## Supporting Information

## Zhao-Hao Li, <sup>a</sup> Li-Ping Xue \*<sup>a</sup>, Bang-Tun Zhao, <sup>a</sup> Jian Kan <sup>b</sup> and Wei-Ping Su\*<sup>b</sup>

<sup>a</sup> College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang, Henan 471022, P. R. China, E-mail:

lpxue@lynu.edu.cn

<sup>b</sup> State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, The Chinese Academy of

Sciences, Fuzhou, Fujian 350002, P. R. China, E-mail: wpsu@fjirsm.ac.cn



**Fig. S1** The (4,4) net where dinuclear SBUs can be viewed as nodes and Hbtca<sup>-</sup>(b) anions as connectors



Fig. S2 XRD curves of 1–5



Fig. S3 The TG curves of 1–5.

Compound 1				
D <b>−</b> H···A	d(D—H)	d(H···A)	$d(D \cdots A)$	<(DHA)
O1−H2W…O7	0.85	1.96	2.766	157
O1-H1W…O2 <sup>#1</sup>	0.85	1.96	2.755	155
$N3-H3N4^{#2}$	0.86	2.05	2.869 (6)	159
N3-H3····N5 <sup>#2</sup>	0.86	2.57	3.196 (6)	130
N6-H6…N2 <sup>#3</sup>	0.86	2.22	3.036 (5)	159
<sup>a</sup> Symmetry codes: #1 -x+1, y+1/2, -z-1/2; #2 -x, -y+1, -z+1; #3 x, y+1, z.				
Compound 2				
D <b>−</b> H···A	d(D—H)	$d(H \cdots A)$	$d(D \cdots A)$	<(DHA)
O1−H2W…O7	0.85	1.96	2.765 (4)	157
$O1-H1W\cdots O2^{\#1}$	0.85	1.97	2.761 (4)	155
N3–H3····N4 <sup>#2</sup>	0.86	2.04	2.861 (6)	160
N3-H3···N5 <sup>#2</sup>	0.86	2.55	3.176 (6)	131
N6-H6…N2 <sup>#3</sup>	0.86	2.20	3.006 (6)	157
<sup>a</sup> Symmetry codes: #1 -x+1, y+1/2, -z-1/2; #2 -x, -y+1, -z+1; #3 x, y+1, z.				
Compound 3				
D <b>−</b> H…A	d(D—H)	$d(H \cdots A)$	$d(D \cdots A)$	<(DHA)
O1−H2W…O7	0.85	1.98	2.782 (6)	157
$O1-H1W\cdots O2^{\#1}$	0.85	1.98	2.781 (5)	156
N3–H3···N4 <sup>#2</sup>	0.86	2.07	2.892 (8)	160
N3-H3···N5 <sup>#2</sup>	0.86	2.57	3.201 (7)	131
N6-H6…N2 <sup>#3</sup>	0.86	2.19	3.001 (7)	158
<sup>a</sup> Symmetry codes: $\#1 - x + 1$ , $y + 1/2$ , $-z - 1/2$ ; $\#2 - x$ , $-y + 1$ , $-z + 1$ ; $\#3 x$ , $y + 1$ , $z$ .				
Compound 4				
D <b>−</b> H···A	d(D—H)	$d(H \cdots A)$	$d(D \cdots A)$	<(DHA)
O1−H2W…O7	0.85	1.96	2.765 (3)	158
$O1-H1W\cdots O2^{\#1}$	0.85	1.98	2.773 (3)	156
N3—H3····N4 <sup>#2</sup>	0.86	2.04	2.864 (4)	160
N3—H3…N5 <sup>#2</sup>	0.86	2.53	3.159 (4)	130
N6-H6…N2 <sup>#3</sup>	0.86	2.19	3.000 (4)	158
<sup>a</sup> Symmetry codes: $#1 - x + 1$ , $y + 1/2$ , $-z - 1/2$ ; $#2 - x$ , $-y + 1$ , $-z + 1$ ; $#3 x$ , $y + 1$ , $z$ .				
Compound 5				
D <b>−</b> H···A	d(D-H)	$d(H \cdots A)$	$d(D \cdots A)$	<(DHA)
01 <b>—</b> H2W…07	0.85	1.96	2.756 (3)	158
O1−H1W…O2 <sup>#1</sup>	0.85	1.97	2.766 (3)	157
N3-H3N4 <sup>#2</sup>	0.86	2.04	2.863 (4)	160
N3-H3N5 <sup>#2</sup>	0.86	2.53	3.148 (4)	130
N6-H6N2 <sup>#3</sup>	0.86	2.17	2.989 (4)	158

Table S1 Hydrogen Bond Lengths (Å) and Bond Angles (°) in  $1-5^{a}$