Bimetallic Coordination Networks based on Al(acacCN)$_3$: A Building Block between Inertness and Lability

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Received Xth XXXXXXXXXX 20XX, Accepted Xth XXXXXXXXX 20XX
First published on the web Xth XXXXXXXXXX 200X
DOI: 10.1039/b000000x

Supplementary Information

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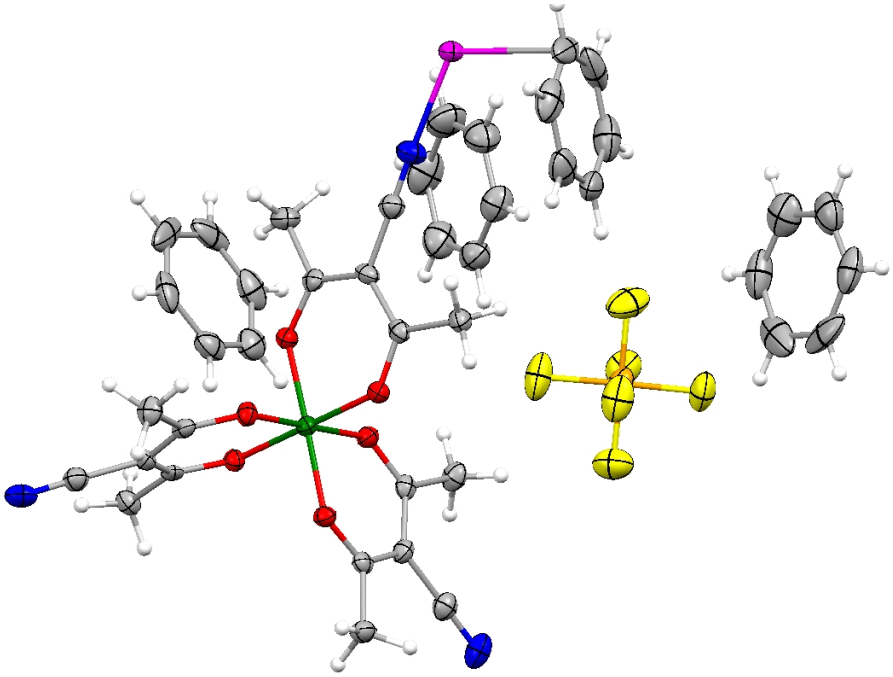

Fig. S1 Displacement ellipsoid plot of the asymmetric unit in **2a**. Ellipsoids are drawn at 50 % probability.

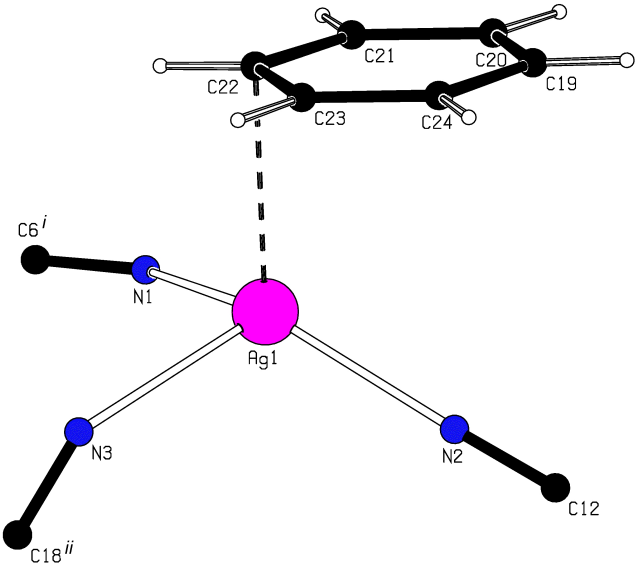

Fig. S2 Ag(I) coordination environment in **2a**. The neighboring benzene molecule induces significant pyramidalization of the Ag(I) coordination environment. Symmetry operations: ^{i}=x-1, $\frac{1}{2}$-y, z-$\frac{1}{2}$, ^{ii}=1-x, $\frac{1}{2}$+y, $\frac{1}{2}$-z. Short contacts: Ag(1)···C(22) 2.541(4) Å, Ag(1)···C(21) 2.782(6) Å, and Ag(1)···C(23) 3.035(4) Å.

