Electronic Supplementary Information

Table S1. Selected bond distances (Å) and angles (°) for **1**.

Cu(1)-O(4)^{i}	1.986(3)	Cu(1)-O(3W)	1.992(3)
Cu(1)-O(1)	1.997(2)	Cu(1)-O(5W)	1.998(3)
Cu(1)-O(4W)	2.427(3)		
O(4)^{i}-Cu(1)-O(3W)	89.73(11)	O(4)^{i}-Cu(1)-O(1)	163.43(8)
O(3W)-Cu(1)-O(1)	90.66(10)	O(4)^{i}-Cu(1)-O(5W)	89.81(11)
O(3W)-Cu(1)-O(5W)	178.49(10)	O(1)-Cu(1)-O(5W)	90.19(10)
O(4)^{i}-Cu(1)-O(4W)	102.71(9)	O(3W)-Cu(1)-O(4W)	89.43(11)
O(1)-Cu(1)-O(4W)	93.86(10)	O(5W)-Cu(1)-O(4W)	89.27(11)

Symmetry codes for **1**: ^{i}x+1/2, -y+1/2, z-1/2

Table S2. Selected bond distances (Å) and angles (°) for **2**.

Ni(1)-O(5)^{i}	2.054(2)	Ni(1)-O(3W)	2.069(3)
Ni(1)-O(2)	2.076(3)	Ni(1)-O(1W)	2.077(3)
Ni(1)-O(5W)	2.082(2)	Ni(1)-O(2W)	2.166(3)
Ni(2)-O(6)^{i}	2.075(2)	Ni(2)-O(1)	2.085(3)
Ni(2)-O(8)^{ii}	2.098(2)	Ni(2)-O(4)^{iii}	2.111(2)
Ni(2)-O(4W)	2.127(3)	Ni(2)-O(5W)	2.129(2)
O(5)^{i}-Ni(1)-O(2)	98.72(11)	O(5)^{i}-Ni(1)-O(1W)	174.77(12)
O(2)-Ni(1)-O(1W)	85.43(11)	O(5)^{i}-Ni(1)-O(3W)	89.43(11)
O(2)-Ni(1)-O(3W)	89.39(11)	O(1W)-Ni(1)-O(3W)	93.81(13)
O(5)^{i}-Ni(1)-O(5W)	88.02(10)	O(2)-Ni(1)-O(5W)	95.64(10)
O(1W)-Ni(1)-O(5W)	88.41(12)	O(3W)-Ni(1)-O(5W)	174.65(12)
O(5)^{i}-Ni(1)-O(2W)	87.38(13)	O(2)-Ni(1)-O(2W)	172.62(13)
O(1W)-Ni(1)-O(2W)	88.72(13)	O(3W)-Ni(1)-O(2W)	86.51(13)
O(5W)-Ni(1)-O(2W)	88.68(12)	O(6)^{i}-Ni(2)-O(1)	92.15(10)
O(6)^{i}-Ni(2)-O(8)^{ii}	91.45(10)	O(1)-Ni(2)-O(8)^{ii}	172.77(10)

O(6)^{i}-Ni(2)-O(4)^{iii}	176.75(10)	O(1)-Ni(2)-O(4)^{iii}	85.80(10)
O(8)^{ii}-Ni(2)-O(4)^{iii}	90.32(10)	O(6)^{i}-Ni(2)-O(4W)	90.40(12)
O(1)-Ni(2)-O(4W)	88.77(11)	O(8)^{ii}-Ni(2)-O(4W)	84.93(11)
O(4)^{iii}-Ni(2)-O(4W)	87.04(12)	O(6)^{i}-Ni(2)-O(5W)	92.42(10)
O(1)-Ni(2)-O(5W)	96.86(10)	O(8)^{ii}-Ni(2)-O(5W)	89.25(10)
O(4)^{iii}-Ni(2)-O(5W)	90.33(9)	O(4W)-Ni(2)-O(5W)	173.60(12)

Symmetry codes for **2**: ^{i}x, y, z+1; ^{ii}-x+3/4, y-1/4, z+5/4; ^{iii}-x+3/4, y-1/4, z+1/4

Table S3. Selected bond distances (Å) and angles (^{o}) for **3**.

