Electronic Supplementary Information

Deciphering the supramolecular isomerization in coordination polymers: connected molecular squares vs fused hexagons

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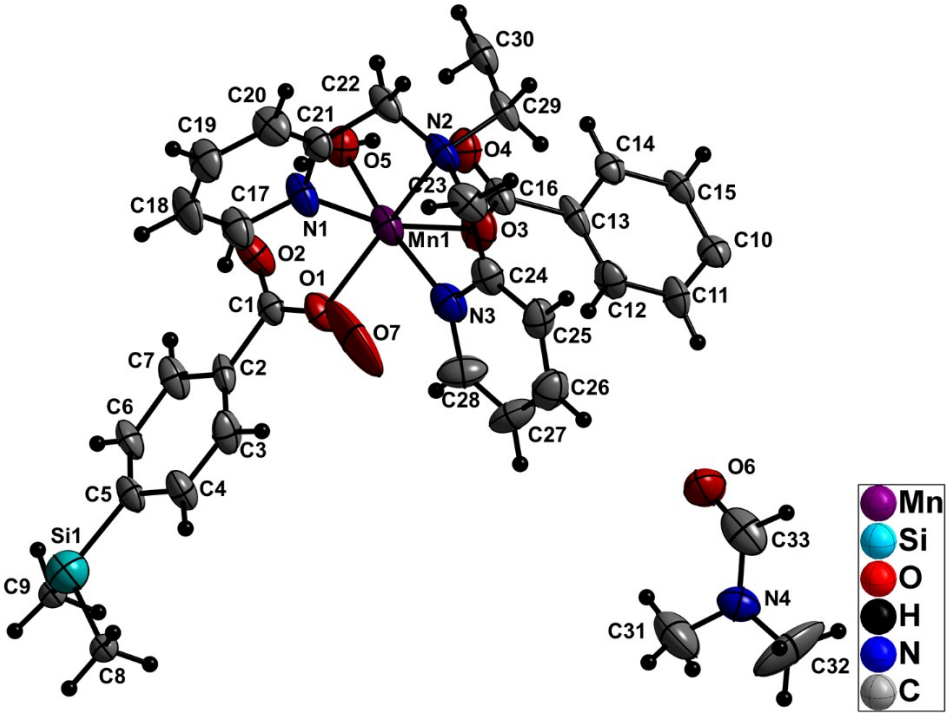
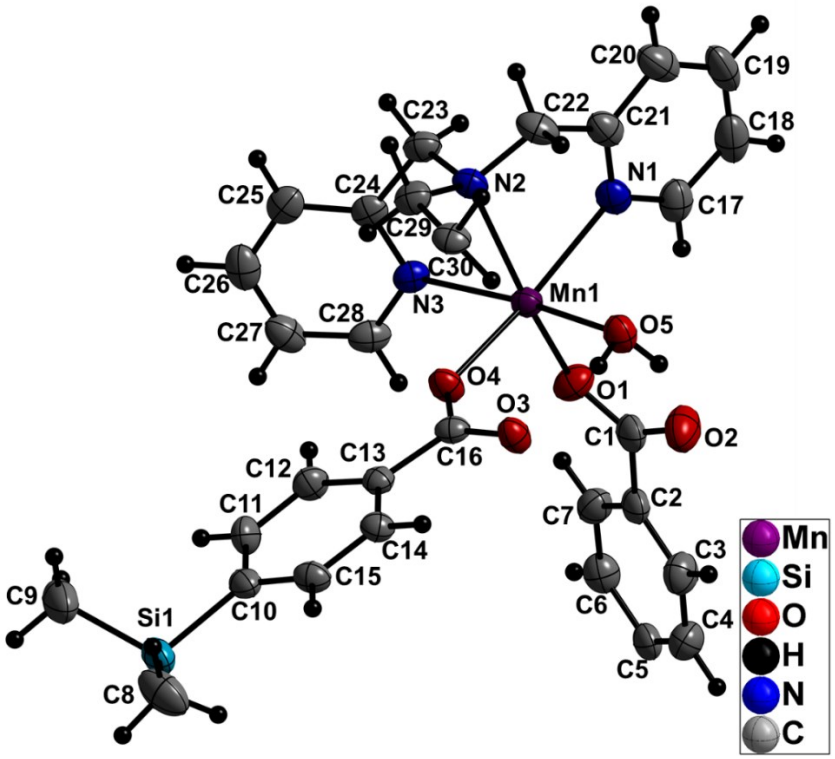


Fig. S1 Coordination environment and the content of asymmetric unit in **1**.



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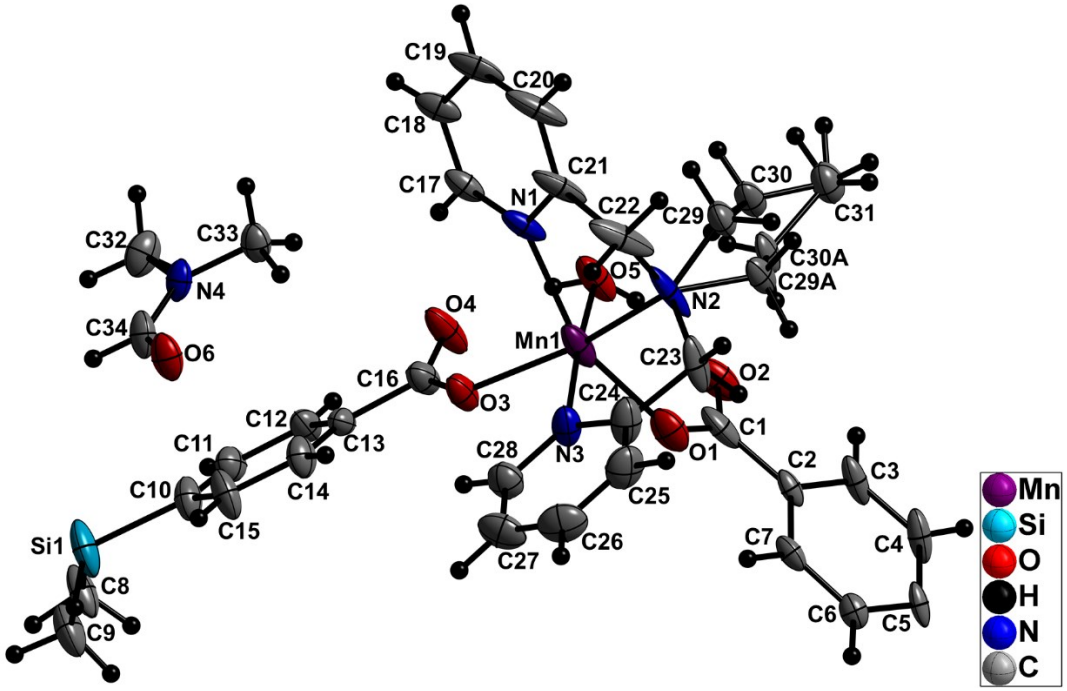

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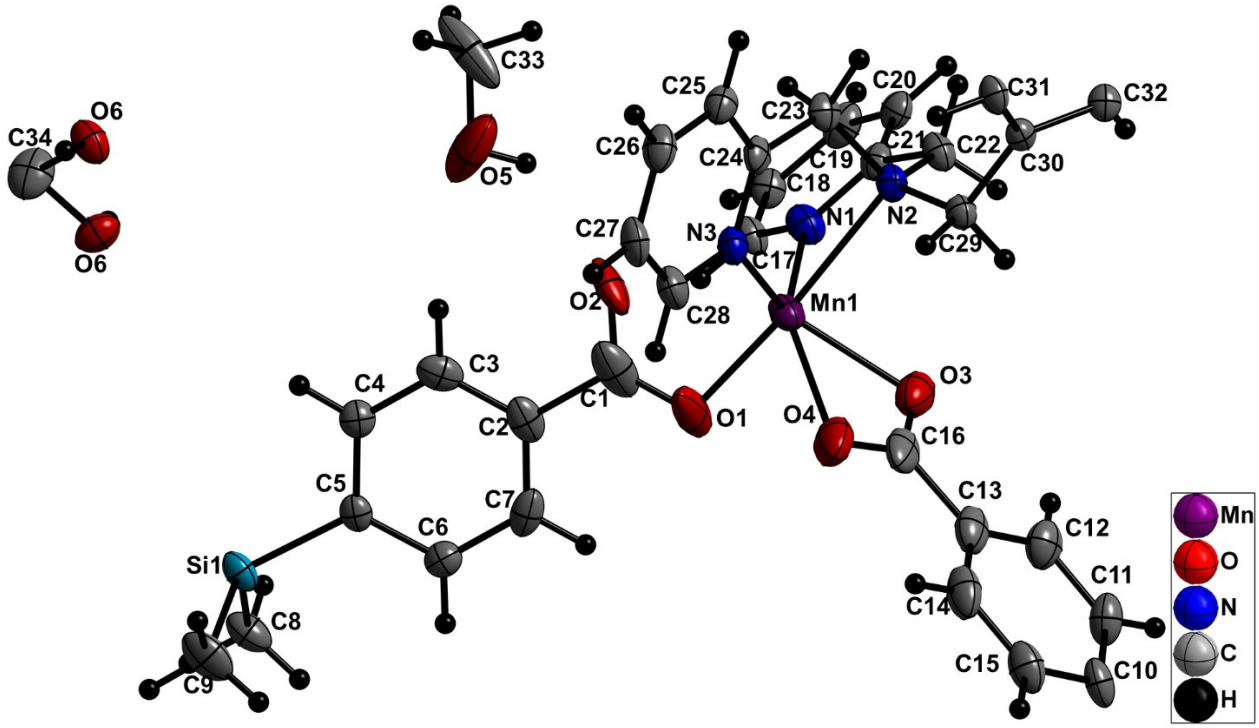

