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Solvent induced mononuclear and dinuclear mixed ligand Cu(II) complex: Structural diversity, supramolecular packing polymorphism and molecular docking studies

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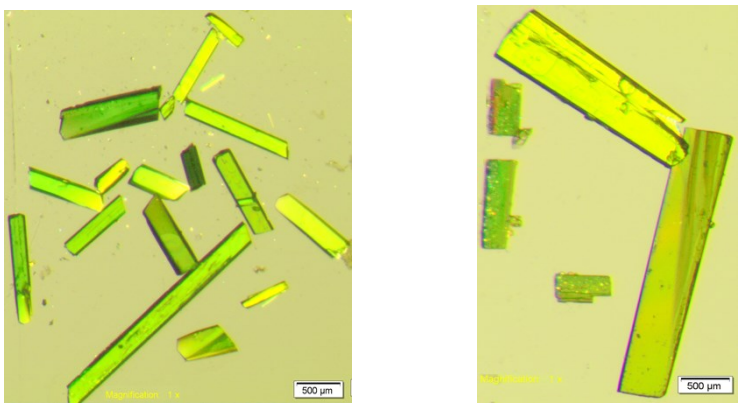

Figure S1: (a) Single crystals of the polymorph **1** and **2**.

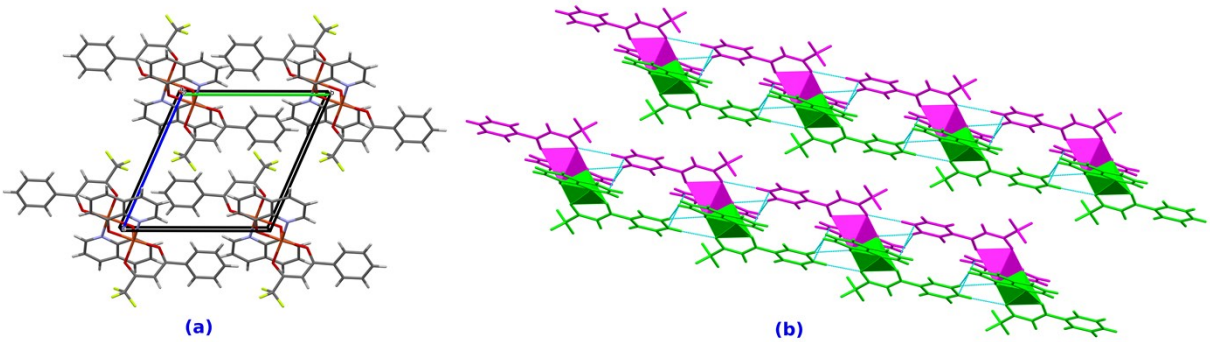

Figure S2: (a) The projection of crystal packing of along *b*-axis (b) an infinite 1-D chain packing of polymorph **1**.

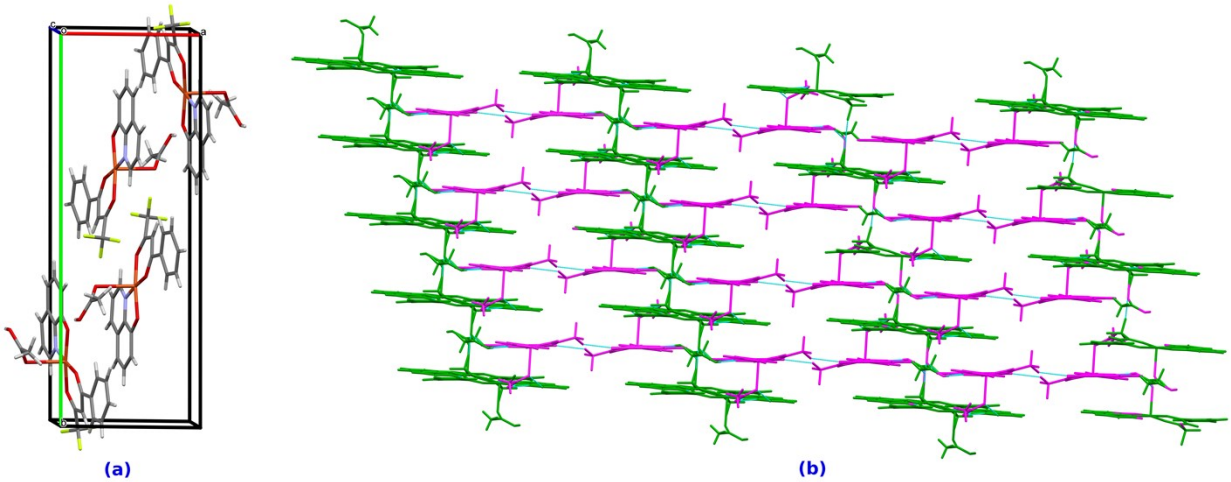

Figure S3: (a) The projection of crystal packing along *c*-axis (b) 2-D ladder like architecture of polymorph **2**.

