A Manganese(II) 3D Metal–Organic Framework with Siloxane-Spaced Dicarboxylic Ligand: Synthesis, Structure, and Properties

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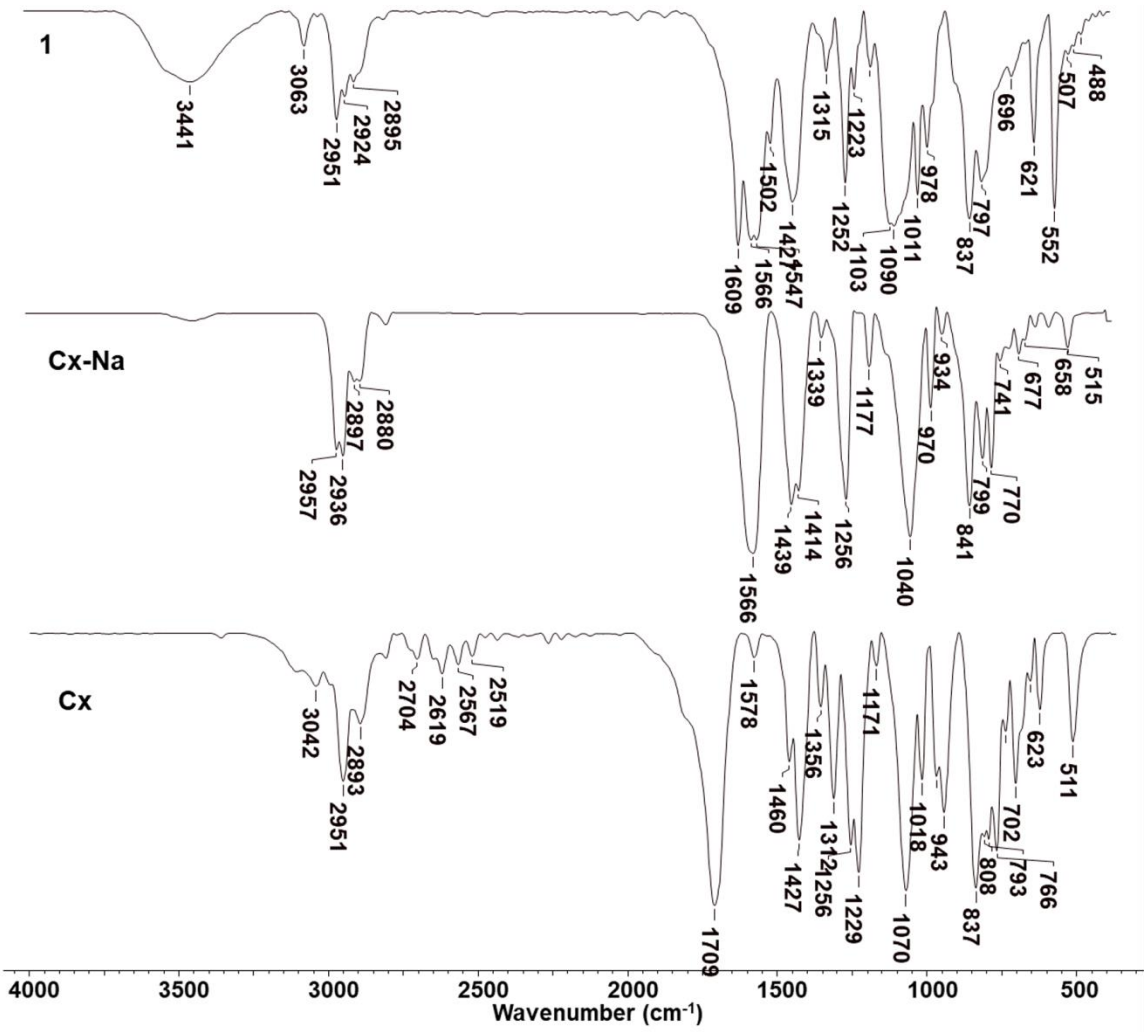