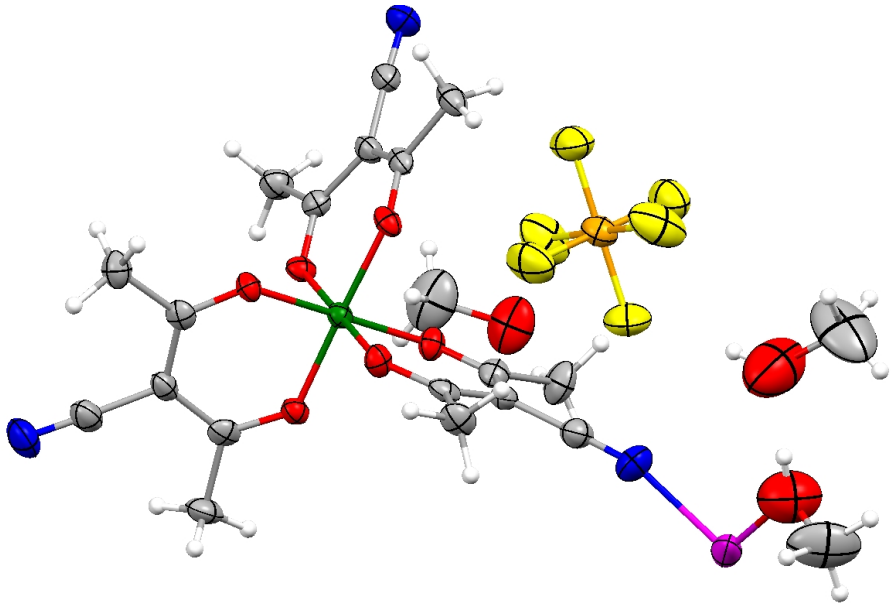

Fig. S3 Displacement ellipsoid plot of the asymmetric unit in **2b**. Ellipsoids are drawn at 50 % probability.

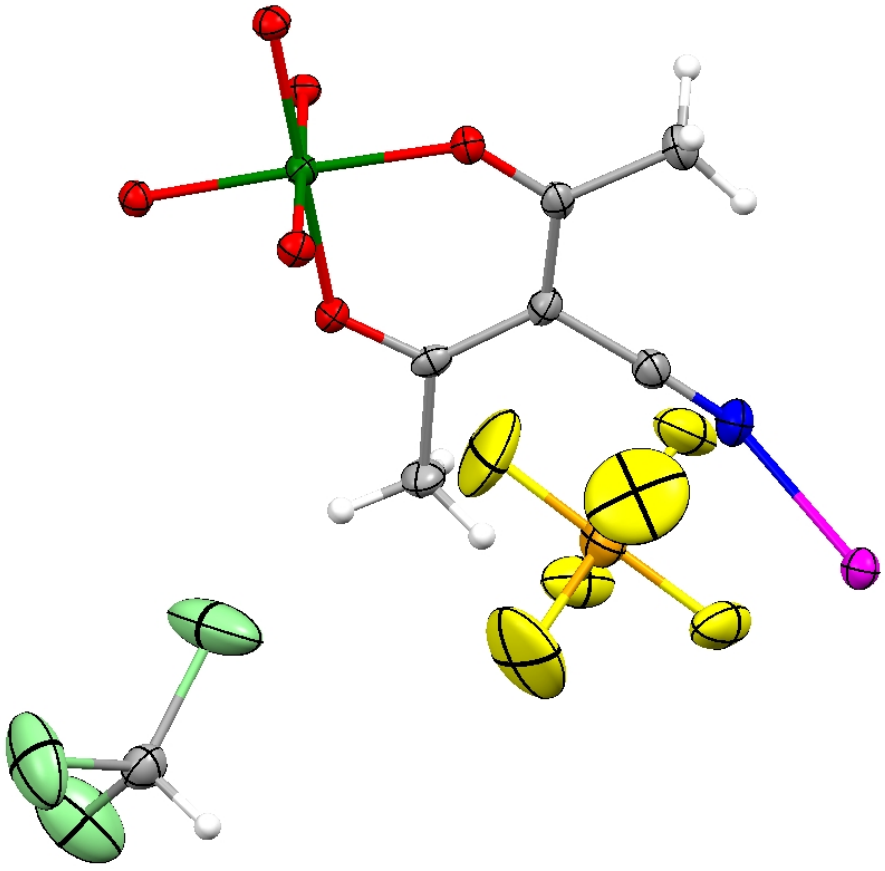

Fig. S4 Displacement ellipsoid plot of a molecular fragment in **2c**. Ellipsoids are drawn at 50 % probability.