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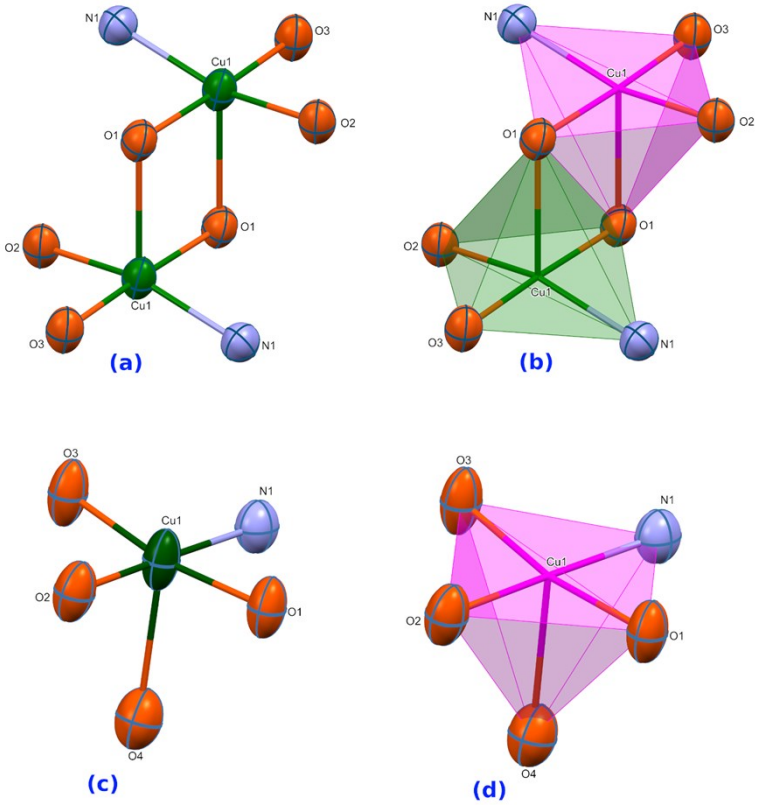

Figure S4: Square pyramidal geometry by (a) doubly phenoxide oxygen bridged dimer in polymorph **1** and (b) apically coordinated acetic acid molecule in polymorph **2**.

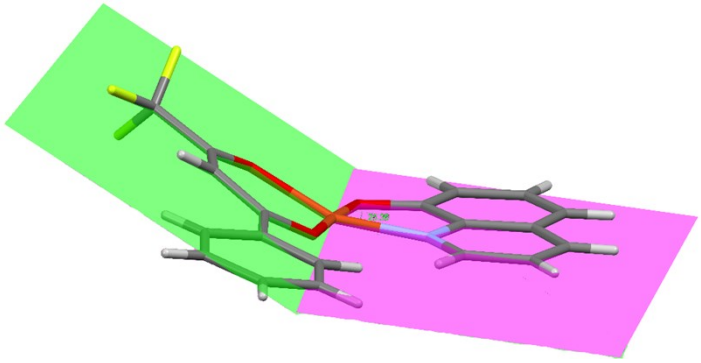

Figure S5: Envelope conformation of Cu(II) complex in polymorph **1**.

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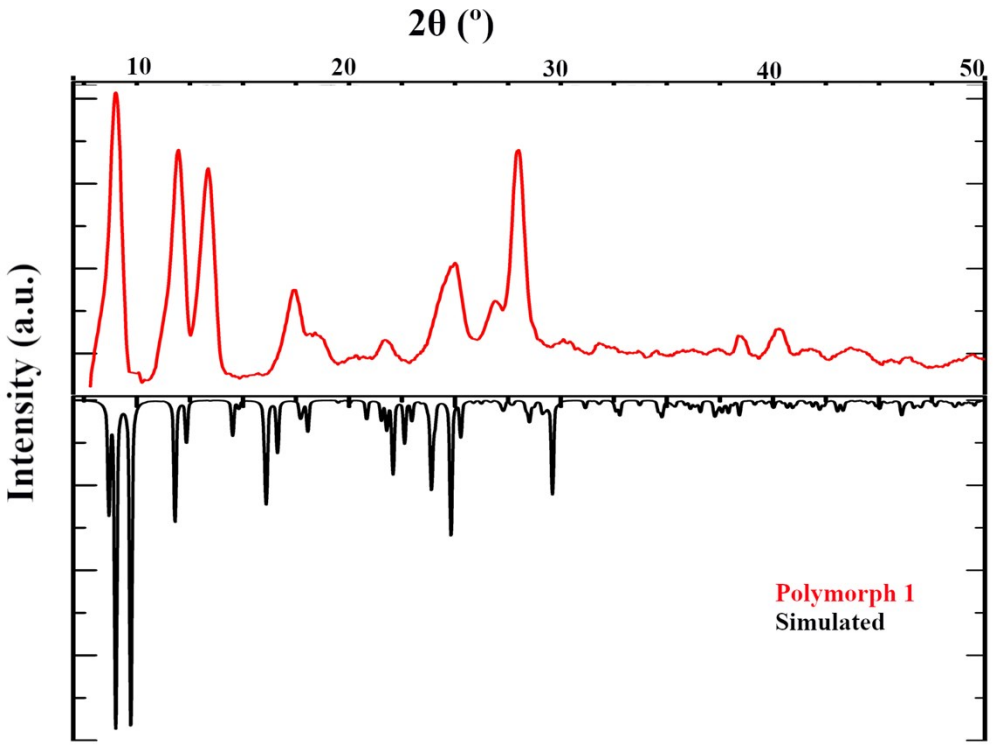

Figure S6a: PXRD pattern of polymorph **1**.