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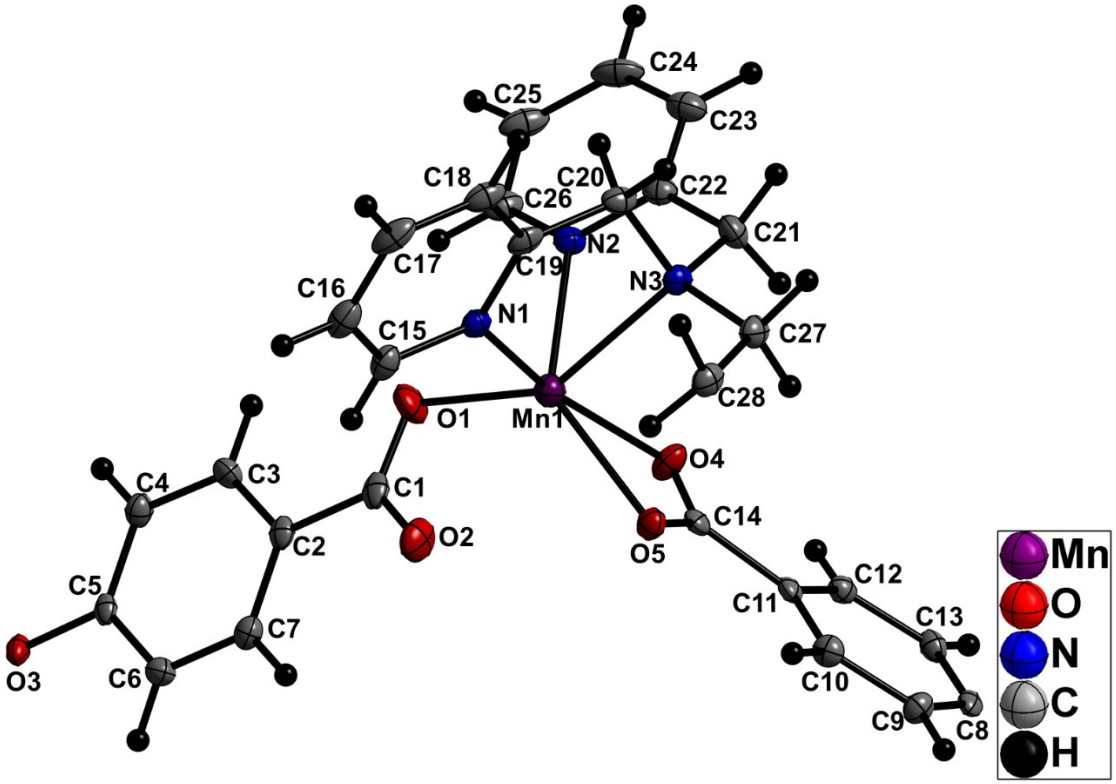

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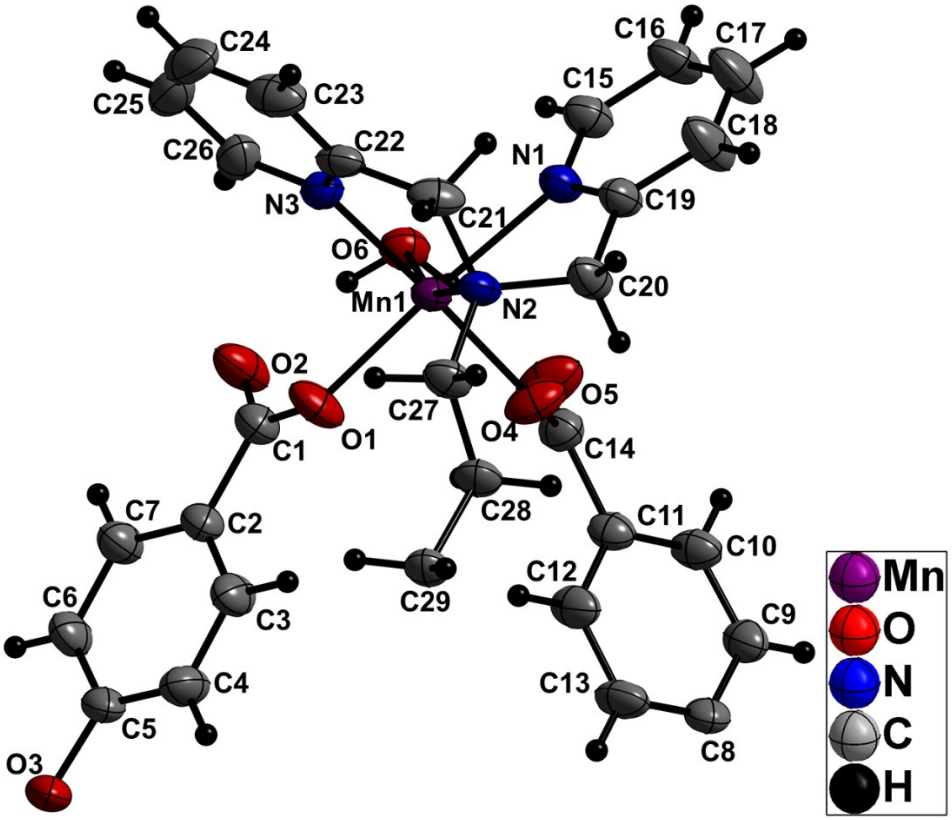
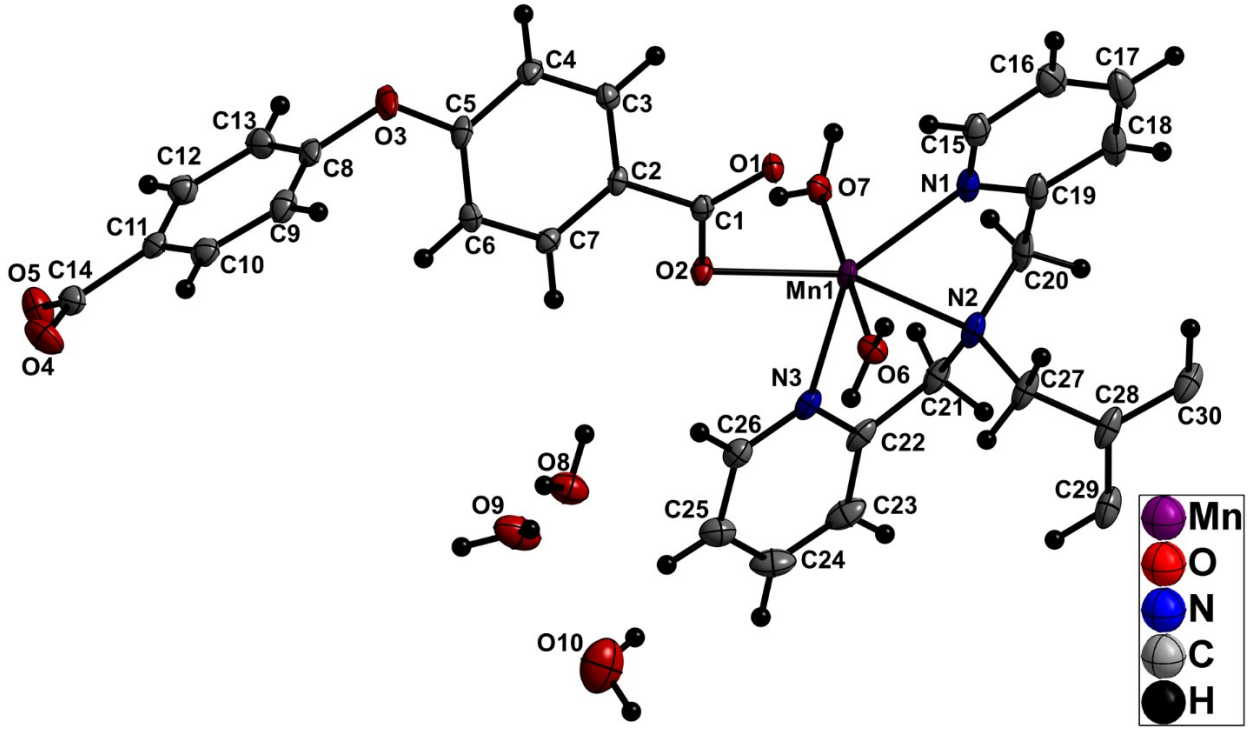


Fig. S6 Coordination environment and the content of asymmetric unit in **5**.