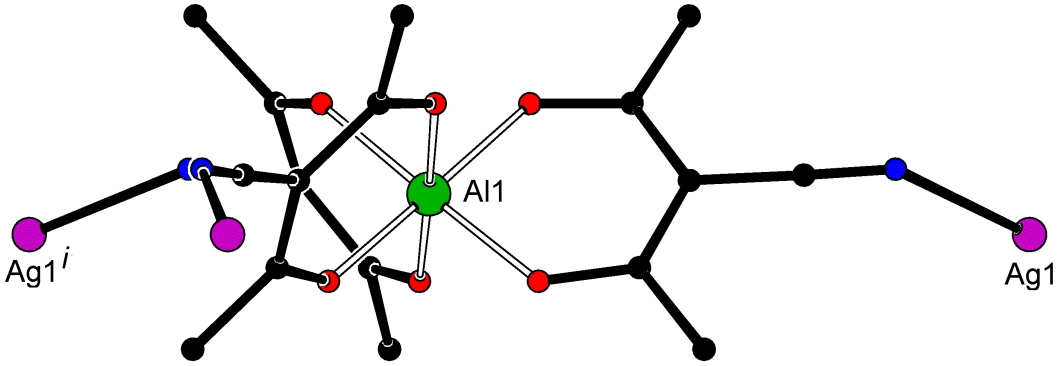

Fig. S5 Al(III) coordination environment in the network of **2c**. The Al(acacCN)$_3$ building block with its peripheric N-donor functionalities coordinates to three Ag(I) cations, with the central Al(III) almost in the plane of the silver cations. Symmetry operations: ^{i} = $\frac{1}{2}$+*y*, $\frac{1}{2}$-*z*, 1-*x*.

