

Supporting Information

for

Modification of structure and magnetic properties in coordination assemblies based on $[\text{Cu}(\text{cyclam})]^{2+}$ and $[\text{W}(\text{CN})_8]^{3-}$

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Table S2. Continuous shape measure parameters for hexa-coordinated Cu centres of **1·5H₂O**, **1** and **2·3H₂O**; OC-6=octahedron.

Figure S4. Inter- and intra-chain H-bonds in **1**.

Figure S5. Inter- and intra-molecular H-bonds in **2·3H₂O**; symmetrically independent molecules marked pink and violet.

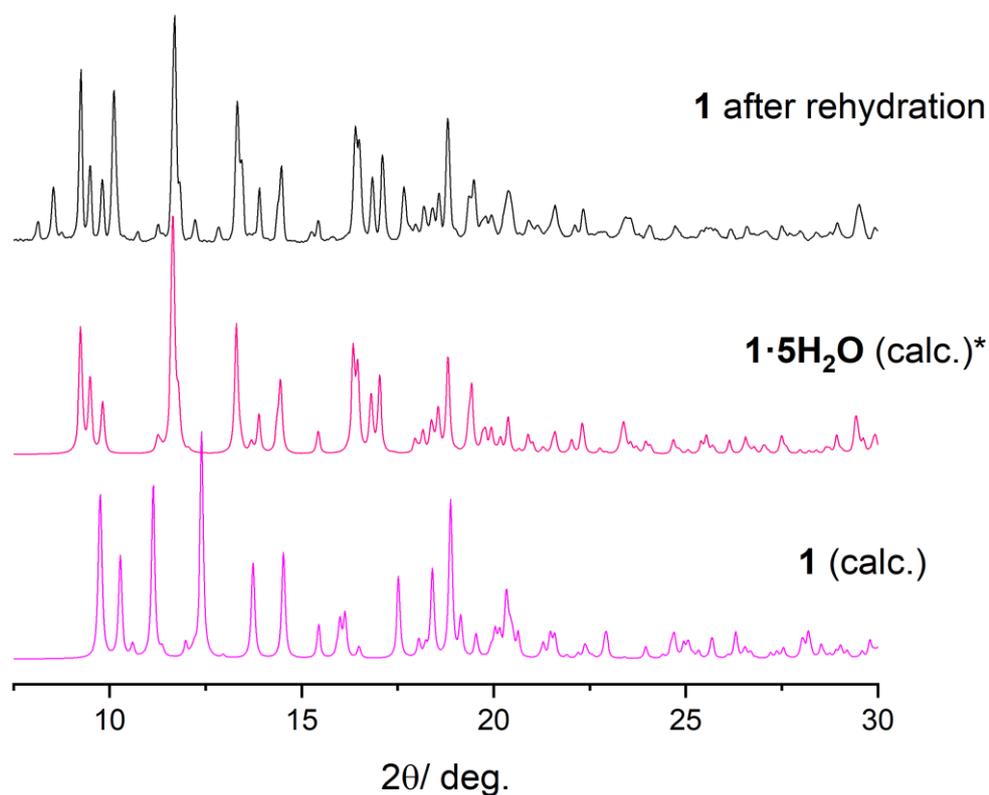


Figure S1. PXRD pattern for the rehydrated sample of **1** in comparison to **1·5H₂O** and **1**.

