ELECTRONIC SUPPLEMENTARY INFORMATION

to

A unique copper(II)-assisted transformation of acetylacetone dioxime in acetone that leads to one-dimensional, quinoxaline-bridged coordination polymers

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This work is dedicated to Professor Jan Reedijk for his great contributions to inorganic chemistry over the last 45 years and on the occasion of his retirement.

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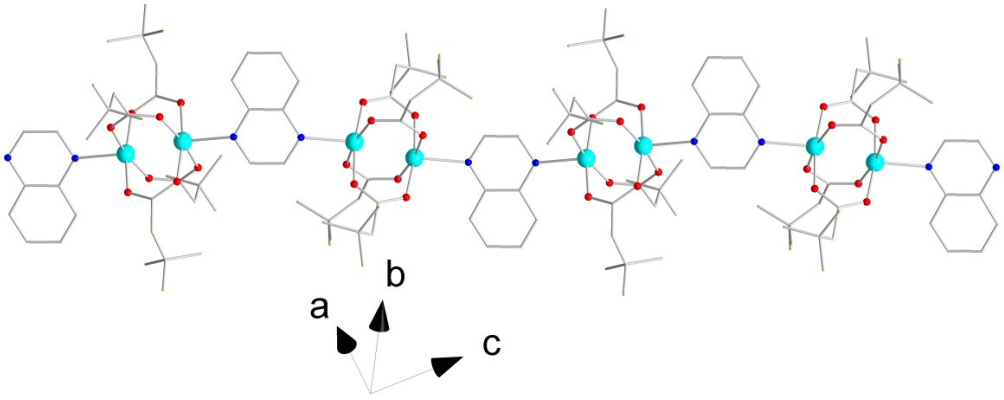

Fig. S1 A portion of a chain that is present in the crystal of $\{[Cu_2(diba)_4(qunx)]\}_n$ (**1**) illustrating four Cu_2 units.

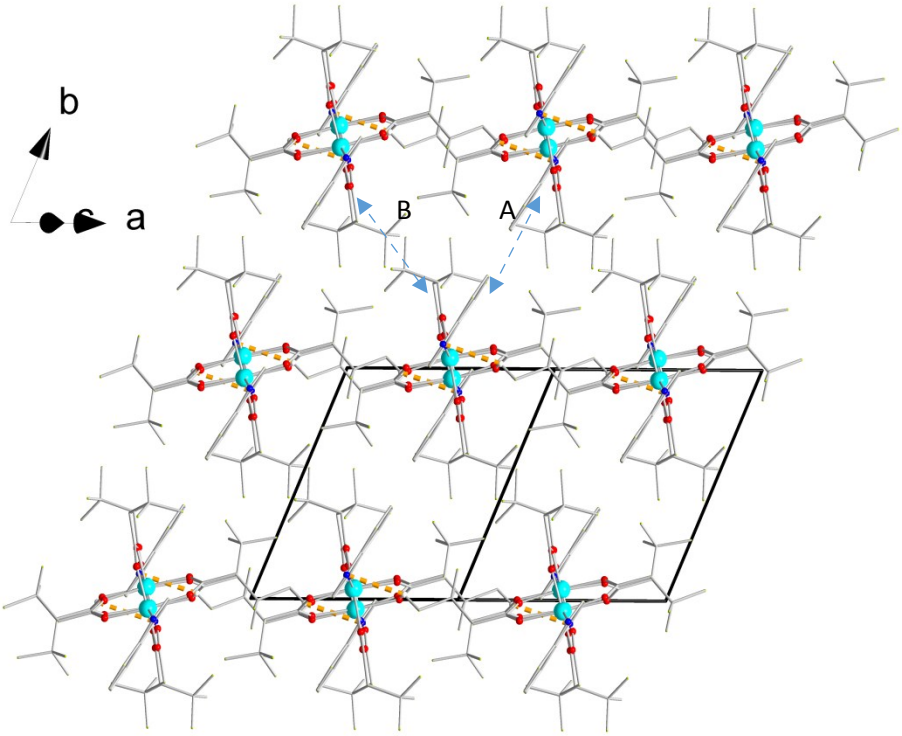

Fig. S2 The arrangement of layers in the structure of $\{[Cu_2(diba)_4(qunx)]\}_n$ (**1**).