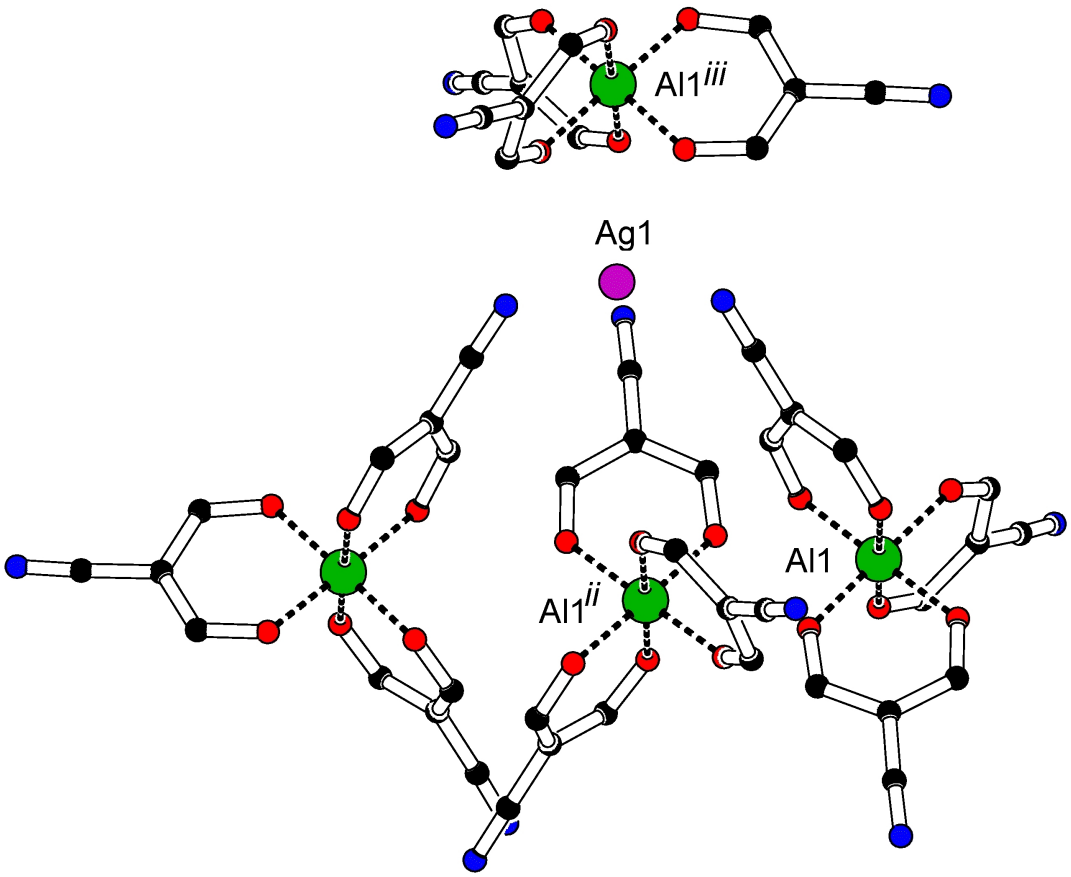

Fig. S6 Ag(I) coordination environment in the network of **2c**; the coordination corresponds to a trigonal pyramidal arrangement. Symmetry operations: ^{ii} = $\frac{3}{2}$-*y*, 1-*z*, x-$\frac{1}{2}$ and ^{iii}=$\frac{1}{2}$+*x*, $\frac{1}{2}$-*y*, 1-*z*.

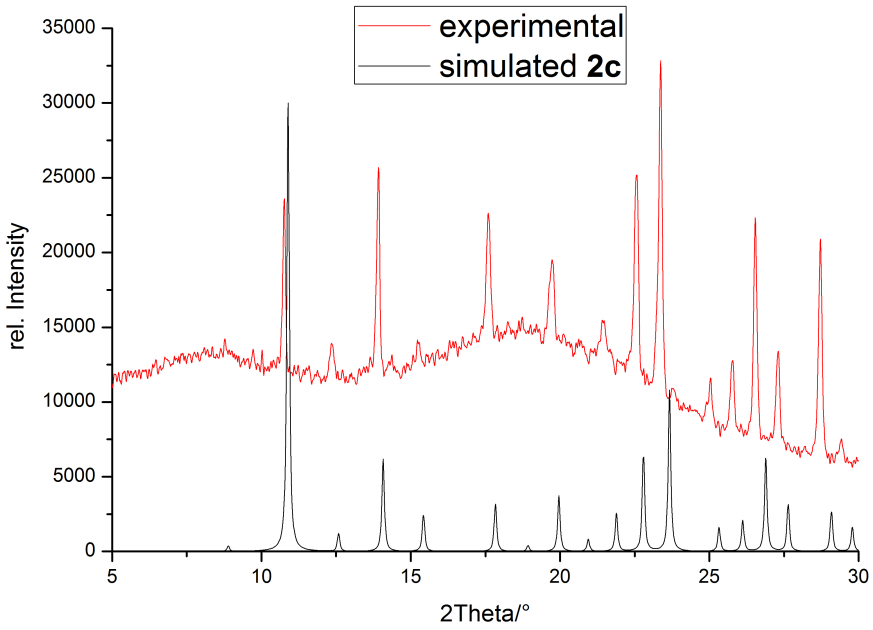

Fig. S7 Experimental and simulated powder pattern of **2c**.

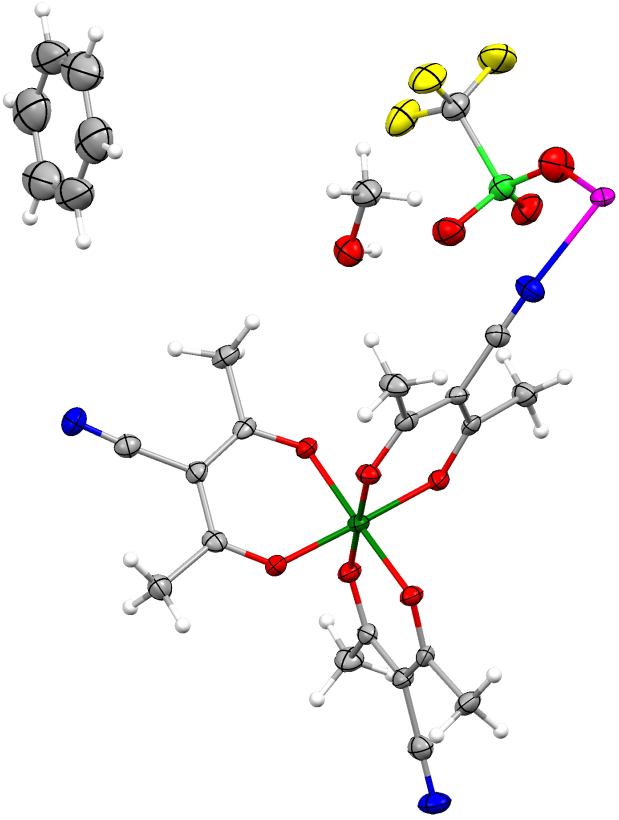

Fig. S8 Displacement ellipsoid plot of a molecular fragment in **3a**. Ellipsoids are drawn at 50 % probability.

