Supplementary Materials: Manganese Fluorene Phosphonates: Formation of Isolated [MnP_2] Chains

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Summary

I. Pattern matching

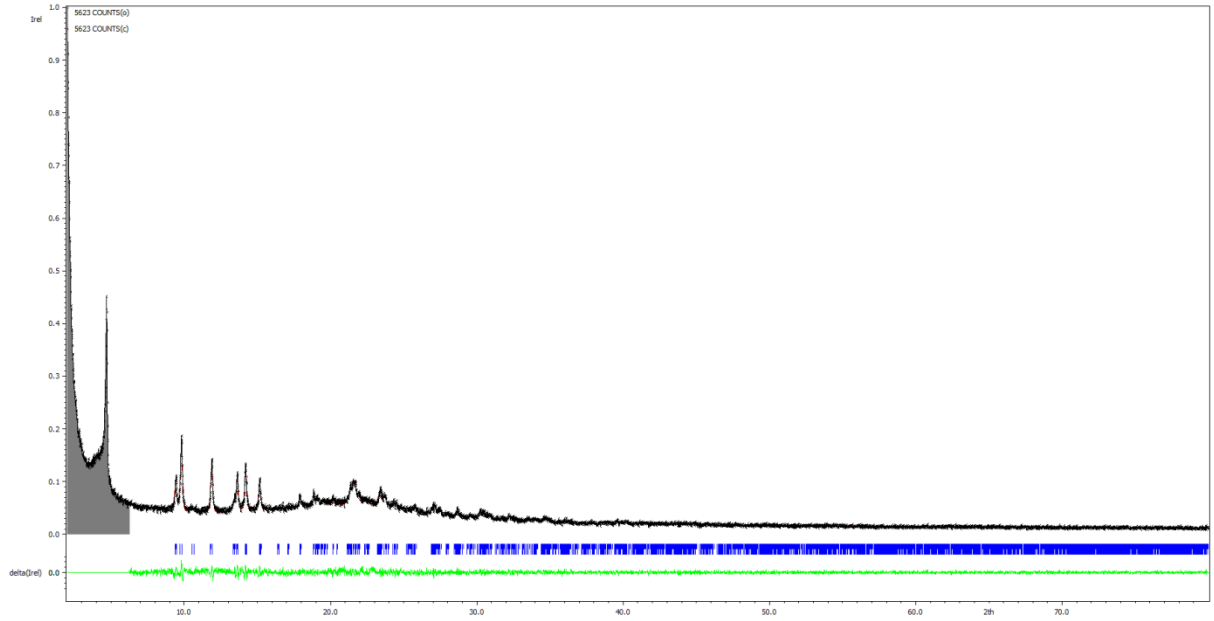

Figure S1. X-ray diffraction data recorded on powder from $Mn(H_2O)_2[O_2(OH)PC_{15}H_{13}]_2{\cdot}2H_2O$ which correspond to the data recorded on single x-ray diffraction. The vertical dashes correspond to the calculated position of the peaks, the bottom line to the difference between experimental and calculated pattern.

II. Thermogravimetric analysis

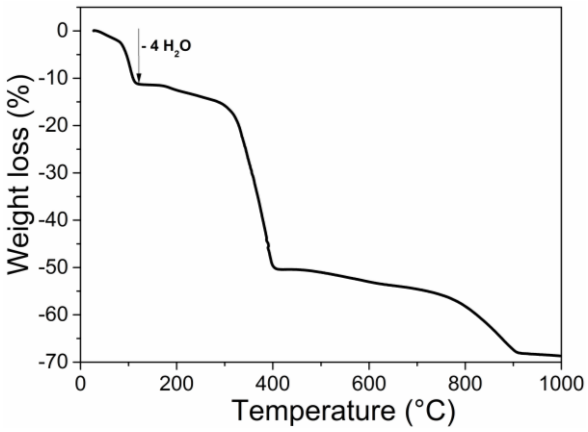

Figure S2. Thermogravimetric analysis curves of $Mn(H_2O)_2[O_2(OH)PC_{15}H_{13}]_2 \cdot 2H_2O$ recorded under air atmosphere from room temperature to 1000 °C.