Figure S1. FTIR spectra for Cx, Cx-Na, and polymer **1**

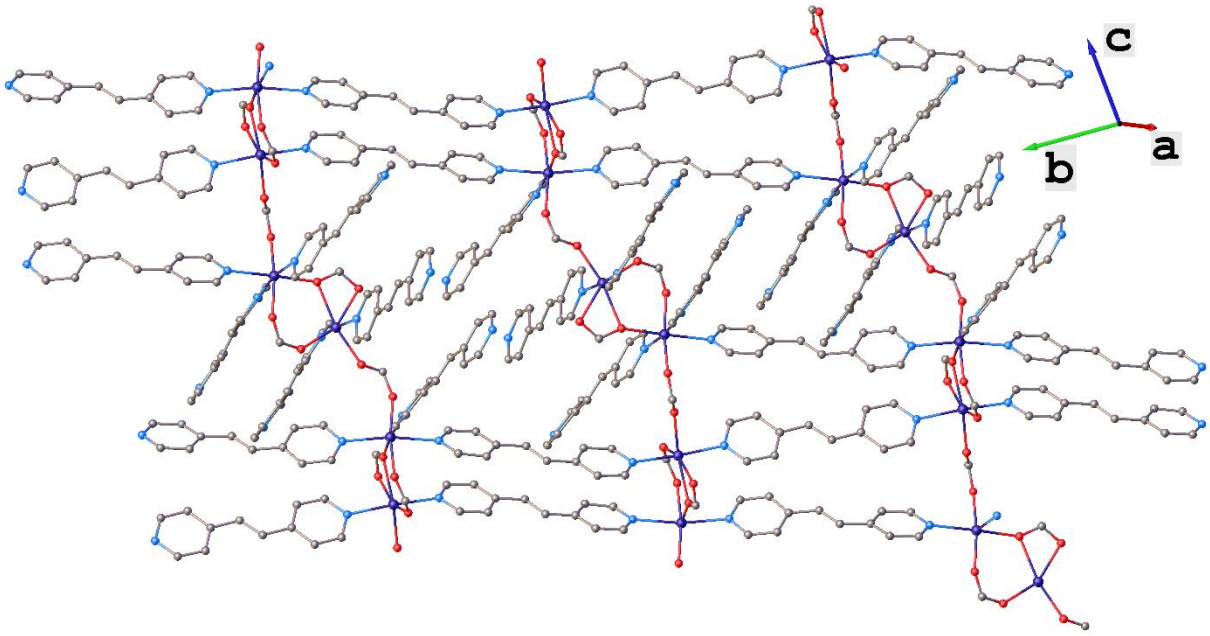

Figure S2. Polymer structure, from the perspective of the etdipy moiety (perchlorate counterion and siloxane moiety were omitted for clarity)

