Supporting information for the article

Unprecedented coordination compounds with 4,4´-diaminodiphenylethane as a supramolecular agent and ditopic ligand: synthesis, crystal structures and Hirshfeld surface analysis

Nicoleta Craciun[1,2], Diana Chisca[1,2], Elena Melnic[1] and Marina S. Fonari[1,*]

1 Institute of Applied Physics USM, Academiei Str. 5, MD-2028 Chisinau, Moldova

2 Faculty of Biology and ChemistryIon Creangă State Pedagogical University, Ion Creangă Str. 1, MD-2069 Chisinau, Moldova

** Correspondence: marina.fonari@ifa.md or fonari.xray@gmail.com*

Table S1. Selected geometric parameters in 1-7.

Parameter	Value	Parameter	Value
1			
Cd(1)-N(5)	2.324(3)	Cd(1)-N(4)	2.369(3)
Cd(1)-N(3)	2.347(3)	Cd(1)-N(2)	2.371(3)
Cd(1)-N(1)	2.356(3)	Cd(1)-N(6)	2.379(3)
N(5)-Cd(1)-N(3)	94.51(11)	N(3)-Cd(1)-N(2)	94.38(11)
N(5)-Cd(1)-N(1)	154.13(10)	N(1)-Cd(1)-N(2)	69.99(10)
N(3)-Cd(1)-N(1)	107.41(11)	N(4)-Cd(1)-N(2)	153.26(12)
N(5)-Cd(1)-N(4)	107.80(11)	N(5)-Cd(1)-N(6)	70.25(11)
N(3)-Cd(1)-N(4)	71.08(11)	N(1)-Cd(1)-N(6)	94.04(11)
N(1)-Cd(1)-N(4)	92.52(11)	N(4)-Cd(1)-N(6)	91.29(11)
N(5)-Cd(1)-N(2)	95.32(11)	N(2)-Cd(1)-N(6)	109.45(11)
N(3)-Cd(1)-N(6)	152.40(12)		
2			
Ni(1)-O(1*w*)	2.046(2)	Ni(1)-N(1)	2.143(3)
Ni(1)-O(2*w*)	2.046(2)		
O(1*w*)-Ni(1)-O(2*w*)	88.88(11)	O(1*w*)-Ni(1)-N(1)	93.44(11)
O(2*w*)-Ni(1)-N(1)	89.23(11)		
3			
Zn(1)-O(4)	2.083(2)	Zn(1)-O(1)	2.132(3)
Zn(1)-N(4)	2.101(3)	Zn(1)-O(2)	2.350(3)
Zn(1)-O(5)	2.114(2)	Zn(1)-N(5)^{a}	2.086(3)
O(4)-Zn(1)-N(4)	91.06(11)	N(4)-Zn(1)-O(5)	87.04(11)
O(4)-Zn(1)-O(5)	176.04(10)	O(4)-Zn(1)-O(1)	90.21(11)
N(4)-Zn(1)-O(1)	105.03(12)	O(5)-Zn(1)-O(1)	86.93(11)
O(4)-Zn(1)-O(2)	85.59(11)	N(4)-Zn(1)-O(2)	161.70(12)
O(5)-Zn(1)-O(2)	95.14(11)	O(1)-Zn(1)-O(2)	57.08(11)
N(5)^{a}-Zn(1)-N(4)	106.62(12)		
^{a}x, -y+1/2, z+1/2			
4			
Cd(1)-N(3)	2.345(5)	Cd(1)-N(4)	2.365(5)
Cd(1)-N(1)	2.356(5)	Cd(1)-N(5)	2.371(5)
Cd(1)-N(6)	2.359(4)		

N(3)-Cd(1)-N(1)	83.4(2)	N(6)-Cd(1)-N(2)	97.7(2)
N(3)-Cd(1)-N(6)	165.3(2)	N(4)-Cd(1)-N(2)	160.4(2)
N(1)-Cd(1)-N(6)	93.0(2)	N(3)-Cd(1)-N(5)	90.9(2)
N(3)-Cd(1)-N(4)	70.6(2)	N(1)-Cd(1)-N(5)	164.9(2)
N(1)-Cd(1)-N(4)	94.4(2)	N(6)-Cd(1)-N(5)	95.8(2)
N(6)-Cd(1)-N(4)	95.5(2)	N(4)-Cd(1)-N(5)	96.9(2)
N(3)-Cd(1)-N(2)	94.5(2)	N(2)-Cd(1)-N(5)	96.1(2)
N(1)-Cd(1)-N(2)	70.6(2)		
5			
Cd(1)-O(1)	2.303(2)	Cd(1)-N(2)	2.360(3)
Cd(1)-N(1)	2.365(2)	Cd(1)-N(3)^{b}	2.316(3)
O(1)-Cd(1)-O(1)^{a}	173.51(12)	O(1)-Cd(1)-N(3)^{b}	86.75(6)
O(1)-Cd(1)-N(2)	93.25(6)	O(1)-Cd(1)-N(1)^{a}	91.40(8)
O(1)-Cd(1)-N(1)	89.20(8)	N(3)^{b}-Cd(1)-N(1)	95.28(6)
N(2)-Cd(1)-N(1)	84.72(6)	N(1)^{a}-Cd(1)-N(1)	169.45(11)
^{a}-*x*+1, *y*, -*z*+1/2; ^{b}*x*, *y*+1, *z*			
6			
Co(1)-O(1*w*)	2.058(2)	Co(1)-N(1)	2.223(2)
Co(1)-N(2)	2.168(3)	Co(1)-N(3)#2	2.185(3)
O(1*w*)-Co(1)-O(1*w*)^{a}	174.27(10)	N(1)^{a}-Co(1)-N(1)	170.55(10)
O(1*w*)-Co(1)-N(2)	87.14(5)	N(2)-Co(1)-N(1)	94.72(5)
O(1*w*)-Co(1)-N(3)^{b}	92.86(5)	N(2)-Co(1)-N(3)^{b}	180.0
O(1*w*)-Co(1)-N(1)	89.62(8)	N(3)^{b}-Co(1)-N(1)	85.28(5)
^{a}-*x*+1, *y*, -*z*+1/2; ^{b}*x*, *y*-1, *z*;			
7			
Cd(1)-N(1)	2.267(2)	Cd(1)-O(2)	2.308(2)
Cd(1)-C(8)	2.753(2)	Cd(1)-O(1)	2.464(2)
N(1)^{a}-Cd(1)-N(1)	111.89(11)	O(2)-Cd(1)-O(1)	53.51(7)
N(1)-Cd(1)-O(2)	132.13(8)	N(1)-Cd(1)-C(8)	100.83(7)
O(1)-Cd(1)-C(8)	146.06(8)	N(1)-Cd(1)-O(1)	84.14(7)
O(2)-Cd(1)-C(8)	103.82(7)		
^{a}-*x*, *y*, -*z*+1/2			

Table S2. Hydrogen bonds for 1-7. [Å and °].

