Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supplementary Information

Exploring biphenyl-2,4,4′-tricarboxylic acid as a flexible building block for the hydrothermal self-assembly of diverse metal-organic and supramolecular networks

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Table S1 Selected bond lengths [Å] and angles [°] for the compounds **1-9**[a].

1					
Zn(1)-O(1)	2.172(4)	Zn(1)-O(2)	2.260(4)	Zn(1)-N(1)	2.113(6)
Zn(1)-N(2)	2.096(5)	Zn(1)-N(3)	2.101(6)	Zn(1)-N(4)	2.156(5)
N(2)-Zn(1)-N(3)	100.2(2)	N(2)-Zn(1)-N(1)	79.2(2)	N(3)-Zn(1)-N(1)	97.4(2)
N(2)-Zn(1)-N(4)	94.0(2)	N(3)-Zn(1)-N(4)	78.6(2)	N(1)-Zn(1)-N(4)	171.4(2)
N(2)-Zn(1)-O(1)	108.0(2)	N(3)-Zn(1)-O(1)	149.2 (2)	N(1)-Zn(1)-O(1)	99.9(2)
N(4)-Zn(1)-O(1)	87.1(2)	N(2)-Zn(1)-O(2)	164.5(2)	N(3)-Zn(1)-O(2)	94.6(2)
N(1)-Zn(1)-O(2)	94.3(2)	N(4)-Zn(1)-O(2)	93.5 (2)	O(1)-Zn(1)-O(2)	59.0(2)
2					
Co(1)-O(1)	2.210(4)	Co(1)-O(1)#1	2.210(4)	Co(1)-N(1)	2.129(5)
Co(1)-N(1)#1	2.129(5)	Co(1)-N(4)	2.126(5)	Co(1)-N(4)#1	2.126(5)
N(4)-Co(1)-N(1)	79.6(2)	N(4)#1-Co(1)-N(1)	100.4(2)	N(4)-Co(1)-O(1)	91.4(2)
N(4)#1-Co(1)-O(1)	88.6(2)	N(1)-Co(1)-O(1)#1	89.9(2)	N(1)-Co(1)-O(1)	90.1(2)
3					
Cd(1)-O(1)	2.443(4)	Cd(1)-O(1)#1	2.443(4)	Cd(1)-N(1)	2.292(4)
Cd(1)-N(1)#1	2.292(4)	Cd(1)-N(4)	2.299(5)	Cd(1)-N(4)#1	2.299(5)
N(1)-Cd(1)-N(4)	75.2(2)	N(1)-Cd(1)-N(4)#1	104.8(2)	N(1)-Cd(1)-O(1)	84.4(2)
N(1)#1-Cd(1)-O(1)	95.6(2)	N(4)-Cd(1)-O(1)	91.2(2)	N(4)#1-Cd(1)-O(1)	88.8(2)
4					
Ni(1)-O(1)	2.079(6)	Ni(1)-O(7)	2.074(6)	Ni(1)-N(1)	2.111(8)
Ni(1)-N(2)	2.095(7)	Ni(1)-N(3)	2.084(7)	Ni(1)-N(4)	2.085(7)
O(1)-Ni(1)-O(7)	90.7(2)	O(1)-Ni(1)-N(3)	93.2(3)	O(7)-Ni(1)-N(3)	100.1(3)
O(1)-Ni(1)-N(1)	87.5(3)	O(7)-Ni(1)-N(1)	168.9(2)	N(3)-Ni(1)-N(1)	90.9(3)
O(1)-Ni(1)-N(2)	90.1(2)	O(7)-Ni(1)-N(2)	88.7(3)	N(3)-Ni(1)-N(2)	170.5(3)
N(1)-Ni(1)-N(2)	80.3(3)	O(1)-Ni(1)-N(4)	173.0(3)	O(7)-Ni(1)-N(4)	90.2(3)
N(3)-Ni(1)-N(4)	79.8(3)	N(1)-Ni(1)-N(4)	92.9(3)	N(2)-Ni(1)-N(4)	96.9(3)
5					
Cd(1)-O(1)	2.377(6)	Cd(1)-O(2)	2.350(8)	Cd(1)-O(3)#1	2.291(7)
Cd(1)-N(1)	2.399(9)	Cd(1)-N(2)	2.399(9)	Cd(1)-Cl(1)	2.628(3)
Cd(2)-O(4)#1	2.294(8)	Cd(2)-O(5)#2	2.271(6)	Cd(2)-O(6)#2	2.468(9)
Cd(2)-N(3)	2.357(9)	Cd(2)-N(4)	2.331(8)	Cd(2)-Cl(1)	2.543(2)
O(3)#1-Cd(1)-O(2)	89.4(3)	O(3)#1-Cd(1)-O(1)	98.9(3)	O(2)-Cd(1)-O(1)	55.3(3)
O(3)#1-Cd(1)-N(1)	102.8(3)	O(2)-Cd(1)-N(1)	92.6(3)	O(1)-Cd(1)-N(1)	140.9(3)
O(3)#1-Cd(1)-N(2)	172.6(3)	O(2)-Cd(1)-N(2)	92.6(3)	O(1)-Cd(1)-N(2)	88.1(3)
N(1)-Cd(1)-N(2)	70.0(3)	O(3)#1-Cd(1)-Cl(1)	97.9(2)	O(2)-Cd(1)-Cl(1)	147.2(2)
O(1)-Cd(1)-Cl(1)	92.0(2)	N(1)-Cd(1)-Cl(1)	116.5(2)	N(2)-Cd(1)-Cl(1)	84.2(2)
O(5)#2-Cd(2)-O(4)#1	87.6(2)	O(5)#2-Cd(2)-N(4)	142.4(3)	O(4)#1-Cd(2)-N(4)	125.4(3)
O(5)#2-Cd(2)-N(3)	100.7(3)	O(4)#1-Cd(2)-N(3)	80.8(3)	N(4)-Cd(2)-N(3)	71.4(3)
O(5)#2-Cd(2)-O(6)#2	54.6(3)	O(4)#1-Cd(2)-O(6)#2	140.5(2)	N(4)-Cd(2)-O(6)#2	94.0(3)
N(3)-Cd(2)-O(6)#2	114.0(3)	O(5)#2-Cd(2)-Cl(1)	110.2(2)	O(4)#1-Cd(2)-Cl(1)	84.75(19)
N(4)-Cd(2)-Cl(1)	92.2(2)	N(3)-Cd(2)-Cl(1)	145.2(2)	O(6)#2-Cd(2)-Cl(1)	97.1(2)
Cd(2)-Cl(1)-Cd(1)	89.02(8)				
6					
Ni(1)-O(1)	2.038(5)	Ni(1)-O(3)#1	2.050(4)	Ni(1)-O(6)#2	2.056(5)
Ni(1)-O(7)	2.144(5)	Ni(1)-O(8)	2.086(5)	Ni(1)-N(1)	2.068(6)
Ni(2)-O(4)#1	2.072(4)	Ni(2)-O(4)#3	2.072(4)	Ni(2)-O(7)	2.071(5)