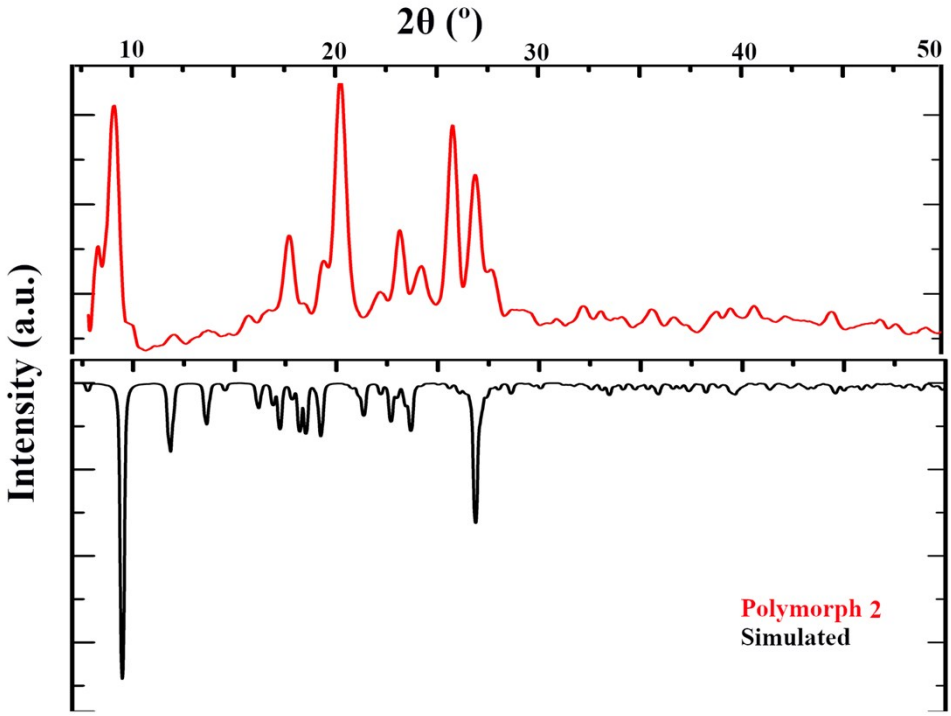

Figure S6b: PXRD pattern of polymorph **2**.

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Table S1: Bond lengths comparison of polymorph **1** and **2** (XRD and DFT).

No.	Polymorph **1**		XRD	DFT		Polymorph **2**		XRD	DFT
1	Cu1	O1	1.944(3)	2.1569		Cu1	O3	1.924(4)	1.9801
2	Cu1	O3	1.930(3)	2.1237		Cu1	O1	1.945(4)	1.9675
3	Cu1	O2	1.955(3)	1.9783		Cu1	O2	1.928(5)	1.9848
4	Cu1	N1	1.978(3)	2.03		Cu1	O4	2.479(4)	2.4366
5	Cu1	O1i	2.387(4)	2.308		Cu1	N1	1.977(5)	2.0215
6	O1	C18	1.328(4)	1.301		O3	C2	1.268(7)	1.2662
7	O1	Cu1i	2.387(4)	2.308		O1	C18	1.332(8)	1.3097
8	O3	C4	1.270(4)	1.258		O2	C4	1.266(8)	1.2639
9	O2	C2	1.272(4)	1.269		C8	C7	1.36(1)	1.3941
10	N1	C19	1.368(5)	1.358		C8	C9	1.38(1)	1.3951
11	N1	C11	1.329(7)	1.326		O4	C21	1.210(9)	1.2141
12	C2	C3	1.374(6)	1.382		N1	C11	1.315(9)	1.3214
13	C2	C1	1.525(7)	1.544		N1	C19	1.367(6)	1.3627
14	C18	C19	1.425(7)	1.445		C11	C12	1.41(1)	1.4092
15	C18	C17	1.391(6)	1.404		O5	C21	1.311(9)	1.3503
16	C19	C14	1.419(5)	1.419		C3	C4	1.428(9)	1.422
17	C4	C5	1.481(6)	1.498		C3	C2	1.37(1)	1.3848
18	C4	C3	1.416(7)	1.429		C4	C5	1.492(9)	1.4949
19	C5	C6	1.395(5)	1.403		C19	C14	1.44(1)	1.4218
20	C5	C10	1.390(8)	1.403		C19	C18	1.391(9)	1.4365
23	C11	C12	1.397(6)	1.406		C14	C15	1.418(8)	1.4156
24	C14	C15	1.409(7)	1.420		C14	C13	1.41(1)	1.4167
25	C14	C13	1.41(1)	1.415		C15	C16	1.34(1)	1.3817
27	C6	C7	1.383(8)	1.393		F1	C1	1.235(9)	1.3497
29	C8	C9	1.364(6)	1.396		C5	C10	1.38(1)	1.4029
30	C8	C7	1.382(8)	1.395		C5	C6	1.38(1)	1.4021
31	C17	C16	1.412(6)	1.404		C16	C17	1.40(1)	1.4089
32	C10	C9	1.373(8)	1.391		C17	C18	1.404(6)	1.3955
33	C15	C16	1.362(9)	1.384		F3	C1	1.29(1)	1.3489
34	C12	C13	1.367(8)	1.378		C2	C1	1.504(9)	1.5428
35	F1	C1	1.321(7)	1.352		C10	C9	1.41(1)	1.3901
36	F2	C1	1.325(8)	1.354		C6	C7	1.37(1)	1.3918
37	F3	C1	1.309(5)	1.349		C1	F2	1.294(9)	1.348
Correlation coefficient			0.9841			**Correlation coefficient**			0.9935

Table S2: Comparison bond angles of polymorph **1** and **2** (XRD and DFT).

