4 (10)
C51 - O10 - C52	115.4 (13)	C38 - C39 - C40	124.6 (9)
Mn1 - N1 - C8	112.0 (6)	C35 - C40 - C39	115.9 (9)
Mn1 - N1 - C7	125.0 (7)	O4 - C40 - C39	118.6 (9)
C7 - N1 - C8	121.6 (9)	O4 - C40 - C35	125.5 (8)
Mn1 - N2 - Mn2	81.0 (3)	O5 - C42 - C43	113.2 (16)
Mn2 - N2 - C14	101.4 (6)	O6 - C43 - C42	119.4 (17)
Mn2 - N2 - C13	119.4 (6)	O7 - C46 - C47	125 (2)
Mn1 - N2 - C14	113.0 (5)	O8 - C47 - C46	113 (2)
Mn1 - N2 - C13	113.6 (6)	O9 - C50 - C51	117 (17)
C13 - N2 - C14	121.1 (8)	O10 - C51 - C50	120.0 (20)
Mn2 - N3 - C28	114.3 (6)		

Table S22. Bond distances (Å) and angles (°) for complex 6.

Mn1	- O1	2.171(4)	O8	- C32	1.397(8)
Mn1	- O2	2.121(3)	N1	- C7	1.439(5)
Mn1	- N1	2.258(3)	N1	- C8	1.360(5)
Mn1	- N1'	2.174(4)	N2	- C13	1.363(5)
Mn1	- N2	2.281(3)	N2	- C14	1.454(5)
Mn1	- N2'	2.154(3)	C1	- C2	1.401(6)
Na1	- O1	2.329(3)	C1	- C6	1.419(6)
Na1	- O2	2.391(3)	C2	- C3	1.373(5)
Na1	- O3	2.514(4)	C3	- C4	1.376(6)
Na1	- O4	2.347(4)	C4	- C5	1.382(6)
Na1	- O5	2.481(6)	C5	- C6	1.377(5)
Na1	- O6	2.416(5)	C6	- C7	1.527(6)
Na2	- O1	2.459(4)	C7	- C14'	1.631(6)
Na2	- O2	2.460(4)	C8	- C9	1.387(6)
Na2	- O7	2.469(4)	C8	- C13	1.478(5)
Na2	- O8	2.400(4)	C9	- C10	1.416(8)
O1	- C1	1.330(5)	C10	- C11	1.355(8)
O2	- C20	1.330(5)	C11	- C12	1.399(8)
O3	- C21	1.407(8)	C12	- C13	1.388(6)
O3	- C22	1.437(9)	C14	- C15	1.532(6)
O4	- C23	1.387(7)	C15	- C16	1.372(6)
O4	- C24	1.426(8)	C15	- C20	1.420(6)
O5	- C25	1.360(10)	C16	- C17	1.399(6)
O5	- C26	1.301(11)	C17	- C18	1.355(8)
O6	- C27	1.376(10)	C18	- C19	1.370(8)
O6	- C28	1.264(11)	C19	- C20	1.411(6)
O7	- C29	1.369(8)	C22	- C23	1.468(14)
O7	- C30	1.381(9)	C26	- C27	1.274(17)
O8	- C31	1.422(10)	C30	- C31	1.384(12)
N2	- Mn1 - N2'	106.1(1)	Na1	- O6 - C27	114.5(5)
N1'	- Mn1 - N2'	70.6(1)	C27	- O6 - C28	117.3(6)
N1'	- Mn1 - N2	68.5(1)	Na2	- O7 - C30	115.2(4)
N1	- Mn1 - N2'	69.3(1)	Na2	- O7 - C29	128.7(4)
N1	- Mn1 - N2	66.9(1)	C29	- O7 - C30	114.4(5)
N1	- Mn1 - N1'	106.0(1)	Na2	- O8 - C32	119.7(3)
O2	- Mn1 - N2'	165.3(1)	Na2	- O8 - C31	113.3(4)
O2	- Mn1 - N2	85.1(1)	C31	- O8 - C32	110.3(5)
O2	- Mn1 - N1'	106.1(1)	Mn1	- N1 - C8	102.0(2)
O2	- Mn1 - N1	124.7(1)	Mn1	- N1 - C7	105.5(2)
O1	- Mn1 - N2'	102.6(1)	C7	- N1 - C8	128.3(3)
O1	- Mn1 - N2	128.1(1)	Mn1	- N1' - C7'	116.2(3)
O1	- Mn1 - N1'	163.3(1)	Mn1	- N2 - C14	104.6(2)
O1	- Mn1 - N1	84.7(1)	Mn1	- N2 - C13	101.8(2)
O1	- Mn1 - O2	76.6(1)	C13	- N2 - C14	127.5(3)
O5	- Na1 - O6	66.8(2)	Mn1	- N2' - C14'	116.9(2)
O4	- Na1 - O6	154.6(2)	O1	- C1 - C6	123.3(3)
O4	- Na1 - O5	88.1(2)	O1	- C1 - C2	118.9(4)
O3	- Na1 - O6	112.1(2)	C2	- C1 - C6	117.8(3)
O3	- Na1 - O5	85.7(2)	C1	- C2 - C3	122.5(4)
O3	- Na1 - O4	67.5(1)	C2	- C3 - C4	119.7(4)
O2	- Na1 - O6	104.0(1)	C3	- C4 - C5	118.5(4)
O2	- Na1 - O5	117.0(2)	C4	- C5 - C6	123.7(4)
O2	- Na1 - O4	83.5(1)	C1	- C6 - C5	117.8(4)
O2	- Na1 - O3	142.9(1)	C5	- C6 - C7	118.5(4)
O1	- Na1 - O6	107.0(2)	C1	- C6 - C7	123.6(3)
O1	- Na1 - O5	172.2(2)	N1	- C7 - C6	118.5(3)
O1	- Na1 - O4	98.3(1)	C6	- C7 - C14'	109.2(3)
O1	- Na1 - O3	92.5(1)	N1	- C7 - C14'	107.0(3)