Ni(2)-O(7)#4	2.071(5)	Ni(2)-N(2)	2.137(5)	Ni(2)-N(2)#4	2.543(2)
O(1)-Ni(1)-O(3)#1	88.6(2)	O(1)-Ni(1)-O(6)#2	93.4(2)	O(1)-Ni(1)-O(7)	92.4(2)
O(1)-Ni(1)-O(8)	173.9(2)	O(1)-Ni(1)-N(1)	86.8(2)	O(1)#1-Ni(1)-O(6)#2	177.9(2)
O(3)#1-Ni(1)-O(7)	89.5(2)	O(3)#1-Ni(1)-O(8)	88.1(2)	O(1)#1-Ni(1)-N(1)	93.2(2)
O(6)#2-Ni(1)-O(7)	90.6(2)	O(6)#2-Ni(1)-O(8)	89.8(2)	O(6)#2-Ni(1)-N(1)	86.7(2)
O(8)-Ni(1)-O(7)	92.8(2)	N(1)-Ni(1)-O(7)	177.1(2)	N(1)-Ni(1)-O(8)	88.2(2)
O(4)#3-Ni(2)-O(4)#1	88.1(3)	O(4)#3-Ni(2)-N(2)#4	176.3(6)	O(4)#3-Ni(2)-N(2)	89.7(2)
O(4)#1-Ni(2)-N(2)#4	89.79(5)	O(4)#1-Ni(2)-N(2)	176.3(2)	O(7)#4-Ni(2)-O(4)#3	91.2(2)
O(7)-Ni(2)-O(4)#3	86.6(2)	O(7)#4-Ni(2)-O(4)#1	86.6(2)	O(7)-Ni(2)-O(4)#1	91.2(2)
O(7)-Ni(2)-O(7)#4	177.0(3)	O(7)-Ni(2)-N(2)	91.7(2)	O(7)#4-Ni(2)-N(2)#4	91.6(7)
O(7)#4-Ni(2)-N(2)	90.4(2)	O(7)-Ni(2)-N(2)#4	90.4(7)	N(2)#4-Ni(2)-N(2)	92.7(6)
Ni(1)-O(7)-Ni(2)	123.7(2)				