III. Single cristal X-Ray diffraction

(1) .Atomic coordinates and thermal parameters

Table S1. Atomic coordinates and thermal parameters of $Mn(H_2O)_2[O_2(OH)PC_{15}H_{13}]_2{\cdot}2H_2O$.

		x/a	y/b	z/c	U_{iso}	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mn1	Mn	0.24701(3)	−0.00559(2)	0.85015(3)		0.02088(12)	0.02844(14)	0.03908(16)	0.00043(9)	−0.00319(10)	−0.00286(10)
P1	P	0.52758(4)	0.04830(2)	0.92399(5)		0.01731(18)	0.0279(2)	0.0385(2)	0.00122(14)	−0.00394(15)	0.00370(16)
P2	P	0.02810(4)	0.05292(2)	1.01820(5)		0.01739(18)	0.02465(19)	0.0446(3)	0.00211(14)	−0.00283(16)	−0.00518(16)
O1	O	0.45104(13)	0.02003(3)	0.83801(15)		0.0245(5)	0.0307(6)	0.0420(7)	−0.0010(5)	−0.0013(5)	−0.0003(5)
H2A	H	0.3541(13)	0.0537(7)	1.046(3)	0.0490						
O4	O	0.17589(13)	0.03956(4)	0.98448(17)		0.0190(5)	0.0318(6)	0.0609(9)	0.0040(5)	−0.0027(5)	−0.0119(6)
O7	O	0.1544(2)	0.02591(6)	0.6673(2)		0.0593(11)	0.0735(13)	0.0614(11)	−0.0075(9)	−0.0210(9)	0.0196(9)
O8	O	0.3358(2)	−0.04673(6)	0.6999(2)		0.0634(12)	0.0708(13)	0.0747(13)	0.0136(10)	−0.0041(10)	−0.0357(10)
O2	O	0.44092(14)	0.05750(4)	1.06601(15)		0.0244(6)	0.0418(7)	0.0405(7)	0.0023(5)	−0.0034(5)	−0.0020(5)
O3	O	0.67754(13)	0.03972(4)	0.97156(16)		0.0174(5)	0.0401(7)	0.0501(8)	0.0015(5)	−0.0040(5)	0.0100(6)
O6	O	−0.04895(13)	0.03415(3)	1.13875(15)		0.0249(6)	0.0288(6)	0.0479(7)	−0.0017(5)	−0.0054(5)	0.0000(5)
O5	O	−0.06152(14)	0.04972(4)	0.87304(16)		0.0252(6)	0.0441(7)	0.0435(8)	0.0005(5)	−0.0029(5)	−0.0064(6)
H5A	H	−0.144(2)	0.0446(12)	0.904(5)	0.122(16)						
C1	C	0.52914(18)	0.08871(5)	0.8182(2)		0.0268(7)	0.0296(8)	0.0409(9)	−0.0005(6)	−0.0063(7)	0.0043(7)
C2	C	0.6153(2)	0.11766(6)	0.8581(2)		0.0459(11)	0.0393(10)	0.0472(11)	−0.0105(9)	−0.0213(9)	0.0069(8)
H21	H	0.68090	0.11510	0.93570	0.0530						
C3	C	0.6057(3)	0.15018(6)	0.7849(2)		0.0524(12)	0.0361(10)	0.0492(12)	−0.0143(9)	−0.0202(9)	0.0057(8)
H20	H	0.66330	0.16990	0.81280	0.0550						
C4	C	0.5106(2)	0.15325(5)	0.6708(2)		0.0353(9)	0.0294(8)	0.0351(9)	−0.0018(7)	−0.0036(7)	0.0016(7)
C5	C	0.4752(2)	0.18387(5)	0.5773(2)		0.0367(9)	0.0314(8)	0.0343(9)	0.0039(7)	0.0013(7)	0.0015(7)
C6	C	0.5264(2)	0.21888(5)	0.5768(2)		0.0484(11)	0.0321(9)	0.0451(11)	−0.0006(8)	0.0045(9)	0.0014(8)
H28	H	0.59570	0.22650	0.64520	0.0500						
C7	C	0.4731(3)	0.24243(6)	0.4728(3)		0.0510(12)	0.0349(10)	0.0576(13)	0.0046(9)	0.0148(10)	0.0095(9)
H27	H	0.50570	0.26650	0.47090	0.0570						
C8	C	0.3735(3)	0.23123(6)	0.3726(3)		0.0524(13)	0.0465(12)	0.0521(13)	0.0141(10)	0.0068(10)	0.0185(10)
H26	H	0.33970	0.24770	0.30210	0.0600						
C9	C	0.3217(3)	0.19638(6)	0.3728(3)		0.0462(12)	0.0501(12)	0.0476(12)	0.0097(10)	−0.0075(9)	0.0108(9)
H25	H	0.25260	0.18900	0.30390	0.0580						
C10	C	0.3733(2)	0.17254(5)	0.4762(2)		0.0349(9)	0.0358(9)	0.0376(9)	0.0069(7)	−0.0024(7)	0.0034(7)
C11	C	0.3364(2)	0.13327(5)	0.4975(2)		0.0340(9)	0.0354(9)	0.0413(10)	0.0034(7)	−0.0113(7)	0.0012(7)