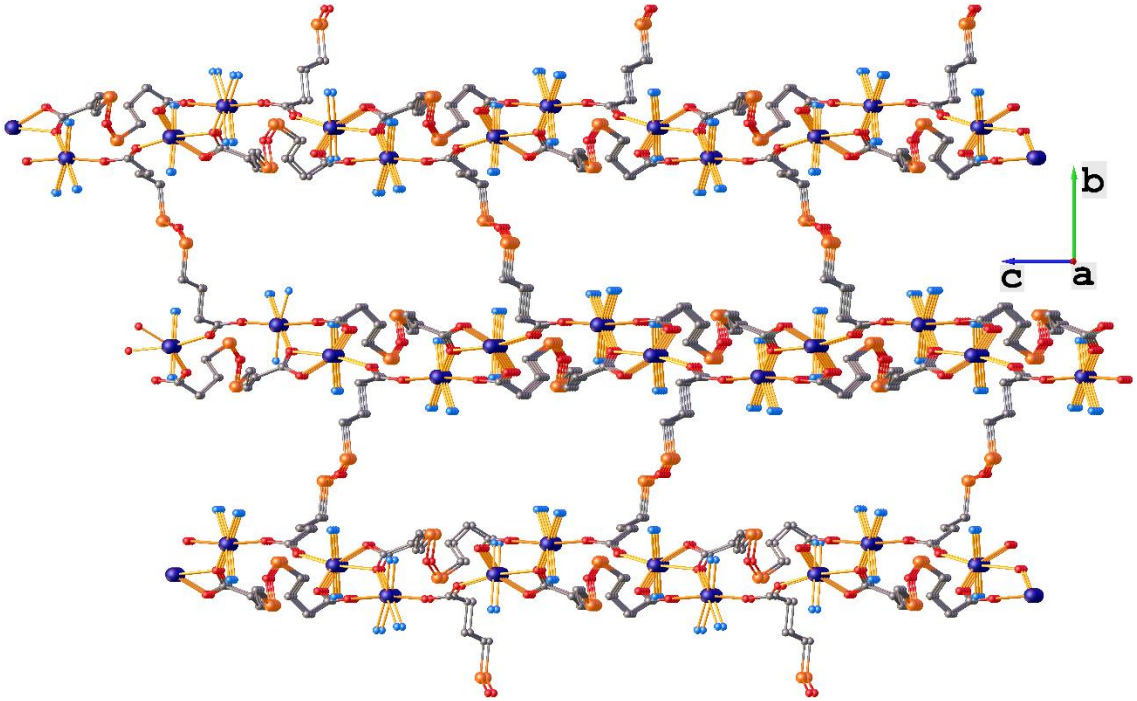

Figure S3. Polymer structure from the perspective of the siloxane moiety (perchlorate counterion and etdipy moiety were omitted for clarity)

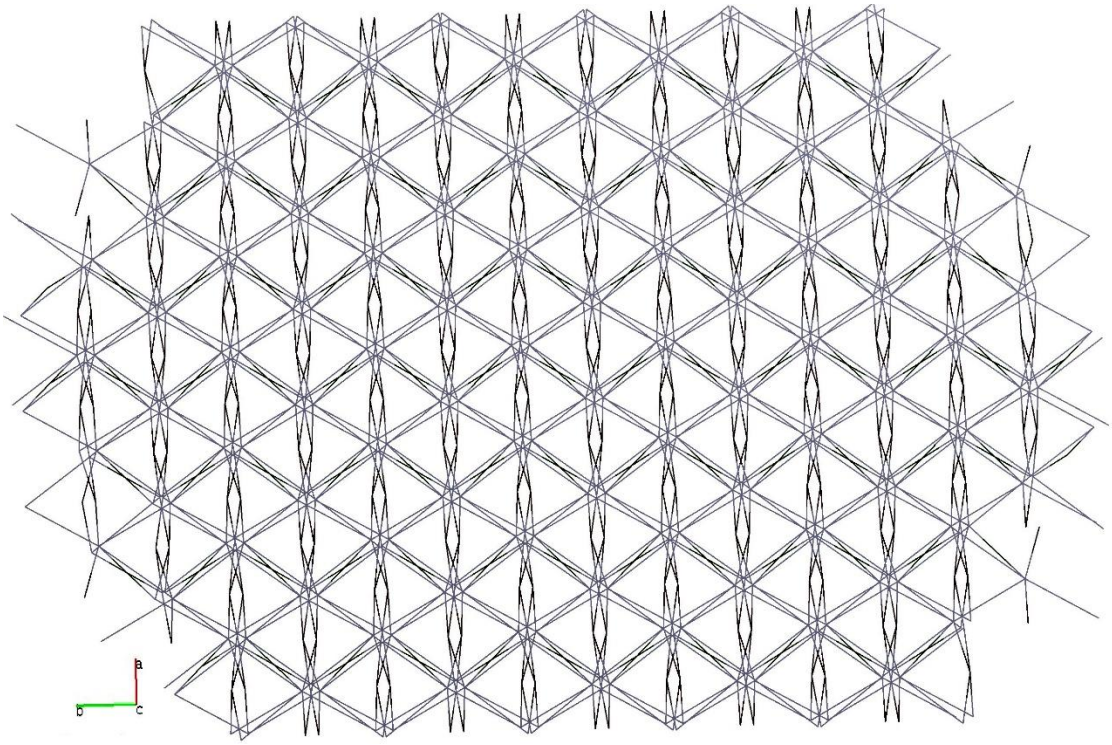

Figure S4. Topology of the polymer network. In the topological analysis, the disordered part of the structure was omitted

