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Supplementary Information

An arsenicniobate-based 3D framework with selective adsorption and anion-exchange properties

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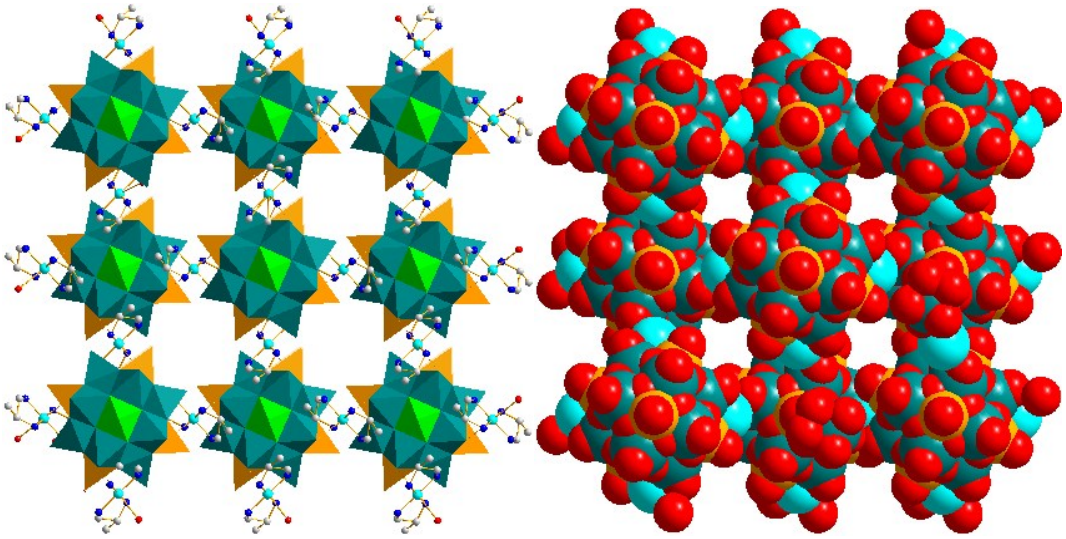

Fig. S1. The 3D porous framework of **1** viewed along the c direction. (color code: NbO_6, teal polyhedron; $V(1)O_5$, green polyhedron; $V(2)O_5$, orange polyhedron; O, red spheres; Cu, turquiose spheres; C, grey spheres; N, blue spheres).

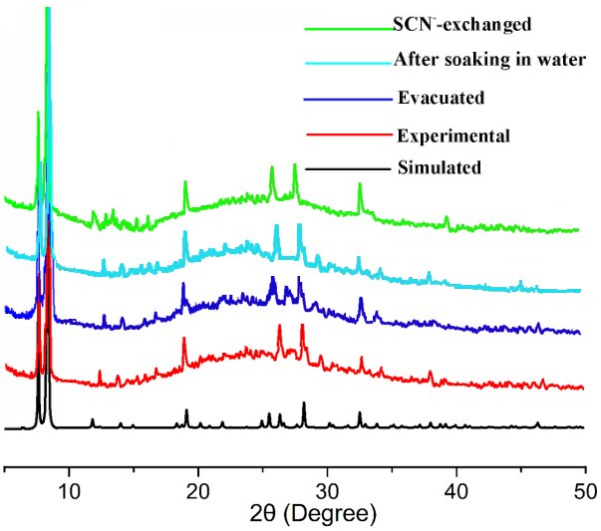

Fig. S2. PXRD patterns of solids **1** (black: calculated; red: as-synthesized sample at room temperature; blue: evacuated sample of 1 after heated at 120℃for 12 h under vacuum; turquoise: after soaking the as-synthesized sample in water for three months; green: SCN^--exchanged samples of **1**.), showing the power product is in good agreement with the calculated pattern from the single-crystal X-ray diffraction.

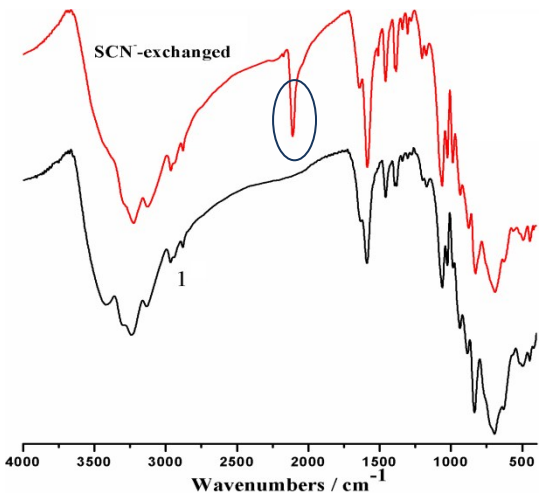

Fig. S3. The IR spectra of **1** from 4000-400 cm^{-1}, the mark indicates that the SCN^- band appears in SCN^--exchanged sample.