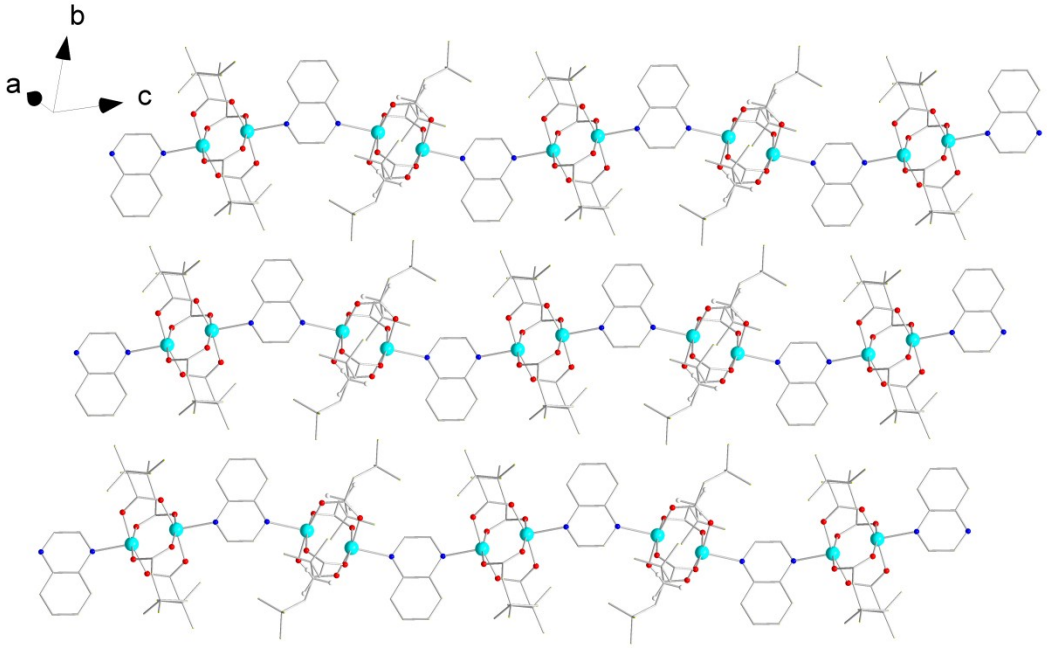

Fig. S3 A view of the arrangement of chains in the structure of $\{[Cu_2(diba)_4(qunx)]\}_n$ (**1**). The chains along the direction indicated with the double dashed arrow A in Fig. S2 are located within the (101) plane and are at distances of 11.0985(2) Å (*b* axis length).

