

Electronic Supplementary Information
to the manuscript

The role of carboxylate ligands in two novel cyanido-bridged 2-D coordination networks Cu^{II}-W^V and Mn^{II}-Nb^{IV}

Tomasz Korzeniak, Dawid Pinkowicz, Wojciech Nitek, Maria Bałanda, Magdalena Fitta and Barbara Sieklucka*

Tab S1. Shape parameters for octacyanidometallate moieties in **(1)**-**(2)**

Metal center	S _{BTPR-8}	S _{SAPR-8}	S _{TDD-8}	Δ _(SAPR,TDD)	φ _(SAPR→TDD)	φ _(TDD→SAPR)
W1 in (1)	2.197	0.178	2.163	0.119	0.249	0.870
W2 in (1)	1.955	0.256	1.938	0.122	0.299	0.823
				Δ _(TDD,BTPR)	φ _(BTPR→TDD)	φ _(TDD→BTPR)
Nb1 in (2)	0.662	2.030	1.565	0.249	0.492	0.757

Abbreviations used: BTPR-8, bicapped trigonal prism; SAPR-8, square antiprism; TDD-8, triangular dodecahedron. S_x denotes the value of the continuous shape measure (CShM) of the coordination sphere relative to the ideal geometry X. The Δ and φ parameters stand for the deviation from minimal distortion path and generalized coordinate along the interconversion path, respectively.

Tab S2. Shape parameters for pentacoordinated Cu3–Cu5 centers in **(1)**.

Metal center	S _{vOC-5}	S _{TBPY-5}	S _{SPY-5}
Cu3	0.847	4.270	0.605
Cu4	0.970	4.694	0.416
Cu5	1.966	3.688	1.177

Abbreviations used: vOC-5, vacant octahedron; TBPY-5, trigonal bipyramide; SPY-5, square pyramide.

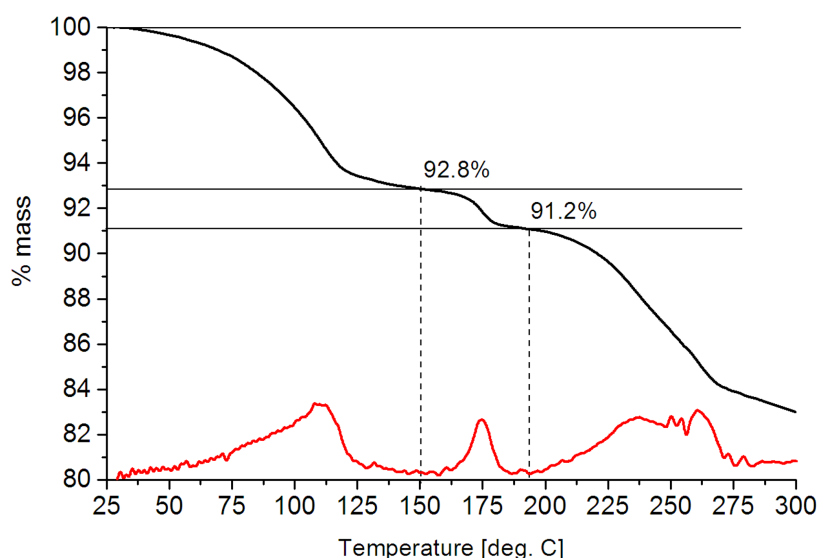


Figure S1. Thermogravimetric analysis for (1): TGA curve is shown in black and derivative in red.

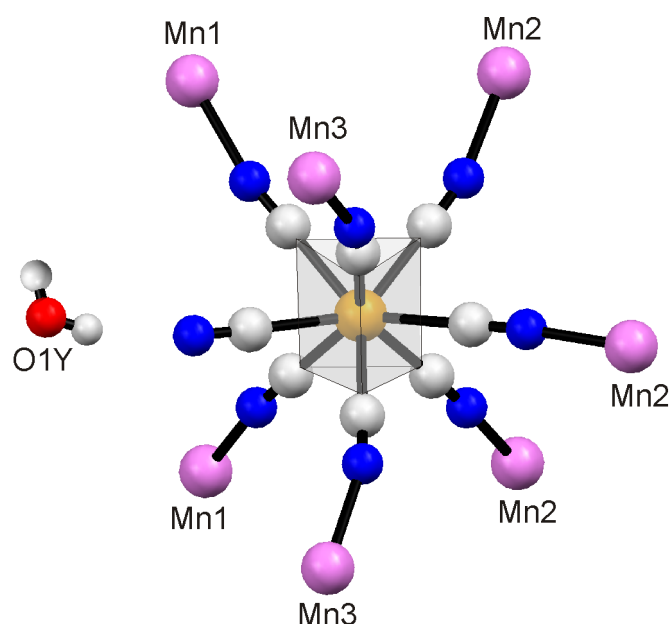


Figure S2. Bicapped trigonal prism geometry of the coordination sphere of $[\text{Nb}^{\text{IV}}(\text{CN})_8]^-$ moiety with Mn-atoms and a water molecule indicating the connectivity of Nb-centre. Nb – orange, Mn– violet, N – blue, C – gray, O – red.

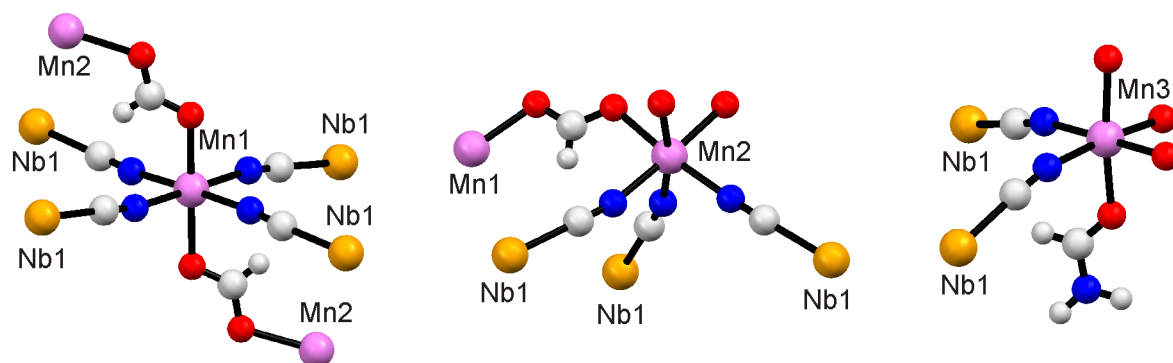


Figure S3. Coordination spheres and connectivity of the manganese centres in (2). Nb – orange, Mn– violet, N – blue, C – gray, O – red.