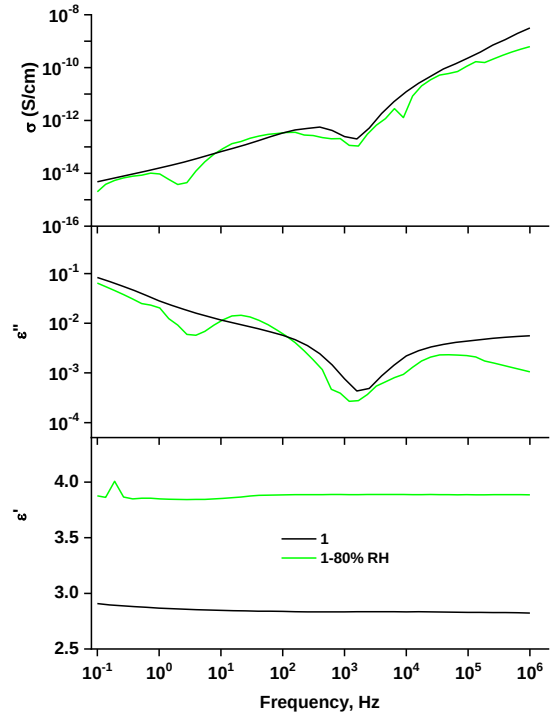

Figure S5. Dielectric properties of compound **1,** including the relative permittivity (ε'), dielectric loss (ε"), and conductivity (σ).

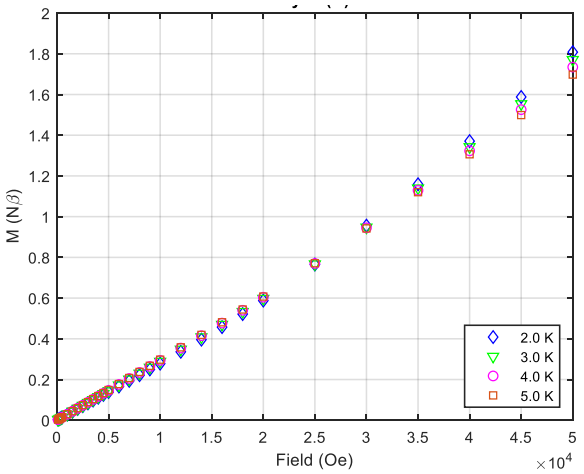

Figure S6. Magnetization curves versus applied magnetic field for compound **1**.

$$\chi = \frac{Ng^2\beta^2 S(S+1)}{3kT} * \left[\frac{1+u_1+u_2+u_1u_2}{1-u_1u_2}\right] \qquad \text{eq-SI-1}$$

$$u_i = \coth(J_i'/kT) - kT/J_i' \;; \qquad J_i' = J_i(S(S+1);\ \text{i=1,2} \qquad \text{eq-SI-2}$$