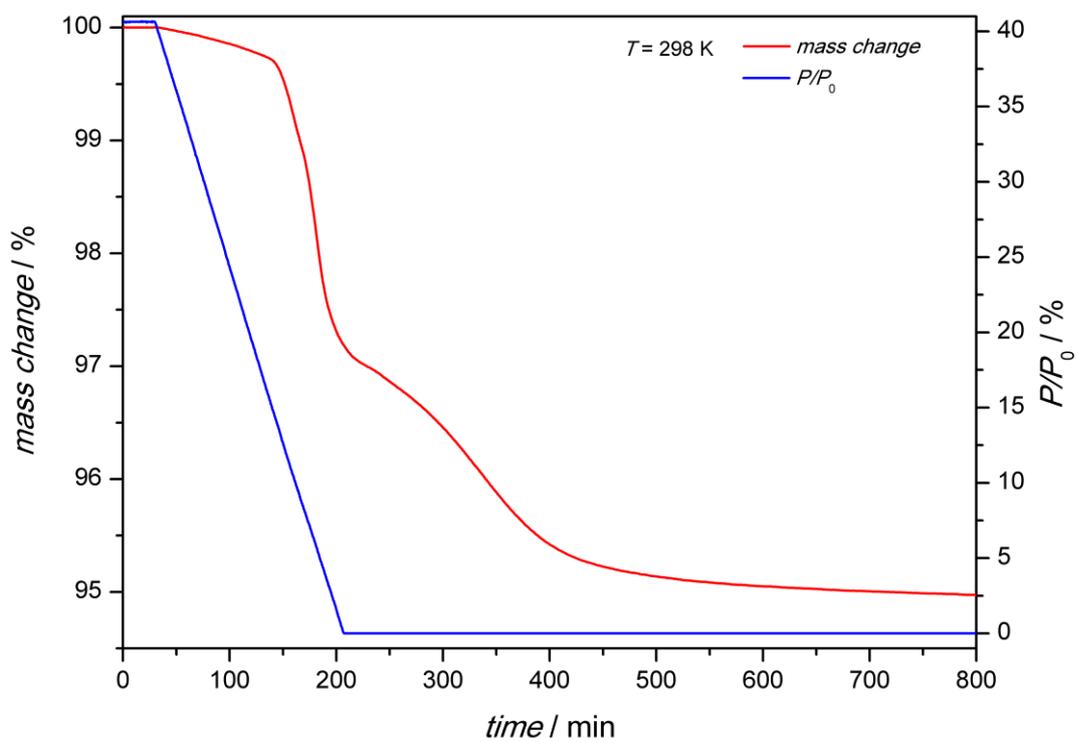


Figure S2. Mass loss upon dehydration of **1·5H₂O** monitored by dynamic vapour sorption method.