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(DHA)	Symmetry transformations for acceptor
1					
C(24)-H(24)···O(2)	0.93	2.56	3.390(6)	149.2	-*x*+1, -*y*+1, -*z*
C(21)-H(21)···O(6)	0.93	2.53	3.279(13)	137.8	-*x*+1, -*y*+1, -*z*+1
C(17)-H(17)···O(6)	0.93	2.50	3.405(16)	163.1	*x*+1, *y*+1, *z*
C(7)-H(7)···O(4)	0.93	2.51	3.396(6)	159.2	*x*, *y*, *z*
2					
N(1)-H(1C)···O(4)	0.89	2.26	3.105(7)	158.7	*x*, -*y*+3/2, *z*+1/2
N(1)-H(1C)···O(3)	0.89	2.40	3.224(13)	153.9	-*x*+2, *y*+1/2, -*z*+3/2
N(1)-H(1D)···O(1)	0.89	2.29	3.100(6)	151.8	-*x*+2, -*y*+1, -*z*+1
N(1)-H(1D)···O(2)	0.89	2.33	3.119(7)	148.4	*x*, *y*, *z*
N(2)-(2N)···O(3*w*)	0.86	2.35	3.119(6)	147.6	*x*, -*y*+3/2, *z*+1/2

O(1*w*)-H(1*w*1)···O(2)	0.81(2)	2.25(4)	2.813(8)	127(4)	-*x*+2, -*y*+1, -*z*+2
O(1*w*)-H(1*w*1)···O(4)	0.81(2)	1.96(2)	2.739(6)	159(4)	*x*, *y*, *z*+1
O(1*w*)-H(2*w*1)···O(3*w*)	0.85(2)	1.88(2)	2.713(4)	168(4)	-*x*+1, *y*-1/2, -*z*+3/2
O(2*w*)-H(1*w*2)···O(2)	0.85(2)	1.79(3)	2.606(7)	161(5)	-*x*+2, *y*-1/2, -*z*+3/2
O(2*w*)-H(1*w*2)···O(3)	0.85(2)	1.98(2)	2.790(10)	159(4)	*x*, -*y*+1/2, *z*+1/2
O(2*w*)-H(2*w*2)···O(1)	0.82(2)	1.91(2)	2.688(6)	160(4)	-*x*+2, -*y*+1, -*z*+1
O(2*w*)-H(2*w*2)···O(3)	0.82(2)	2.30(3)	3.086(15)	160(4)	*x*, *y*, *z*
O(3*w*)-H(1*w*3)···N(2)	0.87(2)	2.05(3)	2.849(5)	152(5)	*x*, *y*, *z*
O(3*w*)-H(2*w*3)···O(1)	0.87(2)	1.91(2)	2.775(8)	172(5)	*x*-1, *y*, *z*
O(3*w*)-H(2*w*3)···O(3)	0.87(2)	2.11(3)	2.841(12)	141(4)	-*x*+1, -*y*+1, -*z*+1
3					
N(4)-H(4A)···O(7)	0.89	2.08	2.935(4)	159.8	*x*, *y*, *z*
N(4)-H(4B)···O(8)	0.89	2.08	2.970(5)	174.9	-*x*+1/2, *y*-1/2, *z*
N(5)-H(5A)···O(8)	0.89	2.09	2.940(4)	159.6	*x*, -*y*+3/2, *z*-1/2
N(5)-H(5B)···O(7)	0.89	2.08	2.967(5)	170.7	-*x*+1/2, -*y*+1, *z*-1/2
C(2)-H(2C)···O(6)	0.96	2.48	3.356(6)	151.2	*x*, *y*-1, *z*
4					
N(5)-H(5A)···O(2)	0.89	2.01	2.87(3)	162.6	*x*, -*y*+3/2, *z*+1/2
N(5)-H(5A)···O(2A)	0.89	2.27	3.14(3)	165.7	*x*, -*y*+3/2, *z*+1/2
N(5)-H(5B)···O(6)	0.89	2.29	3.159(7)	165.5	-*x*, *y*+1/2, -*z*+3/2
N(6)-H(6A)···O(3)	0.89	2.27	3.13(3)	164.5	*x*, -*y*+3/2, *z*+1/2
N(6)-H(6A)···O(3A)	0.89	2.02	2.87(2)	160.1	*x*, -*y*+3/2, *z*+1/2
N(6)-H(6B)···O(7)	0.89	2.29	3.156(7)	163.4	-*x*+1, *y*+1/2, -*z*+3/2
C(1)-H(1)···O(8)	0.93	2.58	3.414(10)	149.4	-*x*+1, *y*+1/2, -*z*+3/2
C(9)-H(9)···O(1A)	0.93	2.42	3.133(11)	133.0	-*x*, -*y*+1, -*z*+1
C(14)-H(14)···O(8)	0.93	2.50	3.369(10)	155.9	*x*, -*y*+3/2, *z*+1/2
C(19)-H(19)···O(4)	0.93	2.48	3.18(2)	131.8	-*x*+1, -*y*+2, -*z*+1
5					
O(1)-H(1*w*)···N(4)	0.87(2)	1.90(2)	2.770(4)	176(3)	*x*, *y*, *z*
O(1)-H(2*w*)···O(2)	0.87(2)	1.98(2)	2.842(9)	177(4)	*x*, *y*, *z*
N(4)-H(1N4)···O(3)	0.85(2)	2.27(2)	3.110(9)	172(5)	-*x*+1/2, *y*+1/2, -*z*+1/2
N(4)-H(2N4)···O(1SS)	0.87(2)	2.19(3)	2.989(13)	151(4)	-*x*+1/2, -*y*+1/2, -*z*+1
6					
O(1*w*)- H(1*w*1)···F(1)	0.86(2)	1.92(2)	2.771(9)	167(3)	*x*, *y*-1, *z*
O(1*w*)-H(2*w*1)···F(1B)	0.86(2)	2.24(3)	3.07(2)	161(3)	*x*, *y*-1, *z*
O(1*w*)-H(1*w*1)···F(4B)	0.86(2)	2.28(3)	3.002(11)	142(3)	*x*, *y*-1, *z*
O(1*w*)-H(2*w*1)···N(4)	0.84(2)	1.92(2)	2.730(4)	167(3)	*x*, *y*, *z*
N(4)-H(1N)···O(1S)	0.88(2)	2.40(3)	3.20(2)	151(4)	*x*, *y*, *z*
N(4)-H(1N)···O(2S)	0.88(2)	2.07(2)	2.893(8)	154(4)	*x*, *y*, *z*
N(4)-H(2N)···F(4)	0.85(2)	2.20(2)	3.022(10)	164(4)	-*x*+3/2, *y*-1/2, -*z*+1/2
N(4)-H(2N)···F(3B)	0.85(2)	2.47(3)	3.29(2)	162(4)	-*x*+3/2, *y*-1/2, -*z*+1/2
C(17)-H(17)···F(2)	0.93	2.55	3.457(11)	163.8	-*x*+3/2, *y*-1/2, -*z*+1/2
C(17)-H(17)···F(4B)	0.93	2.50	3.371(10)	156.6	-*x*+3/2, *y*-1/2, -*z*+1/2
O(1S)-H(1S)···F(2)	0.82	2.25	2.94(2)	141.7	*x*, *y*-1, *z*
7					
N(1)-H(1N)···O(2)	0.84(2)	2.07(2)	2.884(3)	166(3)	-*x*, *y*+1, -*z*+1/2
N(1)-H(2N)···O(4)	0.86(2)	2.14(2)	2.953(3)	159(3)	*x*, -*y*+1, *z*-1/2
O(3)-H(1O)···O(1)	0.82	1.78	2.602(3)	174.4	*x*, -*y*+1, *z*+1/2