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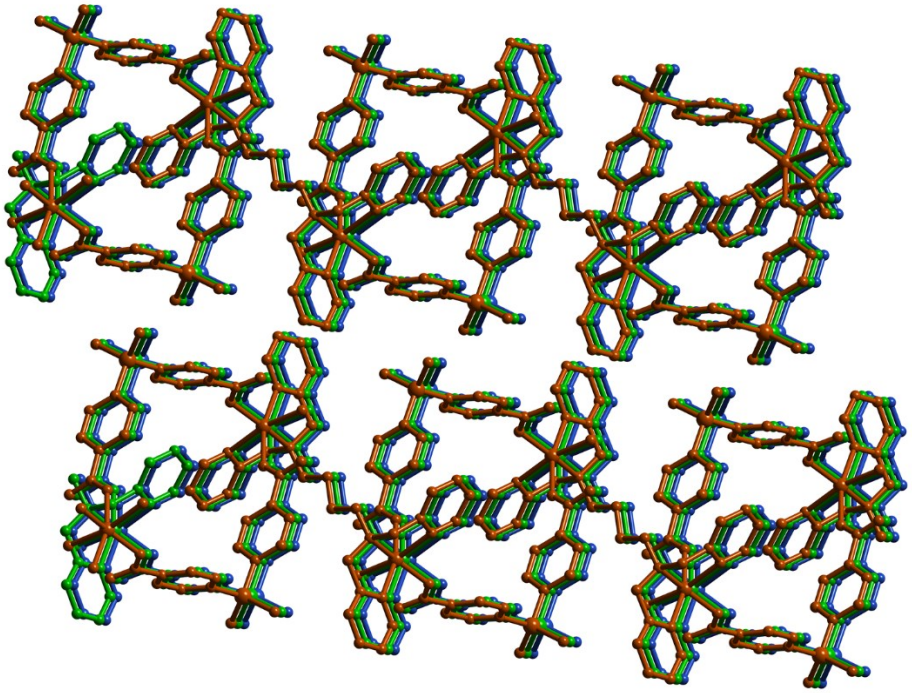

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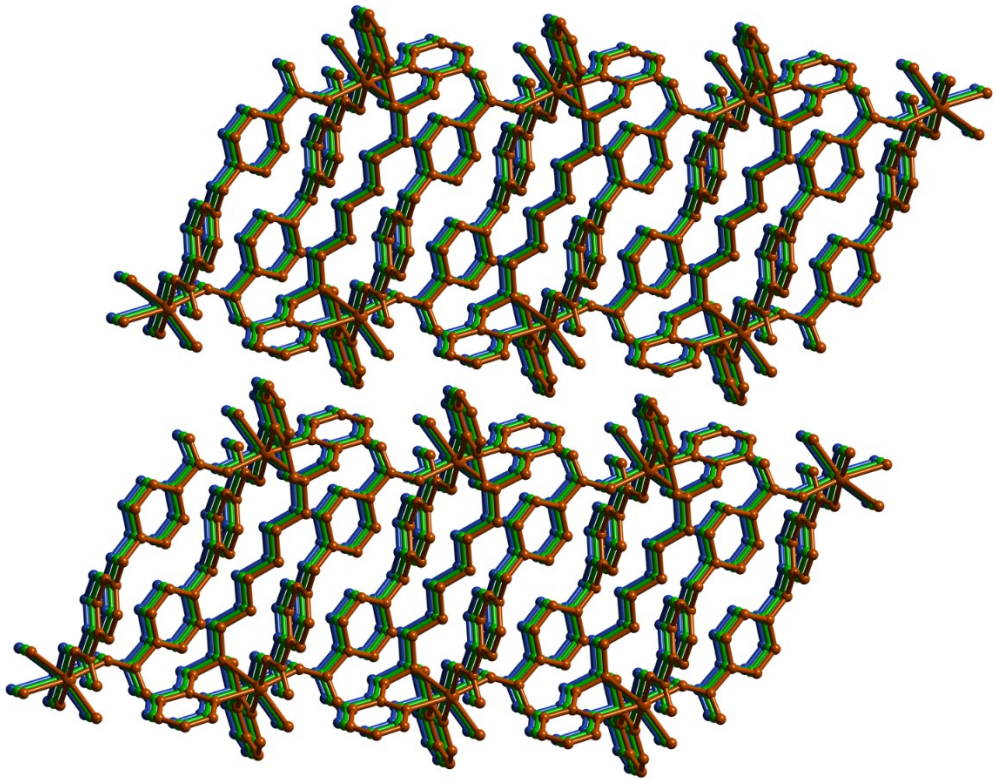

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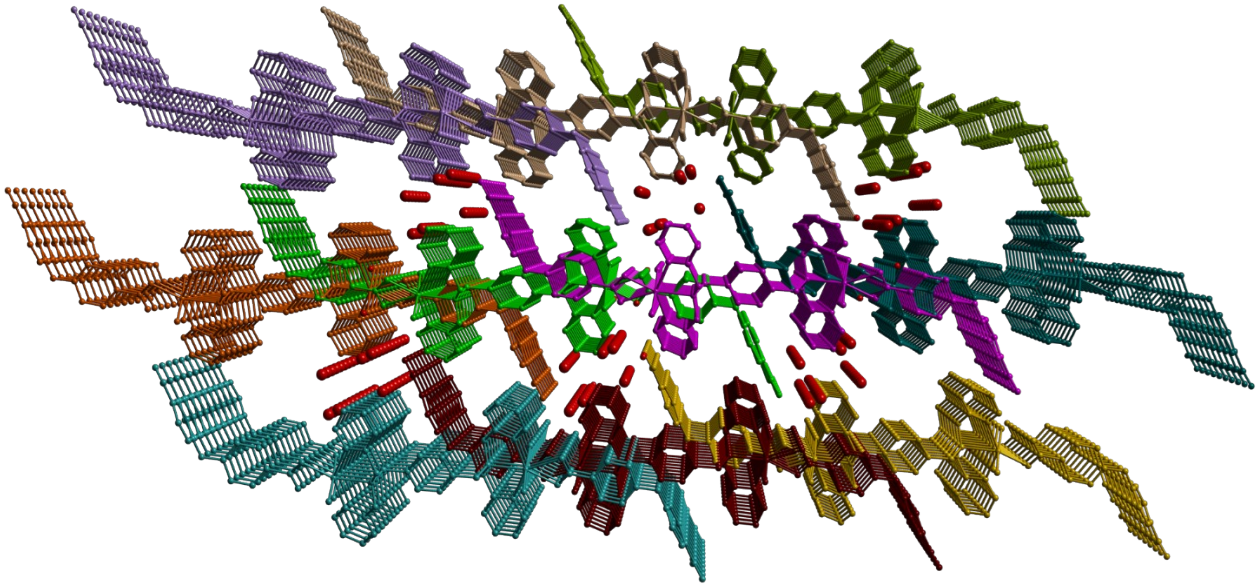

