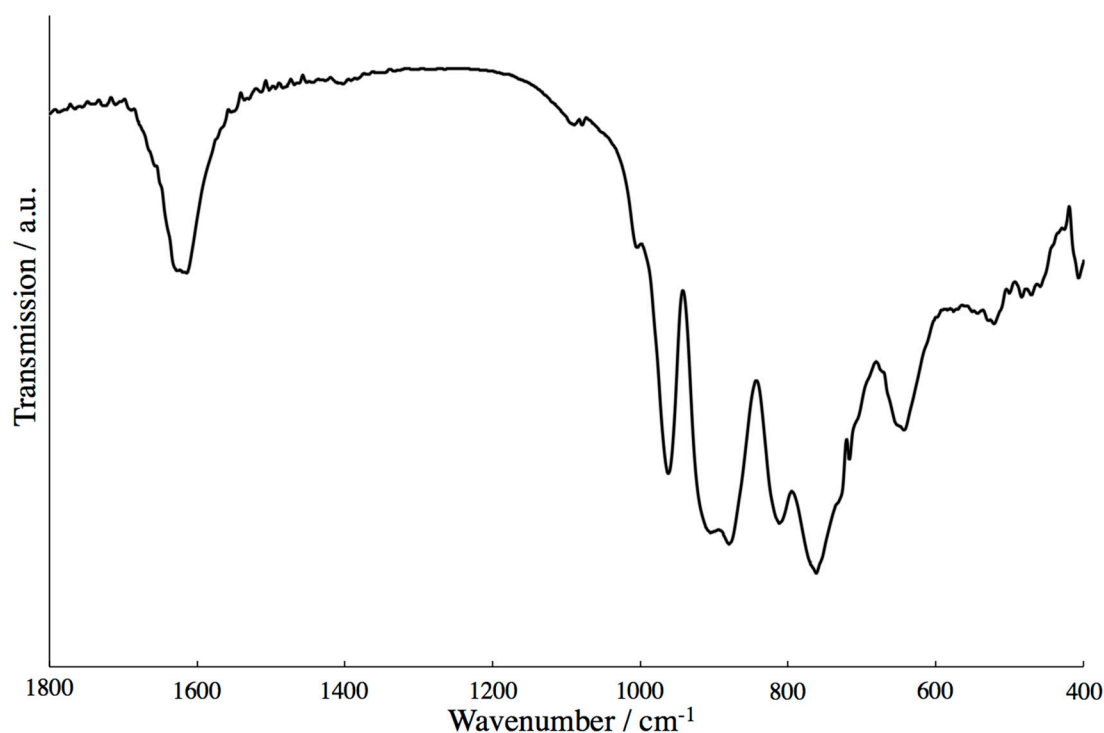


# Supplementary Materials: $\beta,\beta$ -Isomer of Open-Wells-Dawson Polyoxometalate Containing Tetra-Iron(III) Hydroxide Cluster: $[\{\text{Fe}_4(\text{H}_2\text{O})(\text{OH})_5\}(\beta,\beta\text{-Si}_2\text{W}_{18}\text{O}_{66})]^{9-}$

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**Table S1.** Bond valence sum (BVS) calculations of Fe and O atoms of the  $\{\text{Fe}_4(\text{H}_2\text{O})(\text{OH})_5\}$  cluster moieties of  $\beta,\beta\text{-Fe}_4\text{-open}$ .

Fe(1)	2.981	O(67)	1.106
Fe(2)	3.030	O(68)	0.796
Fe(3)	3.018	O(69)	1.157
Fe(4)	3.148	O(70)	0.660
		O(71)	1.170
		O(72)	1.255