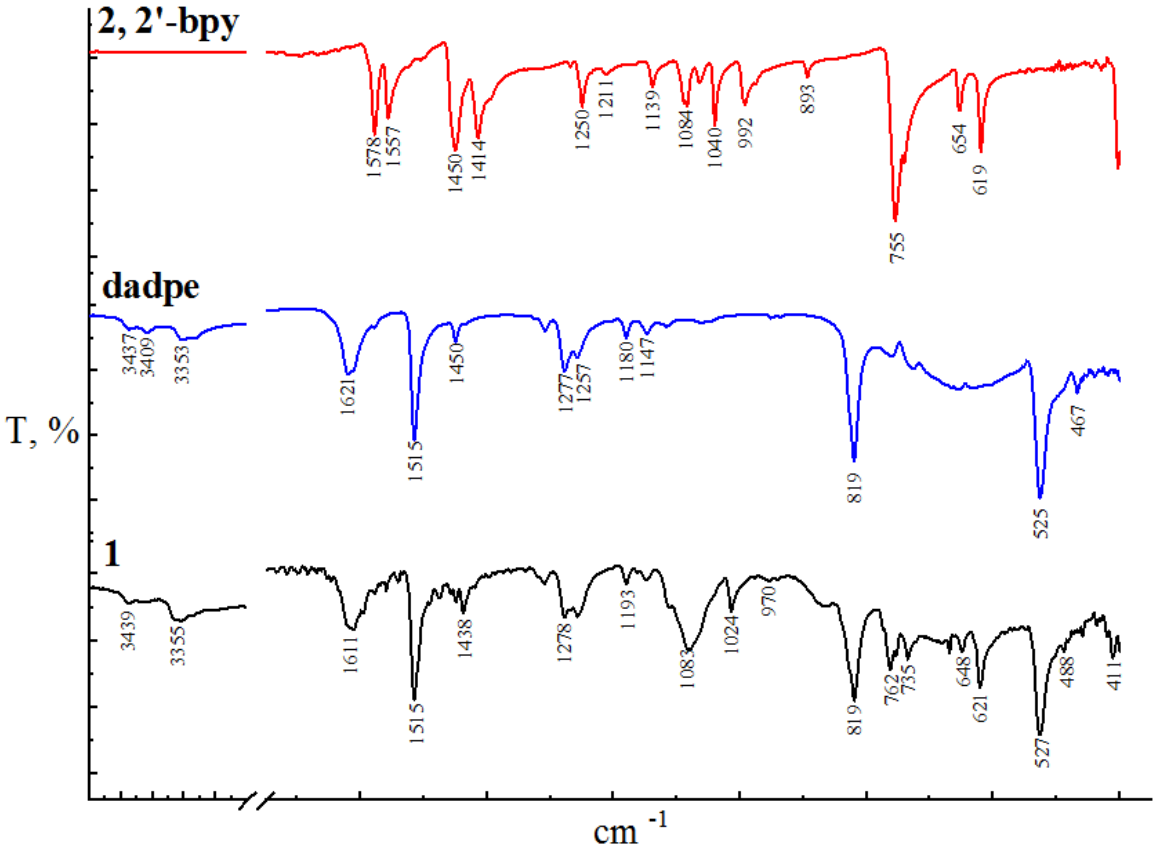


Figure S1. IR spectra for $[Cd(2,2'\text{-bpy})_3](ClO_4)_2](dadpe)(4,4'\text{-bpy})$ (**1**) and starting ligands