Zn(1)-O(4)	1.979(3)	Zn(1)-O(1)^{ii}	2.152(4)
Zn(1)-O(2)^{ii}	2.223(4)	Zn(2)-O(1W)^{iv}	1.970(5)
Zn(2)-O(2W')	2.032(9)	Zn(2)-O(3)	2.061(3)
Zn(2)-O(1W')	2.185(11)	Zn(2)-O(2W)	2.275(17)
O(4)-Zn(1)-O(4)^{i}	100.2(2)	O(4)^{i}-Zn(1)-O(1)^{iii}	91.02(12)
O(4)^{i}-Zn(1)-O(1)^{ii}	113.32(14)	O(1)^{ii}-Zn(1)-O(1)^{iii}	142.38(17)
O(4)-Zn(1)-O(2)^{ii}	149.51(13)	O(4)^{i}-Zn(1)-O(2)^{ii}	96.09(16)
O(1)^{ii}-Zn(1)-O(2)^{ii}	58.76(13)	O(1)^{iii}-Zn(1)-O(2)^{ii}	91.86(14)
O(2)^{ii}-Zn(1)-O(2)^{iii}	82.1(2)	O(1W)^{iv}-Zn(2)-O(1W)	127.1(5)
O(1W)^{iv}-Zn(2)-O(2W')	134.1(3)	O(1W)-Zn(2)-O(2W')	98.7(4)
O(2W')^{iv}-Zn(2)-O(2W')	35.4(5)	O(1W)^{iv}-Zn(2)-O(3)^{iv}	92.1(2)
O(1W)-Zn(2)-O(3)^{iv}	86.0(2)	O(2W')^{iv}-Zn(2)-O(3)^{iv}	93.4(3)
O(2W')-Zn(2)-O(3)^{iv}	90.7(3)	O(1W)^{iv}-Zn(2)-O(3)	86.0(2)
O(1W)-Zn(2)-O(3)	92.1(2)	O(2W')^{iv}-Zn(2)-O(3)	90.7(3)
O(2W')-Zn(2)-O(3)	93.4(3)	O(3)^{iv}-Zn(2)-O(3)	175.7(2)
O(1W)^{iv}-Zn(2)-O(1W')^{iv}	29.0(3)	O(1W)-Zn(2)-O(1W')^{iv}	98.1(4)
O(2W')^{iv}-Zn(2)-O(1W')^{iv}	127.7(4)	O(2W')-Zn(2)-O(1W')^{iv}	163.0(4)
O(3)^{iv}-Zn(2)-O(1W')^{iv}	88.7(3)	O(3)-Zn(2)-O(1W')^{iv}	87.7(3)
O(1W')^{iv}-Zn(2)-O(1W')	69.2(6)	O(1W)^{iv}-Zn(2)-O(2W)	179.0(5)
O(1W)-Zn(2)-O(2W)	53.9(5)	O(2W')^{iv}-Zn(2)-O(2W)	80.2(5)
O(2W')-Zn(2)-O(2W)	44.8(5)	O(3)^{iv}-Zn(2)-O(2W)	87.7(5)

O(3)-Zn(2)-O(2W)	94.3(5)	O(1W')^{iv}-Zn(2)-O(2W)	152.0(5)
O(1W')-Zn(2)-O(2W)	82.9(5)	O(1W)^{iv}-Zn(2)-O(2W)^{iv}	53.9(5)
O(1W)-Zn(2)-O(2W)^{iv}	179.0(5)	O(2W')-Zn(2)-O(2W)^{iv}	80.2(5)
O(3)-Zn(2)-O(2W)^{iv}	87.7(5)	O(2W)-Zn(2)-O(2W)^{iv}	125.1(8)

Symmetry codes for **3**: ^{i}-x+1/2, -y, z; ^{ii}-x+1/2, y, z-1/2; ^{iii}x, -y, z-1/2; ^{iv}-x+1/2, -y+1, z

Table S4. Selected bond distances (Å) and angles (^{o}) for **4**.