C12	C	0.42811(18)	0.12396(5)	0.6276(2)		0.0263(7)	0.0318(8)	0.0360(9)	0.0023(6)	−0.0060(6)	0.0011(7)
C13	C	0.43609(18)	0.09173(5)	0.7015(2)		0.0254(7)	0.0296(8)	0.0427(10)	−0.0010(6)	−0.0073(7)	−0.0008(7)
H17	H	0.37890	0.07200	0.67300	0.0390						
C14	C	0.03558(17)	0.10005(4)	1.0560(2)		0.0231(7)	0.0256(7)	0.0408(9)	0.0014(6)	0.0010(6)	−0.0036(6)
C15	C	0.1387(2)	0.12164(5)	0.9901(2)		0.0318(9)	0.0334(9)	0.0478(11)	0.0015(7)	0.0117(8)	−0.0024(8)
H6	H	0.20920	0.11100	0.93020	0.0450						
C16	C	0.1391(2)	0.15853(5)	1.0115(2)		0.0384(10)	0.0326(9)	0.0540(12)	−0.0040(7)	0.0157(9)	0.0021(8)
H5	H	0.20940	0.17310	0.96670	0.0500						
C17	C	0.0359(2)	0.17368(5)	1.0986(2)		0.0329(8)	0.0260(7)	0.0404(9)	0.0001(6)	0.0010(7)	−0.0003(7)
C18	C	0.0127(2)	0.21101(5)	1.1433(2)		0.0380(9)	0.0264(8)	0.0455(10)	0.0026(7)	−0.0049(8)	0.0000(7)
C19	C	0.0872(3)	0.24189(6)	1.1098(3)		0.0514(12)	0.0312(9)	0.0678(15)	−0.0056(9)	−0.0037(11)	0.0057(9)
H13	H	0.16590	0.24120	1.04520	0.0600						
C20	C	0.0446(3)	0.27395(6)	1.1723(3)		0.0678(17)	0.0271(9)	0.0864(19)	−0.001(1)	−0.0216(14)	0.0010(11)
H12	H	0.09490	0.29540	1.15050	0.0730						
C21	C	−0.0702(3)	0.27508(6)	1.2659(3)		0.0686(16)	0.0308(10)	0.0824(19)	0.0126(10)	−0.0202(14)	−0.0135(11)
H11	H	−0.09720	0.29720	1.30860	0.0730						
C22	C	−0.1461(3)	0.24439(6)	1.2982(3)		0.0495(12)	0.0404(11)	0.0653(15)	0.0142(10)	−0.0070(11)	−0.0136(10)
H10	H	−0.22550	0.24540	1.36170	0.0620						
C23	C	−0.1046(2)	0.21205(5)	1.2364(2)		0.0361(9)	0.0304(8)	0.0454(10)	0.0070(7)	−0.0072(8)	−0.0057(7)
C24	C	−0.17048(19)	0.17523(5)	1.2533(2)		0.0294(8)	0.0323(8)	0.0446(10)	0.0059(7)	0.0037(7)	−0.0043(7)
C25	C	−0.06868(18)	0.15239(5)	1.1647(2)		0.0243(7)	0.0282(8)	0.0378(9)	0.0031(6)	0.0021(6)	−0.0024(6)
C26	C	−0.06852(18)	0.11567(5)	1.1440(2)		0.0223(7)	0.0280(8)	0.0449(10)	0.0001(6)	0.0044(6)	−0.0011(7)
H2	H	−0.13870	0.10120	1.18920	0.0380						
C111	C	0.3800(3)	0.11099(7)	0.3644(3)		0.0822(19)	0.0482(13)	0.0456(12)	0.0081(12)	−0.0136(12)	−0.0082(10)
H29A	H	0.32890	0.11970	0.27890	0.0880						
H29B	H	0.35590	0.08580	0.38090	0.0880						
H29C	H	0.48280	0.11320	0.34870	0.0880						
C112	C	0.1786(2)	0.12727(7)	0.5288(4)		0.0315(10)	0.0553(14)	0.092(2)	0.0022(10)	−0.0182(11)	0.0146(13)
H30A	H	0.14960	0.14210	0.61110	0.0900						
H30B	H	0.16240	0.10200	0.55200	0.0900						
H30C	H	0.12240	0.13380	0.44340	0.0900						
C241	C	−0.3202(2)	0.17486(7)	1.1849(3)		0.0302(9)	0.0523(12)	0.0692(15)	0.0075(9)	−0.0024(9)	−0.0114(11)
H14A	H	−0.38270	0.19120	1.23850	0.0760						
H14B	H	−0.35920	0.15050	1.18900	0.0760						
H14C	H	−0.31390	0.18260	1.08380	0.0760						
C242	C	−0.1787(3)	0.16320(7)	1.4118(3)		0.0569(14)	0.0548(13)	0.0482(12)	0.0178(11)	0.0106(10)	0.0004(10)
H15A	H	−0.08270	0.16280	1.45340	0.0800						
H15B	H	−0.22030	0.13920	1.41670	0.0800						
H15C	H	−0.23830	0.18000	1.46640	0.0800						