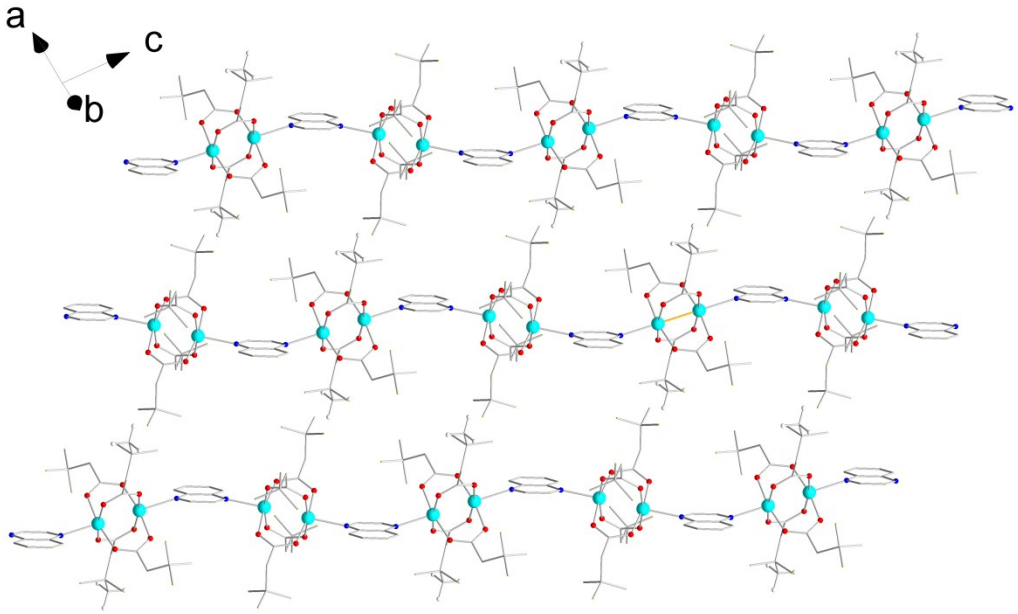

Fig. S4 Another view of the arrangement of chains in the structure of $\{[Cu_2(diba)_4(qunx)]\}_n$ (**1**). The chains along the direction indicated with the double dashed arrow B in Fig. S2 are located within the (111) plane and are at distances of 11.738(2) Å.

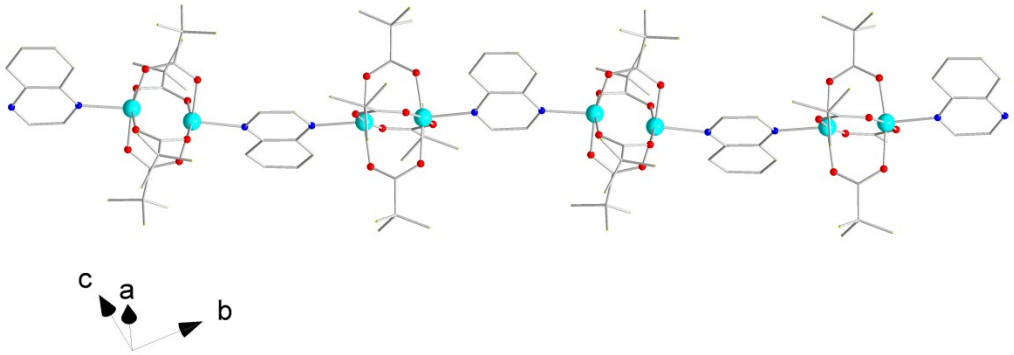

Fig. S5 A portion of a chain that is present in the crystal of $\{[Cu_2(piv)_4(qunx)]\}_n$ (**2**) illustrating four Cu_2 units.