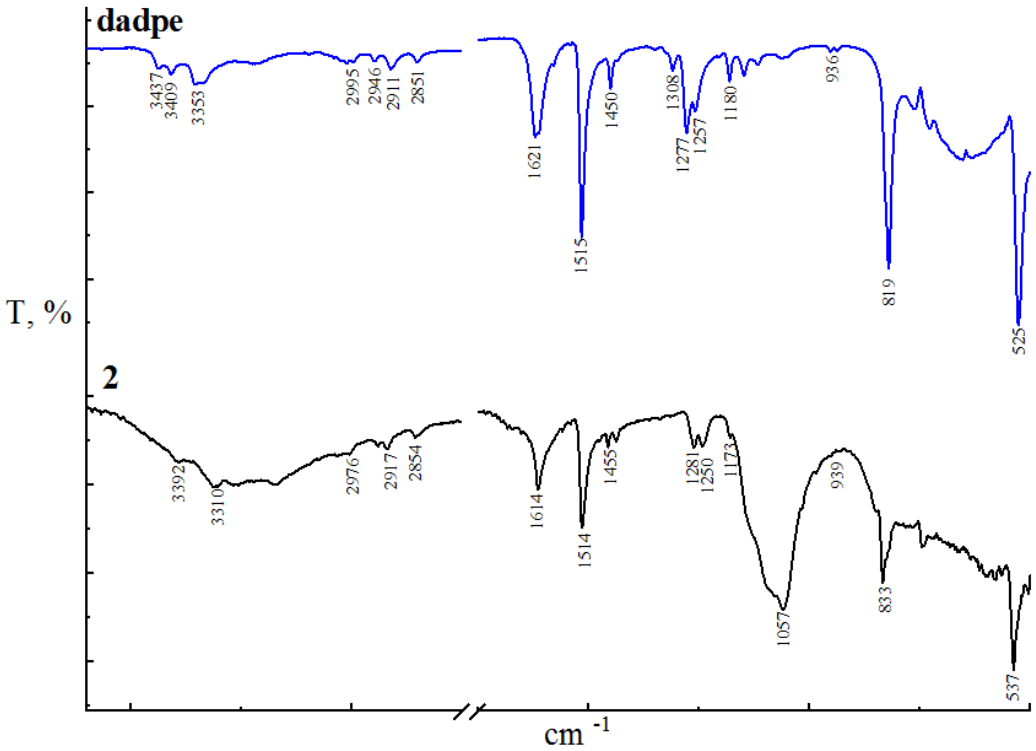


Figure S2. IR spectra for $[Ni(dadpe)_2(H_2O)_4](SO_4)\cdot H_2O$ (**2**) and dadpe ligand

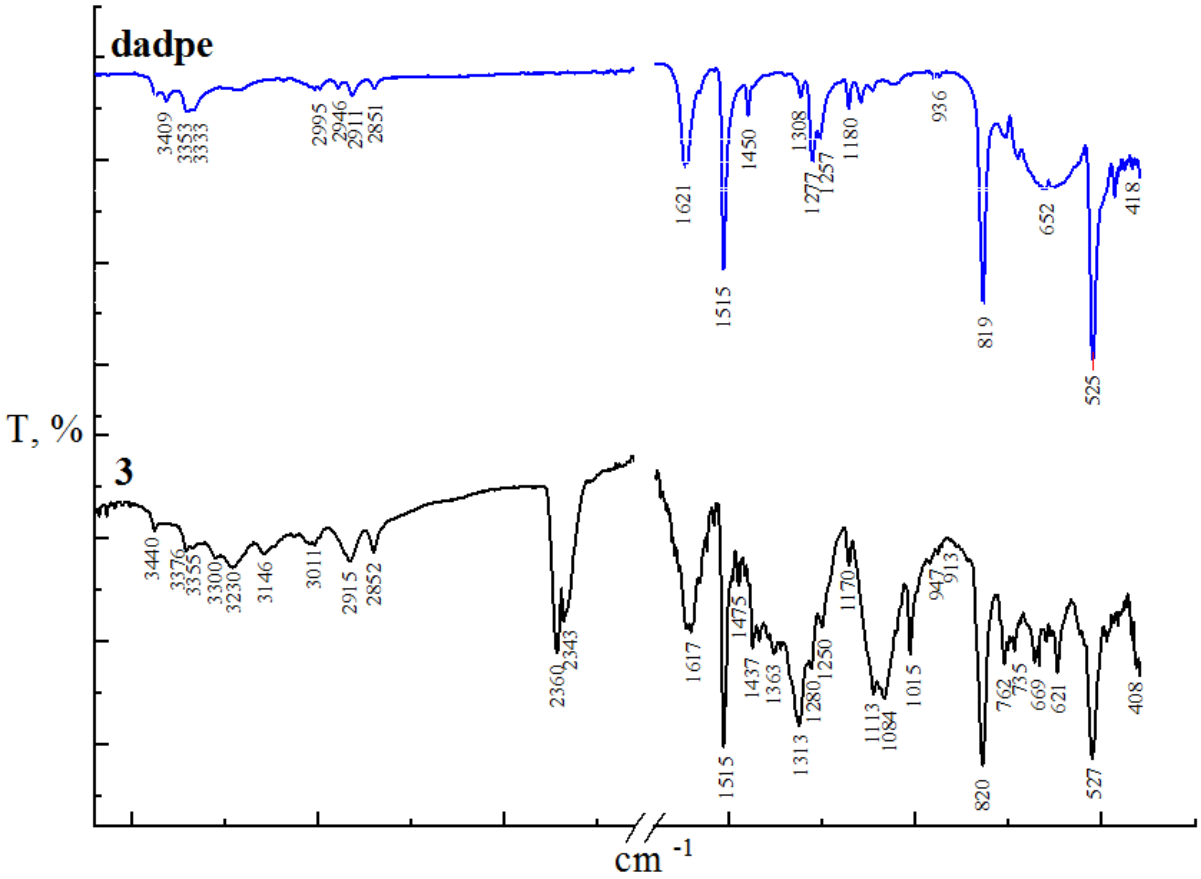


Figure S3. IR spectra for {[Zn(NO_3)(dadpe)($dmf)_2$](NO_3)}n (**3**) and dadpe ligand