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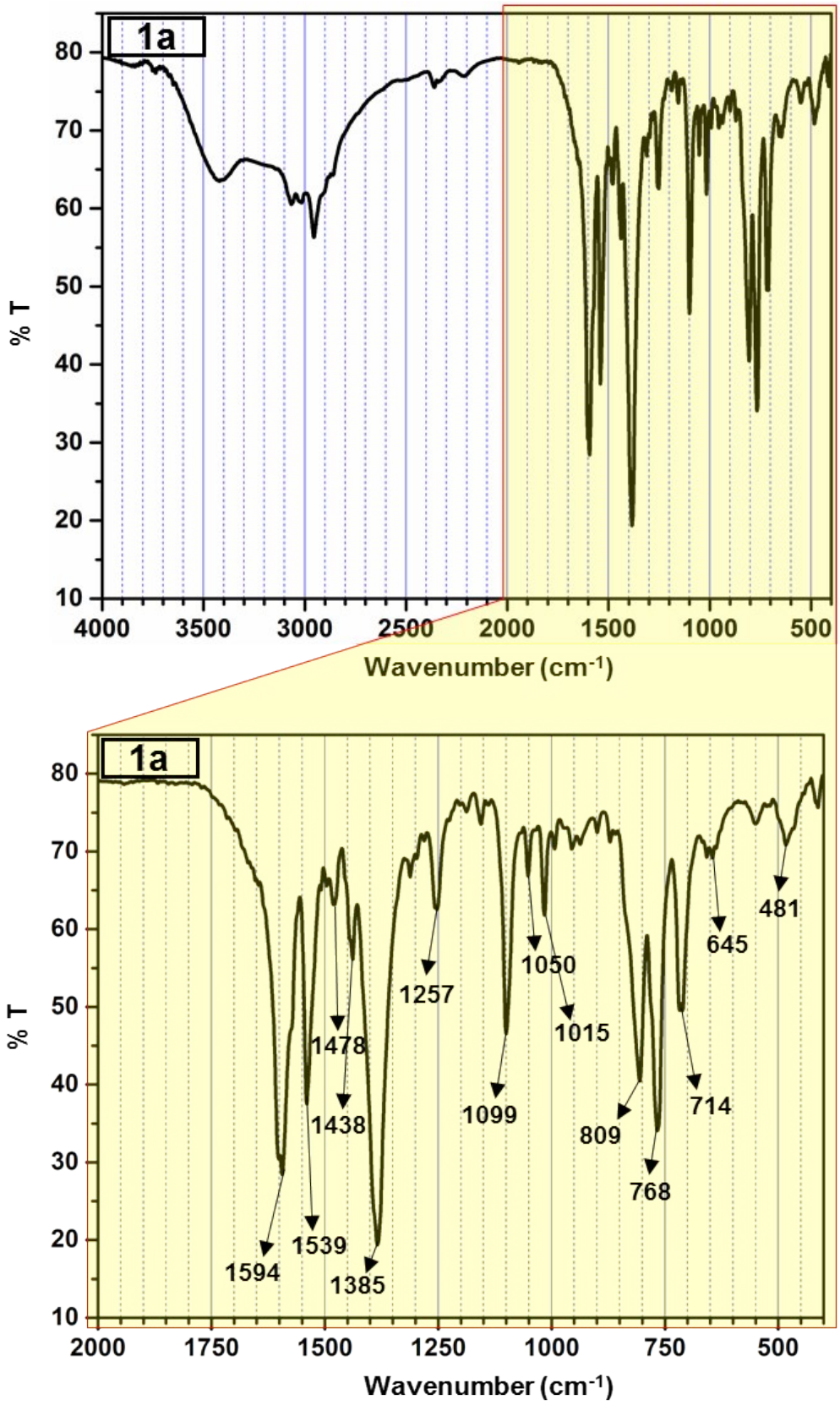
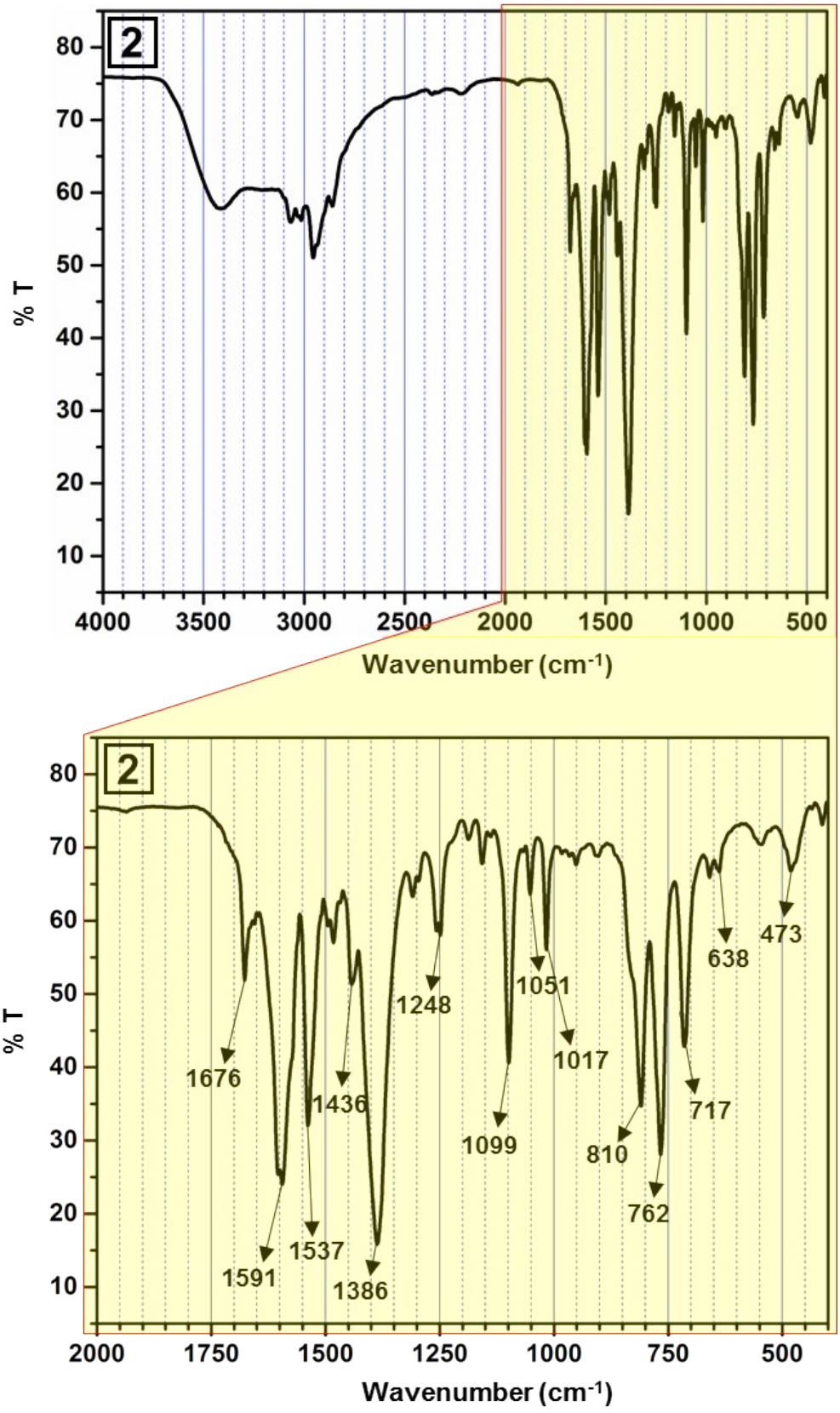


Fig. S11 FTIR spectrum of **1a**.



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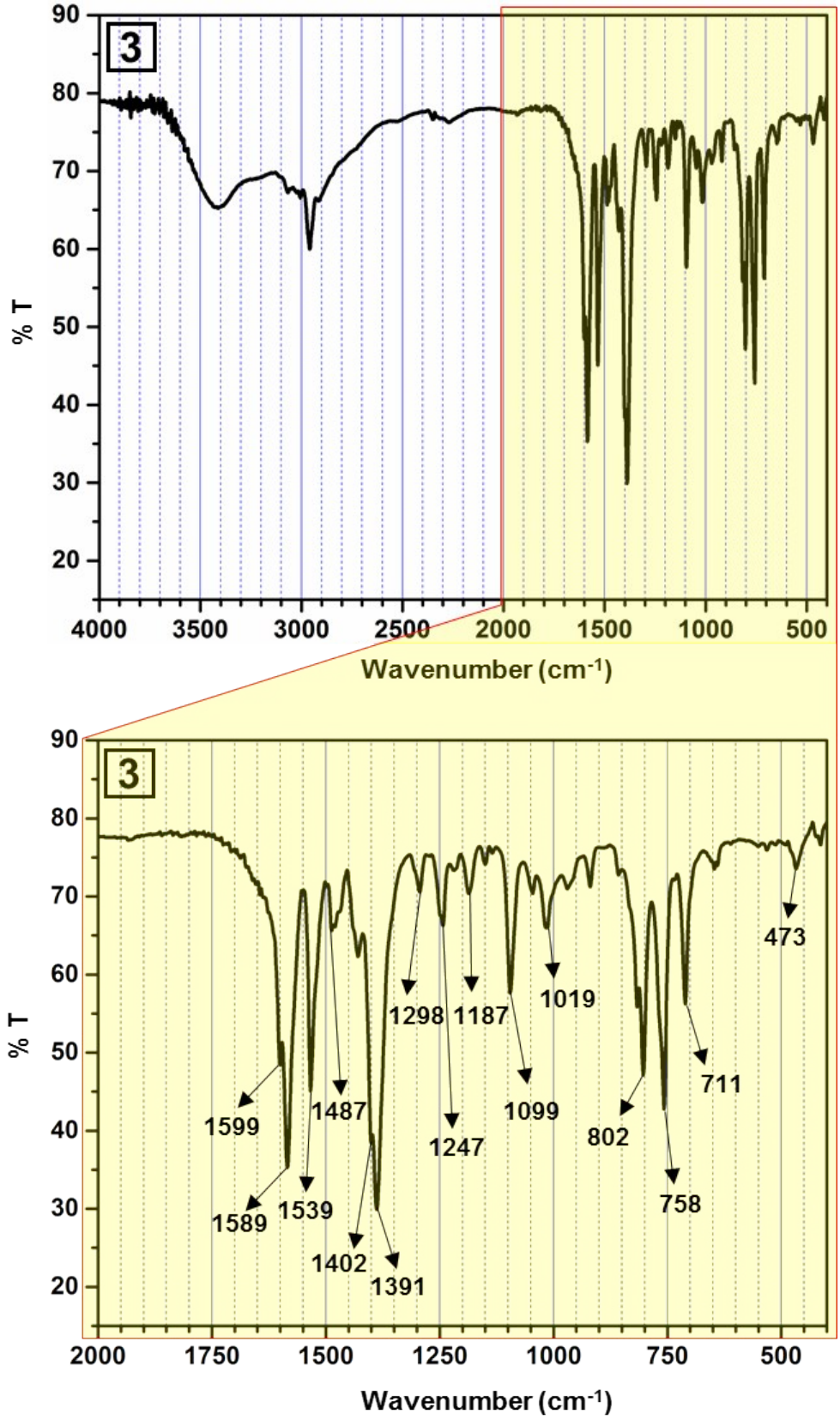