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Co(1)-O(1)	2.107(5)	Co(1)-O(1)#1	2.107(5)	Co(1)-O(8)	2.092(5)
Co(1)-O(8)#1	2.092(5)	Co(1)-N(1)	2.179(6)	Co(1)-N(1)#1	2.179(6)
Co(2)-O(2)	2.067(5)	Co(2)-O(4)#2	2.040(5)	Co(2)-O(6)#3	2.087(5)
Co(2)-O(7)	2.091(5)	Co(2)-O(8)	2.214(5)	Co(2)-N(2)	2.122(7)
O(1)-Co(1)-O(1)#1	87.4(3)	O(1)-Co(1)-N(1)#1	175.3(2)	O(1)#1-Co(1)-N(1)#1	90.6(2)
O(1)#1-Co(1)-N(1)	175.3(2)	O(1)-Co(1)-N(1)	90.6(2)	O(8)#1-Co(1)-O(1)	86.8(2)
O(8)-Co(1)-O(1)#1	86.8(2)	O(8)#1-Co(1)-O(1)#1	92.0(2)	O(8)-Co(1)-O(1)	92.0(2)
O(8)-Co(1)-O(8)#1	178.3(3)	O(8)-Co(1)-N(1)	89.1(2)	O(8)#1-Co(1)-N(1)#1	89.1(2)
O(8)#1-Co(1)-N(1)	92.2(2)	O(8)-Co(1)-N(1)#1	92.2(2)	N(1)-Co(1)-N(1)#1 92.2(2)	91.7(4)
O(2)-Co(2)-O(6)#2	176.7(2)	O(2)-Co(2)-O(7)	86.4(2)	O(2)-Co(2)-O(8)	90.3(2)
O(2)-Co(2)-N(2)	93.8(2)	O(4)#3-Co(2)-O(2)	89.4(2)	O(4)#3-Co(2)-O(6)#2	93.9(2)
O(4)#3-Co(2)-O(7)	174.7(2)	O(4)#3-Co(2)-O(8)	92.4(2)	O(4)#3-Co(2)-N(2)	86.9(2)
O(6)#2-Co(2)-O(7)	90.4(2)	O(6)#2-Co(2)-O(8)	88.9(2)	O(6)#2-Co(2)-N(2)	87.1(3)
O(7)-Co(2)-O(8)	90.8(2)	O(7)-Co(2)-N(2)	90.3(2)	N(2)-Co(2)-O(8)	175.8(2)
Co(1)-O(8)-Co(2)	122.4(2)				