Mn(1)-O(1)	2.110(3)	Mn(1)-O(1W)	2.141(3)
Mn(1)-O(3)^{i}	2.156(3)	Mn(1)-N(2)	2.247(3)
Mn(1)-N(1)	2.279(3)	Mn(1)-O(4)^{i}	2.458(3)
O(1)-Mn(1)-O(1W)	88.83(11)	O(1)-Mn(1)-O(3)^{i}	104.52(10)
O(1W)-Mn(1)-O(3)^{i}	88.56(12)	O(1)-Mn(1)-N(2)	89.75(10)
O(1W)-Mn(1)-N(2)	131.99(12)	O(3)^{i}-Mn(1)-N(2)	137.75(11)
O(1)-Mn(1)-N(1)	149.80(11)	O(1W)-Mn(1)-N(1)	86.60(11)
O(3)^{i}-Mn(1)-N(1)	105.19(10)	N(2)-Mn(1)-N(1)	71.69(10)
O(1)-Mn(1)-O(4)^{i}	93.93(10)	O(1W)-Mn(1)-O(4)^{i}	143.89(11)
O(3)^{i}-Mn(1)-O(4)^{i}	55.89(9)	N(2)-Mn(1)-O(4)^{i}	84.07(10)
N(1)-Mn(1)-O(4)^{i}	107.14(10)		

Symmetry code for **4**: ^{i}x+1, y, z

Table S5. Selected bond distances (Å) and angles (^{o}) for **5**.

Mn(1)-O(2)	2.102(2)	Mn(1)-O(1W)	2.127(2)
Mn(1)-O(3)^{i}	2.135(2)	Mn(1)-N(2)	2.241(3)
Mn(1)-N(1)	2.288(3)		
O(2)-Mn(1)-O(1W)	88.68(10)	O(2)-Mn(1)-O(3)^{i}	103.00(9)
O(1W)-Mn(1)-O(3)^{i}	94.36(10)	O(2)-Mn(1)-N(2)	93.11(8)
O(1W)-Mn(1)-N(2)	130.07(10)	O(3)^{i}-Mn(1)-N(2)	133.23(9)
O(2)-Mn(1)-N(1)	155.07(9)	O(1W)-Mn(1)-N(1)	84.91(10)
O(3)^{i}-Mn(1)-N(1)	101.49(10)	N(2)-Mn(1)-N(1)	73.15(9)

Symmetry code for **5**: ^{i}x+1, y, z

Table S6. Selected bond distances (Å) and angles (°) for **6**.

Zn(1)-O(1)	1.974(3)	Zn(1)-O(3)^{i}	1.986(3)
Zn(1)-N(1)^{ii}	2.003(3)	Zn(1)-N(3)	2.018(3)
O(1)-Zn(1)-O(3)^{i}	115.88(13)	O(1)-Zn(1)-N(1)^{ii}	119.87(13)
O(3)^{i}-Zn(1)-N(1)^{ii}	107.35(13)	O(1)-Zn(1)-N(3)	102.62(13)
O(3)^{i}-Zn(1)-N(3)	100.06(14)	N(1)^{ii}-Zn(1)-N(3)	108.87(13)

Symmetry codes for **6**: ^{i}-x, y-1/2, -z+3/2; ^{ii}-x+1, y+1/2, -z+3/2

Table S7. Selected bond distances (Å) and angles (°) for **7**.

Zn(1)-O(1)	1.962(2)	Zn(1)-O(3)^{i}	1.970(2)
Zn(1)-N(1)	1.991(3)	Zn(1)-O(4)^{ii}	1.999(2)
O(1)-Zn(1)-O(3)^{i}	125.75(9)	O(1)-Zn(1)-N(1)	115.45(10)
O(3)^{i}-Zn(1)-N(1)	111.64(10)	O(1)-Zn(1)-O(4)^{ii}	100.16(10)
O(3)^{i}-Zn(1)-O(4)^{ii}	90.67(8)	N(1)-Zn(1)-O(4)^{ii}	106.58(10)

Symmetry codes for **7**: ^{i}-x, y+1/2, -z+3/2; ^{ii} x, y+1, z

Table S8. Selected bond distances (Å) and angles (°) for **8**.