**Figure S1.** FT-IR spectrum of potassium salt of  $\beta,\beta\text{-Fe}_4\text{-open}$  (KBr disk).

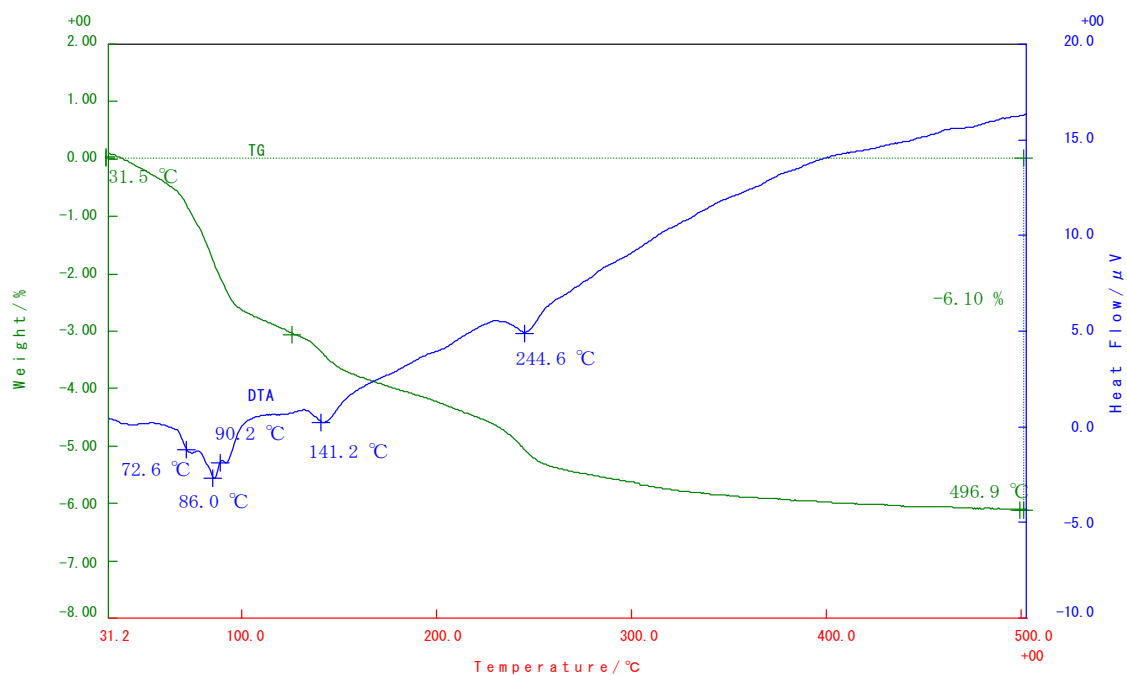


Figure S2. TG/DTA data of potassium salt of  $\beta,\beta\text{-Fe}_4\text{-open}$ .