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Co(1)-O(2)	2.136(5)	Co(1)-O(7)	2.071(5)	Co(1)-O(8)	2.169(5)
Co(1)-O(9)	2.056(5)	Co(1)-O(11)	2.144(5)	Co(1)-O(16)#1	2.028(5)
Co(2)-O(1)	2.091(5)	Co(2)-O(5)#2	2.046(5)	Co(2)-O(7)	2.090(5)
Co(2)-O(10)	2.182(5)	Co(2)-O(11)	2.133(5)	Co(2)-N(1)	2.110(7)
Co(3)-O(6)#2	2.224(6)	Co(3)-O(6)#5	2.224(6)	Co(3)-O(7)	1.964(5)
Co(3)-O(7)#3	1.964(5)	Co(3)-O(15)#1	2.153(5)	Co(3)-O(15)#4	2.153(5)
Co(4)-O(3)#7	2.024(6)	Co(4)-O(4)#6	2.002(6)	Co(4)-O(13)	2.035(5)
Co(4)-O(14)#8	2.026(5)	Co(4)-N(2)	2.074(6)		
O(16)#1-Co(1)-O(9)	89.0(2)	O(16)#1-Co(1)-O(7)	92.1(2)	O(9)-Co(1)-O(7)	178.0(2)
O(16)#1-Co(1)-O(2)	175.8(2)	O(9)-Co(1)-O(2)	94.3(2)	O(7)-Co(1)-O(2)	84.7(2)
O(16)#1-Co(1)-O(11)	91.2(2)	O(9)-Co(1)-O(11)	93.9(2)	O(7)-Co(1)-O(11)	84.4(2)
O(2)-Co(1)-O(11)	91.0(2)	O(16)#1-Co(1)-O(8)	94.2(2)	O(9)-Co(1)-O(8)	86.3(2)
O(7)-Co(1)-O(8)	95.2(2)	O(2)-Co(1)-O(8)	83.6(2)	O(11)-Co(1)-O(8)	174.6(2)
O(5)#2-Co(2)-O(7)	91.9(2)	O(5)#2-Co(2)-O(1)	176.1(2)	O(7)-Co(2)-O(1)	84.2(2)
O(5)#2-Co(2)-N(1)	91.1(2)	O(7)-Co(2)-N(1)	176.7(2)	O(1)-Co(2)-N(1)	92.8(2)
O(5)#2-Co(2)-O(11)	88.3(2)	O(7)-Co(2)-O(11)	84.3(2)	O(1)-Co(2)-O(11)	91.8(2)
N(1)-Co(2)-O(11)	97.1(2)	O(5)#2-Co(2)-O(10)	92.0(2)	O(7)-Co(2)-O(10)	90.2(2)
O(1)-Co(2)-O(10)	87.5(2)	N(1)-Co(2)-O(10)	88.4(2)	O(11)-Co(2)-O(10)	174.5(2)
O(7)-Co(3)-O(15)#1	93.6(2)	O(7)-Co(3)-O(15)#4	86.4(2)	O(7)#3-Co(3)-O(6)#5	94.1(2)
O(7)-Co(3)-O(6)#5	85.9(2)	O(15)#4-Co(3)-O(6)#5	86.0(2)	O(15)#1-Co(3)-O(6)#5	94.0(2)

O(4)#6-Co(4)-O(3)#7	163.3(2)	O(4)#6-Co(4)-O(14)#8	88.3(3)	O(3)#7-Co(4)-O(14)#8	90.5(3)
O(4)#6-Co(4)-O(13)	88.7(2)	O(3)#7-Co(4)-O(13)	87.8(3)	O(14)#8-Co(4)-O(13)	163.5(2)
O(4)#6-Co(4)-N(2)	102.1(3)	O(3)#7-Co(4)-N(2)	94.5(2)	O(14)#8-Co(4)-N(2)	99.9(2)
O(13)-Co(4)-N(2)	96.6(2)	Co(3)-O(7)-Co(1)	126.9(3)	Co(3)-O(7)-Co(2)	123.6(2)
Co(1)-O(7)-Co(2)	95.9(2)				
9					
Pb(1)-O(1)	2.614(5)	Pb(1)-O(2)	2.369(5)	Pb(1)-O(5)#3	2.643(5)
Pb(1)-O(9)#1	2.613(5)	Pb(1)-O(10)#1	2.477(5)	Pb(1)-O(10)#2	2.555(5)
Pb(2)-O(5)	2.412(5)	Pb(2)-O(6)#4	2.484(5)	Pb(2)-O(7)	2.379(5)
Pb(2)-O(9)#8	2.863(5)	Pb(2)-O(13)	2.495(5)	Pb(3)-O(3)#6	2.468(5)
Pb(3)-O(4)#6	2.493(5)	Pb(3)-O(4)#7	2.566(5)	Pb(3)-O(8)	2.543(5)
Pb(3)-O(11)#5	2.319(5)	O(2)-Pb(1)-O(10)#2	79.4(2)	O(10)#1-Pb(1)-O(10)#2	65.2(2)
O(2)-Pb(1)-O(10)#1	78.2(2)	O(10)#1-Pb(1)-O(1)	124.5(2)	O(10)#2-Pb(1)-O(1)	80.9(2)
O(2)-Pb(1)-O(1)	52.2(2)	O(10)#1-Pb(1)-O(9)#1	51.0(2)	O(10)#2-Pb(1)-O(9)#1	115.3(2)
O(2)-Pb(1)-O(9)#1	78.6(2)	O(2)-Pb(1)-O(5)#3	75.0(2)	O(10)#1-Pb(1)-O(5)#3	120.3(2)
O(1)-Pb(1)-O(9)#1	125.4(2)	O(1)-Pb(1)-O(5)#3	73.6(2)	O(9)#1-Pb(1)-O(5)#3	71.8(2)
O(10)#2-Pb(1)-O(5)#3	151.5(2)	O(7)-Pb(2)-O(6)#4	130.8(2)	O(5)-Pb(2)-O(6)#4	81.9(2)
O(7)-Pb(2)-O(5)	75.8(2)	O(5)-Pb(2)-O(13)	114.2(2)	O(6)#4-Pb(2)-O(13)	72.4(2)
O(7)-Pb(2)-O(13)	77.7(2)	O(11)#5-Pb(3)-O(4)#6	80.4(2)	O(3)#6-Pb(3)-O(4)#6	51.9(2)
O(11)#5-Pb(3)-O(3)#6	94.5(2)	O(3)#6-Pb(3)-O(8)	73.3(2)	O(4)#6-Pb(3)-O(8)	119.1(2)
O(11)#5-Pb(3)-O(8)	79.6(2)	O(3)#6-Pb(3)-O(4)#7	115.2(2)	O(4)#6-Pb(3)-O(4)#7	63.4(2)
O(11)#5-Pb(3)-O(4)#7	76.2(2)	Pb(2)-O(5)-Pb(1)#5	102.3(2)	Pb(1)#9-O(10)-Pb(1)#7	114.8(2)
O(8)-Pb(3)-O(4)#7	154.8(2)	Pb(3)#8-O(4)-Pb(3)#2	116.6(2)		