No.	Polymorph **1**			XRD	DFT		Polymorph **2**			XRD	DFT
1	O1	Cu1	O3	176.5(1)	171.94		O3	Cu1	O1	170.4(2)	172.49
2	O1	Cu1	O2	91.6(1)	97.36		O3	Cu1	O2	92.4(2)	90.73
3	O1	Cu1	N1	84.3(1)	79.46		O3	Cu1	O4	100.3(2)	91.76
4	O1	Cu1	O1	85.4(1)	86.99		O3	Cu1	N1	90.8(2)	92.86
5	O3	Cu1	O2	91.8(1)	89.31		O1	Cu1	O2	92.5(2)	92.25
6	O3	Cu1	N1	92.5(2)	94.20		O1	Cu1	O4	88.1(2)	95.08
7	O3	Cu1	O1	94.3(1)	99.40		O1	Cu1	N1	84.0(2)	83.22
8	O2	Cu1	N1	159.7(2)	157.56		O2	Cu1	O4	87.8(2)	90.83

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9	O2	Cu1	O1	91.4(1)	94.72		O2	Cu1	N1	176.2(2)	170.99
10	N1	Cu1	O1	108.0(1)	103.90		O4	Cu1	N1	93.5(2)	97.31
11	Cu1	O1	C18	111.3(3)	109.44		Cu1	O3	C2	124.1(4)	124.59
12	Cu1	O1	Cu1	94.6(1)	93.01		Cu1	O1	C18	111.5(4)	112.46
13	C18	O1	Cu1	112.6(3)	116.90		Cu1	O2	C4	128.4(4)	128.44
14	Cu1	O3	C4	129.1(3)	126.73		C7	C8	C9	119.7(8)	119.82
15	Cu1	O2	C2	123.6(3)	125.37		Cu1	O4	C21	118.0(5)	130.13
16	Cu1	N1	C19	110.4(3)	113.21		Cu1	N1	C11	129.1(4)	129.28
17	Cu1	N1	C11	130.7(3)	126.91		Cu1	N1	C19	110.0(4)	110.31
18	C19	N1	C11	118.6(4)	119.67		C11	N1	C19	120.9(5)	120.41
19	O2	C2	C3	129.1(4)	130.68		N1	C11	C12	121.1(6)	121.34
20	O2	C2	C1	112.3(4)	111.49		C4	C3	C2	122.8(6)	122.87
21	C3	C2	C1	118.6(4)	117.8		O2	C4	C3	122.9(6)	124.02
22	O1	C18	C19	118.2(4)	118.5		O2	C4	C5	117.3(5)	116.02
23	O1	C18	C17	124.7(4)	124.1		C3	C4	C5	119.5(5)	119.95
24	C19	C18	C17	117.1(4)	117.4		N1	C19	C14	120.6(5)	122.08
25	N1	C19	C18	115.0(4)	116.5		N1	C19	C18	116.3(5)	115.48
26	N1	C19	C14	122.5(4)	122.1		C14	C19	C18	123.1(5)	122.44
27	C18	C19	C14	122.4(4)	121.4		C19	C14	C15	116.2(6)	118.49
28	O3	C4	C5	116.6(4)	117.3		C19	C14	C13	117.1(6)	116.3
29	O3	C4	C3	122.9(4)	123.9		C15	C14	C13	126.7(6)	125.2
30	C5	C4	C3	120.5(4)	118.8		C14	C15	C16	120.1(6)	118.94
31	C4	C5	C6	122.7(4)	122.3		C4	C5	C10	117.6(6)	118.22
32	C4	C5	C10	119.8(4)	118.7		C4	C5	C6	122.8(6)	122.83
33	C6	C5	C10	117.4(5)	119.0		C10	C5	C6	119.5(6)	118.94
34	C2	C3	C4	123.2(4)	123.8		C15	C16	C17	124.0(6)	122.66
35	N1	C11	C12	122.4(5)	122.1		C16	C17	C18	118.6(6)	120.73
36	C19	C14	C15	117.6(4)	118.7		O3	C2	C3	128.8(6)	129.31
37	C19	C14	C13	116.7(5)	117.1		O3	C2	C1	112.5(5)	112.2
38	C15	C14	C13	125.7(5)	124.2		C3	C2	C1	118.7(6)	118.5
39	C5	C6	C7	120.9(5)	120.4		C5	C10	C9	118.7(6)	120.5
40	C9	C8	C7	119.6(5)	119.8		C5	C6	C7	121.5(7)	120.44
41	C18	C17	C16	120.7(5)	120.8		F1	C1	F3	106.6(7)	107.23
42	C5	C10	C9	121.5(5)	120.6		F1	C1	C2	116.6(7)	113.45
43	C14	C15	C16	120.5(5)	119.8		F1	C1	F2	105.4(7)	107.3
44	C11	C12	C13	119.9(5)	119.3		F3	C1	C2	115.7(7)	110.49
45	C17	C16	C15	121.7(5)	121.9		F3	C1	F2	101.0(7)	107.43
46	C8	C9	C10	120.6(5)	120.1		C2	C1	F2	110.1(6)	110.69
47	C14	C13	C12	119.9(5)	119.8		O4	C21	O5	123.6(7)	120.91
48	C6	C7	C8	120.1(5)	120.2		O4	C21	C20	123.5(7)	126.22
49	C2	C1	F1	111.1(4)	110.9		O5	C21	C20	112.8(6)	112.85
50	C2	C1	F2	111.3(4)	110.5		C14	C13	C12	120.0(6)	120.36
51	C2	C1	F3	114.8(4)	114.2		O1	C18	C19	118.1(5)	118.52
52	F1	C1	F2	104.2(4)	106.9		O1	C18	C17	123.9(5)	124.73
53	F1	C1	F3	107.7(4)	107.1		C19	C18	C17	118.0(5)	116.74
Correlation coefficient				**0.9911**			**Correlation coefficient**				**0.9830**

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Table S3: Comparison of torsion angles of polymorph **1** and **2** (XRD and DFT).