(2) .Bond Valence Sum

Table S2. Bond valence sum of $Mn(H_2O)_2[O_2(OH)PC_{15}H_{13}]_2{\cdot}2H_2O$.

Valence Bond	Mn1	P1	P2	H_w(x 2)	H8	H5A	BVS
O1	0.384	1.358					**1.742**
O2		1.099					
O3	0.331	1.339					**1.670**
O4	0.332		1.349				**1.681**
O5			1.084				
O6	0.383		1.364				**1.747**
O7	0.302			0.813			**1.928**
O8	0.306			0.813			**1.932**
C14			1.224				
C1		1.212					
BVS	**2.038**	**5.008**	**5.021**				
*** The O···H distance used in the calculation for the water molecules is equal to 0.9584 Å.**							

(3) Interatomic distances

Table S3. Interatomic distances of $Mn(H_2O)_2[O_2(OH)PC_{15}H_{13}]_2 \cdot 2H_2O$.

$Mn(H_2O)_2[O_2(OH)PC_{15}H_{13}]_2.2H_2O$									
Atoms 1,2	**d1,2 [Å]**	**Atoms 1,2**	**d1,2 [Å]**	**Atoms 1,2**	**d1,2 [Å]**	**Atoms 1,2**	**d1,2 [Å]**	**Atoms 1,2**	**d1,2 [Å]**
Mn1—O1	2.1441(12)	C1—C13	1.392(2)	C10—C11	1.519(3)	C20—C21	1.382(4)	C241—H14A	0.9800
Mn1—O6^{i}	2.1461(13)	C1—C2	1.400(3)	C11—C12	1.519(2)	C20—H12	0.9500	C241—H14B	0.9800
Mn1—O4	2.1972(13)	C2—C3	1.393(3)	C11—C112	1.526(3)	C21—C22	1.382(4)	C241—H14C	0.9800
Mn1—O3^{ii}	2.2000(13)	C2—H21	0.9500	C11—C111	1.540(3)	C21—H11	0.9500	C242—H15A	0.9800
Mn1—O8	2.2319(18)	C3—C4	1.387(3)	C12—C13	1.386(3)	C22—C23	1.391(3)	C242—H15B	0.9800
Mn1—O7	2.2347(18)	C3—H20	0.9500	C13—H17	0.9500	C22—H10	0.9500	C242—H15C	0.9800
P1—O1	1.5038(14)	C4—C12	1.398(3)	C14—C26	1.399(2)	C23—C24	1.516(3)	(i) -x, -y, 2-z; (ii) 1-x, -y, 2-z.	
P1—O3	1.5092(12)	C4—C5	1.471(3)	C14—C15	1.399(2)	C24—C25	1.520(2)		
P1—O2	1.5817(15)	C5—C6	1.393(3)	C15—C16	1.392(3)	C24—C242	1.533(3)		
P1—C1	1.7977(18)	C5—C10	1.403(3)	C15—H6	0.9500	C24—C241	1.541(3)		
P2—O6	1.5018(14)	C6—C7	1.396(3)	C16—C17	1.381(3)	C25—C26	1.384(2)		
P2—O4	1.5072(13)	C6—H28	0.9500	C16—H5	0.9500	C26—H2	0.9500		
P2—O5	1.5879(15)	C7—C8	1.380(4)	C17—C25	1.404(2)	C111—H29A	0.9800		
P2—C14	1.7954(17)	C7—H27	0.9500	C17—C18	1.470(2)	C111—H29B	0.9800		
O2—H2A	0.847(10)	C8—C9	1.389(4)	C18—C19	1.383(3)	C111—H29C	0.9800		
O3—Mn1^{ii}	2.2001(13)	C8—H26	0.9500	C18—C23	1.398(3)	C112—H30A	0.9800		
O6—Mn1^{i}	2.1461(12)	C9—C10	1.393(3)	C19—C20	1.388(3)	C112—H30B	0.9800		
O5—H5A	0.849(10)	C9—H25	0.9500	C19—H13	0.9500	C112—H30C	0.9800		