[a] Symmetry transformations used to generate equivalent atoms: #1 –*x*+1, –*y*+2, –*z* for **2**; #1 –*x*+1, –*y*+1, –*z*+1 for **3**; #1 *x*, *y*–1, *z*; #2 –*x*+1, –*y*, *z*+1/2 for **5**; #1 –*x*+1/2, *y*–1/2, –*z*+1/2; #2 –*x*+1/2, –*y*+3/2, –*z*; #3 *x*+1/2, *y*–1/2, *z*; #4 –*x*+1, *y*, –*z*+1/2 for **6**; #1 –*x*, *y*, –*z*+1/2; #2 *x*, –*y*+2, *z*+1/2 ; #3 –*x*+1/2, *y*–1/2, –*z*+1/2 for **7**; #1 –*x*, –*y*+1, –*z*+1; #2 *x*, *y*, *z*+1; #3 –*x*, –*y*+2, –*z*; #4 *x*, *y*+1, *z*–1; #5 –*x*, –*y*+2, –*z*–1 ; #6 –*x*+1, –*y*+1, –*z*; #7 *x*, *y*–1, *z*+1; #8 –*x*+1, –*y*, –*z*+1 for **8**; #1 –*x*–1/2, *y*–1/2, –*z*+3/2; #2 *x*–1/2, –*y*+3/2, *z*–1/2; #3 *x*–1, *y*, *z*; #4 –*x*+1, –*y*+2, –*z*+1; #5 *x*+1, *y*, *z* ; #6 –*x*+1/2, *y*+1/2, –*z*+3/2; #7 *x*+1/2, –*y*+3/2, *z*+1/2; #8 –*x*+1/2, *y*–1/2, –*z*+3/2; #9 –*x*–1/2, *y*+1/2, –*z*+3/2 for **9**.

Table S2 Conventional hydrogen bonds in crystal packing [Å, °] of **1**–**4** and **6**–**9**.

Complexes	D-H···A	*d*(D-H)	*d*(H…A)	*d*(D…A)	∠DHA	Symmetry code
1	O(4)-H(4)···O(5)	0.82	1.81	2.593	160.5	*x*, *y*, *z*+1
	O(6)-H(6)···O(10	0.82	1.70	2.463	153.1	-*x*+1, -*y*, -*z*
	O(7)-H(7)···O(3)	0.82	1.93	2.711	157.8	-*x*+2,-*y*,-*z*+1
	O(12)-H(12)···O(9)	0.82	1.79	2.593	166.4	*x*, *y*, *z*+1
	O(13)-H(1W)···O(1)	0.85	2.00	2.824	163.7	*x*-1,*y*,*z*