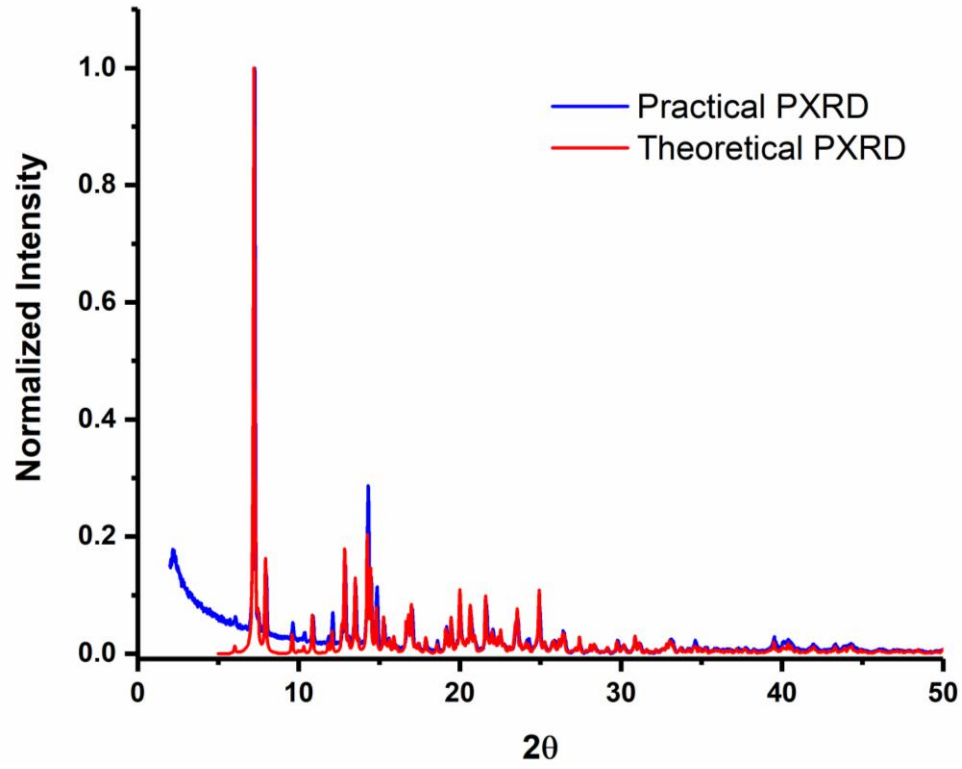

Figure S7. PXRD diffractogram (blue) vs. the one simulated based on single crystal X-ray diffraction data (red).

Table S1. Selected bond lengths [Å], angles [°] and hydrogen bonds for compound **1**.

Mn1-O1	2.180(4)	C11-C12	1.394(10)
Mn1-O5[1]	2.131(5)	C13-C14	1.507(8)
Mn1-O6	2.107(5)	C24-C23	1.497(8)
Mn1-N1[2]	2.295(5)	C25-C26	1.509(8)
Mn1-N2	2.302(5)	C31-C32	1.377(9)
Mn1-N3[3]	2.322(5)	C31-C35	1.399(10)
Mn2-O1[4]	2.291(4)	C33-C34	1.367(9)
Mn2-O2[4]	2.255(5)	C34-C35	1.364(10)
Mn2-O4[5]	2.093(5)	C35-C36	1.488(9)
Mn2-O7	2.109(4)	C36-C37	1.278(10)
Mn2-N4	2.280(5)	C37-C38	1.472(9)
Mn2-N5	2.265(5)	C38-C39	1.403(10)
O1-Mn2[6]	2.291(4)	C38-C42	1.359(10)
O1-C13	1.292(8)	C39-C40	1.391(9)
O2-Mn2[6]	2.255(5)	C41-C42	1.372(9)
O2-C13	1.251(7)	C43-C44	1.368(10)
O4-Mn2[7]	2.093(5)	C44-C45	1.371(10)
O4-C24	1.259(8)	C45-C46	1.368(10)
O5-Mn1[8]	2.131(5)	C45-C48	1.485(9)
O5-C24	1.242(7)	C46-C47	1.385(9)
O6-C25	1.260(7)	C48-C48[11]	1.302(13)
O7-C25	1.237(7)	Si1-O3	1.606(9)
N1-Mn1[9]	2.295(5)	Si1-C16	1.837(12)
N1-C2	1.341(9)	Si1-C17	1.833(12)
N1-C3	1.310(9)	Si1-C18	1.824(12)
N2-C10	1.328(9)	Si2-O3	1.606(9)
N2-C11	1.311(9)	Si2-C19	1.826(12)
N3-Mn1[10]	2.322(5)	Si2-C20	1.830(12)
N3-C32	1.328(9)	Si2-C21	1.832(11)
N3-C33	1.323(8)	Si3-O8	1.608(10)
N4-C40	1.339(8)	Si3-C28	1.87(2)
N4-C41	1.335(9)	Si3-C29	1.88(2)
N5-C43	1.348(9)	Si3-C30	1.67(3)
N5-C47	1.332(8)	C14-C15	1.504(9)
C1-C2	1.372(9)	C15-C16	1.500(9)
C1-C5	1.376(10)	C21-C22	1.426(13)
C3-C4	1.386(10)	C22-C23	1.434(14)
C4-C5	1.362(10)	C26-C27	1.592(19)
C5-C6	1.454(9)	C27-C28	1.53(2)
C6-C7	1.306(10)	Cl1-O9	1.366(9)