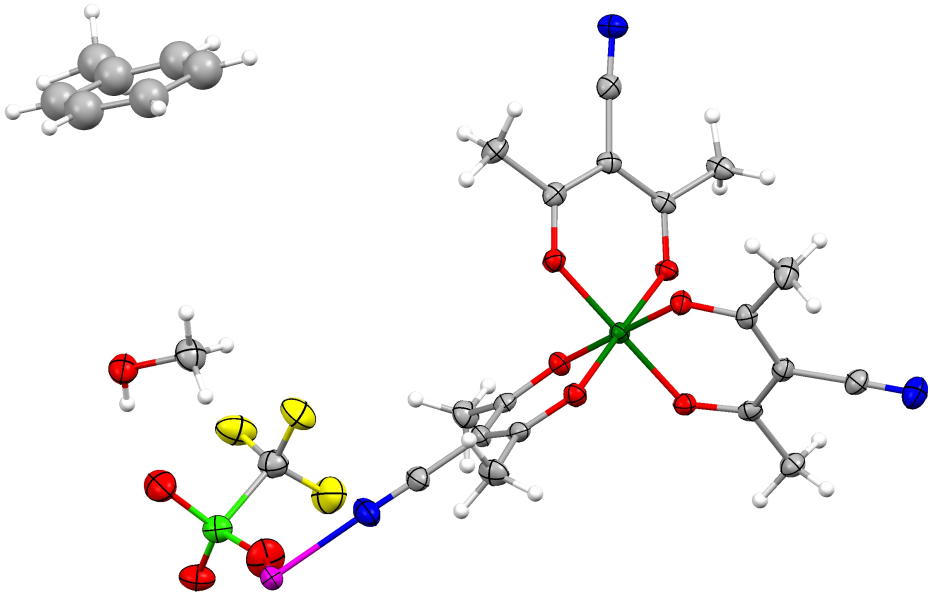

Fig. S9 Displacement ellipsoid plot of a molecular fragment in **3b**. Ellipsoids are drawn at 50 % probability.

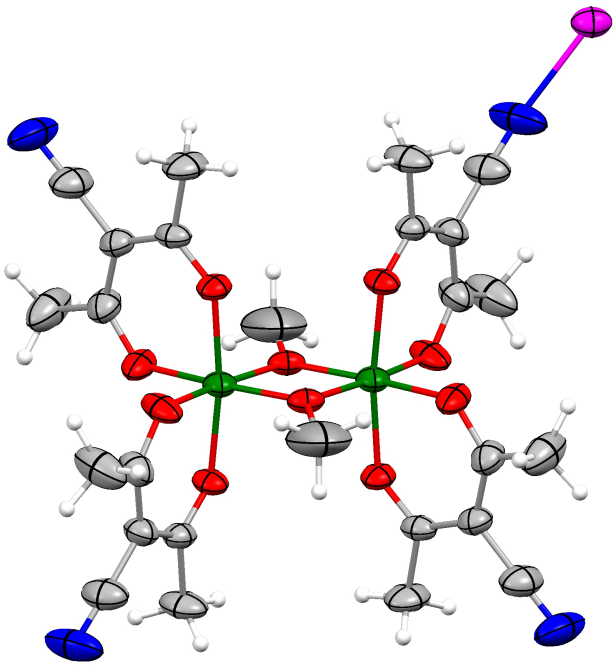

Fig. S10 Displacement ellipsoid plot of a molecular fragment in **3c**. Ellipsoids are drawn at 50 % probability.