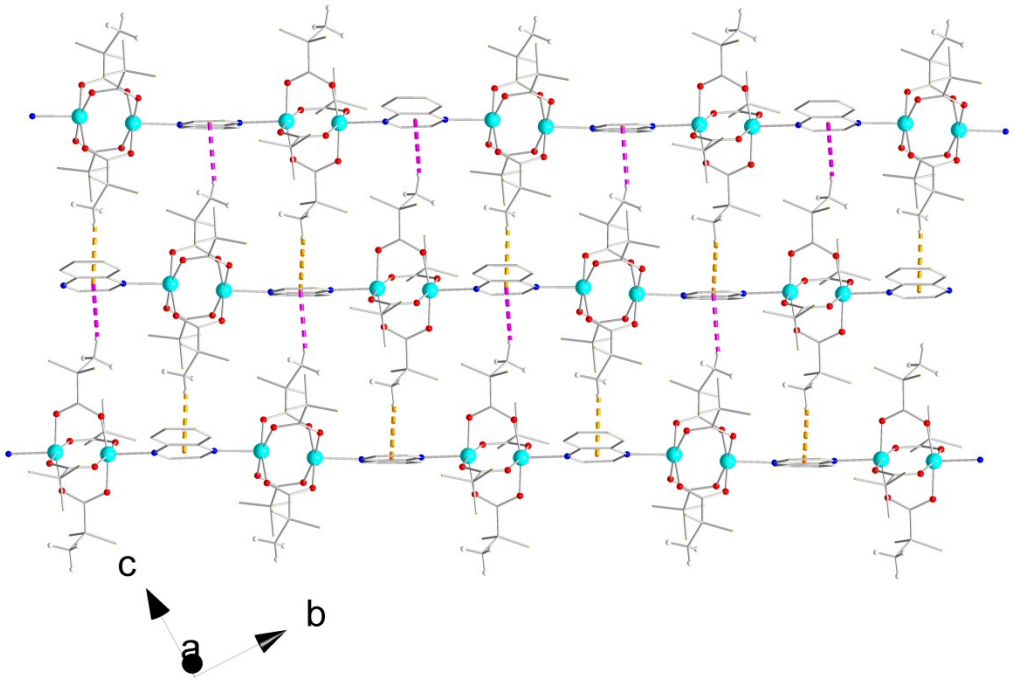

Fig. S6 The formation of a layer parallel to the (100) plane through C (methyl)−H···π (diazine) interactions; the interactions are shown with dashed orange and dashed magenta lines.

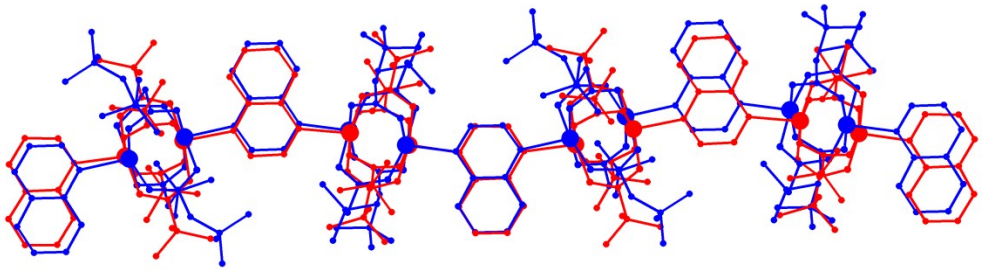

Fig. S7 Portions of the chains of complexes **1** (blue) and **2** (red) in an overlapped mode.

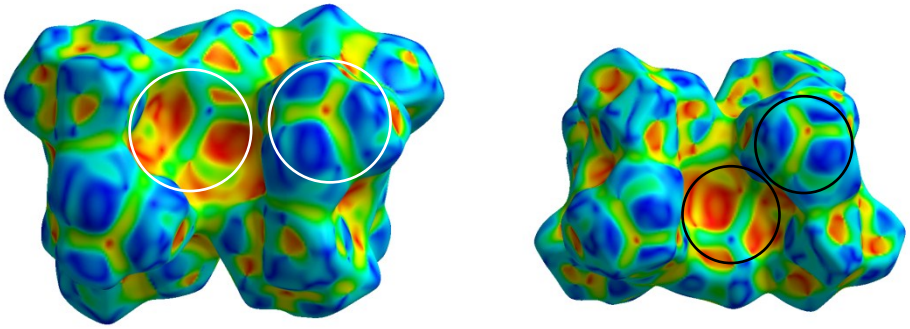

Fig. S8 *S* map for **2**. Circled with white lines (a) and black lines (b) are the contact areas of HS which indicate the C5−H5A···Cg1 and C14−H14A···Cg1 interactions, respectively.