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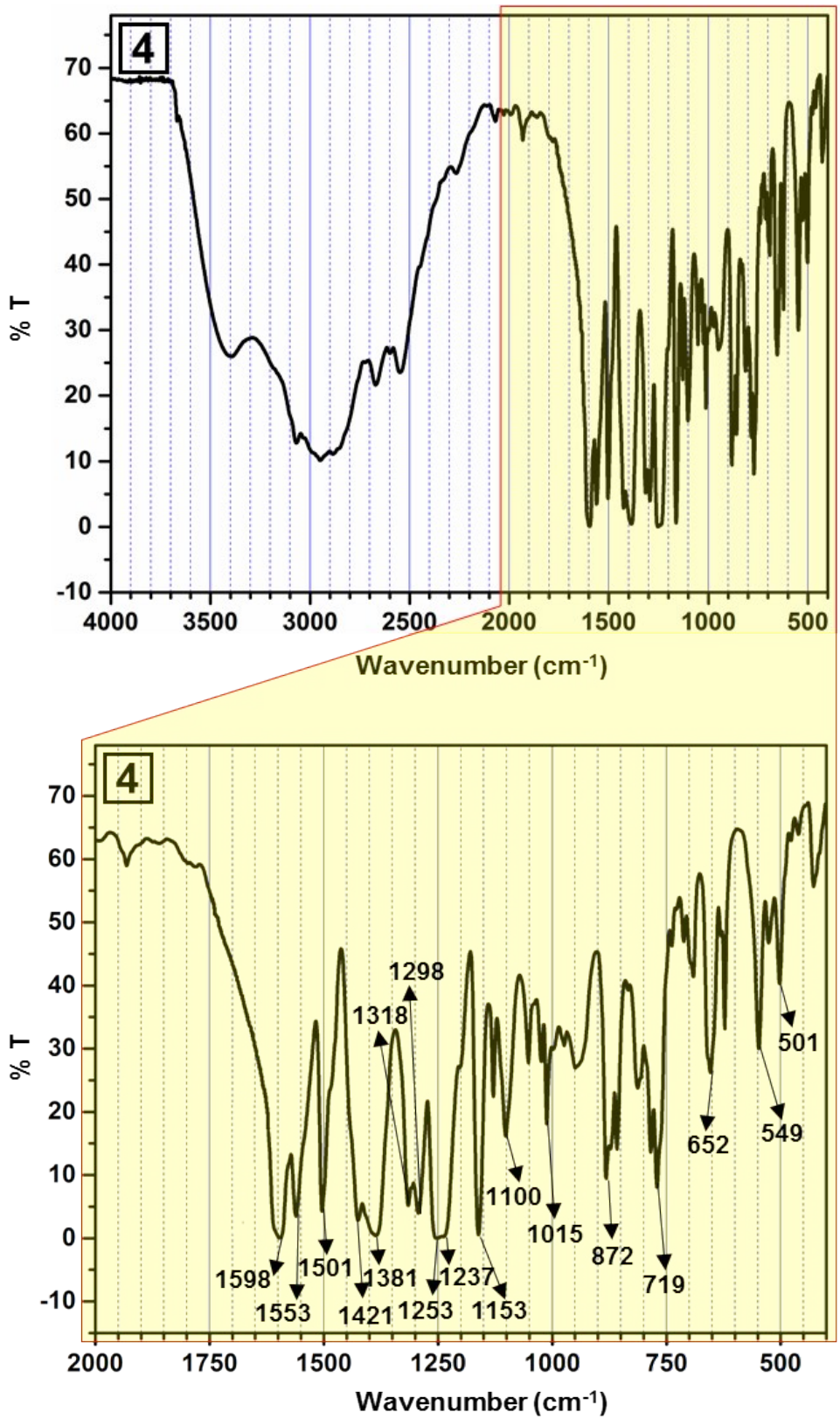

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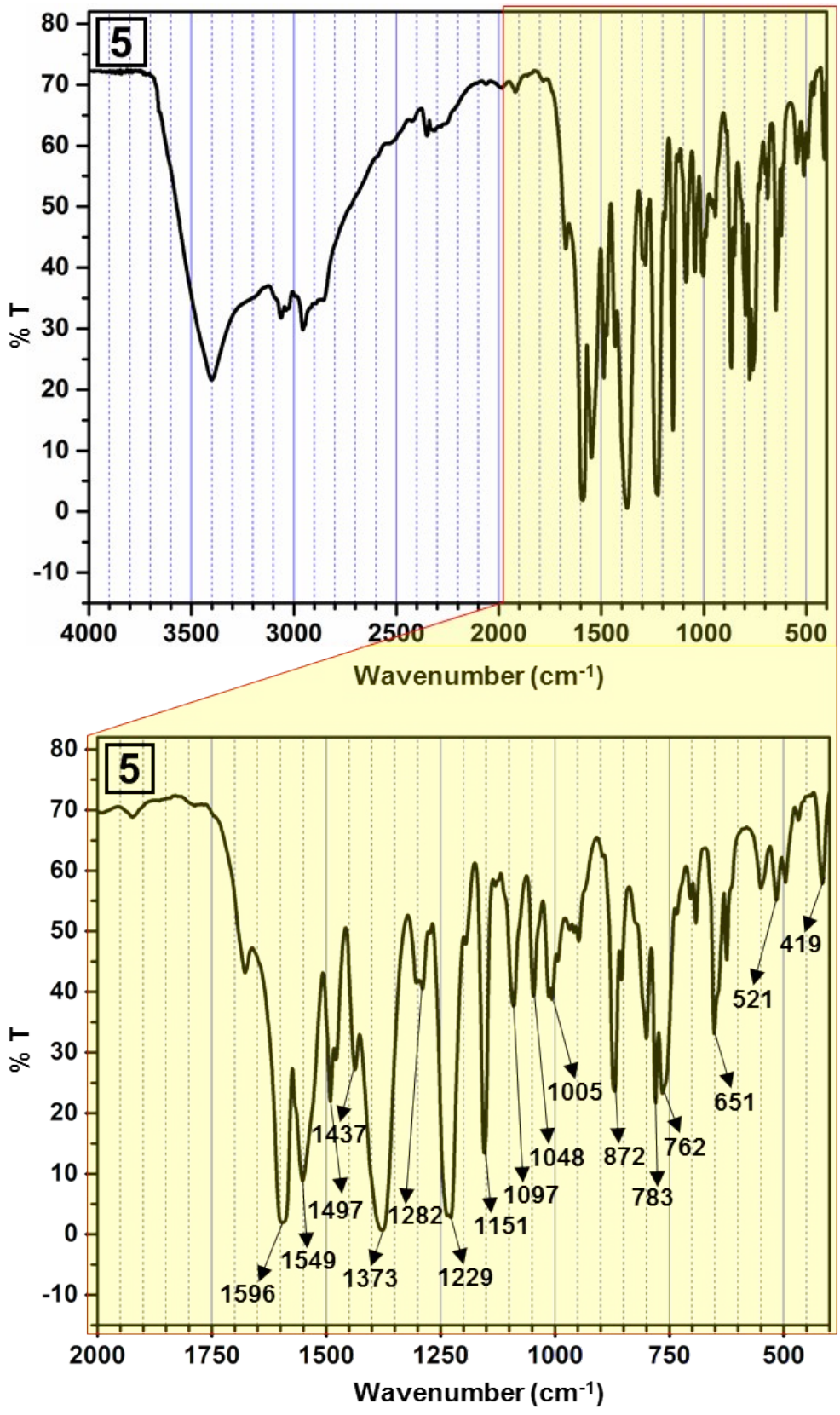