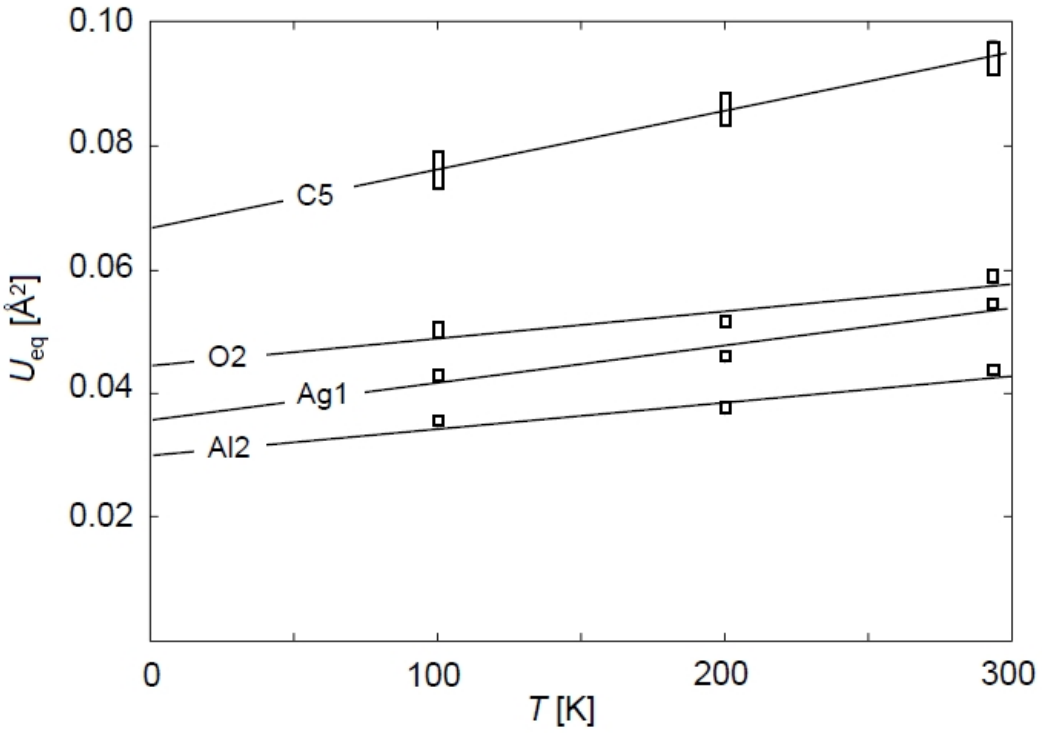

Fig. S11 All atoms of the network structure **3c** show unusual large U_{eq}. Temperature dependent single crystal X-ray diffraction experiments and void anlaysis of the network indicate statically disordered solvent molecules which affect the displacement parameters of the well-ordered framework atoms.

Table 1 Comparison of the refinement results for the framework **3c** after and before treatment with the BYPASS procedure.

Compound	BYPASS procedure	assignment of well-ordered electron-density
wR_2 (all reflections)	0.1547	0.4700
R_1 (all/obs)	0.0832/0.0615	0.2091/0.1901
GOF on F^2	1.085	3.474
Diff. peak/hole (e Å^{-3})	0.913 and -1.024	9.603 and -0.972

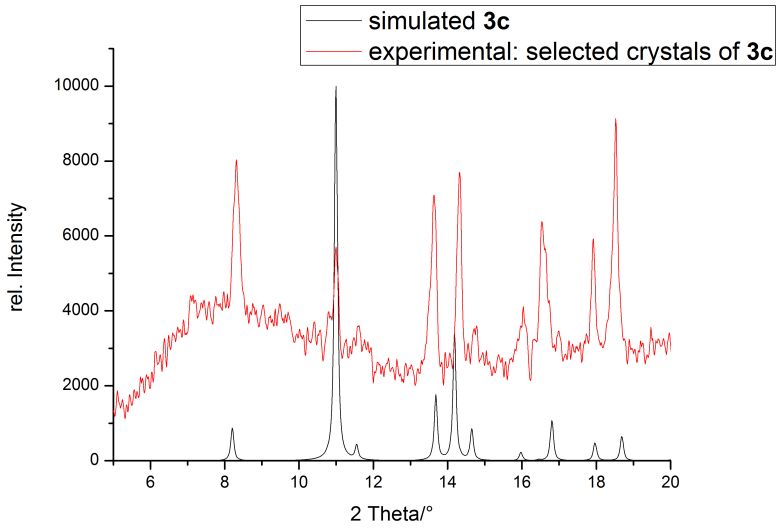

Fig. S12 Simulated and experimental powder pattern of selected crystals of **3c**.