	O(13)-H(2W)···O(5)	0.85	2.01	2.855	169.9	-*x*+1,-*y*,-*z*
2	N(2)-H(4)···O(3)	0.86	1.84	2.696	173.4	*x*+1,*y*+1,*z*
	N(3)-H(5)···O(4)	0.86	1.90	2.762	174.3	*x*+1,*y*+1,*z*
	O(2)-H(1)···O(4)	0.82	1.68	2.482	166.8	-*x*+1,-*y*+1,-*z*
	O(6)-H(2)···O(5)	0.82	1.82	2.629	168.4	-*x*+2,-*y*+2,-*z*+1
3	N(2)-H(4)···O(6)	0.86	1.92	2.774	172.2	-*x*,-*y*,-*z*+1
	N(3)-H(5)···O(5)	0.86	1.85	2.699	169.2	-*x*,-*y*,-*z*+1
	O(2)-H(1)···O(6)	0.82	1.71	2.517	169.4	-*x*+1,-*y*,-*z*+1
	O(4)-H(2)···O(3)	0.82	1.82	2.625	168.0	-*x*+2,-*y*+1,-*z*+2
4	O(5)-H(5)···O(3)	0.82	1.68	2.482	166.0	*x*,*y*-1,*z*
	O(7)-H(1W)···O(4)	0.85	1.80	2.646	179.3	-*x*+1/2,*y*-1/2,*z*+1/2
	O(7)-H(2W)···O(2)	0.85	1.83	2.677	179.0	
	O(8)-H(3W)···O(2)	0.85	2.03	2.875	179.8	
	O(8)-H(4W)···O(6)	0.85	2.08	2.926	179.8	*x*-1/2,-*y*+1/2,*z*
	O(9)-H(6W)···O(4)	0.85	2.07	2.917	179.5	-*x*+1,-*y*+1,*z*+1/2
6	O(8)-H(8A)···O(3)	0.85	2.33	2.876	122.5	-*x*+2,*y*-1/2,-*z*+1/2
	O(8)-H(8B)···O(4)	0.70	2.12	2.794	163.6	*x*+1/2, *y*-1/2,*z*
	O(7)-H(7A)···O(2)	0.86	1.73	2.551	159.0	
	O(7)-H(7B)···O(5)	0.85	1.76	2.578	160.0	-*x*+1/2,-*y*+3/2,-*z*
7	O(7)-H(7A)···N(3)	0.89	1.85	2.739	173.1	-*x*,*y*,-*z*+1/2
	O(7)-H(7B)···O(1)	0.89	1.92	2.776	160.1	-*x*,*y*,-*z*+1/2
	O(8)-H(8A)···O(5)	0.86	1.72	2.575	169.0	*x*,-*y*+2,*z*+1/2
	O(8)-H(8B)···O(3)	0.86	1.73	2.585	169.0	-*x*+1/2,*y*-1/2,-*z*+1/2
8	O(8)-H(1W···O(6)	0.82	1.95	2.743	163.1	-*x*,-*y*+2,-*z*-1
	O(8)-H(2W)···O(2)	0.85	2.02	2.869	179.6	
	O(9)-H(3W)···O(12)	0.82	1.81	2.629	173.8	-*x*,-*y*+1,-*z*
	O(9)-H(4W)···O(2)	0.76	2.08	2.778	152.3	-*x*,-*y*+1,-*z*
	O(10)-H(5W)···O(15)	0.82	1.99	2.800	168.5	*x*,*y*+1,*z*-1
9	O(13)-H(1W)···O(6)	0.85	2.09	2.941	179.2	-*x*+1,-*y*+2,-*z*+1
	O(13)-H(2W)···O(8)	0.88	1.87	2.636	144.9	