C7-C8	1.467(9)	Cl1-O10	1.493(11)
C8-C9	1.365(10)	Cl1-O11	1.390(9)
C8-C12	1.340(10)	Cl1-O12	1.389(8)
C9-C10	1.388(10)		

[1] – 1 + *x*, ½ – *y*, – ½ + *z*; [2] – *x*, – ½ + *y*, ½ – *z*; [3] 1 – *x*, ½ + *y*, ½ – *z*; [4] + *x*, ½ – *y*, ½ + *z*; [5] – 1 + *x*, + *y*, + *z*; [6] + *x*, ½ – *y*, – ½ + *z*; [7] 1 + *x*, + *y*, + *z*; [8] 1 + *x*, ½ – *y*, ½ + *z*; [9] – *x*, ½ + *y*, ½ – *z*; [10] 1 – *x*, – ½ + *y*, ½ – *z*; [11] – *x*, 1 – *y*, 1 – *z*

O1-Mn1-N1[1]	89.10(18)	C8-C12-C11	121.3(8)
O1-Mn1-N2	174.82(17)	O1-C13-C14	117.9(8)
O1-Mn1-N3[2]	86.70(18)	O2-C13-O1	118.2(6)
O5[3]-Mn1-O1	94.29(17)	O2-C13-C14	122.5(8)
O5[3]-Mn1-N1[1]	85.43(19)	O4-C24-C23	115.4(11)
O5[3]-Mn1-N2	86.3(2)	O5-C24-O4	125.3(6)
O5[3]-Mn1-N3[2]	86.86(19)	O5-C24-C23	119.3(11)
O6-Mn1-O1	89.37(17)	O6-C25-C26	119.1(8)
O6-Mn1-O5[3]	171.23(17)	O7-C25-O6	122.6(6)
O6-Mn1-N1[1]	102.62(19)	O7-C25-C26	116.7(8)
O6-Mn1-N2	89.3(2)	C32-C31-C35	119.2(7)
O6-Mn1-N3[2]	85.40(19)	N3-C32-C31	123.4(8)
N1[1]-Mn1-N2	96.08(19)	N3-C33-C34	124.0(7)
N1[1]-Mn1-N3[2]	170.9(2)	C35-C34-C33	120.2(7)
N2-Mn1-N3[2]	88.19(19)	C31-C35-C36	124.8(7)
O2[4]-Mn2-O1[4]	57.37(15)	C34-C35-C31	116.6(6)
O2[4]-Mn2-N4	87.51(18)	C34-C35-C36	118.6(7)
O2[4]-Mn2-N5	89.4(2)	C37-C36-C35	127.3(8)
O4[5]-Mn2-O1[4]	97.73(17)	C36-C37-C38	125.8(9)
O4[5]-Mn2-O2[4]	154.83(18)	C39-C38-C37	121.2(7)
O4[5]-Mn2-O7	93.41(18)	C42-C38-C37	121.6(7)
O4[5]-Mn2-N4	92.18(19)	C42-C38-C39	117.2(6)
O45-Mn2-N5	93.7(2)	C40-C39-C38	119.2(7)
O7-Mn2-O1[4]	168.14(17)	N4-C40-C39	123.1(7)
O7-Mn2-O2[4]	111.70(17)	N4-C41-C42	124.4(7)
O7-Mn2-N4	87.41(18)	C38-C42-C41	120.0(7)
O7-Mn2-N5	87.08(18)	N5-C43-C44	123.7(7)
N4-Mn2-O1[4]	96.19(17)	C43-C44-C45	120.1(7)
N5-Mn2-O1[4]	88.15(18)	C44-C45-C48	119.9(7)
N5-Mn2-N4	172.2(2)	C46-C45-C44	117.1(6)
Mn1-O1-Mn2[6]	119.16(19)	C46-C45-C48	123.0(6)
C13-O1-Mn1	149.8(4)	C45-C46-C47	119.8(7)
C13-O1-Mn2[6]	90.9(3)	N5-C47-C46	123.7(7)