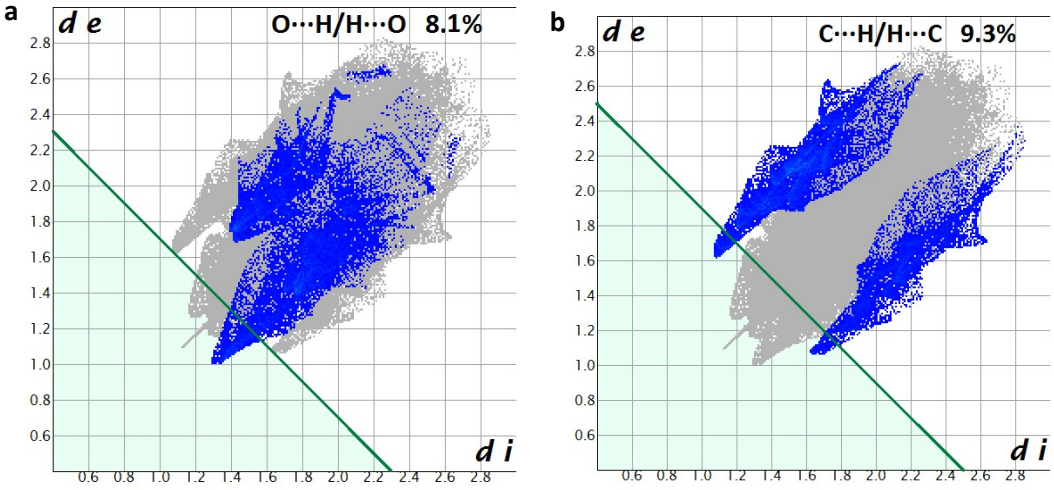

Fig. S9 O···H/ H···O (a) and C···H/H···C (b) contributions (blue areas), along with the other kinds of contacts (gray area), into the 2D fingerprint plot for compound **2**. For the meaning of the green line, see text of the main ms.

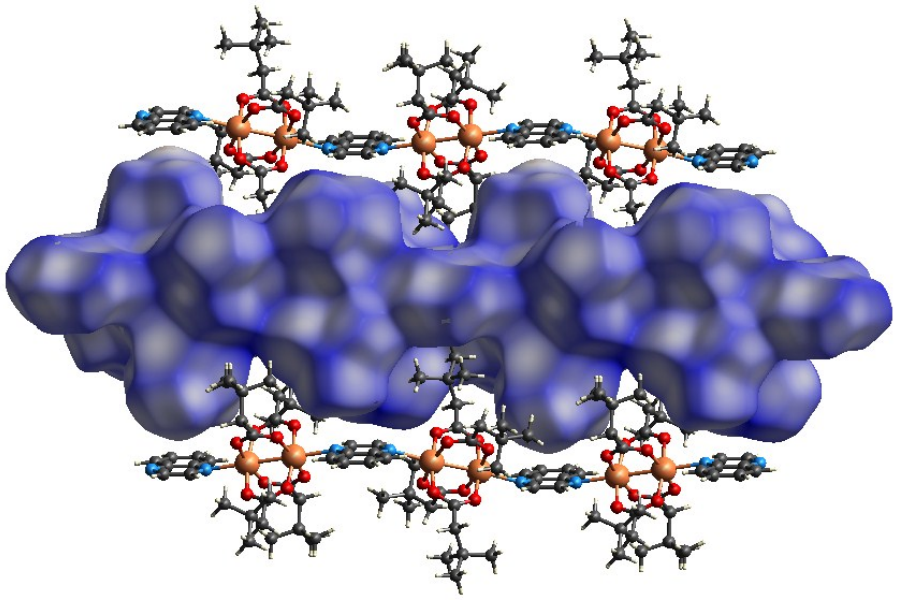

Fig. S10 A combined HS d_{norm} map and the molecular representation of neighbouring chains within the layers of complex **1**.

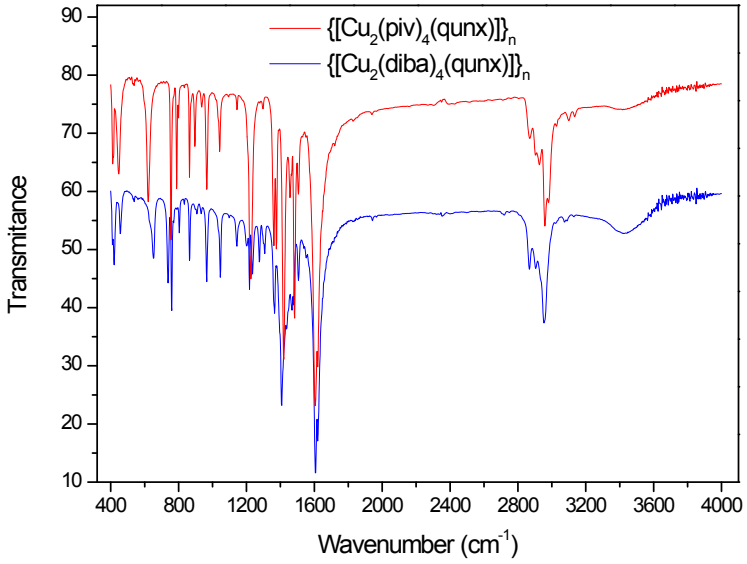

Fig. S11 The FT-IR (KBr) spectra of $\{[Cu_2(diba)_4(qunx)]\}_n$ (**1**, bottom plot) and $\{[Cu_2(piv)_4(qunx)]\}_n$ (**2**, upper plot).