IV Fingerprint plots of $Mn(H_2O)_2[O_2(OH)PC_{15}H_{13}]_2 \cdot 2H_2O$

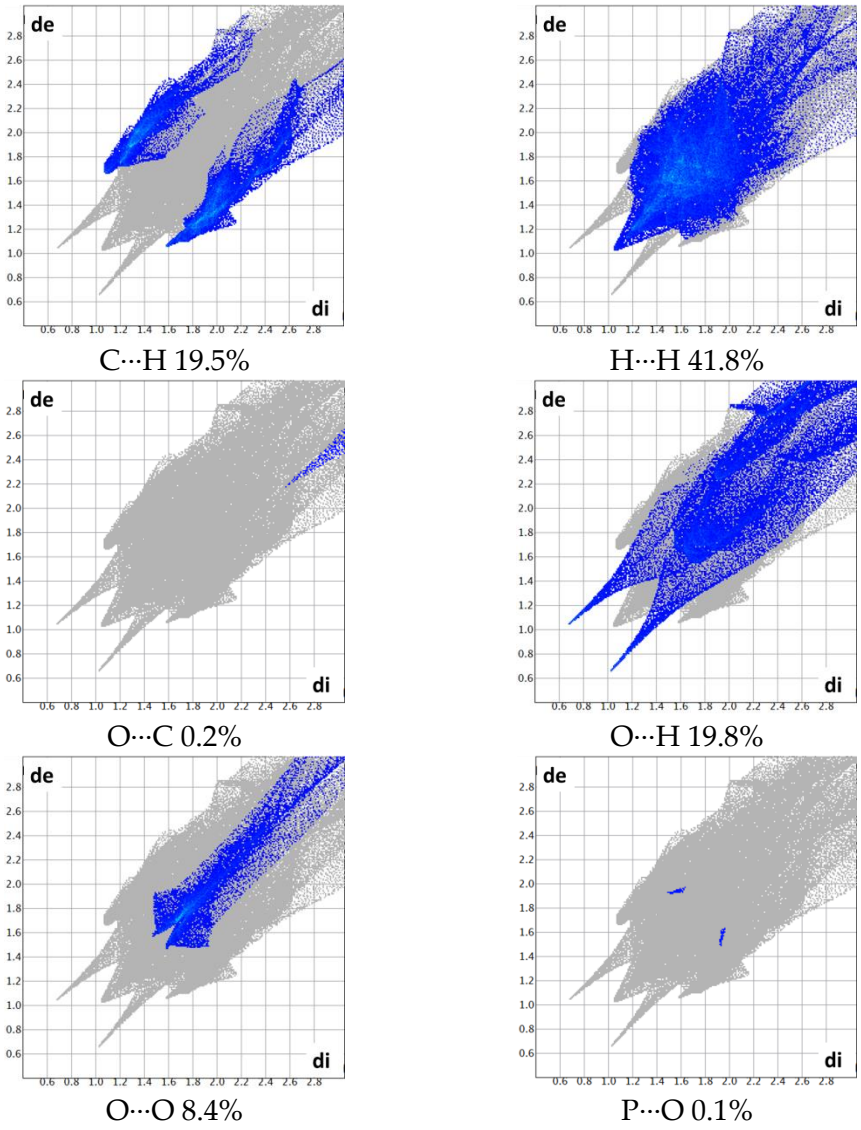

Figure S3. Fingerprint plots of $Mn(H_2O)_2[O_2(OH)PC_{15}H_{13}]_2 \cdot 2H_2O$ highlighting the different intermolecular interactions with their percentage of contribution on the orientation I of the organic sub-network. Manganese atoms and water molecules are not taken in account in the calculations. Pictures generated with CrystalExplorer software [1].