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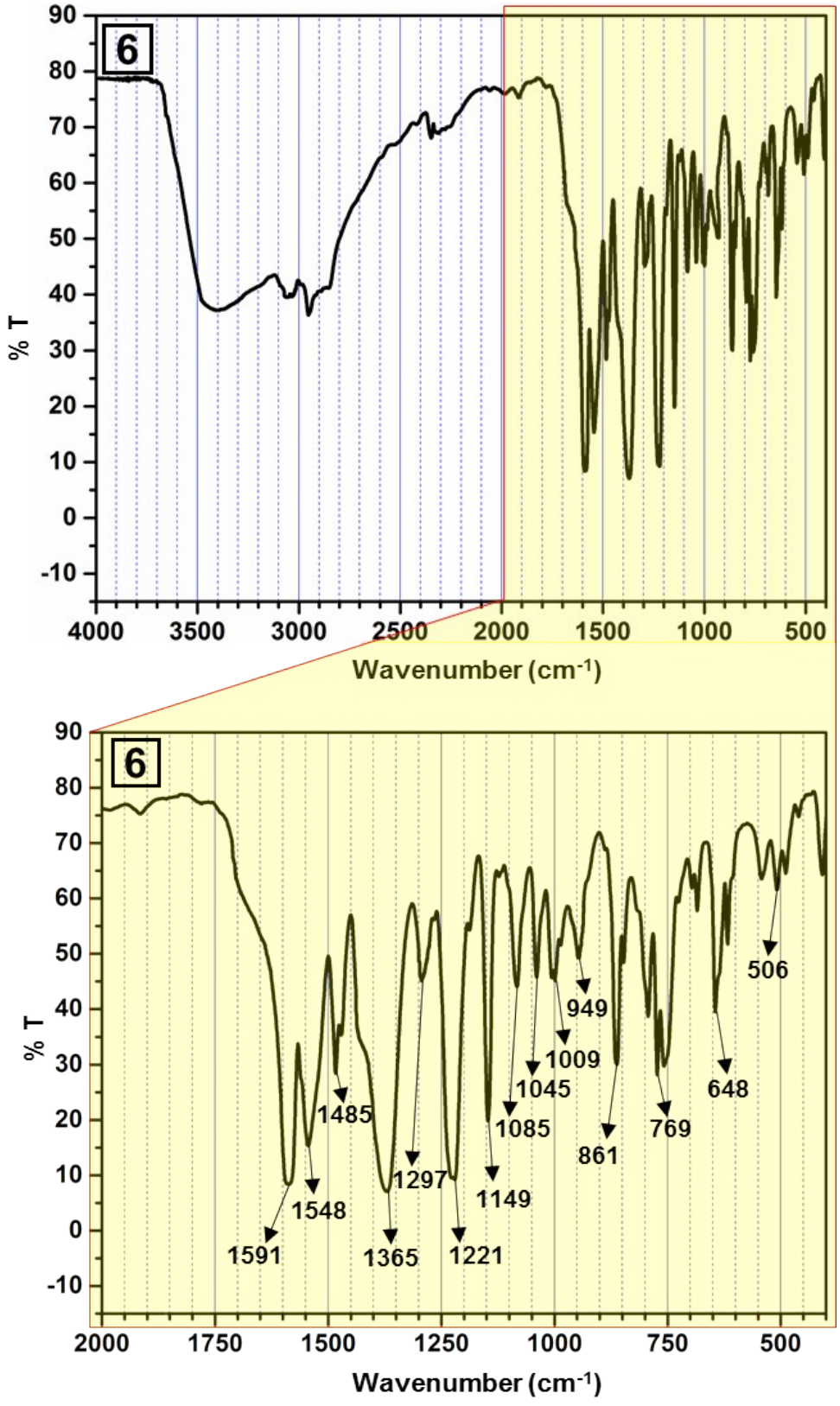

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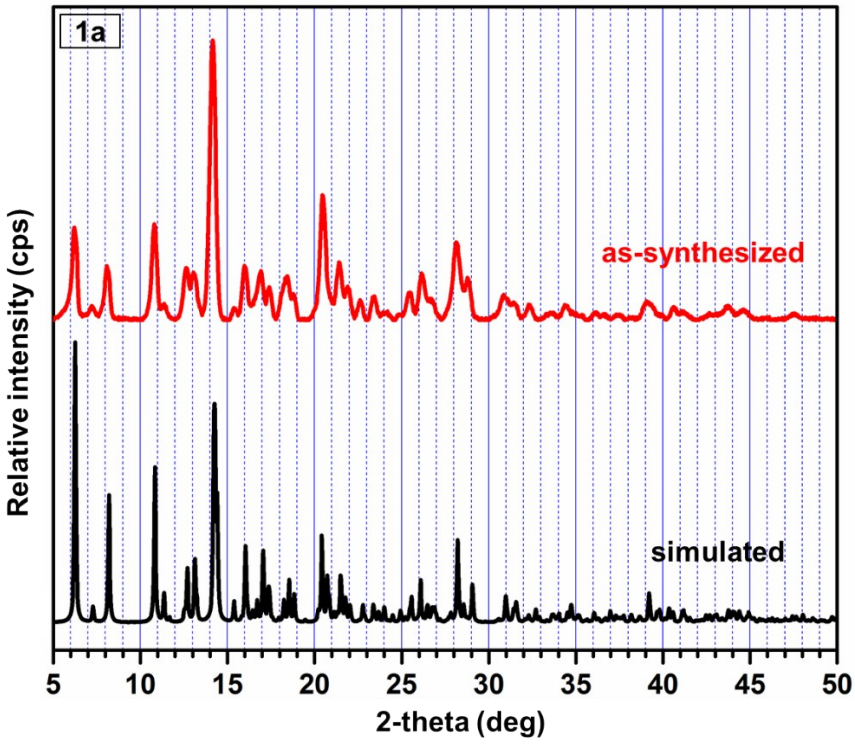
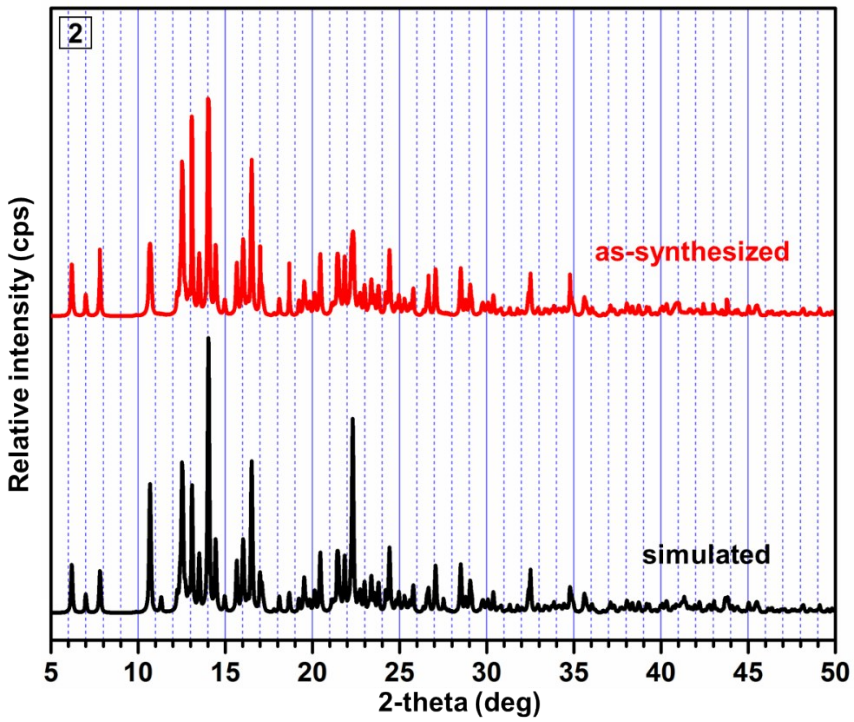


Fig. S17 PXRD patterns of the as synthesized **1a** compared with the simulated powder patterns obtained from single crystal structures.



