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Table S1. Hydrogen Bonds (Angstrom, Deg)

D-H···A	D-H	H···A	D···A	D-H···A	Symmetry Transformation
Compound 1					
O3--H3A..O4	0.72(5)	2.18(5)	2.898(9)	170(5)	1-x,1-y,1-z
O3--H3B..O2	0.79(5)	1.98(5)	2.756(4)	167(4)	-1+x,y,z
Compound 2					
O3--H3A..O2	0.78(7)	2.00(6)	2.775(6)	172(6)	1/2+x,1/2-y,1/2+z
Compound 3					
O3--H3A..O2	0.83(3)	1.94(3)	2.770(3)	177(7)	-1+x,y,z
O3--H3B..O6	0.85(3)	1.97(3)	2.811(4)	171(5)	.
O6--H6A..O5	0.85(4)	2.23(5)	2.988(5)	149(4)	-1+x,y,z
O6--H6B..O4	0.85(4)	2.15(4)	2.990(5)	170(5)	.
O7--H7A..O4	0.85(5)	1.90(5)	2.727(5)	167(6)	.
O7--H7B..O8	0.85(4)	1.99(3)	2.783(6)	156(6)	2-x,-y,2-z
O8--H8A..O5	0.85(5)	2.02(5)	2.826(5)	157(6)	.
O8--H8B..O7	0.84(6)	2.18(5)	2.815(6)	132(5)	1+x,y,z
Compound 4					
O3--H3A..O10	0.74(5)	1.83(5)	2.560(6)	171(7)	1+x,y,z
O5--H5A..O2	1.10(4)	1.51(4)	2.602(5)	172(3)	-1+x,y,z
O5--H5B..O7	0.79(5)	1.92(5)	2.697(5)	167(5)	x,y,-1+z
O6--H6..O8	0.86(5)	1.53(5)	2.392(6)	173(5)	.
O10--H10A..O2	0.77(5)	1.99(5)	2.753(7)	171(5)	4_455
O10--H10B..O6	0.69(6)	2.16(6)	2.830(6)	166(7)	4_554
Compound 5					
O5--H5A..O2	0.83(5)	2.08(5)	2.858(5)	156(5)	-1+x,y,z
O5--H5B..O4	0.80(5)	1.97(5)	2.726(5)	157(6)	-1+x,y,z
O9--H9..O16	0.80(6)	1.73(7)	2.521(6)	174(9)	.
O10--H10A..O7	0.86(5)	1.97(5)	2.827(4)	171(5)	-1+x,y,z
O10--H10B..O14	0.74(5)	2.27(5)	3.007(5)	178(10)	x,y,1+z
O15--H15A..O3	0.99(6)	1.89(6)	2.872(6)	169(6)	1-x,1/2+y,1-z
O15--H15B..O11	1.00(6)	2.00(6)	2.975(8)	165(6)	.
O16--H16A..O3	0.99(6)	1.79(7)	2.761(6)	164(9)	.
O17--H17A..O4	0.78(9)	2.04(9)	2.806(6)	172(11)	-1+x,y,z
O17--H17B..O16	1.02(8)	2.23(8)	2.636(8)	102(5)	.
Compound 6					
O3--H3A..O2	0.8400	2.0600	2.791(4)	146.00	1+x,y,z
O3--H3B..O6	0.8400	1.8600	2.697(5)	174.00	1+x,y,z
O6--H6A..O7	0.8600	2.3500	2.875(6)	120.00	-1+x,y,z
O6--H6B..O5	0.8600	1.8800	2.734(6)	173.00	.
O7--H7A..O4	0.8500	1.8600	2.701(6)	170.00	.
O7--H7B..O9	0.8400	2.2100	2.786(12)	126.00	.
O9--H9A..O5	0.8500	2.0000	2.855(10)	180.00	.

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Table S2. Analysis of Short Ring-Interactions

- Cg(I) = Plane number I
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-Cg(J) or Cg(I)-Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)

Cg(I)	Cg(J)	Symmetry code	Cg-Cg	Alpha	Gamma	Gamma	CgI_Perp	CgJ_Perp
Compound 1								
N2-C7-C8-C9-C10-C11	N3-C12-C13-C14-C15-C16	1-x, -y, 1-z	3.833(2)	0.53	21.63	22.05	3.552	3.563
Compound 2								
N1-C9-C10-C11-C12-C13	N3-C19-C20-C21-C22-C23	1+x, y, z	3.630(4)	2.71	18.97	18.51	3.442	3.433
C17-C18-C19-C20-C21-C22	C17-C18-C19-C20-C21-C22	-x, 1-y, -z	3.804(4)	0.00	23.65	23.65	3.484	3.485
Compound 3								
N2-C8-C9-C10-C11-C12	N3-C14-C15-C16-C17-C18-	1-x, 1-y, 2-z	3.695(2)	2.02	23.89	24.75	3.355	3.378
N1-C2-C3-C4-C5-C6	C19-C20-C21-C22-C23-C24	1-x,1-y,1-z	3.869(2)	3.22	25.36	28.16	3.411	3.496
Compound 4								
N1-C1-C2-C3-C4-C5	C16-C17-C18-C19-C20-C21	x, y, z	3.703(3)	2.24	22.93	22.95	3.410	3.410
C24-C25-C26-C27-C28-C29	C24-C25-C26-C27-C28-C29	-x, -y, 2-z	3.675(3)	0.03	16.88	16.88	3.517	3.517
Compound 5								
N4-C32-C33-C34-C35-C36	N2-C14-C15-C16-C17-C18	1-x, 1/2+y, 1-z	3.670(3)	0.91	18.58	18.36	3.483	3.479
N3-C19-C20-C21-C22-C23	N5-C37-C38-C39-C40-C41	1-x,1/2+y,1-z	3.714(3)	3.04	19.85	20.40	3.481	3.493
Compound 6								
N1-C2-C3-C4-C5-C6	N1-C2-C3-C4-C5-C6	-x, 1-y, 2-z	3.670(3)	0.00	19.68	19.68	3.455	3.455
N3-C14-C15-C16-C17-C18	C19-C20-C21-C22-C28-C27	1-x,1-y,1-z	3.673(2)	15.44	27.37	11.93	3.594	3.262