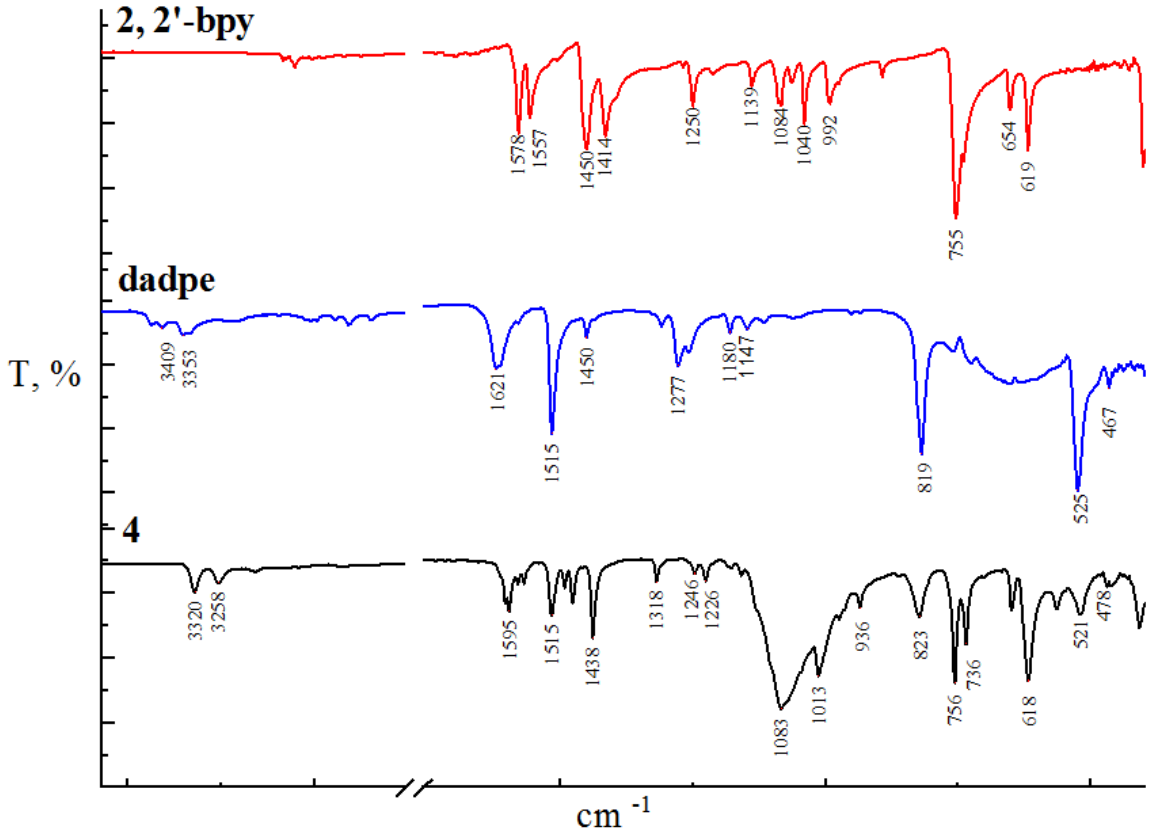


Figure S4. IR spectra for {[Cd(2,2′-bpy)$_2$(dadpe)]($ClO_4)_2$}$_n$ (**4**) and ligands

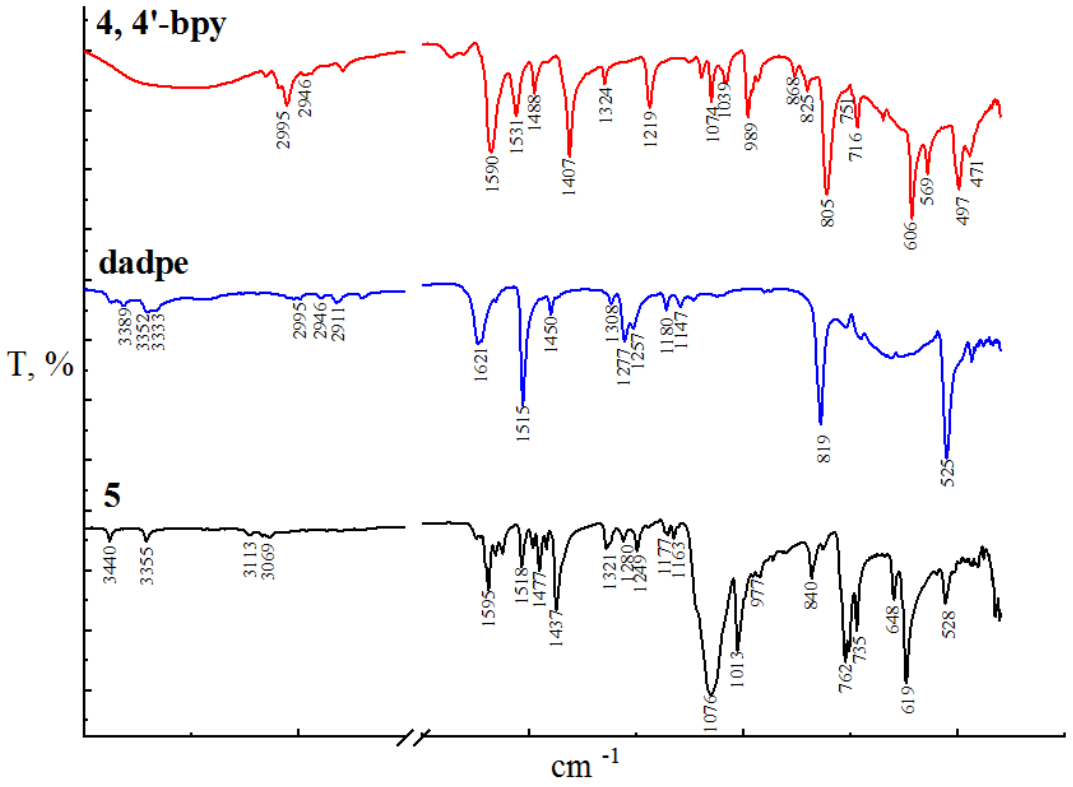


Figure S5. IR spectra for $\{[Cd(4,4'\text{-bpy})_2(H_2O)_2](ClO_4)_2(dadpe)(EtOH)_2\}_n$ (**5**) and ligands

