

Table SII. Crystallographic data for complexes 3-5, 8, 13, 21, 22.

	3	4	5	8
Formula ^a	C ₇₂ H ₈₄ Mn ₆ N ₆ O ₂₈	C ₇₂ H ₆₈ Mn ₆ N ₁₄ O ₂₀	C ₆₄ H ₈₀ Mn ₆ N ₆ O ₂₄	C ₇₀ H ₉₆ Mn ₆ N ₆ O ₂₄
<i>M</i> _w	1811.05	1778.98	1646.93	1735.13
Crystal System	Triclinic	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1	P-1
<i>a</i> /Å	11.9177(3)	12.1880(3)	12.7404(3)	13.521(2)
<i>b</i> /Å	12.7405(3)	12.2015(3)	15.4280(4)	13.6880(19)
<i>c</i> /Å	13.5095(3)	13.3261(3)	19.0456(5)	13.814(2)
<i>α</i> ^o	80.875(1)	101.143(1)	90.075(2)	112.975(9)
<i>β</i> ^o	77.238(1)	96.929(1)	103.2920(10)	95.825(9)
<i>γ</i> ^o	80.941(1)	106.861(1)	98.8750(10)	118.889(7)
<i>V</i> /Å ³	1959.23(8)	1827.56(8)	3597.04(16)	1923.0(6)
<i>Z</i>	1	1	2	1
<i>T</i> /K	150	150	150	150
<i>λ</i> ^b /Å	0.71073	0.71073	0.71073	0.71073
<i>D</i> _c /g cm ⁻³	1.535	1.620	1.520	1.498
<i>μ</i> (Mo-Kα)/mm ⁻¹	1.022	1.090	1.101	1.034
Meas./indep.(<i>R</i> _{int}) refl.	33921 / 10895 (0.042)	27345 / 7457 (0.041)	48617 / 20054 (0.042)	17799 / 10695 (0.0864)
Obs. refl. [<i>I</i> >2σ(<i>I</i>)]	8549	5865	15709	9800
<i>wR</i> 2 ^{c,d}	0.1068	0.0883	0.1305	0.1886
<i>R</i> 1 ^{d,e}	0.0437	0.0358	0.0541	0.0757
Goodness of fit on <i>F</i> ²	0.9321	0.8895	1.0171	1.0423
<i>Δρ</i> _{max,min} /eÅ ⁻³	0.89 / -0.69	0.51 / -0.50	0.75 / -0.73	1.27 / -0.96

	13	21	22
Formula ^a	C ₆₅ H ₉₂ Mn ₆ N ₆ O ₂₇	C ₈₀ H ₉₇ Mn ₆ N ₆ O ₂₆	C ₆₈ H _{74.5} Cl ₄ Mn ₆ N ₆ O _{24.5}
<i>M</i> _w	1719.04	1888.24	1839.24
Crystal System	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1
<i>a</i> /Å	12.2582(4)	12.1777(3)	11.9218(2)
<i>b</i> /Å	12.3804(4)	12.3384(2)	12.0379(2)
<i>c</i> /Å	14.8895(5)	14.4043(3)	13.6675(3)
<i>α</i> ^o	91.749(2)	84.4970(10)	85.793(1)
<i>β</i> ^o	107.077(2)	89.042(2)	85.319(1)
<i>γ</i> ^o	115.261(2)	75.2140(10)	75.513(1)
<i>V</i> /Å ³	1921.47(12)	2082.91(8)	1889.92(6)
<i>Z</i>	1	1	1
<i>T</i> /K	150	150	150
<i>λ</i> ^b /Å	0.71073	0.71073	0.71073
<i>D</i> _c /g cm ⁻³	1.490	1.505	1.616
<i>μ</i> (Mo-Kα)/mm ⁻¹	1.037	0.963	1.194
Meas./indep. (<i>R</i> _{int}) refl.	41182 / 10653 (0.058)	49999 / 8507 (0.054)	22561 / 7715 (0.035)
Obs. refl. [<i>I</i> > 2σ(<i>I</i>)]	8300	5460	6111
<i>wR</i> 2 ^{c,d}	0.0489	0.1085	0.0780
<i>R</i> 1 ^{d,e}	0.1220	0.0345	0.0330
Goodness of fit on <i>F</i> ²	1.0096	0.8922	0.8767
Δρ _{max,min} /eÅ ⁻³	1.05 / -0.76	0.81 / -0.62	0.68 / -0.50

^a Including solvate molecules. ^b Mo-Kα radiation, graphite monochromator. ^c $wR2 = [\sum w(IF_o^2 - IF_c^2)^2 / \sum wIF_o^2]^2$.
^d For observed data. ^e $R1 = \sum IF_o - IF_c / \sum IF_o$. SQUEEZE (P. van der Sluis and A. L. Spek, *Acta Cryst.* 1990, **A46**, 194) was employed for 4 and 13 - see CIF files for full details.