Zn(1)-O(3)^{i}	1.949(3)	Zn(1)-O(1)	1.999(3)
Zn(1)-N(1)^{ii}	2.017(3)	Zn(1)-N(1')^{ii}	2.028(14)
Zn(1)-N(3)	2.028(3)		
O(3)^{i}-Zn(1)-O(1)	105.09(11)	O(3)^{i}-Zn(1)-N(1)^{ii}	121.8(3)
O(1)-Zn(1)-N(1)^{ii}	113.4(4)	O(3)^{i}-Zn(1)-N(1')^{ii}	113.0(3)
O(1)-Zn(1)-N(1')^{ii}	117.0(4)	O(3)^{i}-Zn(1)-N(3)	110.08(14)
O(1)-Zn(1)-N(3)	102.75(13)	N(1)^{ii}-Zn(1)-N(3)	102.1(3)
N(1')^{ii}-Zn(1)-N(3)	108.4(4)		

Symmetry code for **8**: ^{i}-x+2, -y, -z+2; ^{ii} -x+3/2, y-1/2, -z+1/2

Table S9. Selected bond distances (Å) and angles (°) for **9**.

Co(1)-O(2)	1.963(3)	Co(1)-O(4)^{i}	2.021(3)

Co(1)-N(1)^{ii}	2.034(3)	Co(1)-N(3)	2.042(3)
O(2)-Co(1)-O(4)^{i}	103.38(12)	O(2)-Co(1)-N(1)^{ii}	121.35(13)
O(4)^{i}-Co(1)-N(1)^{ii}	115.77(12)	O(2)-Co(1)-N(3)	110.00(13)
O(4)^{i}-Co(1)-N(3)	100.83(12)	N(1)^{ii}-Co(1)-N(3)	103.66(13)

Symmetry code for **9**: ^{i}-x+2, -y+1, -z+1; ^{ii}-x+3/2, y+1/2, -z-1/2

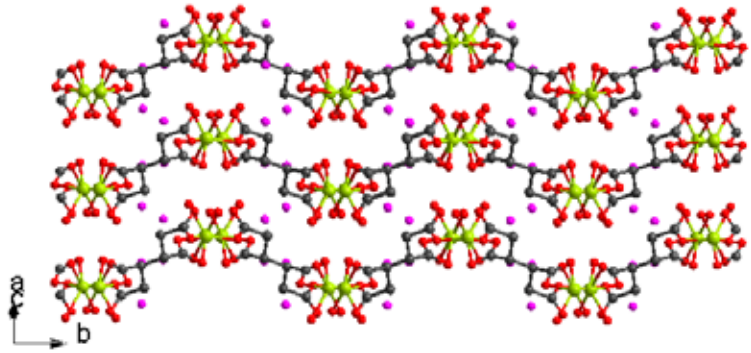


Fig. S1 View of the 3D supramolecular network of **1** (pink dots represent free water molecules).

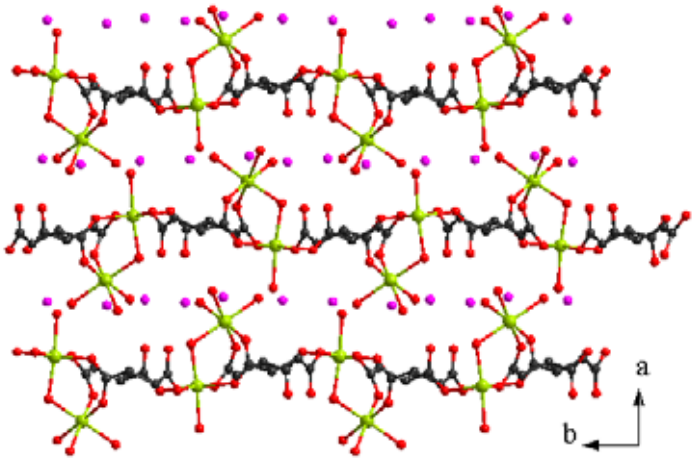


Fig. S2 View of the 3D supramolecular network of **2** (pink dots represent free water molecules).

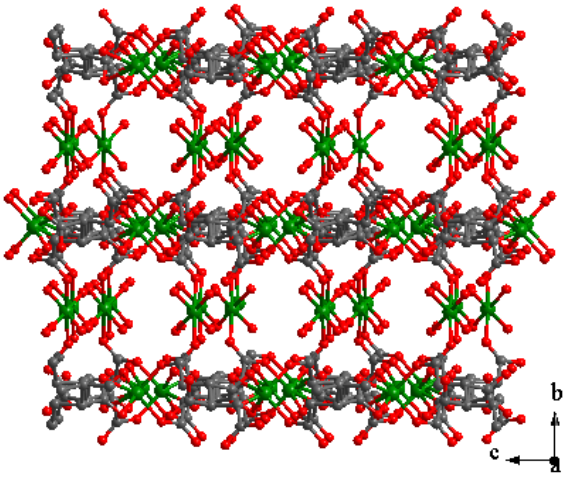


Fig. S3 View of the 3D network of **3**.