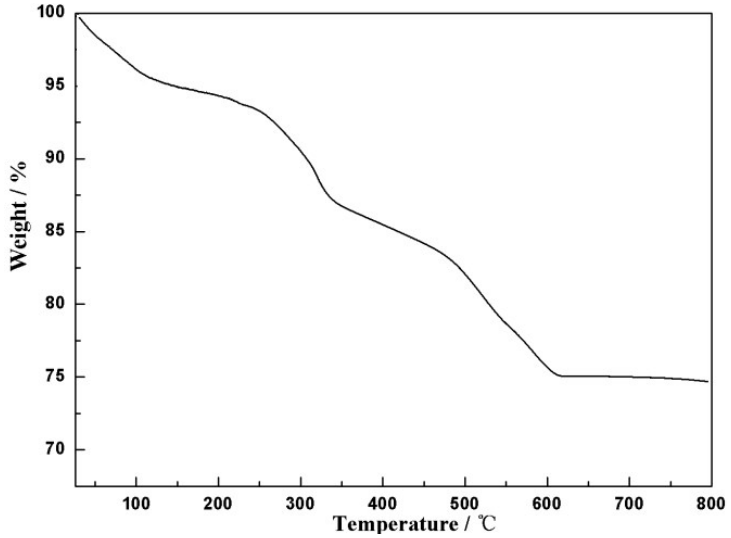

Fig. S4. The thermogravimetric (TG) curves of **1** measured from 30 to 800 ºC under N_2 atmosphere with the heating rate of 10 ºC/min.

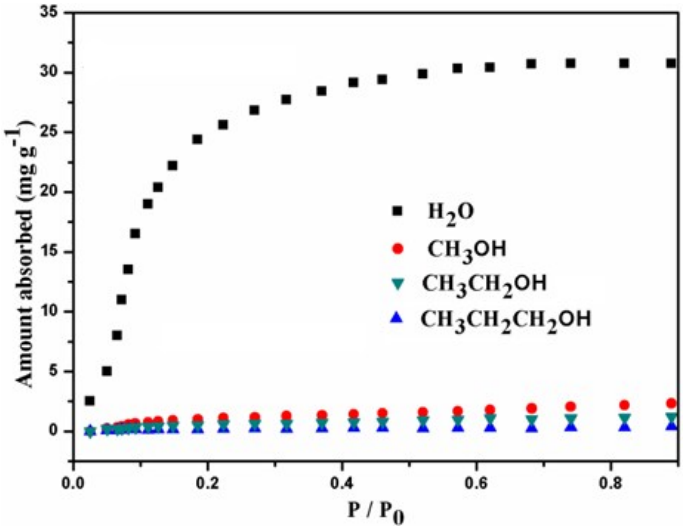

Fig. S5. Water and alcohols adsorption isotherms of **1** at 298 K.