Table S22. Bond distances (Å) and angles (°) for complex 6 (cont.).

O1	-	Na1	-	O2	68.5(1)	N1	-	C8	-	C13	112.3(3)
O7	-	Na2	-	O8	68.1(1)	N1	-	C8	-	C9	129.8(4)
O2	-	Na2	-	O8	107.3(1)	C9	-	C8	-	C13	117.9(3)
O2	-	Na2	-	O7	154.4(2)	C8	-	C9	-	C10	121.1(4)
O1	-	Na2	-	O8	149.6(1)	C9	-	C10	-	C11	120.3(5)
O1	-	Na2	-	O7	105.1(1)	C10	-	C11	-	C12	121.1(5)
O1	-	Na2	-	O2	65.4(1)	C11	-	C12	-	C13	120.9(5)
Na1	-	O1	-	Na2	94.3(1)	C8	-	C13	-	C12	118.6(4)
Mn1	-	O1	-	Na2	87.3(1)	N2	-	C13	-	C12	129.5(4)
Mn1	-	O1	-	Na1	89.7(1)	N2	-	C13	-	C8	111.8(3)
Na2	-	O1	-	C1	107.8(2)	N2	-	C14	-	C7'	106.0(3)
Na1	-	O1	-	C1	136.3(3)	C7'	-	C14	-	C15	110.8(3)
Mn1	-	O1	-	C1	127.5(3)	N2	-	C14	-	C15	116.4(3)
Na1	-	O2	-	Na2	92.7(1)	C14	-	C15	-	C20	124.8(4)
Mn1	-	O2	-	Na2	88.4(1)	C14	-	C15	-	C16	117.2(4)
Mn1	-	O2	-	Na1	89.3(1)	C16	-	C15	-	C20	117.9(4)
Na2	-	O2	-	C20	111.4(3)	C15	-	C16	-	C17	123.3(4)
Na1	-	O2	-	C20	135.2(3)	C16	-	C17	-	C18	118.9(4)
Mn1	-	O2	-	C20	127.0(3)	C17	-	C18	-	C19	119.9(4)
Na1	-	O3	-	C22	103.3(3)	C18	-	C19	-	C20	122.6(5)
Na1	-	O3	-	C21	125.6(4)	C15	-	C20	-	C19	117.5(4)
C21	-	O3	-	C22	113.7(5)	O2	-	C20	-	C19	118.9(4)
Na1	-	O4	-	C24	121.9(3)	O2	-	C20	-	C15	123.6(4)
Na1	-	O4	-	C23	119.4(4)	O3	-	C22	-	C23	108.1(6)
C23	-	O4	-	C24	112.4(5)	O4	-	C23	-	C22	108.8(5)
Na1	-	O5	-	C26	112.7(6)	O5	-	C26	-	C27	123.8(8)
Na1	-	O5	-	C25	123.3(4)	O6	-	C27	-	C26	120.3(7)
C25	-	O5	-	C26	118.1(7)	O7	-	C30	-	C31	115.4(6)
Na1	-	O6	-	C28	126.3(4)	O8	-	C31	-	C30	115.7(7)

Prime denotes a transformation of 1-x, y, 1-z.