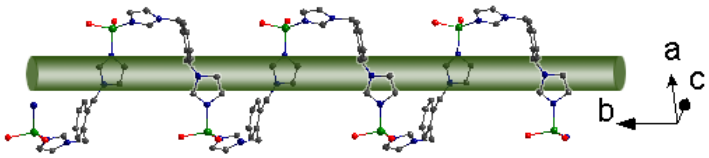


Fig. S4 The helical chain of the '*trans*' shaped obib ligands in **6**.

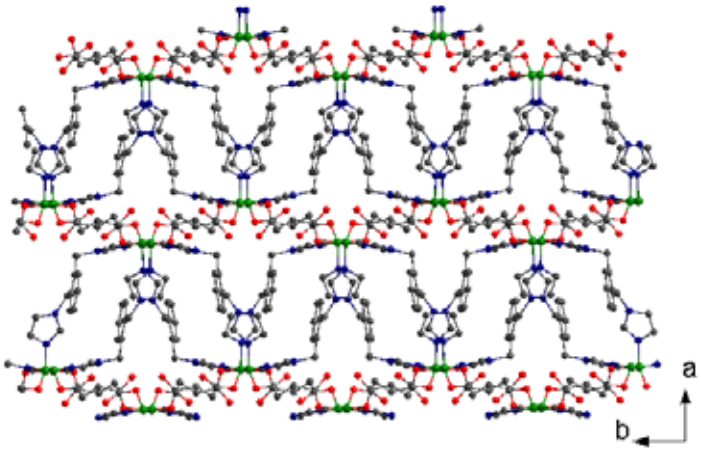


Fig. S5 View of the 3D network of **6**.

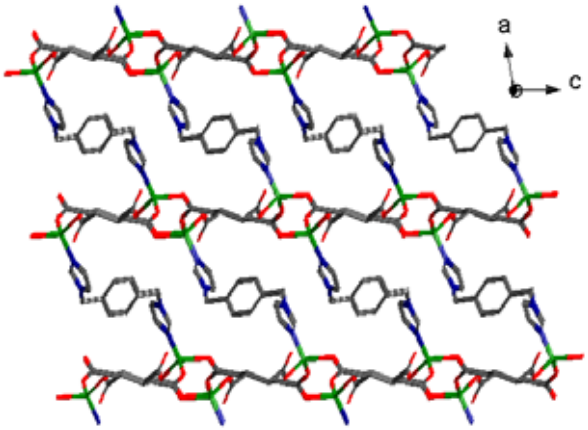


Fig. S6 View of the 3D network of **7**.

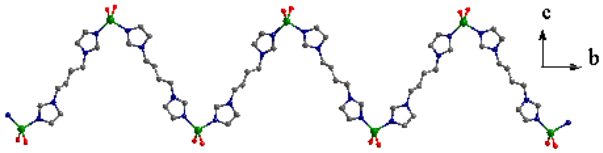


Fig. S7 The infinite zigzag chain of the bbi ligands in **8**.

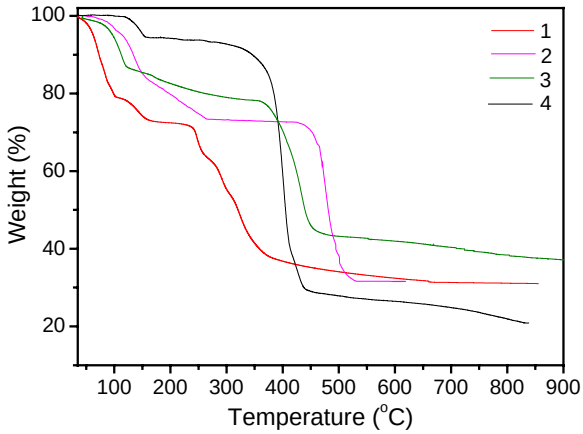


Fig. S8 TGA curves of **1-4**.