No.	Polymorph **1**				XRD	DFT		Polymorph **2**				XRD	DFT
1	O3	Cu1	O1	C18	-32(2)	23.13		O1	Cu1	O3	C2	-113(1)	-115.59
2	O3	Cu1	O1	Cu1	84(2)	143.07		O2	Cu1	O3	C2	7.4(5)	-2.2
3	O2	Cu1	O1	C18	152.2(3)	142.92		O4	Cu1	O3	C2	95.6(5)	88.65
4	O2	Cu1	O1	Cu1	-91.3(1)	94.37		N1	Cu1	O3	C2	-170.7(5)	-173.94
5	N1	Cu1	O1	C18	-7.8(3)	-15.2		O3	Cu1	O1	C18	-59(1)	-59.48
6	N1	Cu1	O1	Cu1	108.7(1)	104.73		O2	Cu1	O1	C18	-179.7(4)	-172.77
7	O1i	Cu1	O1	C18	-116.5(3)	-119.93		O4	Cu1	O1	C18	92.6(4)	96.19
8	O1	Cu1	O1	Cu1	-0.0(1)	0		N1	Cu1	O1	C18	-1.1(4)	-0.59
9	O1	Cu1	O3	C4	-179(2)	119.24		O3	Cu1	O2	C4	-2.7(5)	2.5
10	O2	Cu1	O3	C4	-3.6(4)	-0.87		O1	Cu1	O2	C4	169.1(5)	175.61
11	N1	Cu1	O3	C4	156.5(4)	156.93		O4	Cu1	O2	C4	-102.9(5)	-89.27
12	O1	Cu1	O3	C4	-95.2(4)	-98.22		N1	Cu1	O2	C4	146(3)	116.02
13	O1	Cu1	O2	C2	-174.2(3)	-168.81		O3	Cu1	O4	C21	-159.0(5)	-149.67
14	O3	Cu1	O2	C2	6.0(4)	4.19		O1	Cu1	O4	C21	25.6(5)	33.42
15	N1	Cu1	O2	C2	-96.3(5)	-95.12		O2	Cu1	O4	C21	-67.0(5)	-58.92
16	O1	Cu1	O2	C2	100.4(3)	103.62		N1	Cu1	O4	C21	109.5(5)	117.22
17	O1	Cu1	N1	C19	7.5(3)	11.18		O3	Cu1	N1	C11	-7.0(5)	-6.28
18	O1	Cu1	N1	C11	-179.0(4)	-174.26		O3	Cu1	N1	C19	173.3(4)	174.25
19	O3	Cu1	N1	C19	-173.9(3)	-163.82		O1	Cu1	N1	C11	-178.9(5)	-179.85
20	O3	Cu1	N1	C11	-0.5(4)	10.75		O1	Cu1	N1	C19	1.4(4)	0.68
21	O2	Cu1	N1	C19	-71.7(5)	-65.46		O2	Cu1	N1	C11	-156(3)	-119.64
22	O2	Cu1	N1	C11	101.8(6)	109.11		O2	Cu1	N1	C19	24(3)	60.89
23	O1	Cu1	N1	C19	90.7(3)	95.38		O4	Cu1	N1	C11	93.4(5)	85.87
24	O1	Cu1	N1	C11	-95.8(4)	-90.05		O4	Cu1	N1	C19	-86.3(4)	-93.6
25	O1	Cu1	O1	Cu1	0.0(1)	0		Cu1	O3	C2	C3	-8.4(9)	1.3
26	O1	Cu1	O1	C18	-115.4(3)	-113.6		Cu1	O3	C2	C1	169.9(4)	-178.94
27	O3	Cu1	O1	Cu1	-176.5(1)	-175.1		Cu1	O1	C18	C19	0.7(6)	0.4
28	O3	Cu1	O1	C18	68.1(3)	71.3		Cu1	O1	C18	C17	179.9(5)	-179.6
29	O2	Cu1	O1	Cu1	91.5(1)	-97.15		Cu1	O2	C4	C3	-1.8(9)	-1.72
30	O2	Cu1	O1	C18	-23.9(3)	-19.23		Cu1	O2	C4	C5	-175.5(4)	179.3
31	N1	Cu1	O1	Cu1	-82.5(2)	-78.37		C9	C8	C7	C6	-4(1)	-0.5
32	N1	Cu1	O1	C18	162.2(3)	168.03		C7	C8	C9	C10	3(1)	-0.1
33	Cu1	O1	C18	C19	6.8(5)	16.89		Cu1	O4	C21	O5	-101.7(7)	179.12
34	Cu1	O1	C18	C17	-174.4(4)	-165.3		Cu1	O4	C21	C20	76.5(8)	0.22
35	Cu1	O1	C18	C19	-98.1(4)	-87.09		Cu1	N1	C11	C12	-178.7(5)	-179.27
36	Cu1	O1	C18	C17	80.8(5)	90.73		C19	N1	C11	C12	0.9(9)	0.15
37	Cu1	O1	Cu1	O1	0.0(1)	0		Cu1	N1	C19	C14	179.0(4)	179.55
38	Cu1	O1	Cu1	O3	176.5(1)	175.1		Cu1	N1	C19	C18	-1.5(6)	-0.66
39	Cu1	O1	Cu1	O2	-91.5(1)	-94.37		C11	N1	C19	C14	-0.6(8)	0.03
40	Cu1	O1	Cu1	N1	82.5(2)	78.37		C11	N1	C19	C18	178.8(5)	179.82
41	C18	O1	Cu1	O1	115.4(3)	113.6		N1	C11	C12	C13	0(1)	-0.16
42	C18	O1	Cu1	O3	-68.1(3)	-71.3		C2	C3	C4	O2	3(1)	-0.22
43	C18	O1	Cu1	O2	23.9(3)	19.23		C2	C3	C4	C5	176.9(6)	178.72
44	C18	O1	Cu1	N1	-162.2(3)	-168.03		C4	C3	C2	O3	2(1)	0.42
45	Cu1	O3	C4	C5	179.8(3)	179.1		C4	C3	C2	C1	-176.0(6)	-179.33
46	Cu1	O3	C4	C3	-0.8(6)	-2.12		O2	C4	C5	C10	14.2(9)	17
47	Cu1	O2	C2	C3	-4.7(7)	-5.15		O2	C4	C5	C6	-165.4(6)	-162.38
48	Cu1	O2	C2	C1	175.3(3)	174.47		C3	C4	C5	C10	-159.8(6)	-162.03
49	Cu1	N1	C19	C18	-5.9(5)	-6.04		C3	C4	C5	C6	20.6(9)	18.6
50	Cu1	N1	C19	C14	174.4(4)	172.22		N1	C19	C14	C15	180.0(5)	179.89
51	C11	N1	C19	C18	179.7(4)	178.96		N1	C19	C14	C13	-0.9(9)	-0.18
52	C11	N1	C19	C14	0.1(7)	-2.78		C18	C19	C14	C15	0.5(9)	0.11