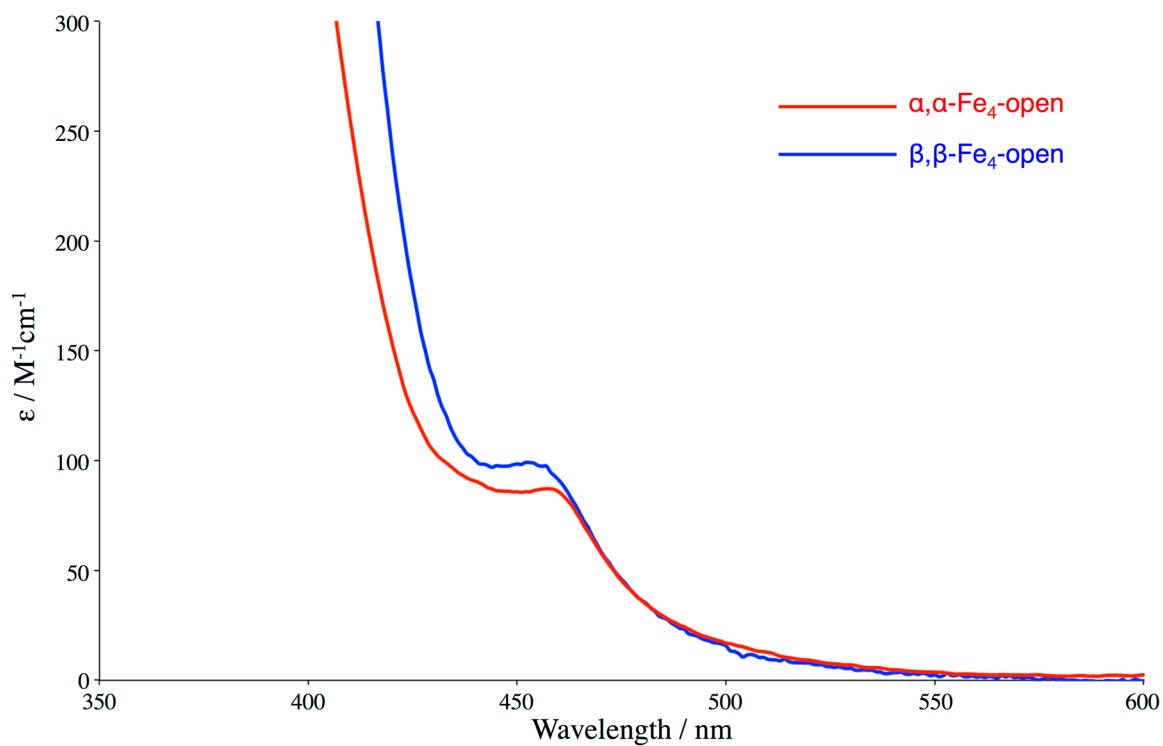
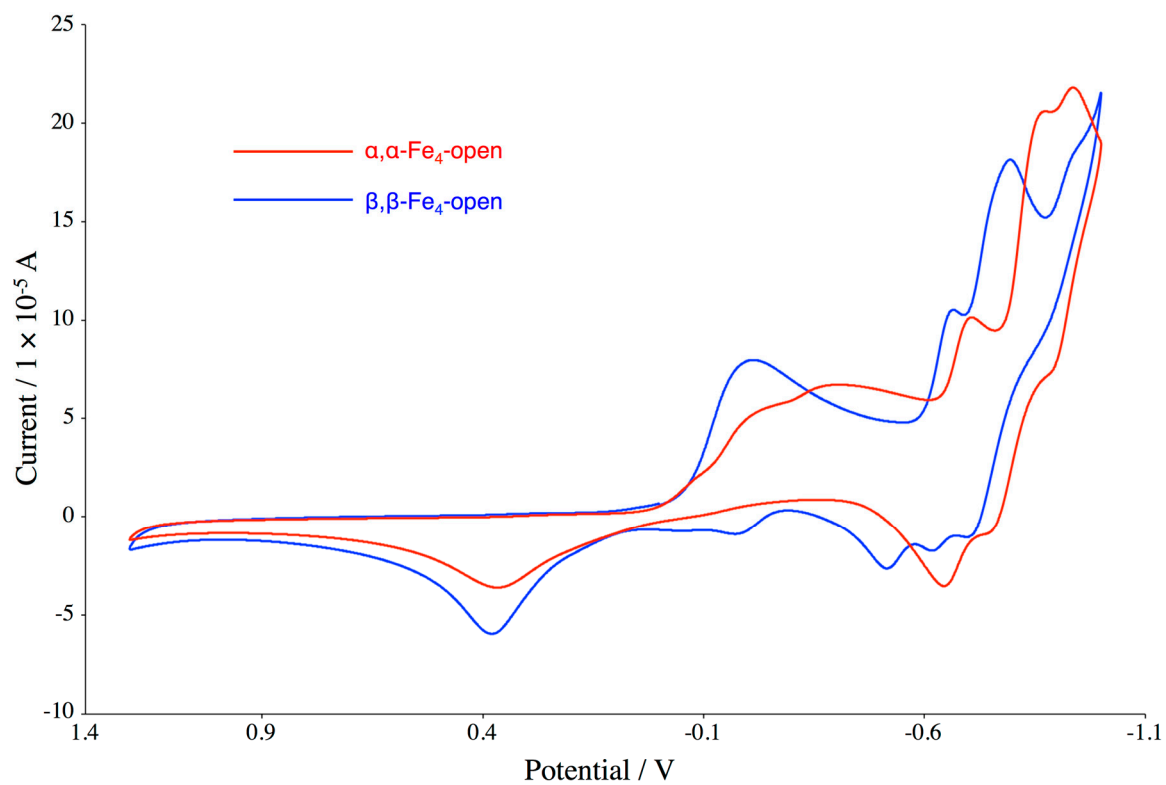


Figure S3. UV/VIS absorption spectra of potassium salt of  $\alpha,\alpha\text{-Fe}_4\text{-open}$  (red line) and  $\beta,\beta\text{-Fe}_4\text{-open}$  (blue line) in  $\text{H}_2\text{O}$ .



**Figure S4.** Cyclic voltammograms (CV) of 0.5 mM potassium salt of  $\alpha,\alpha$ - (red line) and  $\beta,\beta$ -Fe<sub>4</sub>-open (blue line) in 0.5 M potassium acetate buffer, pH 4.8, scan rate 25 mV·s<sup>-1</sup>, under N<sub>2</sub>.