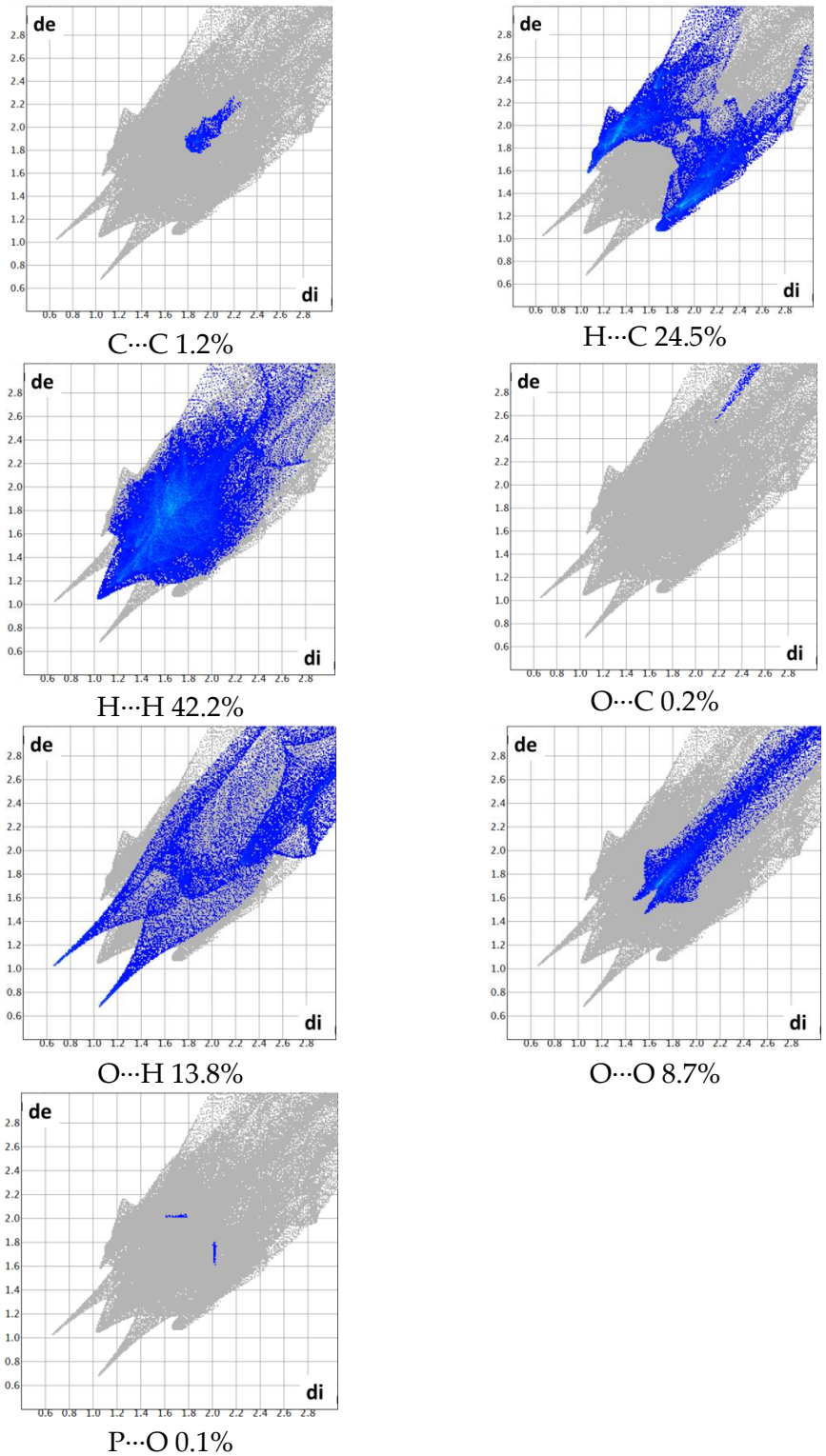

Figure S4. Fingerprint plots of $Mn(H_2O)_2[O_2(OH)PC_{15}H_{13}]_2{\cdot}2H_2O$ highlighting the different intermolecular interactions with their percentage of contribution on the orientation II of the organic sub-network. Manganese atoms and water molecules are not taken in account in the calculations. Pictures generated with CrystalExplorer software [1].

1. Wolff, S.K.; Grimwood, D.J.; McKinnon, J.J.; Turner, M.J.; Jayatilaka, D.; Spackman, M.A. *CrystalExplorer*; University of Western Australia, Crawley, WA, Australia, 2012.