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53	Cu1	N1	C11	C12	-173.3(4)	-172.03	
54	C19	N1	C11	C12	-0.3(7)	2.22	
5	O2	C2	C3	C4	-1.5(8)	1.15	
56	C1	C2	C3	C4	178.5(4)	-178.45	
57	O2	C2	C1	F1	57.8(5)	57.5	
58	O2	C2	C1	F2	-57.9(5)	-60.88	
59	O2	C2	C1	F3	-179.7(4)	178.5	
60	C3	C2	C1	F1	-122.2(5)	-122.83	
61	C3	C2	C1	F2	122.1(5)	118.8	
62	C3	C2	C1	F3	0.3(6)	-1.82	
63	O1	C18	C19	N1	-0.5(6)	-8.26	
64	O1	C18	C19	C14	179.2(4)	173.46	
65	C17	C18	C19	N1	-179.4(4)	173.78	
66	C17	C18	C19	C14	0.2(7)	-4.5	
67	O1	C18	C17	C16	-179.6(4)	-173.77	
68	C19	C18	C17	C16	-0.8(7)	4.06	
69	N1	C19	C14	C15	179.7(4)	-175.75	
70	N1	C19	C14	C13	0.2(7)	1.81	
71	C18	C19	C14	C15	0.1(7)	2.43	
72	C18	C19	C14	C13	-179.4(5)	179.99	
73	O3	C4	C5	C6	-161.8(5)	-155.46	
74	O3	C4	C5	C10	15.3(6)	23.43	
75	C3	C4	C5	C6	18.8(7)	25.69	
76	C3	C4	C5	C10	-164.1(5)	-155.42	
77	O3	C4	C3	C2	4.6(7)	2.82	
78	C5	C4	C3	C2	-176.1(4)	-178.41	
79	C4	C5	C6	C7	178.4(5)	178.89	
80	C10	C5	C6	C7	1.2(8)	0	
81	C4	C5	C10	C9	-179.0(5)	-179.74	
82	C6	C5	C10	C9	-1.8(8)	-0.81	
83	N1	C11	C12	C13	0.3(8)	-0.74	
84	C19	C14	C15	C16	0.2(8)	0.15	
85	C13	C14	C15	C16	179.6(6)	-177.22	
86	C19	C14	C13	C12	-0.2(8)	-0.3	
87	C15	C14	C13	C12	-179.6(6)	177.11	
88	C5	C6	C7	C8	0.2(9)	0.68	
89	C7	C8	C9	C10	0.5(9)	-0.26	
90	C9	C8	C7	C6	-1.1(9)	-0.55	
91	C18	C17	C16	C15	1.1(8)	-1.65	
92	C5	C10	C9	C8	1.0(9)	0.95	
93	C14	C15	C16	C17	-0.8(8)	-0.57	
94	C11	C12	C13	C14	-0.0(9)	-0.22	
Correlation coefficient					**0.9912**		

C18	C19	C14	C13	179.6(6)	-179.96
N1	C19	C18	O1	0.6(8)	0.2
N1	C19	C18	C17	-178.7(5)	-179.8
C14	C19	C18	O1	-179.9(5)	179.99
C14	C19	C18	C17	0.7(9)	-0.01
C19	C14	C15	C16	-0.9(9)	-0.13
C13	C14	C15	C16	-179.9(7)	179.95
C19	C14	C13	C12	2(1)	0.17
C15	C14	C13	C12	-178.8(7)	-179.91
C14	C15	C16	C17	-0(1)	0.05
C4	C5	C10	C9	179.7(6)	179.79
C6	C5	C10	C9	-1(1)	-0.81
C4	C5	C6	C7	178.7(7)	179.58
C10	C5	C6	C7	-1(1)	0.2
C15	C16	C17	C18	1(1)	0.06
C16	C17	C18	O1	179.0(6)	179.93
C16	C17	C18	C19	-1.7(9)	-0.07
O3	C2	C1	F1	161.9(7)	-178.88
O3	C2	C1	F3	35.5(9)	60.68
O3	C2	C1	F2	-78.2(8)	-58.2
C3	C2	C1	F1	-20(1)	0.92
C3	C2	C1	F3	-146.0(7)	-119.53
C3	C2	C1	F2	100.4(8)	121.6
C5	C10	C9	C8	-0(1)	0.77
C5	C6	C7	C8	3(1)	0.45
C14	C13	C12	C11	-2(1)	0
Correlation coefficient				**0.9795**	