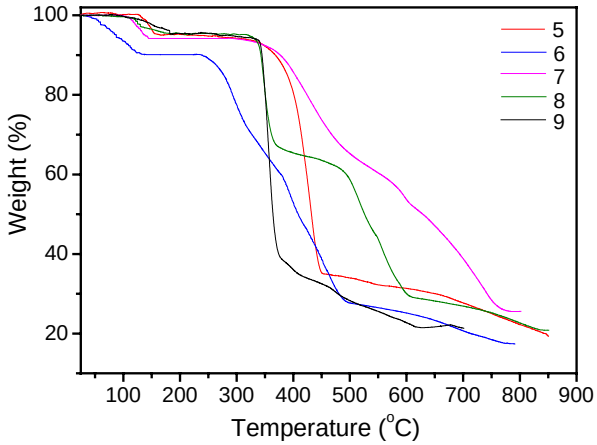


Fig. S9 TGA curves of **5-9**.

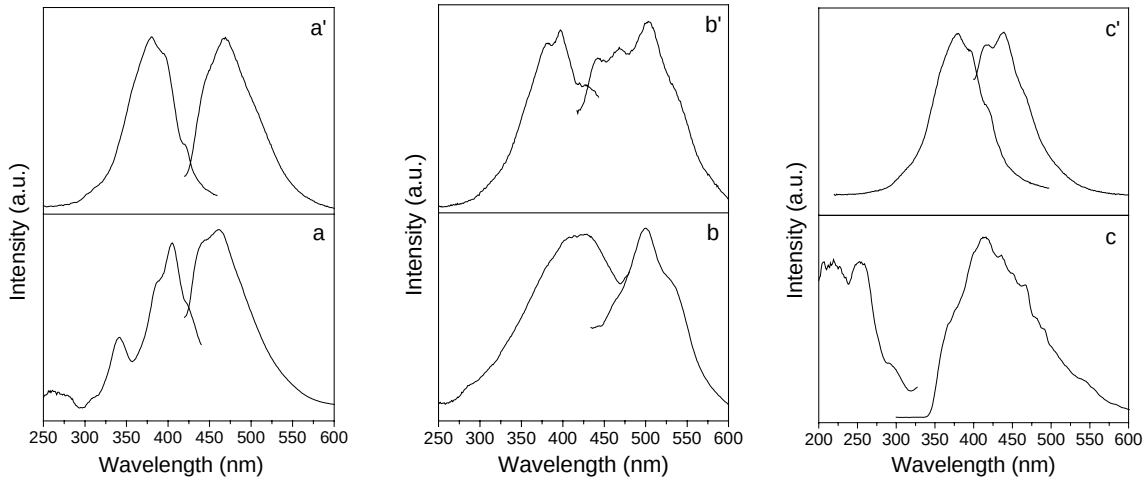
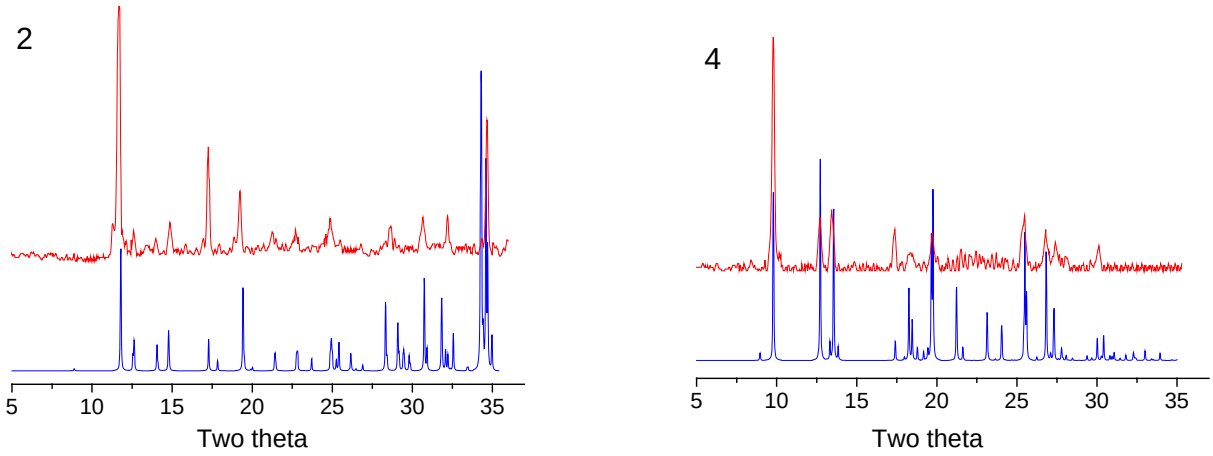


Fig. S10 Solid-state photoluminescent spectra of **6** (a), **7** (b) and **8** (c) and free ligands obib (a'), pbib (b') and bbi (c') at room temperature.