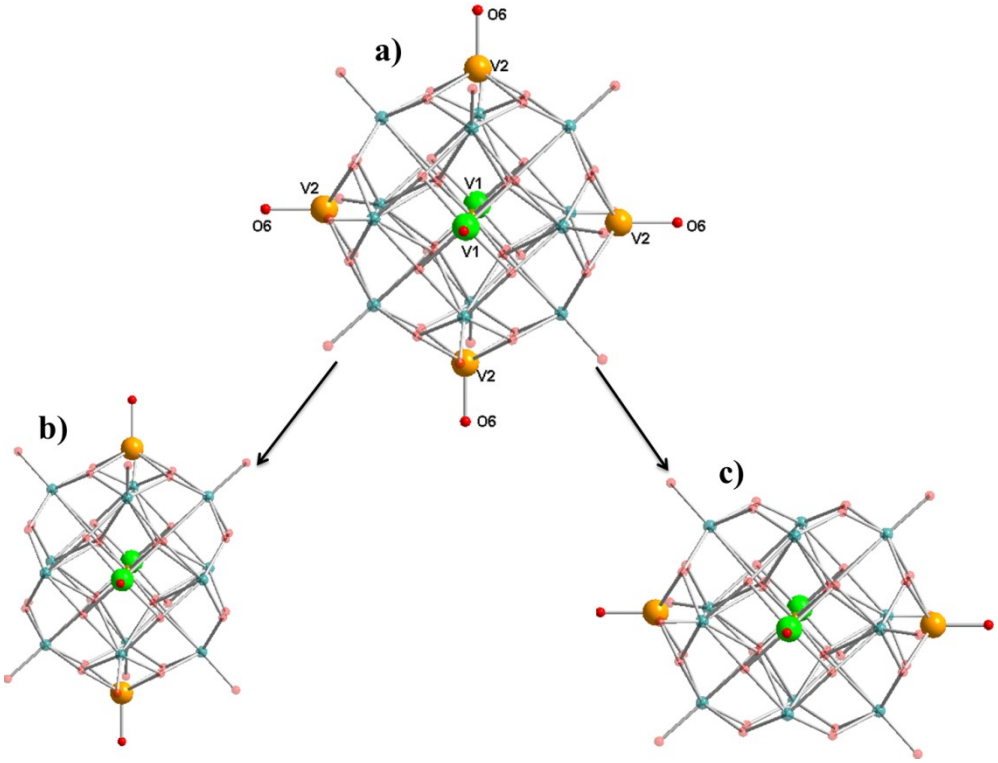

Fig. S6. (a) Ball-and-stick view of the disordered $[AsNb_{12}O_{40}(VO)_4]^{7-}$ cluster (color code: V1, green spheres; V2, orange spheres), in which all V1 centers are full-occupancy and all V2 centers are half-occupancy; (b) and (c) Ball-and-stick view of two possible actual configurations of $[AsNb_{12}O_{40}(VO)_4]^{7-}$ cluster in compound **1**. Both configurations possess 50% opportunity of appearance in the same position of **1**.

Such site-occupancy disorder of vanadium atom also can be seen in other reported literatures (A. J. Jacobson et. al, Inorg. Chem, 2003, 42, 3728-3733; G. -Y. Yang et. al, Inorg. Chem, 2007, 46, 9503−9508).

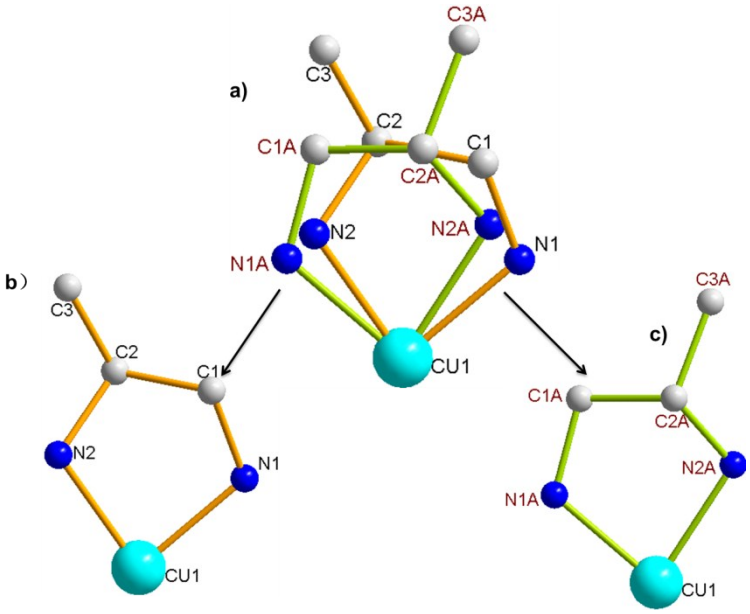

Fig. S7. The disordered dap molecules coordinated to Cu atoms.

As shown in Fig. S7, the dap molecule coordinated to Cu atoms have been refined as two sets of atoms with 50% occupancy for each. The atom labelings and bonds of two sets of atoms are distinguished in different colors (b and c).

Table S1. Bond-valence sum calculations for **1.**

Bonds	Bond length (Å)	BVS	Bonds	Bond length (Å)	BVS
V(1)-O(3)	1.596(11)	1.616	V(2)-O(6)	1.628(11)	1.482
V(1)-O(5)	1.973(5)	0.583	V(2)-O(7)	1.972(10)	0.585
V(1)-O(5) #2	1.973(5)	0.583	V(2)-O(7) #4	1.972(10)	0.585
V(1)-O(5) #3	1.973(5)	0.583	V(2)-O(4)	1.971(12)	0.587
V(1)-O(5) #6	1.973(5)	0.583	V(2)-O(4) #4	1.971(12)	0.587
	sum	3.948		sum	3.826