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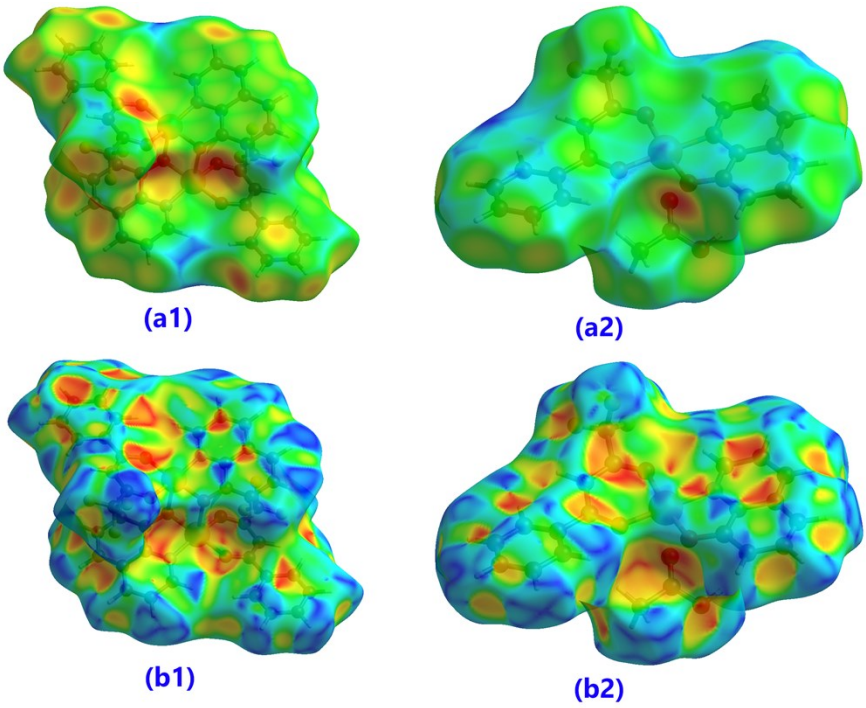

Figure S7 : d_e surface and shape index surface of polymorph **1** (a) and **2** (b).

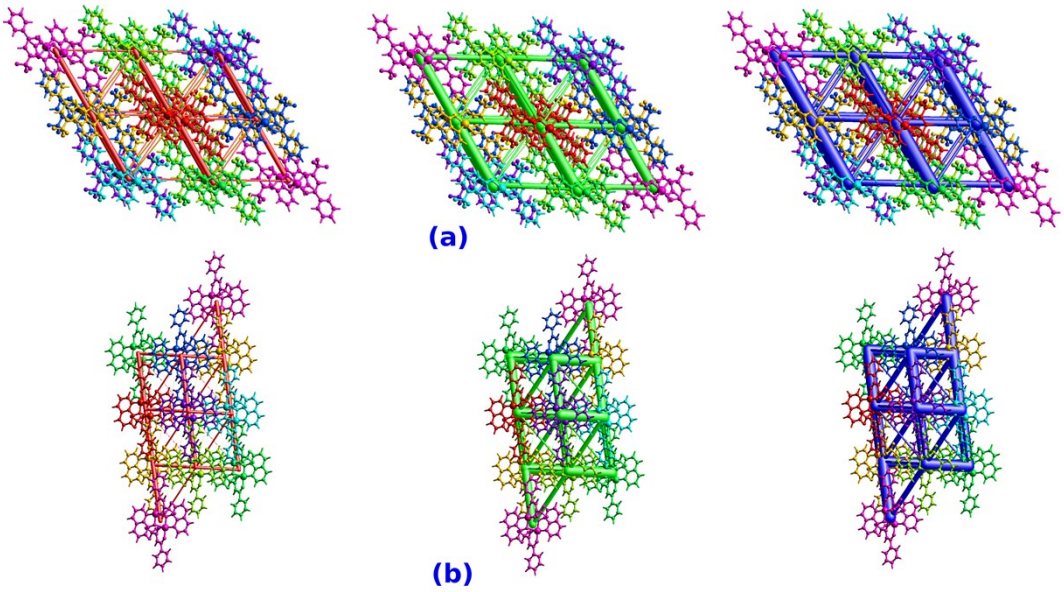

Figure S8: Energy frameworks of polymorph **1** corresponding to the different energy components viewed along *a* and *c*-axis.