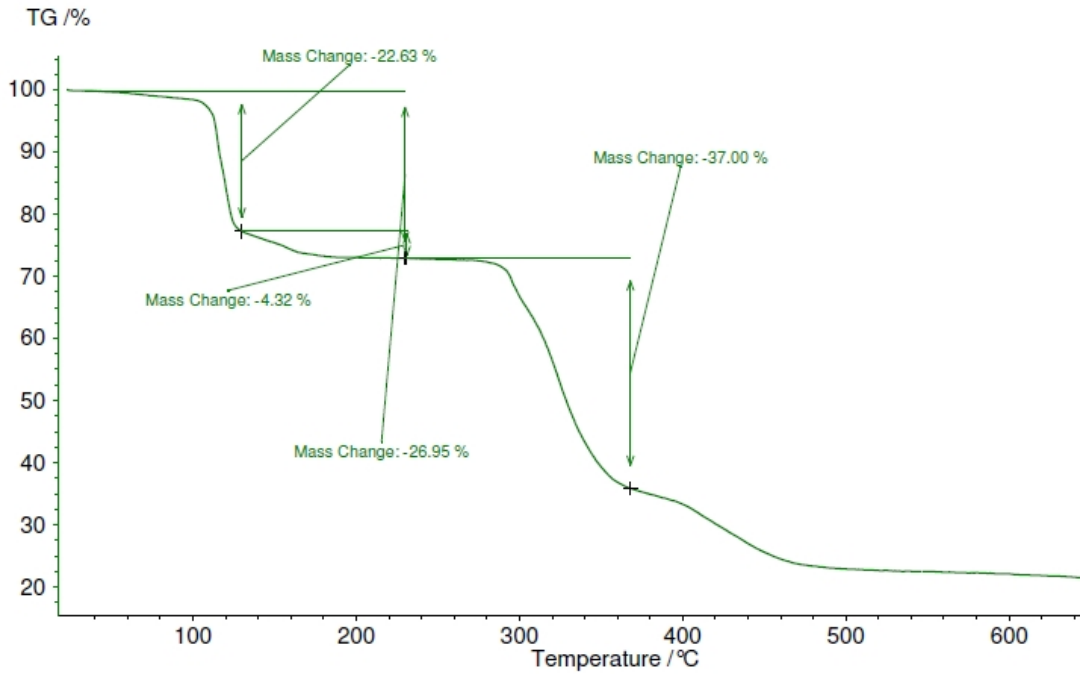

Fig. S13 TG measurement of selected crystals of **3c**. The molecular weight of the network structure is 720.4 g mol^{-1}. The assumed solvent content of eleven water molecules and one hydoxide molecule corresponds to a molecular weight of 215.2 g mol^{-1}. Elimination of the solvent within the voids of the network corresponds to a weight loss of 23 %.

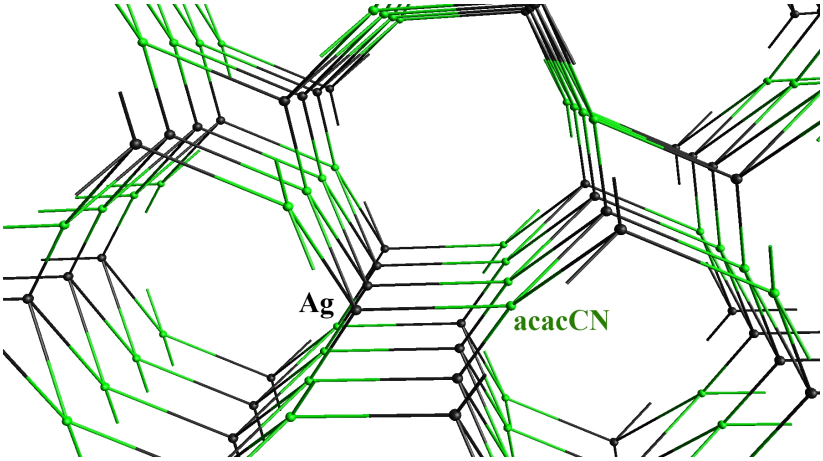

Fig. S14 Topology analysis of [Ag(acacCN)] with GTECS3D. The acacCN ligand is treated as a single node. Color code: Ag node: black and acacCN node: green.