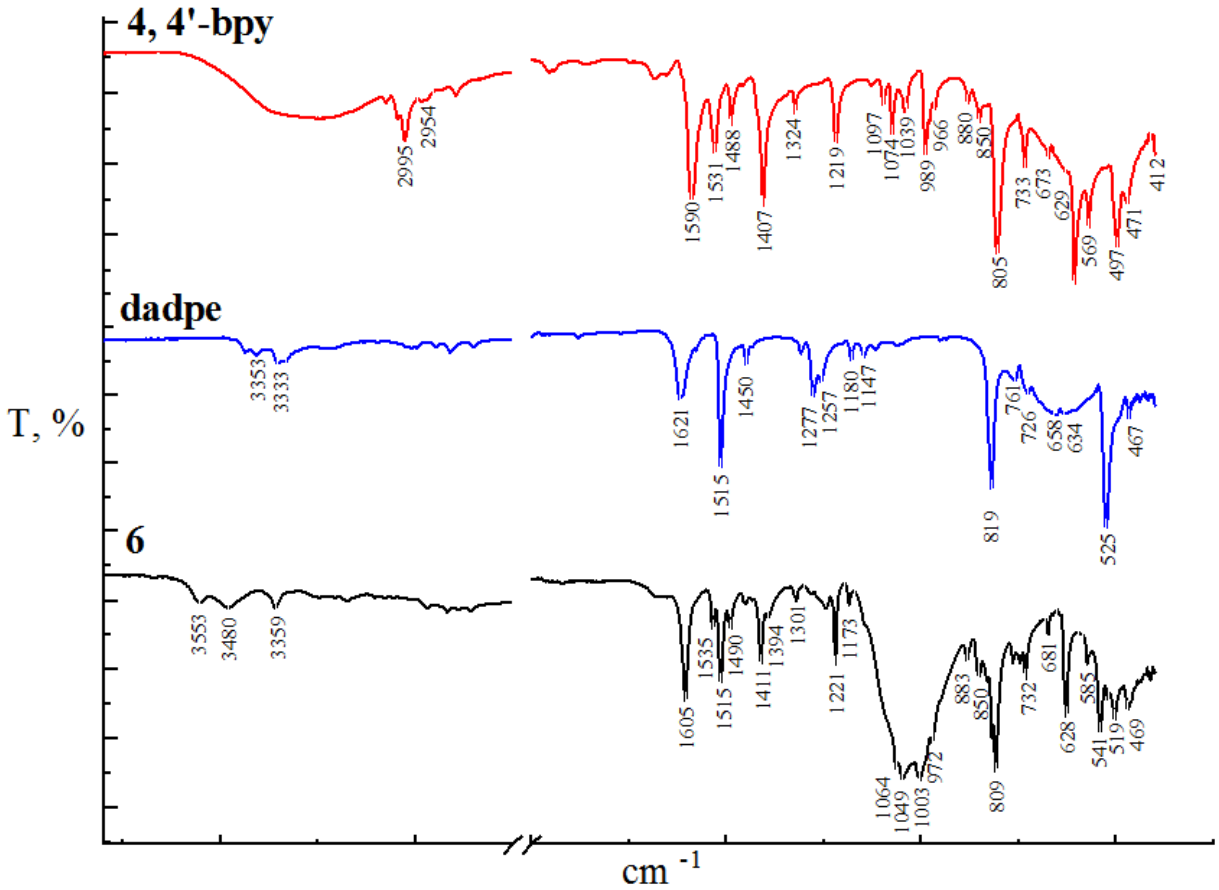


Figure S6. IR spectra for $\{[Co(4,4'\text{-bpy})_2(H_2O)_2](BF_4)_2(dadpe)(EtOH)_2\}_n$ (**6**) and ligands