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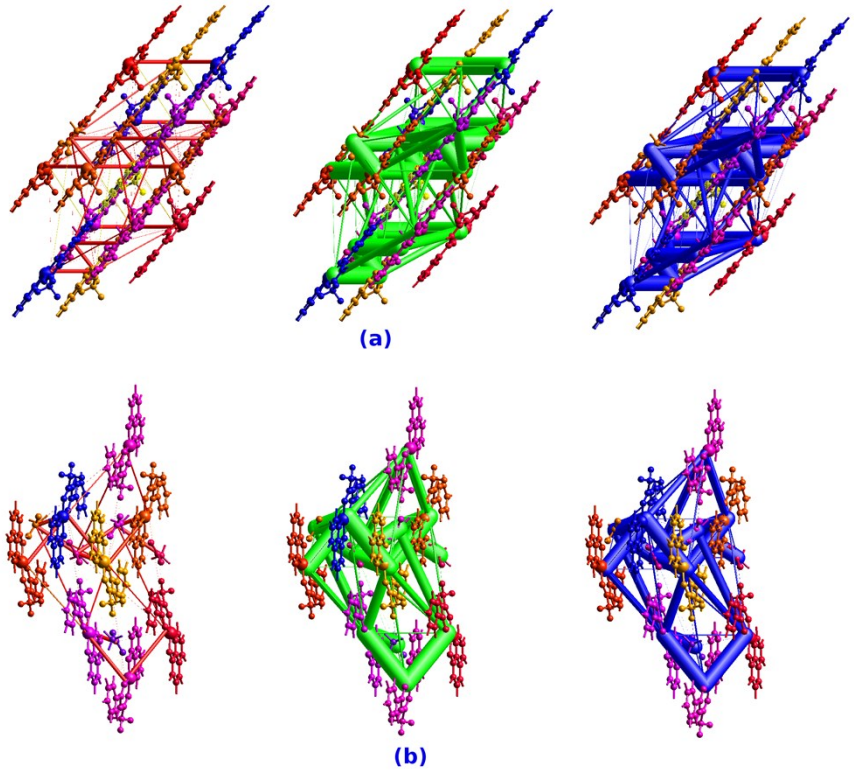

Figure S9: Packing of molecules and energy frameworks corresponding to the different energy components viewed along *a* and *c*-axis for polymorph **2**.

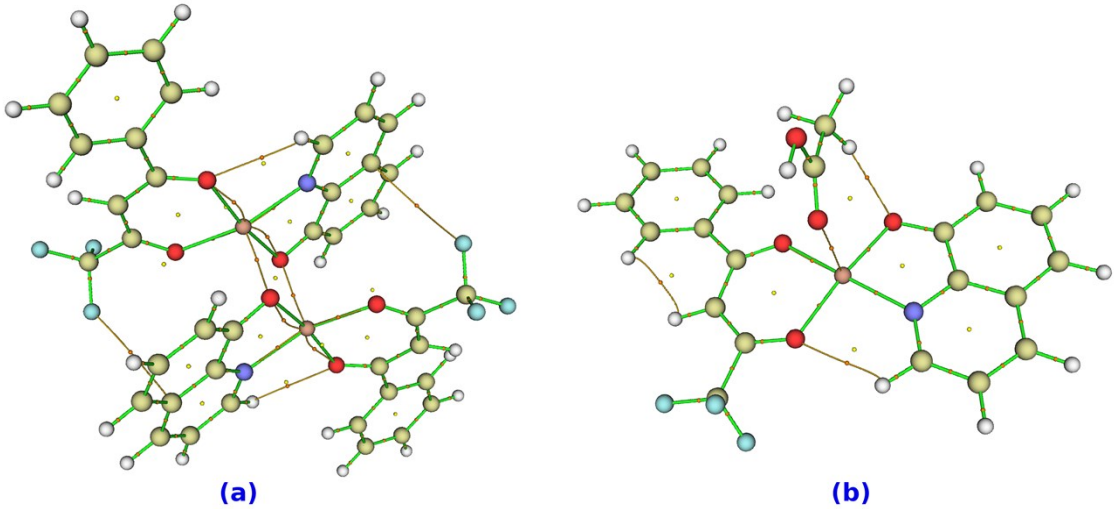

Figure S10: 3D plot of the interactions in the polymorph **1** and **2** showing the connecting bond critical points as orange points.

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Table S4: Mulliken and natural charges of the polymorphs **1** and **2**.

Polymorph 1				Polymorph 2		
Atom	NBO	Mulliken		Atom	NBO	Mulliken
Cu1	0.914	-2.230		Cu1	1.067	-0.420
O1	-0.682	0.222		O1	-0.73	-0.026
O2	-0.641	0.103		O2	-0.652	0.055
O3	-0.651	0.035		O3	-0.668	-0.068
N1	-0.489	0.322		N1	-0.508	0.517
C1	1.031	0.764		O4	-0.616	-0.115
C2	0.402	0.206		O5	-0.679	-0.161
C3	-0.458	-0.981		C1	1.020	0.722
C4	0.511	0.286		C2	0.406	-0.300
C5	-0.110	1.206		C3	-0.451	-0.700
C6	-0.175	-0.910		C4	0.516	-0.093
C7	-0.203	-0.443		C5	-0.119	1.229
C8	-0.186	-0.169		C6	-0.169	-1.137
C9	-0.203	0.291		C7	-0.205	-0.419
C10	-0.163	0.367		C8	-0.18	-0.145
C11	0.103	0.067		C9	-0.203	-0.24
C12	-0.241	-0.452		C10	-0.157	0.608
C13	-0.106	0.222		C11	0.09	-0.125
C14	-0.086	0.540		C12	-0.249	-0.467
C15	-0.194	-0.350		C13	-0.116	-0.123
C16	-0.181	-0.229		C14	-0.079	0.517
C17	-0.232	0.059		C15	-0.25	-0.302
C18	0.362	0.535		C16	-0.166	-0.31
C19	0.162	0.158		C17	-0.276	-0.353
F1	-0.353	-0.041		C18	0.350	-0.028
F2	-0.360	-0.049		C19	0.137	-0.048
F3	-0.348	-0.134		C20	0.692	-0.504
				C21	0.829	0.212
				F1	-0.357	-0.145
				F2	-0.350	-0.068
				F3	-0.350	-0.068