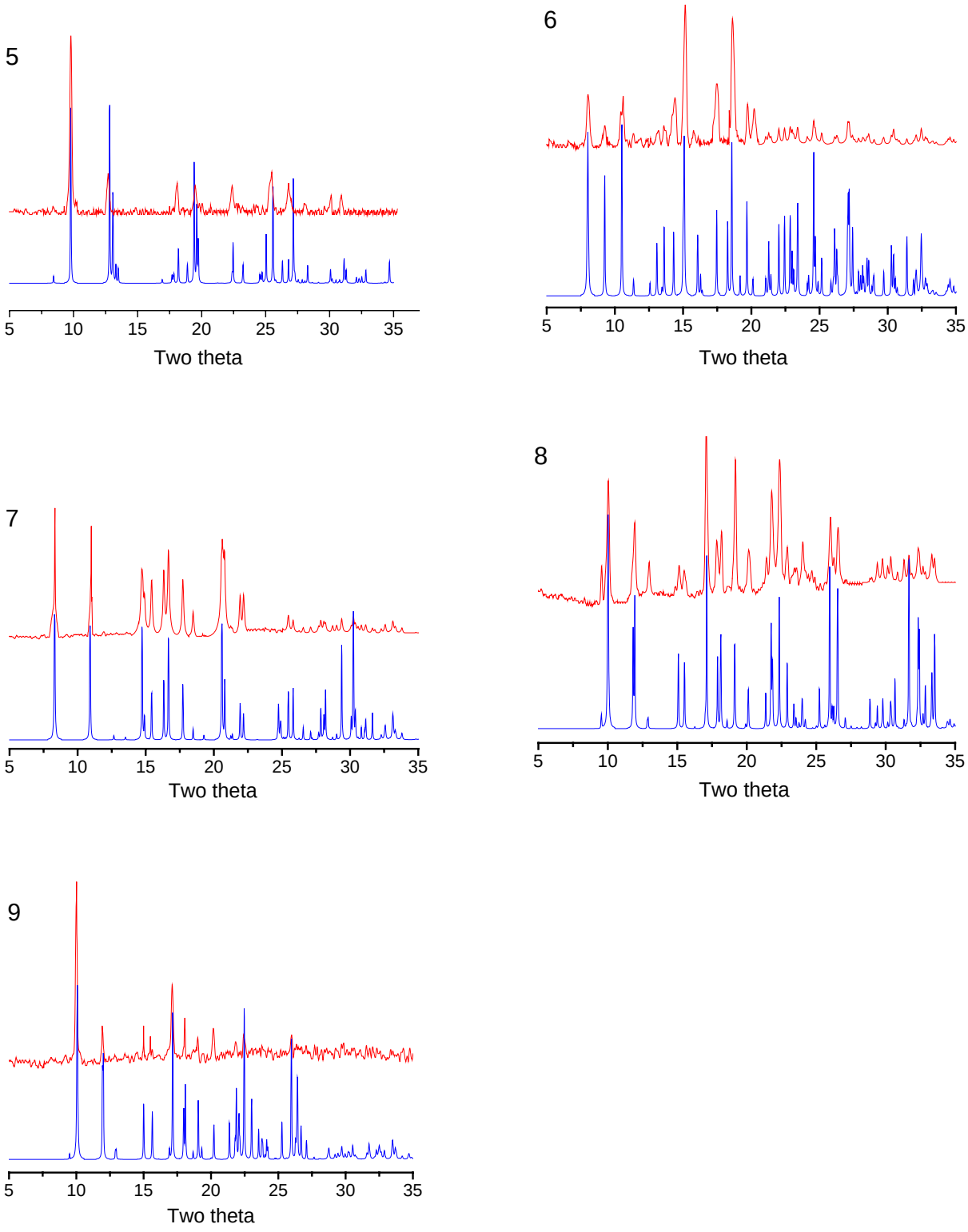


Fig. S11. The simulated (blue) and experimental (red) XRPD patterns for the compounds.