C13-O2-Mn2[6]	93.6(4)	C48[11]-C48-C45	124.3(9)
C24-O4-Mn2[7]	135.2(4)	O3-Si1-C16	89.7(11)
C24-O5-Mn1[8]	138.4(5)	O3-Si1-C17	124.8(17)
C25-O6-Mn1	144.8(4)	O3-Si1-C18	104.5(17)
C25-O7-Mn2	134.8(4)	C17-Si1-C16	113(2)
C2-N1-Mn1[9]	119.6(5)	C18-Si1-C16	118(2)
C3-N1-Mn1[9]	124.2(5)	C18-Si1-C17	106(2)
C3-N1-C2	116.1(6)	O3-Si2-C19	105.1(15)
C10-N2-Mn1	119.4(5)	O3-Si2-C20	99.8(17)
C11-N2-Mn1	124.4(5)	O3-Si2-C21	117.4(12)
C11-N2-C10	115.8(6)	C19-Si2-C20	118(2)
C32-N3-Mn1[10]	125.6(5)	C19-Si2-C21	113.6(18)
C33-N3-Mn1[10]	117.8(4)	C20-Si2-C21	102.7(17)
C33-N3-C32	116.6(6)	O8-Si3-C28	105.1(15)
C40-N4-Mn2	116.3(5)	O8-Si3-C29	110.5(13)
C41-N4-Mn2	127.1(4)	O8-Si3-C30	116.5(14)
C41-N4-C40	116.1(5)	C28-Si3-C29	102.8(14)
C43-N5-Mn2	118.8(4)	C30-Si3-C28	111.2(15)
C47-N5-Mn2	125.6(5)	C30-Si3-C29	109.8(15)
C47-N5-C43	115.5(6)	Si2-O3-Si1	143.4(15)
C2-C1-C5	120.4(7)	C15-C14-C13	111.5(12)
N1-C2-C1	123.3(8)	C16-C15-C14	121.3(15)
N1-C3-C4	123.6(7)	C15-C16-Si1	112.3(15)
C5-C4-C3	120.6(8)	C22-C21-Si2	112.8(15)
C1-C5-C6	123.0(7)	C21-C22-C23	113.0(17)
C4-C5-C1	116.0(6)	C22-C23-C24	113.8(12)
C4-C5-C6	121.0(7)	C25-C26-C27	109.6(13)
C7-C6-C5	126.9(8)	C28-C27-C26	118(2)
C6-C7-C8	128.4(8)	C27-C28-Si3	114(2)
C9-C8-C7	123.1(7)	O9-Cl1-O10	101.7(8)
C12-C8-C7	122.0(7)	O9-Cl1-O11	114.6(6)
C12-C8-C9	114.8(6)	O9-Cl1-O12	115.8(7)
C8-C9-C10	122.0(7)	O11-Cl1-O10	103.6(8)
N2-C10-C9	122.2(7)	O12-Cl1-O10	106.4(7)
N2-C11-C12	123.8(7)	O12-Cl1-O11	112.9(6)

[1] $-x, -\frac{1}{2}+y, \frac{1}{2}-z$; [2] $1-x, \frac{1}{2}+y, \frac{1}{2}-z$; [3] $-1+x, \frac{1}{2}-y, -\frac{1}{2}+z$; [4] $+x, \frac{1}{2}-y, \frac{1}{2}+z$; [5] $-1+x, +y, +z$; [6] $+x, \frac{1}{2}-y, -\frac{1}{2}+z$; [7] $1+x, +y, +z$; [8] $1+x, \frac{1}{2}-y, \frac{1}{2}+z$; [9] $-x, \frac{1}{2}+y, \frac{1}{2}-z$; [10] $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$; [11] $-x, 1-y, 1-z$

D-H···A	d(D-H)/Å	d(H···A)/Å	d(D-A)/Å	D-H···A/°	Symmetry code

C3-H···O5	0.93	2.48	3.060(8)	120.2	1 – *x*, 1 – *y*, 1 – *z*
C33-H···O6	0.93	2.59	3.093(7)	114.3	1 – *x*, – ½ + *y*, ½ – *z*
C26-H···O2	0.97	2.56	3.413(16)	147.4	+ *x*, ½ – *y*, ½ + *z*