Table SI2 Individual bond lengths making up each Mn-N-O-Mn bridge in complexes **1-24**

Complex	Mn1-N-O-Mn2 (t.a)	Mn1-N-O-Mn3 (t.a)	Mn2-N-O-Mn3 (t.a)
(1)	2.002 / 1.376 / 1.918 (25.57)	1.997 / 1.388 / 1.948 (18.01)	2.006 / 1.375 / 1.898 (10.42)
(2)	2.013 / 1.371 / 1.906 (25.50)	1.915 / 1.369 / 2.004 (29.74)	1.998 / 1.397 / 1.955 (42.44)
(3)	1.993 / 1.378 / 1.929 (18.74)	1.932 / 1.390 / 2.011 (18.91)	2.005 / 1.374 / 1.910 (11.99)
(4)	1.960 / 1.387 / 2.009 (28.18)	1.898 / 1.372 / 2.005 (8.38)	1.996 / 1.373 / 1.905 (16.18)
(5)†	2.004 / 1.379 / 1.895 (9.66)	1.918 / 1.373 / 2.000 (15.60)	2.014 / 1.380 / 1.948 (29.83)
	1.993 / 1.382 / 1.910 (13.53)	1.918 / 1.376 / 1.997 (37.33)	2.017 / 1.383 / 1.972 (23.80)
(6)	1.938 / 1.362 / 2.008 (27.40)	2.011 / 1.382 / 1.904 (36.35)	1.909 / 1.398 / 1.988 (31.10)
(7)	2.018 / 1.373 / 1.922 (27.83)	1.944 / 1.391 / 1.994 (41.46)	2.017 / 1.374 / 1.918 (40.07)
(8)	2.015 / 1.368 / 1.918 (26.93)	1.952 / 1.387 / 1.986 (40.70)	2.003 / 1.375 / 1.904 (34.53)
(9)	1.909 / 1.370 / 2.019 (36.92)	1.990 / 1.380 / 1.947 (42.12)	1.916 / 1.376 / 2.029 (23.27)
	2.011 / 1.376 / 1.911 (32.33)	1.947 / 1.392 / 1.989 (42.24)	2.014 / 1.372 / 1.904 (16.76)
(10)	1.998 / 1.352 / 1.962 (47.56)	1.894 / 1.368 / 2.002 (23.75)	2.010 / 1.385 / 1.908 (31.76)
(11)	2.000 / 1.370 / 1.931 (30.36)	1.960 / 1.398 / 1.985 (43.71)	2.021 / 1.374 / 1.909 (38.33)
(12)	1.871 / 1.388 / 2.022 (30.43)	1.957 / 1.434 / 1.954 (31.91)	2.014 / 1.338 / 2.049 (42.94)
(13)	2.007 / 1.371 / 1.924 (29.68)	1.965 / 1.392 / 1.993 (44.47)	2.016 / 1.378 / 1.910 (38.51)
(14)	1.997 / 1.375 / 1.925 (31.26)	1.957 / 1.391 / 1.999 (39.92)	2.006 / 1.376 / 1.924 (38.20)
(15)	2.004 / 1.376 / 1.918 (39.10)	1.915 / 1.366 / 2.003 (43.04)	2.001 / 1.391 / 1.951 (34.86)
(16)	1.955 / 1.396 / 1.991 (42.61)	2.007 / 1.396 / 1.931 (34.07)	1.914 / 1.379 / 2.017 (36.73)
(17)	1.942 / 1.395 / 1.984 (47.16)	2.000 / 1.372 / 1.932 (30.37)	1.916 / 1.371 / 2.027 (38.19)
(18)	1.996 / 1.395 / 1.958 (41.09)	1.932 / 1.381 / 1.990 (40.50)	2.011 / 1.369 / 1.911 (33.28)
(19)	1.941 / 1.390 / 1.996 (42.32)	2.015 / 1.370 / 1.928 (25.60)	1.918 / 1.367 / 2.010 (39.28)
(20)	1.943 / 1.394 / 1.989 (38.85)	1.993 / 1.371 / 1.911 (32.06)	1.916 / 1.379 / 1.998 (38.67)
(21)	1.981 / 1.396 / 1.966 (43.61)	2.000 / 1.374 / 1.932 (33.72)	2.015 / 1.374 / 1.899 (29.53)
(22)	1.969 / 1.395 / 1.991 (43.48)	1.990 / 1.370 / 1.922 (31.03)	1.897 / 1.370 / 2.007 (27.70)
(23)	2.020 / 1.373 / 1.907 (33.40)	1.927 / 1.369 / 2.001 (33.00)	1.991 / 1.393 / 1.957 (43.89)
(24)	2.001 / 1.372 / 1.926 (33.01)	1.943 / 1.399 / 1.979 (37.16)	2.000 / 1.379 / 1.892 (31.28)