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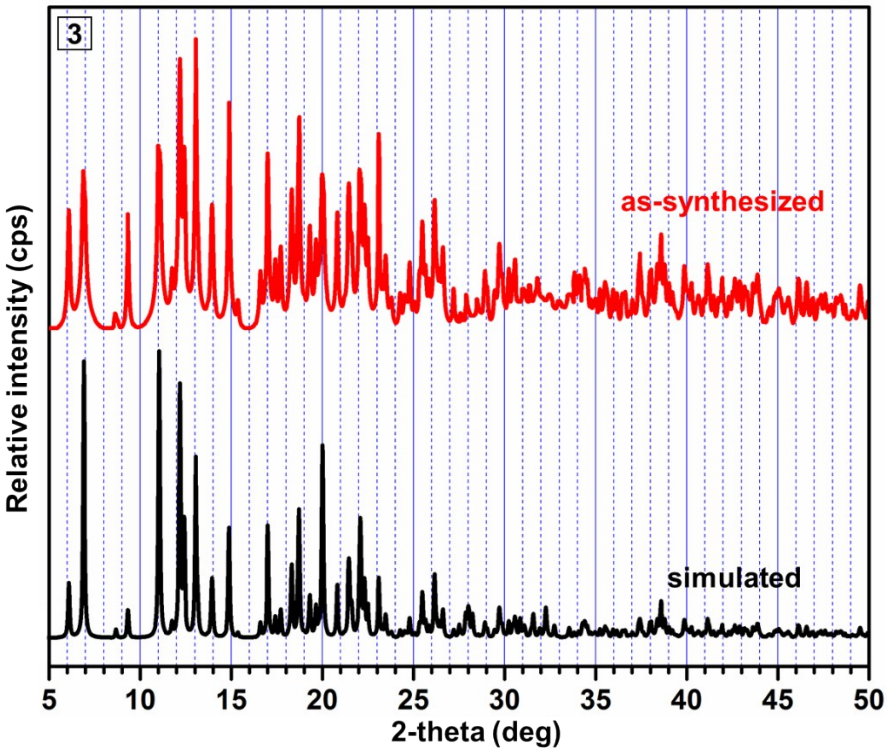

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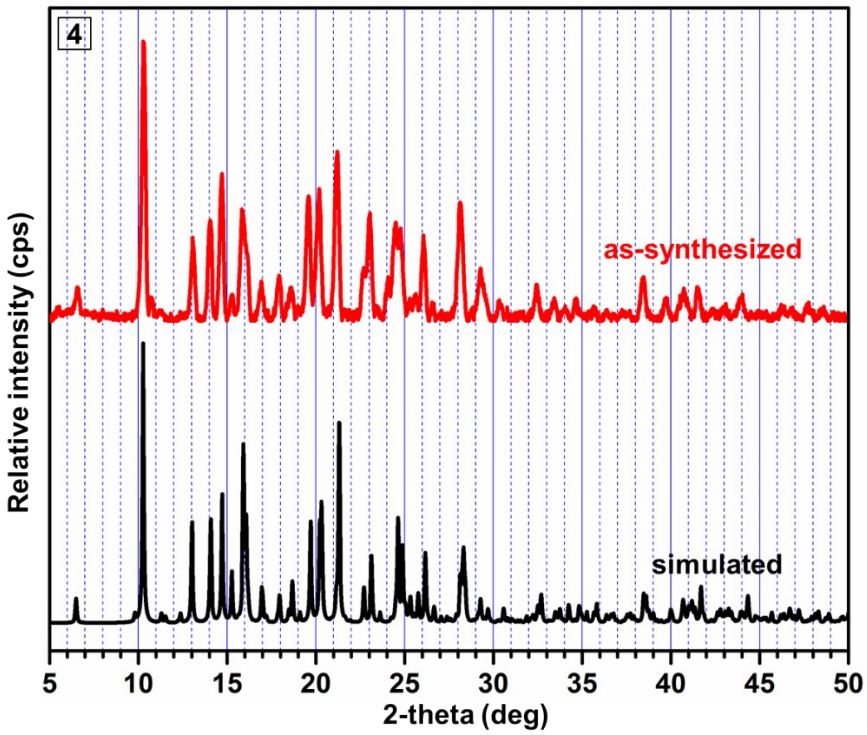

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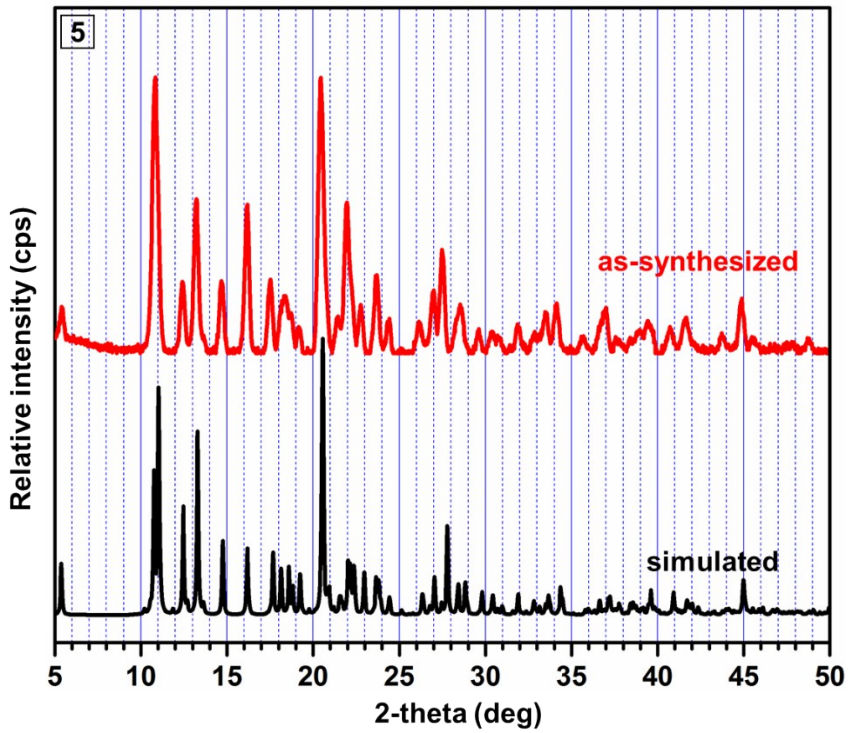

Fig. S21 PXRD patterns of the as synthesized **5** compared with the simulated powder patterns obtained from single crystal structures.

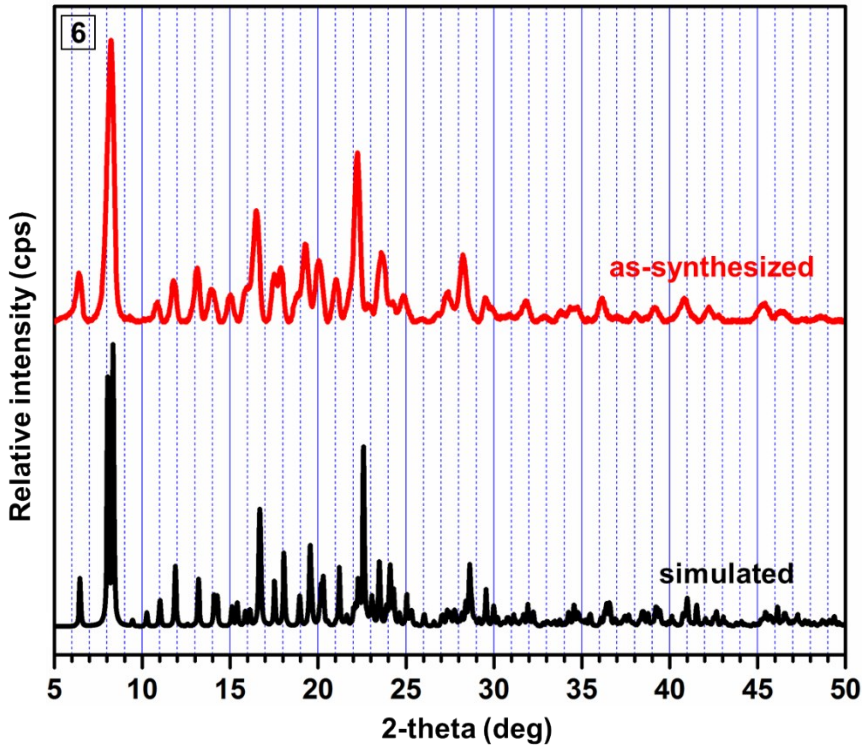

Fig. 22 PXRD patterns of the as synthesized **6** compared with the simulated powder patterns obtained from single crystal structures.

Section-S5

Table S1 Selected bond lengths (Å) and bond angles (degree) in **1-6**.