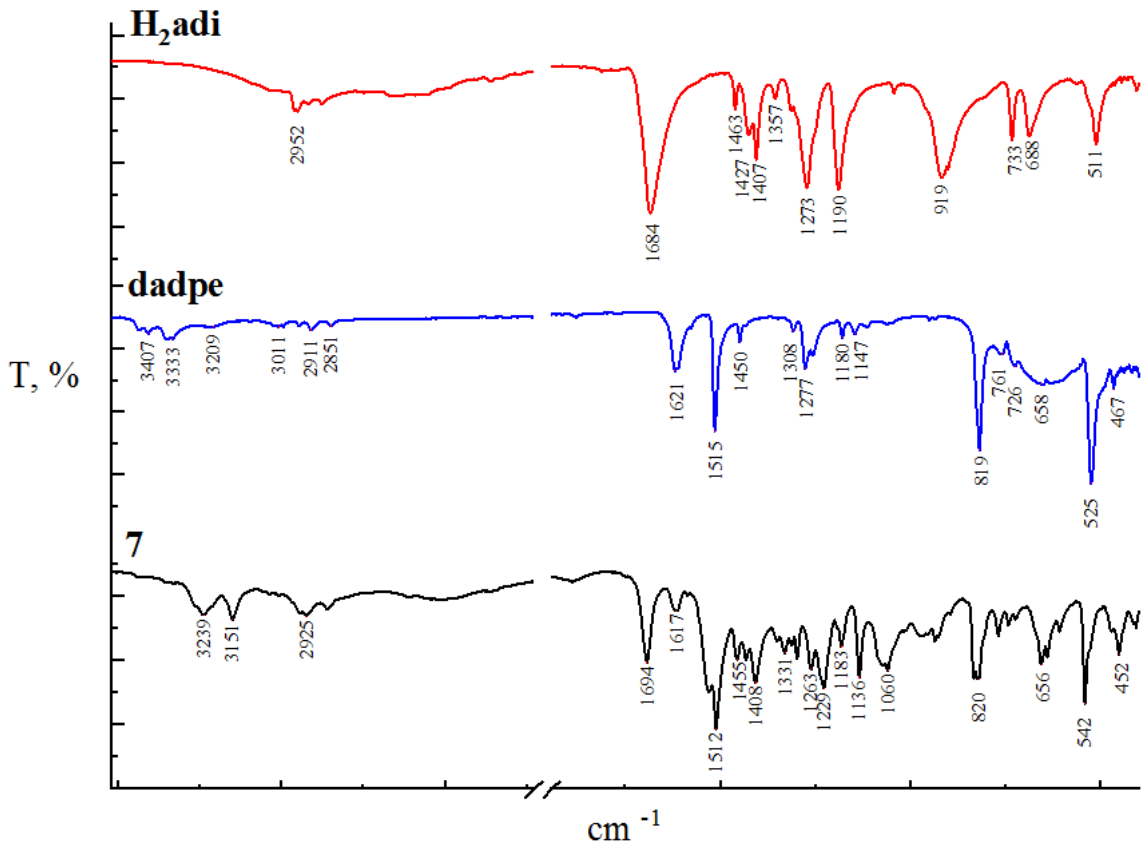


Figure S7. IR spectra for {[Cd(adi)(dadpe)](H_2adi)}$_n$ (**7**) and ligands

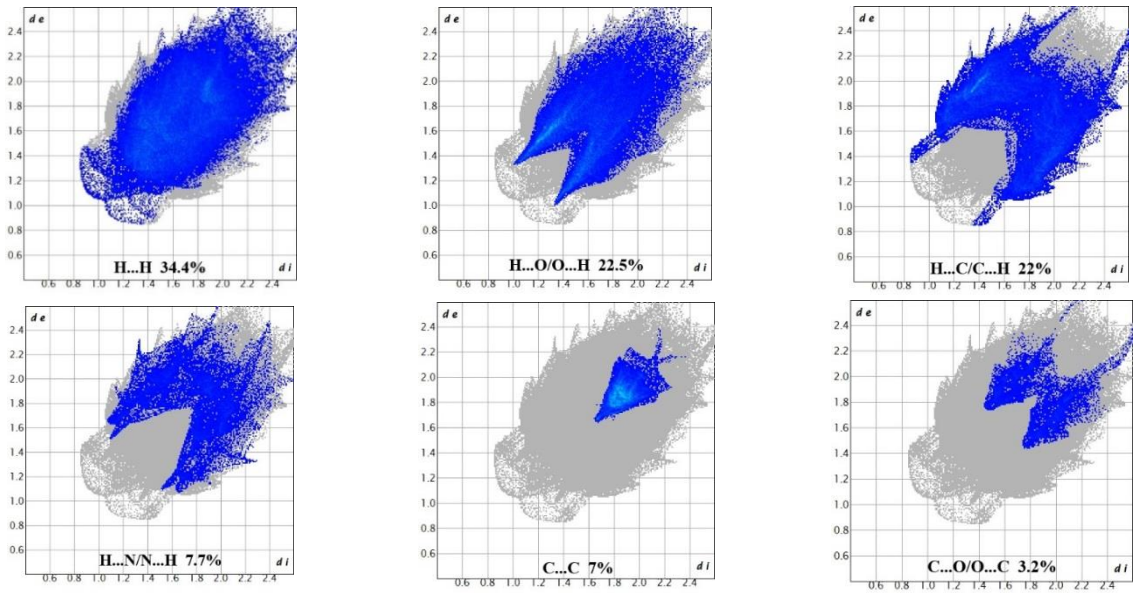


Figure S8. 2D fingerprint plots of contacts in **1**

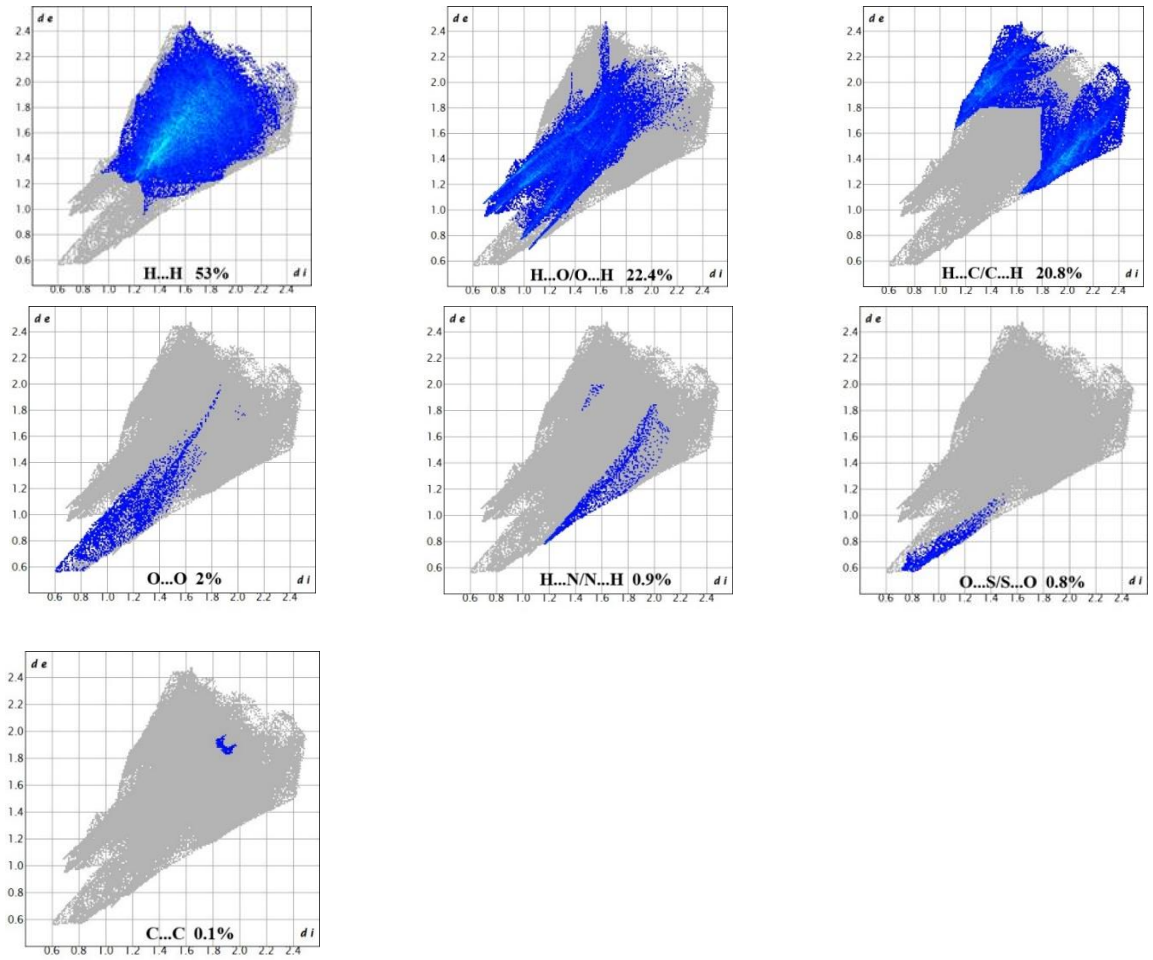
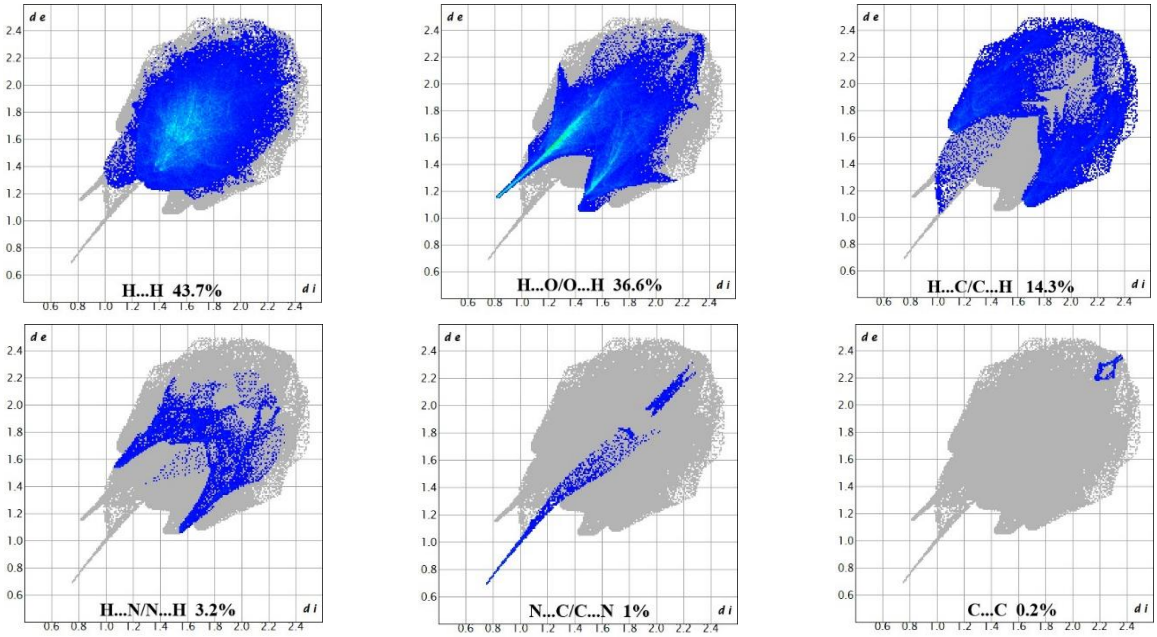