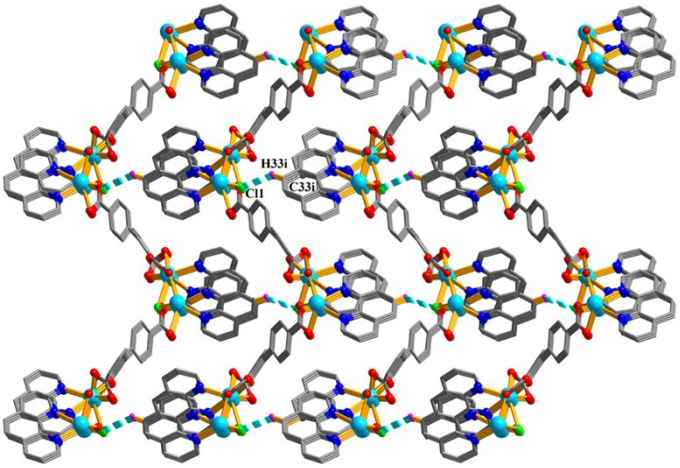
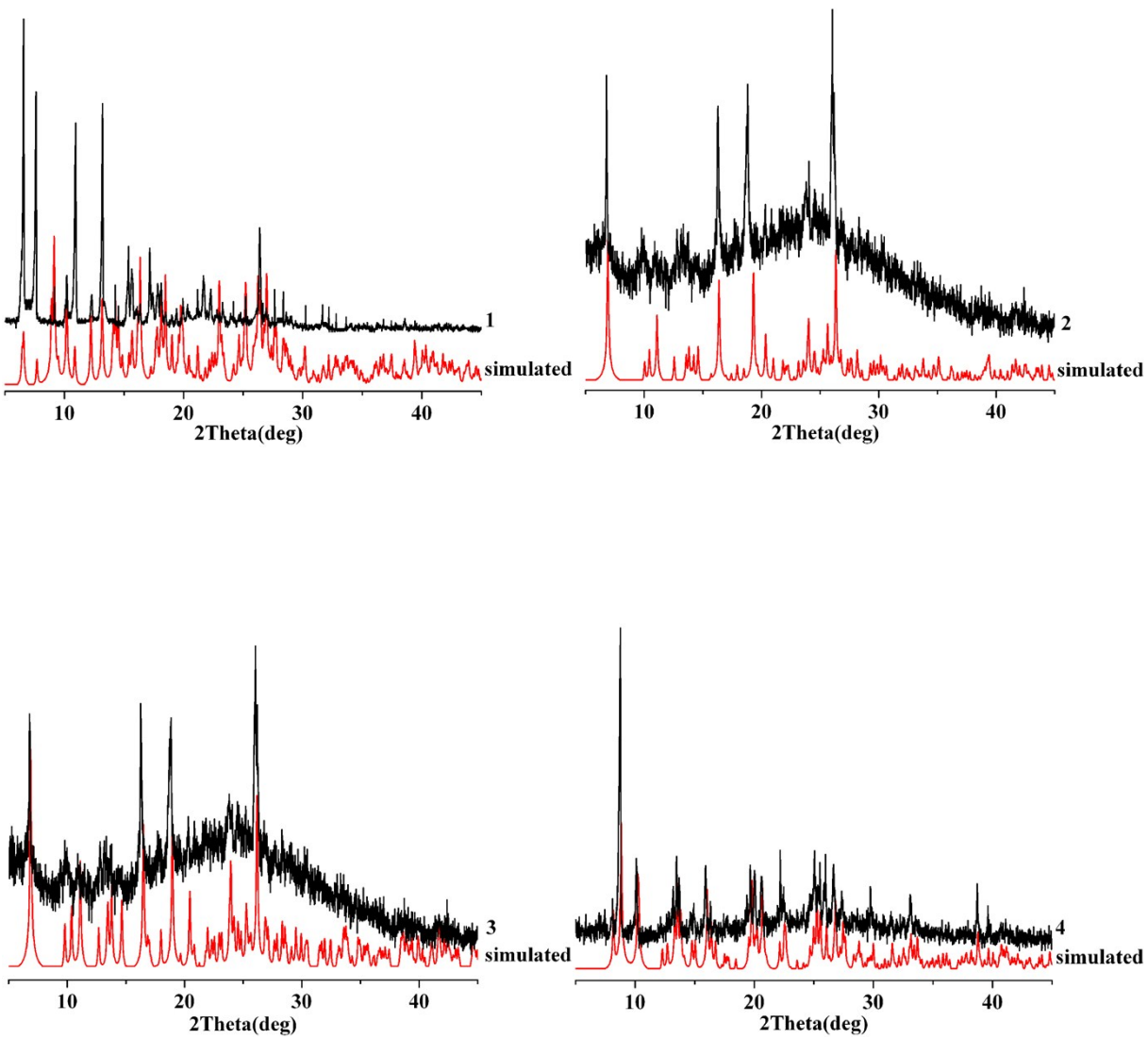


Fig. S1 3D structure formed by the hydrogen bonds in **5** (blue dashed lines present the H-bond).