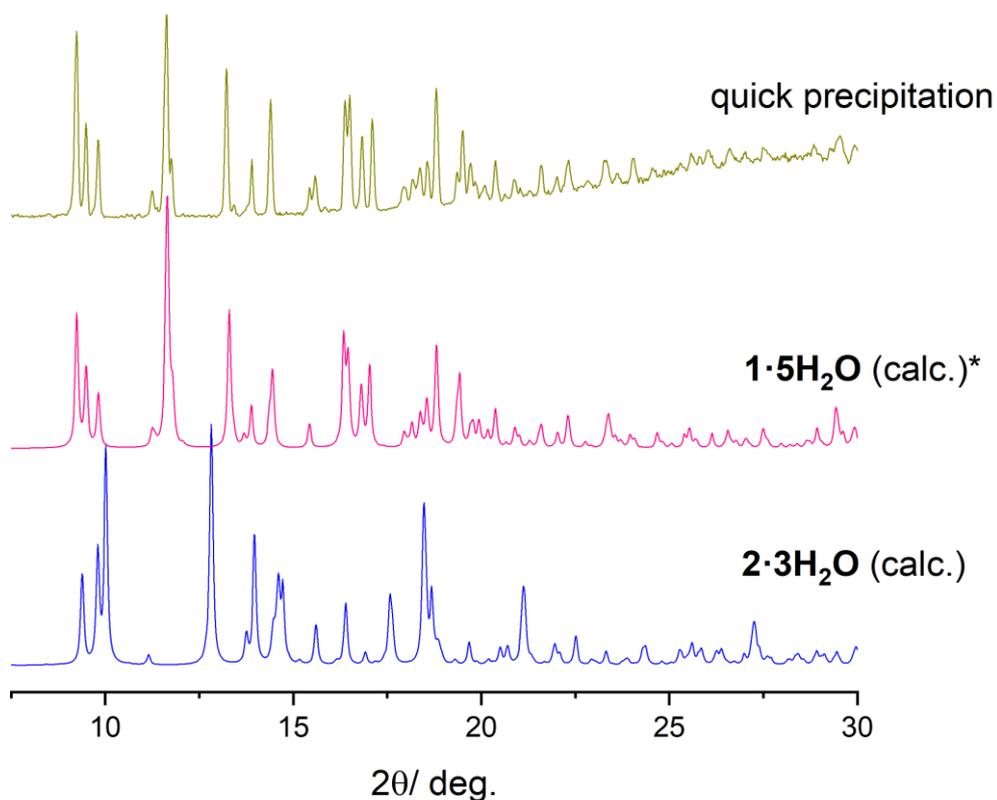


Figure S3. PXRD pattern for sample obtained from $[\text{Cu}(\text{cyclam})](\text{NO}_3)_2$ and $\text{Na}_3[\text{W}(\text{CN})_8]$ by quick precipitation from water solution in comparison to $1\cdot 5\text{H}_2\text{O}$ and $2\cdot 3\text{H}_2\text{O}$.

Table S1. Continuous shape measure parameters for octa-coordinated W centres in the structures of $1\cdot 5\text{H}_2\text{O}$, **1** and $2\cdot 3\text{H}_2\text{O}$; SAPR-8 = square antiprism, TDD-8 = triangular dodecahedron, BTR-8 = biaugmented trigonal prism.

Atom	$1\cdot 5\text{H}_2\text{O}$			1			$2\cdot 3\text{H}_2\text{O}$		
	SAPR-8	TDD-8	BTPR-8	SAPR-8	TDD-8	BTPR-8	SAPR-8	TDD-8	BTPR-8
W1	0.546	1.363	1.468	1.497	0.675	1.351	0.405	1.542	1.505
W2							0.264	1.722	1.647

Table S2. Continuous shape measure parameters for hexa-coordinated Cu centres of $1\cdot 5\text{H}_2\text{O}$, **1** and $2\cdot 3\text{H}_2\text{O}$; OC-6=octahedron.

Atom	$1\cdot 5\text{H}_2\text{O}$	1	$2\cdot 3\text{H}_2\text{O}$
	OC-6	OC-6	OC-6
Cu1	1.841	1.679	1.448
Cu2	1.435	1.218	1.631
Cu3	-	-	1.388
Cu4	-	-	0.985