1							
Mn1	O1	2.109(8)		Mn1	O3	2.116(8)	
Mn1	O5	2.193(9)		Mn1	N1	2.259(9)	
Mn1	N2	2.361(9)		Mn1	N3	2.195(11)	
O1	Mn1	O3	103.8(4)	O1	Mn1	O5	94.5(3)
O1	Mn1	N1	90.6(4)	O1	Mn1	N2	154.0(3)
O1	Mn1	N3	89.0(3)	O3	Mn1	O5	86.2(3)
O3	Mn1	N1	165.5(3)	O3	Mn1	N2	95.6(4)
O3	Mn1	N3	84.6(3)	O5	Mn1	N1	90.8(3)
O5	Mn1	N2	104.1(3)	O5	Mn1	N3	170.7(3)
N1	Mn1	N2	71.4(4)	N3	Mn1	N1	97.7(3)
N3	Mn1	N2	75.5(3)				
Symmetry codes: (#1) +x,+y,1+z; (#2) +x,+y,-1+z; (#3) -x,-y,-z							
1a							
Mn1	O1		2.1222(17)	Mn1	O4(#1)		2.1355(16)
Mn1	O5		2.2425(17)	Mn1	N1		2.289(2)
Mn1	N2		2.358(2)	Mn1	N3		2.3026(19)
O1	Mn1	O4(#1)	98.46(7)	O1	Mn1	O5	95.43(7)
O1	Mn1	N1	95.98(7)	O1	Mn1	N2	159.21(7)
O1	Mn1	N3	91.92(7)	O41	Mn1	O5	87.37(6)
O41	Mn1	N1	163.74(6)	O41	Mn1	N2	95.73(7)
O41	Mn1	N3	81.82(7)	O5	Mn1	N1	83.87(7)
O5	Mn1	N2	100.34(7)	O5	Mn1	N3	167.73(6)
N1	Mn1	N2	72.52(7)	N1	Mn1	N3	105.16(7)
N3	Mn1	N2	75.12(7)				
Symmetry codes: (#1) -x,1-y,1-z;							
2							
Mn1	O1		2.124(3)	Mn1	O3(#1)		2.144(2)
Mn1	O5		2.227(3)	Mn1	N1		2.271(4)
Mn1	N2		2.404(4)	Mn1	N3		2.257(3)
O1	Mn1	O3(#)1	106.99(10)	O1	Mn1	O5	87.88(11)
O1	Mn1	N1	158.68(12)	O1	Mn1	N2	91.35(17)
O1	Mn1	N3	86.09(11)	O31	Mn1	O5	91.40(9)
O31	Mn1	N1	93.29(12)	O31	Mn1	N2	152.21(15)
O31	Mn1	N3	87.66(10)	O5	Mn1	N1	85.08(12)
O5	Mn1	N2	110.38(11)	O5	Mn1	N3	173.35(13)
N1	Mn1	N2	72.44(18)	N3	Mn1	N1	101.54(12)
N3	Mn1	N2	72.62(12)				
Symmetry codes: (#1) +x,+y,1+z;							

Table S1 Continued:

3							
Mn1	O1		2.182(4)	Mn1	O3(#1)		2.179(3)
Mn1	O4(#1)		2.408(4)	Mn1	N1		2.236(3)
Mn1	N2		2.430(3)	Mn1	N3		2.221(3)
O1	Mn1	O4(#1)	87.34(12)	O1	Mn1	N1	93.33(13)
O1	Mn1	N2	165.98(13)	O1	Mn1	N3	116.24(15)
O31	Mn1	O1	96.19(14)	O31	Mn1	O4(#1)	57.02(12)
O31	Mn1	N1	94.27(13)	O31	Mn1	N2	85.71(11)
O31	Mn1	N3	129.57(12)	O41	Mn1	N2	105.16(11)
N1	Mn1	O4(#1)	151.11(12)	N1	Mn1	N2	72.66(11)
N3	Mn1	O4(#1)	85.57(11)	N3	Mn1	N1	119.35(12)
N3	Mn1	N2	71.86(10)				

Symmetry codes:
(#1) +x,1+y,+z;

4							
Mn1	O1		2.1659(16)	Mn1	O4		2.2693(15)
Mn1	O5		2.2692(14)	Mn1	N2		2.4352(17)
Mn1	N3		2.3121(18)	Mn1	N1		2.2611
O1	Mn1	O4	101.61(6)	O1	Mn1	O5	125.51(6)
O1	Mn1	N2	148.56(6)	O1	Mn1	N3	82.37(6)
O1	Mn1	N1	97.69(5)	O4	Mn1	N2	92.39(6)
O4	Mn1	N3	86.76(6)	O5	Mn1	O4	58.05(5)
O5	Mn1	N2	85.77(5)	O5	Mn1	N3	136.83(6)
N3	Mn1	N2	70.35(6)	N1	Mn1	O4	160.38(5)
N1	Mn1	O5	107.22(5)	N1	Mn1	N2	72.50(5)
N1	Mn1	N3	99.33(5)				

5							
Mn1	O1		2.1108(12)	Mn1	O4		2.0888(13)
Mn1	O6		2.2209(13)	Mn1	N1		2.2655(14)
Mn1	N2		2.3544(14)	Mn1	N3		2.2303(14)
O1	Mn1	O6	94.07(5)	O1	Mn1	N1	174.70(5)
O1	Mn1	N2	102.82(5)	O1	Mn1	N3	87.72(6)
O4	Mn1	O1	90.18(6)	O4	Mn1	O6	89.40(6)
O4	Mn1	N1	87.95(6)	O4	Mn1	N2	98.53(5)
O4	Mn1	N3	171.99(5)	O6	Mn1	N1	90.87(5)
O6	Mn1	N2	161.24(4)	O6	Mn1	N3	98.45(5)
N1	Mn1	N2	72.58(5)	N3	Mn1	N1	93.46(5)
N3	Mn1	N2	74.45(5)				

Table S1 Continued:

6							
Mn1	O2		2.2512(14)	Mn1	O6		2.1469(14)
Mn1	O7		2.1446(14)	Mn1	N1		2.3175(16)
Mn1	N2		2.4155(16)	Mn1	N3		2.3041(16)
O2	Mn1	N1	136.31(5)	O2	Mn1	N2	152.15(5)
O2	Mn1	N3	81.82(5)	O6	Mn1	O2	90.85(5)
O6	Mn1	N1	90.64(5)	O6	Mn1	N2	95.09(5)
O6	Mn1	N3	87.95(5)	O7	Mn1	O2	87.39(5)
O7	Mn1	O6	175.02(5)	O7	Mn1	N1	87.43(6)
O7	Mn1	N2	88.62(5)	O7	Mn1	N3	96.40(6)
N1	Mn1	N2	70.93(6)	N3	Mn1	N1	141.87(5)
N3	Mn1	N2	71.26(5)				

Table S2 Hydrogen bonding parameters in **1**-**6**.

D-H-A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°	symmetry
1					
O5 -- H5A .. O2	0.9000	1.9000	2.647(12)	140.00	.
O5 -- H5B .. O4	0.9000	1.8700	2.696(14)	152.00	.
C8 -- H8B .. O6	0.9800	2.5900	3.56(2)	169.00	x,y,1+z
C31 -- H31B .. O6	0.9800	2.3500	2.77(2)	106.00	.
1a					
O5 -- H5A .. O2	0.8700	1.9500	2.678(3)	140.00	.
O5 -- H5B .. O3	0.8700	1.8900	2.686(2)	151.00	-x,1-y,1-z
2					
O5 -- H5A .. O4	0.8700	1.8900	2.677(4)	149.00	x,y,1+z
O5 -- H5B .. O2	0.8700	1.8600	2.651(4)	150.00	.
C25 -- H25 .. O6	0.9500	2.5300	3.404(6)	152.00	-x,1-y,1-z
C33 -- H33C .. O6	0.9800	2.4200	2.804(6)	103.00	.
3					
O5 -- H5 .. O2	0.8400	2.2700	2.978(9)	142.00	.
O6 -- H6A .. O3	0.8400	2.1300	2.938(7)	161.00	.
5					
O6 -- H6A .. O5	0.83(3)	1.91(3)	2.722(2)	167(3)	.
O6 -- H6B .. O2	0.89(3)	1.84(3)	2.688(2)	160(3)	.
6					
O6 -- H6A .. O9	0.820(19)	1.894(19)	2.708(2)	171(2)	-1+x,y,z
O6 -- H6B .. O1	0.824(19)	1.935(19)	2.753(2)	171.9(19)	-x,-y,1-z
O7 -- H7A .. O2	0.78(3)	1.96(3)	2.738(2)	177(3)	1-x,-y,1-z
O7 -- H7B .. O4	0.89(4)	1.75(4)	2.635(2)	175(3)	x,y,-1+z
O8 -- H8A .. O1	0.87(2)	1.98(2)	2.851(2)	172.4(18)	1-x,-y,1-z
O8 -- H8B .. O4	0.88(2)	1.91(2)	2.772(2)	166(2)	1-x,-y,2-z
O9 -- H9A .. O10	0.87(2)	1.97(3)	2.806(3)	160(2)	2-x,1-y,1-z
O9 -- H9B .. O8	0.88(2)	1.89(2)	2.739(3)	163(2)	.
O10 -- H10B .. O5	0.88(3)	2.00(3)	2.826(3)	157(3)	x,1+y,-1+z