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Table S3: Distortion Parameter τ and Angular Coordinates for Structures Reported on CSD

Structure	τ	ϕ_x	O-Cu-O'	ϕ'_x	Structure	τ	ϕ_x	O-Cu-O'	ϕ'_x
Compound **1**	0.16(1)	98.6	86.91	11.69	IFODOW [10]	0.026(12)	103	96.6	6.4
Compound **2**	0.23(2)	86.3	88.54	-2.24	IFODUC [10]	0.063(9)	100.7	97.1	3.6
Compound **3**	0.17(1)	96.4	82.15	14.25	IWINEH [11]	0.040(7)	95.2	92.3	2.9
Compound **4**	0.08(2)	102.3	89.94	12.36	IWINOR [12]	0.142(6)	106.0	90.0	16.0
Compound **5**	0.22(2)	93.8	89.46	4.34		0.072(10)	110.4	94.0	16.4
	0.24(2)	92.5	86.69	5.81		0.026(9)	101.4	84.9	16.5
Compound **6**	0.26(2)	91.5	89.52	1.98	JEDOIQ [13]	0.232(15)	92.5	88.4	4.1
AGOYEA [1]	0.091(3)	118.3	93.4	24.9	JEZJAZ [14]	0.167(12)	93.1	91.5	1.6
	0.160(3)	116.7	91.9	24.8	JEZJAZ01 [15]	0.160(2)	92.9	90.5	2.4
	0.126(3)	125.4	93.5	31.9		0.172(2)	92.8	91.8	1.0
	0.238(3)	100.5	92.0	8.5	JOQKAB [16]	0.013(4)	105.1	90.0	15.1
DEXPIG [2]	0.149(10)	98.1	94.5	3.6	KEBYUL [17]	0.043(3)	104.1	100.1	4.0
EJAFAW [3]	0.183(10)	89.9	99.3	-9.4		0.084(3)	102.4	99.2	3.2
EROQUX [4]	0.003(10)	109.2	97.0	12.2	LUBZEN [18]	0.065(2)	102.9	95.4	7.5
	0.018(10)	102.5	94.7	7.8		0.013(2)	106.4	95.0	11.4
ETAWAX [5]	0.163(11)	92.9	92.7	0.2	NATHAR [19]	0.090(11)	101.8	90.2	11.6
FEGTAN [6]	0.117(12)	92.6	86.3	6.3	NESDOE [20]	0.290(5)	104.1	85.7	18.4
	0.093(11)	95.4	90.6	4.8	NEWDEZ [21]	0.045(7)	101.8	88.9	12.9
	0.232(13)	93.1	86.3	6.8	PAPNAW [22]	0.285(19)	94.8	90.6	4.2
	0.239(12)	93.8	83.0	10.8	RELTUY [23]	0.236(15)	97.1	85.2	11.9
FETGUH [7]	0.0182(7)	105.5	97.2	8.3	SISCUS [24]	0.278(2)	115.9	96.3	19.6
GITLOK [8]	0.5330(3)	105.1	193.9	11.2	UCUMOU [25]	0.241(18)	91.4	92.9	-1.5
GITLUQ [8]	0.235(9)	90.9	91.3	-0.4	WIPPUG [26]	0.024(16)	109.1	90.5	18.6
	0.163(2)	91.9	92.1	-0.2	XAFKUL [27]	0.134(8)	96.4	93.1	3.3
HUJSOU [9]	0.214(18)	104.8	93.6	11.2	YOBLIK [28]	0.188(5)	100.9	88.8	12.1
	0.036(18)	108.5	103.9	4.6					

Table S4: Intermolecular Interactions. Hydrogen Bonds Geometries (Å, °) for Structures Reported on CSD

Structure	D-H···A	D-H	H···A	D···A	D-H···A	Symmetry Transform.
EJAFAW	O5-H1···O2	0.8400	1.9300	2.7572	166.00	½ + x, 3/2 - y, ½ +z
ETAWAX	O5-H35···O2	0.8700	2.0400	2.8592	159.00	-1 + x, y, z
IFODUC	O2-H2···O5	0.8900	1.8800	2.7648	171.00	x, ½ - y, ½ +z
IWINEH	O5-H23···O4	0.8400	2.0400	2.8484	162.00	1 - x, 1 - y, -z
JEDOIQ	O1-H1···O3	1.1800	1.5300	2.6990	172.00	1 + x, y, z
NATHAR	O3-H1···O1	0.9500	1.8000	2.7454	177.00	1 + x, y, z
NESDOE	O6-H2···O5	0.6800	2.3700	2.7889	122.00	½ + x, ½ + y, z
PAPNAW	O4-H1···O3	0.8500	2.4500	2.8165	107.00	x, -1 + y, z
WIPPUG	O1-H9···O3	0.6500	2.1900	2.8283	171.00	3/2 - x,- ½ + y, ½ -z
XAFKUL	O1-H1···O5	0.8200	2.0200	2.7970	159.00	½ - x,- ½ + y, ½ -z

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