Figure S9. 2D fingerprint plots of contacts in **2**



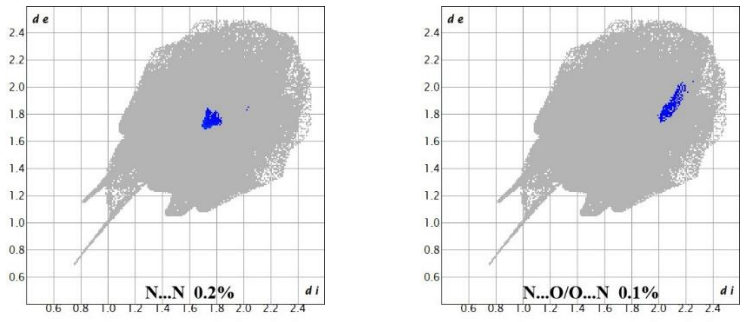


Figure S10. 2D fingerprint plots of contacts in **3**

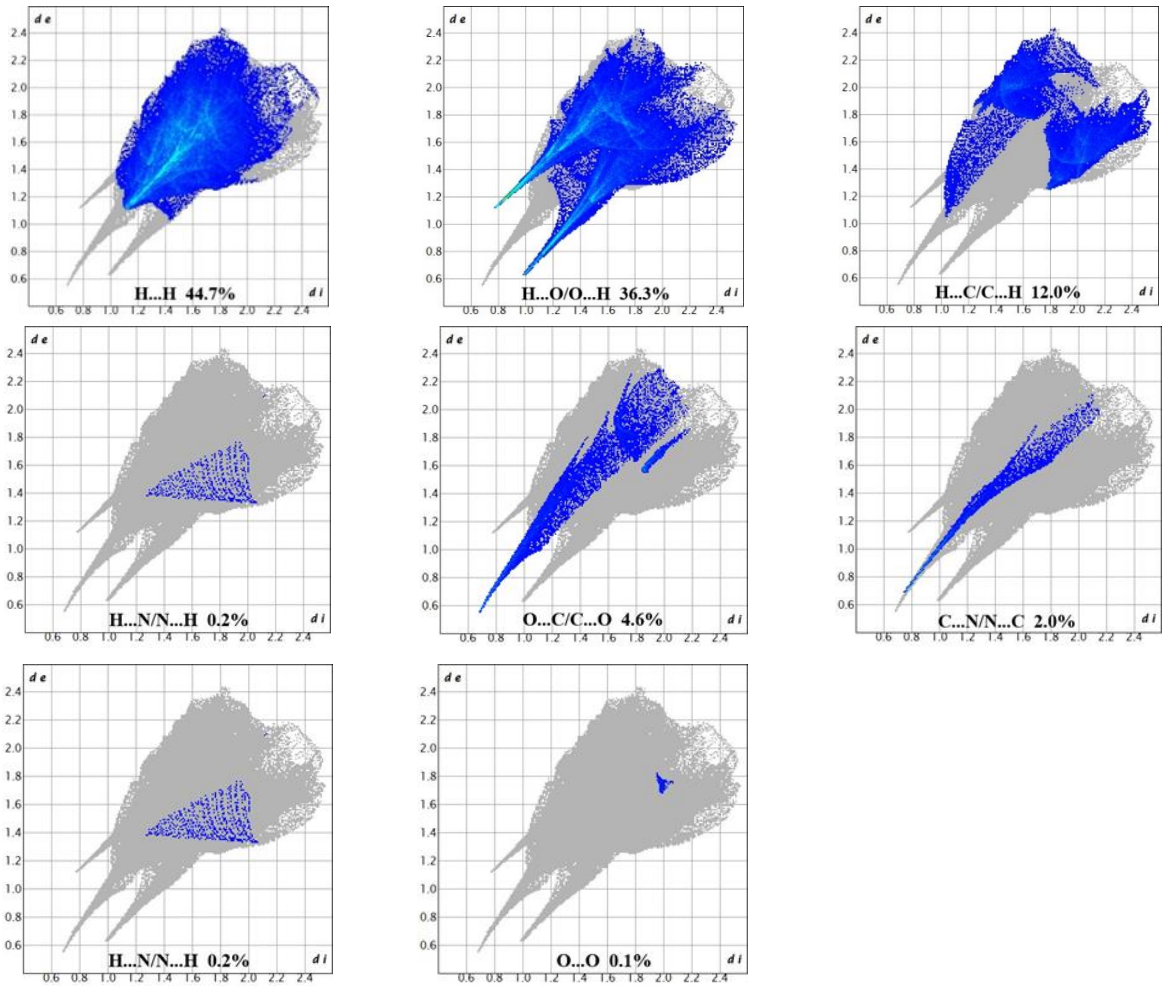


Figure S11. 2D fingerprint plots of contacts in **7**