Electronic Supplementary Information

Ferromagnetic interactions through triple hydrogen bonds in the coordination polymers of α, α' - dihydroxy-bibenzyl-4,4'-dicarboxylate

Yu Ma, Ai-Ling Cheng, and En-Qing Gao*



Fig. S1 Comparison of the PXRD patterns measured for 3 (black) and that calculated from the single-crystal data of 1 (red)



Fig. S2 the 3D packing of the layers through hydrogen bonds in compound 1



Fig. S3. The 3,5-connectted $(4.6^2)(4.6^6.8^3)$ net in compound **1**

Tuble 52. Selected hydrogen bond lengths [11] and angles [] for 2				
A [Transformation]	d(D-H)	$d(H \cdots A)$	$d(D \cdots A)$	<(DHA)
O2	0.77(2)	1.99(2)	2.7376(16)	165(2)
O4 [-x+1, -y+1, -z+2]	0.74(3)	2.35(3)	3.0548(16)	160(3)
O6 [x-1, -y+1/2, z-3/2]	0.86(2)	1.91(2)	2.7552(16)	168(2)
O3 [x-1, -y+1/2, z-1/2]	0.76(3)	2.24(3)	2.9752(15)	163(2)
OW2 [-x+1, y+1/2, -z+5/2]	0.81(2)	2.11(2)	2.8831(14)	159.5(19)
OW1 [x, y, z+1]	0.747(19)	2.033(19)	2.7621(15)	165(2)
O2	0.87(2)	1.88(2)	2.6851(14)	153.0(18)
O9 [x, -y+1/2, z-1/2]	0.78(2)	1.94(2)	2.7118(14)	174(2)
O1 [x, -y+1/2, z-1/2]	0.81(3)	2.20(3)	3.0031(16)	178(2)
OW1 [-x+1, y-1/2, -z+3/2]	0.82(2)	2.04(2)	2.8522(17)	166.6(19)
O4 [-x+1, y-1/2, -z+5/2]	0.82(2)	1.96(2)	2.7750(14)	175.5(18)
O6 [x-1, -y+1/2, z-3/2]	0.85(2)	1.81(2)	2.6376(13)	164.6(18)
O5 [x-1, -y+1/2, z-3/2]	0.85(2)	2.635(19)	3.0127(13)	108.3(14)
O5 [x-1, y, z-1]	0.79(2)	2.07(2)	2.8490(15)	172.5(19)
OW2 [-x, y+1/2, -z+3/2]	0.80(2)	2.05(2)	2.8477(17)	173(2)
D = donor, A = acceptor.				
	A [Transformation] O2 O4 [-x+1, -y+1, -z+2] O6 [x-1, -y+1/2, z-3/2] O3 [x-1, -y+1/2, z-1/2] OW2 [-x+1, y+1/2, -z+5/2] OW1 [x, y, z+1] O2 O9 [x, -y+1/2, z-1/2] O1 [x, -y+1/2, z-1/2] OW1 [-x+1, y-1/2, -z+3/2] O4 [-x+1, y-1/2, -z+5/2] O6 [x-1, -y+1/2, z-3/2] O5 [x-1, -y+1/2, z-3/2] O5 [x-1, y, z-1] OW2 [-x, y+1/2, -z+3/2] nor, A = acceptor.	A [Transformation]d(D-H)O2 $0.77(2)$ O4 $[-x+1, -y+1, -z+2]$ $0.74(3)$ O6 $[x-1, -y+1/2, z-3/2]$ $0.86(2)$ O3 $[x-1, -y+1/2, z-1/2]$ $0.76(3)$ OW2 $[-x+1, y+1/2, -z+5/2]$ $0.81(2)$ OW1 $[x, y, z+1]$ $0.747(19)$ O2 $0.87(2)$ O9 $[x, -y+1/2, z-1/2]$ $0.78(2)$ O1 $[x, -y+1/2, z-1/2]$ $0.81(3)$ OW1 $[-x+1, y-1/2, -z+3/2]$ $0.82(2)$ O4 $[-x+1, y-1/2, -z+5/2]$ $0.82(2)$ O5 $[x-1, -y+1/2, z-3/2]$ $0.85(2)$ O5 $[x-1, y, z-1]$ $0.79(2)$ OW2 $[-x, y+1/2, -z+3/2]$ $0.80(2)$ nor, A = acceptor. $x = 0$	A [Transformation]d(D-H)d(H···A)O2 $0.77(2)$ $1.99(2)$ O4 $[-x+1, -y+1, -z+2]$ $0.74(3)$ $2.35(3)$ O6 $[x-1, -y+1/2, z-3/2]$ $0.86(2)$ $1.91(2)$ O3 $[x-1, -y+1/2, z-1/2]$ $0.76(3)$ $2.24(3)$ OW2 $[-x+1, y+1/2, -z+5/2]$ $0.81(2)$ $2.11(2)$ OW1 $[x, y, z+1]$ $0.747(19)$ $2.033(19)$ O2 $0.87(2)$ $1.88(2)$ O9 $[x, -y+1/2, z-1/2]$ $0.78(2)$ $1.94(2)$ O1 $[x, -y+1/2, z-1/2]$ $0.81(3)$ $2.20(3)$ OW1 $[-x+1, y-1/2, -z+3/2]$ $0.82(2)$ $2.04(2)$ O4 $[-x+1, y-1/2, -z+5/2]$ $0.85(2)$ $1.81(2)$ O5 $[x-1, -y+1/2, z-3/2]$ $0.85(2)$ $1.81(2)$ O5 $[x-1, -y+1/2, z-3/2]$ $0.85(2)$ $2.035(19)$ O5 $[x-1, y, z-1]$ $0.79(2)$ $2.07(2)$ OW2 $[-x, y+1/2, -z+3/2]$ $0.80(2)$ $2.05(2)$	A [Transformation]d(D-H)d(H···A)d(D···A)O20.77(2)1.99(2)2.7376(16)O4[-x+1, -y+1, -z+2]0.74(3)2.35(3)3.0548(16)O6[x-1, -y+1/2, z-3/2]0.86(2)1.91(2)2.7552(16)O3[x-1, -y+1/2, z-1/2]0.76(3)2.24(3)2.9752(15)OW2[-x+1, y+1/2, -z+5/2]0.81(2)2.11(2)2.8831(14)OW1[x, y, z+1]0.747(19)2.033(19)2.7621(15)O20.87(2)1.88(2)2.6851(14)O9[x, -y+1/2, z-1/2]0.78(2)1.94(2)2.7118(14)O1[x, -y+1/2, z-1/2]0.81(3)2.20(3)3.0031(16)OW1[-x+1, y-1/2, -z+3/2]0.82(2)2.04(2)2.8522(17)O4[-x+1, y-1/2, -z+5/2]0.85(2)1.81(2)2.6376(13)O5[x-1, -y+1/2, z-3/2]0.85(2)1.81(2)2.6376(13)O5[x-1, y, z-1]0.79(2)2.07(2)2.8490(15)OW2[-x, y+1/2, -z+3/2]0.80(2)2.05(2)2.8477(17)

Table S2. Selected hydrogen-bond lengths [Å] and angles [°] for **2**