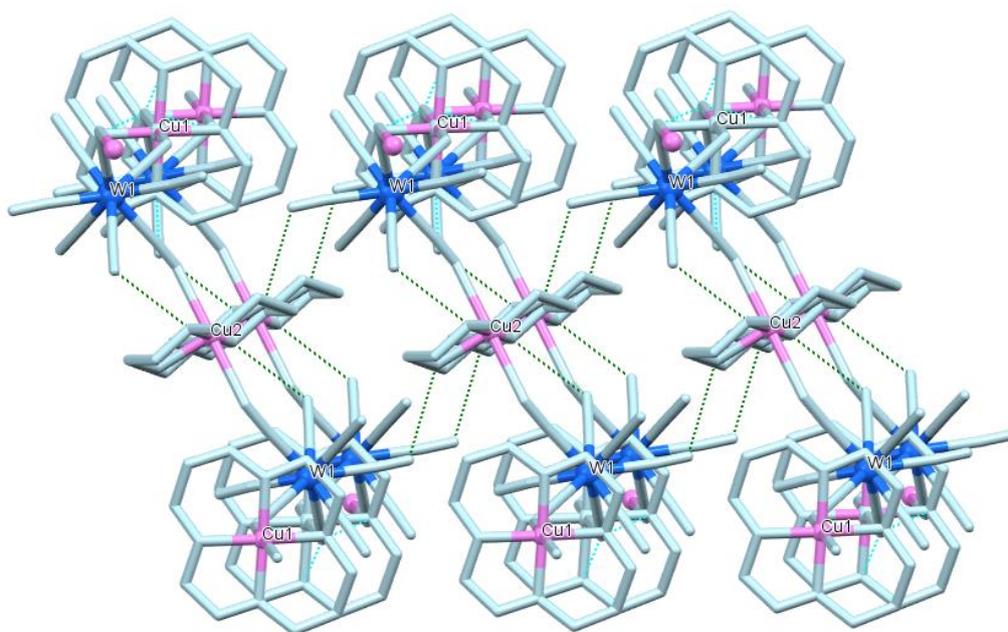


Figure S4. Inter- and intra-chain H-bonds in **1**.

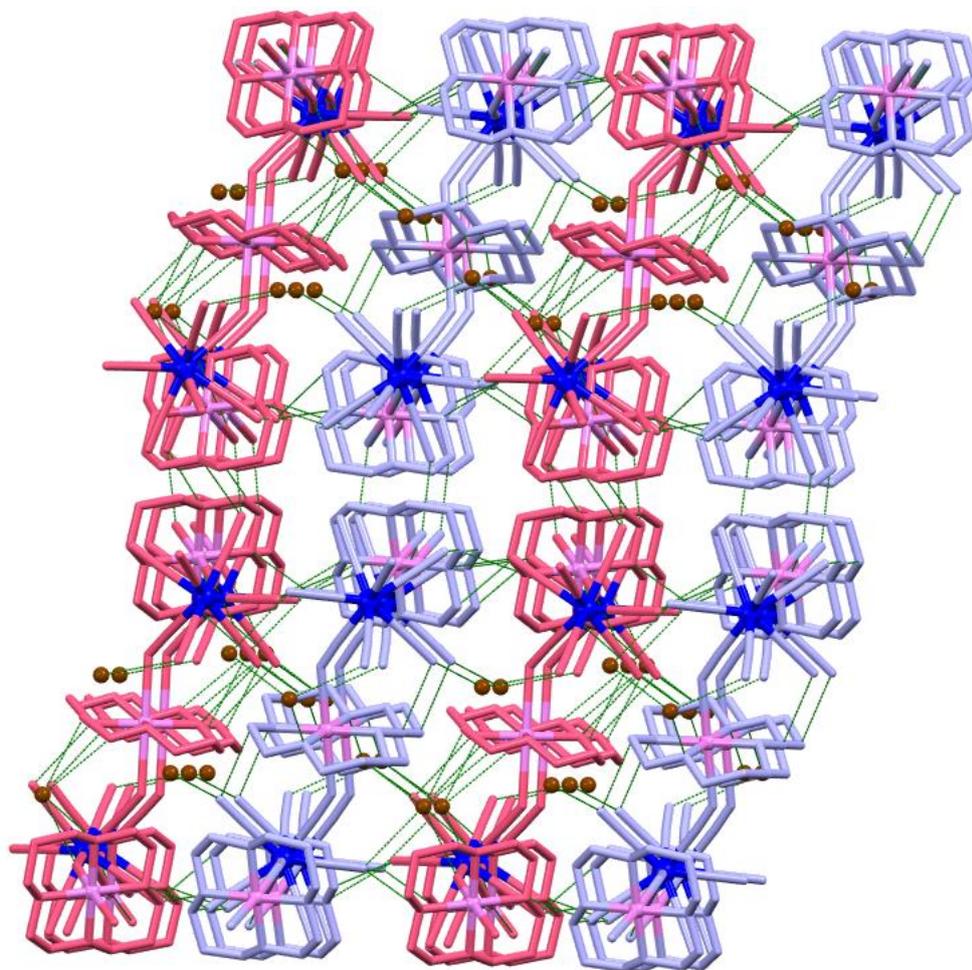


Figure S5. Inter- and intra-molecular H-bonds in **2·3H₂O**; symmetrically independent molecules marked pink and violet.