Table S1 Selected interatomic distances and angles for complex **1**[a]

	Distances (Å)		
Cu1···Cu1’	2.609(2)	Cu1−N1	2.261(2)
Cu2···Cu2’	2.611(1)	Cu2−O5	1.964(2)
Cu1···Cu2	7.159(2)	Cu2−O6’’	1.960(2)
Cu1−O1	1.971(2)	Cu2−O7	1.978(2)
Cu1−O2’	1.958(2)	Cu2−O8’’	1.962(2)
Cu1−O3	1.945(2)	Cu2−N2	2.245(2)
Cu1−O4’	1.950(2)		
	Angles (°)		
O1−Cu1−O2’	169.1(1)	O5−Cu2−O6’’	169.4(1)
O1−Cu1−O3	89.5(1)	O5−Cu2−O7	88.1(1)
O1−Cu1−O4’	87.8(1)	O5−Cu2−O8’’	90.1(1)
O1−Cu1−N1	91.0(1)	O5−Cu2−N2	90.6(1)
O2’−Cu1−O3	88.4(1)	O6’’−Cu2−O7	90.8(1)
O2’−Cu1−O4’	92.3(1)	O6’’−Cu2−O8’’	88.3(1)
O2’−Cu1−N1	99.9(1)	O6’’−Cu2−N2	99.9(1)
O3−Cu1−O4’	169.1(1)	O7−Cu2−O8’’	169.1(1)
O3−Cu1−N1	101.1(1)	O7−Cu2−N2	90.6(1)
O4’−Cu1−N1	89.5(1)	O8’’−Cu2−N2	100.2(1)
Cu1···Cu2···Cu2’’	160.3(1)	Cu1’···Cu1···Cu2	158.2(1)

[a] Symmetry operations used to generate equivalent atoms: (‘) *-x*,*-y*+2, *-z*; (”) *-x*, *-y*+2, *-z*+1.

Table S2 Selected interatomic distances and angles for complex **2**[a]

Distances (Å)			
Cu1···Cu2	2.606(2)	Cu1−N2’	2.247(13)
Cu1’’···Cu2	7.274(2)	Cu2−O2	1.954(11)
Cu1−O1	1.945(10)	Cu2−O4	1.957(10)
Cu1−O3	1.941(10)	Cu2−O5	1.938(11)
Cu1−O6	1.943(10)	Cu2−O7	1.939(10)
Cu1−O8	1.955(10)	Cu2−N1	2.233(13)
Angles (°)			
O1−Cu1−O3	89.2(5)	O2−Cu2−O4	87.8(5)
O1−Cu1−O6	169.1(4)	O2−Cu2−O5	167.6(4)
O1−Cu1−O8	90.1(5)	O2−Cu2−O7	89.9(5)
O1−Cu1−N2’	95.4(5)	O2−Cu2−N1	97.1(5)
O3−Cu1−O6	89.1(5)	O4−Cu2−O5	90.1(5)
O3−Cu1−O8	167.7(4)	O4−Cu2−O7	170.4(4)
O3−Cu1−N2’	103.9(5)	O4−Cu2−N1	90.4(5)
O6−Cu1−O8	89.3(5)	O5−Cu2−O7	90.1(5)
O6−Cu1−N2’	95.5(5)	O5−Cu2−N1	95.1(4)
O8−Cu1−N2’	88.5(5)	O7−Cu2−N1	99.1(5)
Cu1···Cu2···Cu1’’	166.5(4)	Cu2···Cu1’’···Cu2’’	164.2(4)

[a] Symmetry operations used to generate equivalent atoms: (‘) -*x*+3/2, *y*+1/2, *z*+1/2; (’’) -*x*+3/2, *y*-1/2, *z*-1/2 .