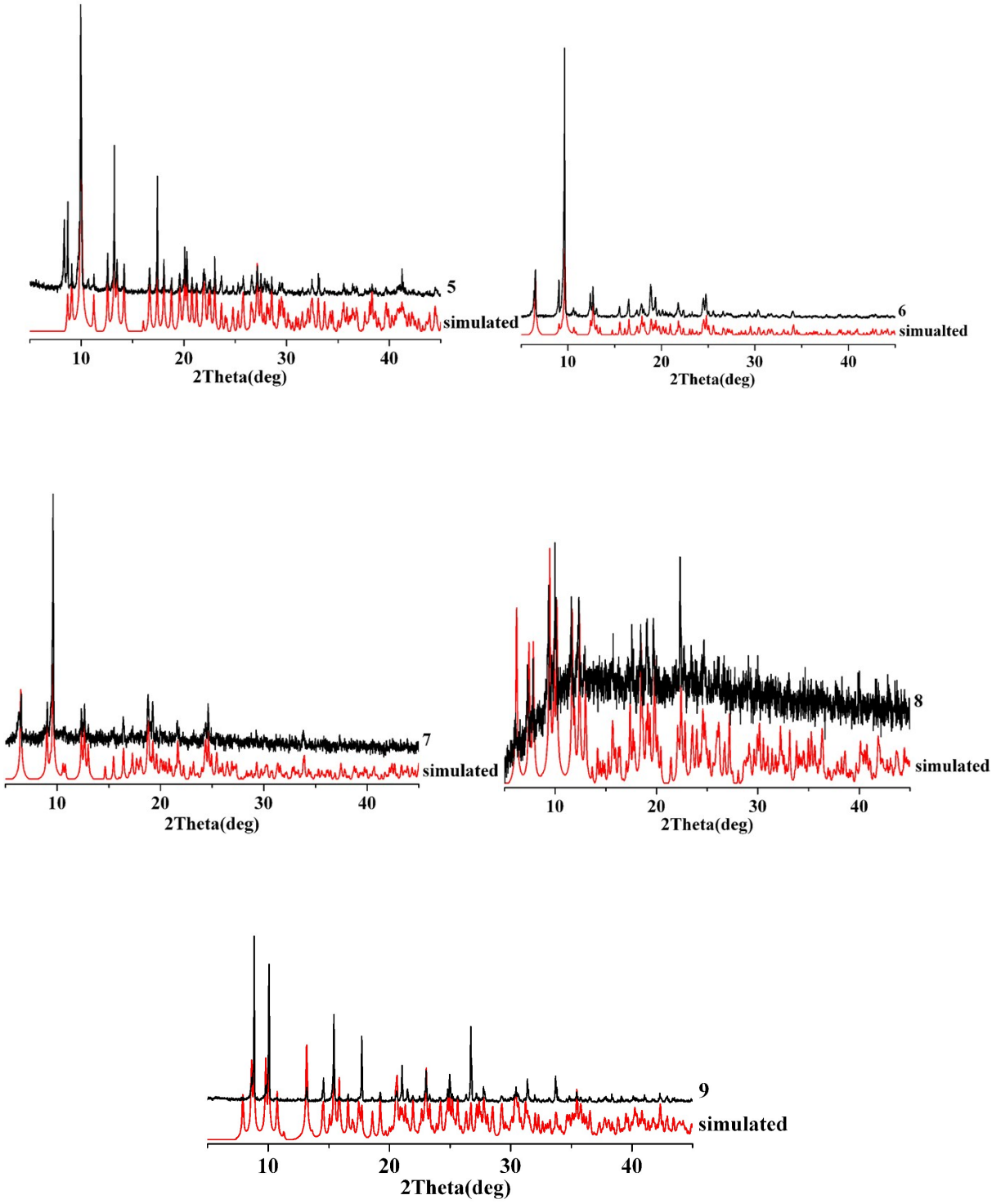


Fig. S2 The PXRD patterns of compounds **1**–**9** at room temperature. Black paterns correspnond to the experimental data obtained using the as-synthesized bulk samples. Red patterns have been simulated from the single crystal X-ray data.