

Supporting Information

Alpha and Beta Isomers of Tetrahafnium(IV) Containing Decatungstosilicates, [Hf₄(OH)₆(CH₃COO)₂(x-SiW₁₀O₃₇)₂]¹²⁻ (x = α, β)

Awatef S. Assran,^{a,b} Sib Sankar Mal,^{a,c} Natalya V. Izarova,^{a,d} Abhishek Banerjee,^a Andreas Suchopar,^a Masahiro Sadakane,^e and Ulrich Kortz^{a,*}

^a Jacobs University, School of Engineering and Science, P.O. Box 750 561, 28725 Bremen, Germany;

^b Permanent address: South Valley University, Faculty of Science at Qena, Chemistry department, 83523 Qena, Egypt;

^c Current address: Center For Catalysis Research and Innovation, Department of Chemistry, University of Ottawa, 10 Marie Curie, K1N 6N5, ON, Canada;

^d Permanent address: Nikolaev Institute of Inorganic Chemistry, Prospekt Lavrentyeva 3, 630090 Novosibirsk, Russia;

^e Chemistry and Chemical Engineering, Graduate School of Engineering, Hiroshima University, 1-4-1 Kagamiyama, Higashi-Hiroshima, 739-8527, Japan.

E-mail: u.kortz@jacobs-university.de; Fax: +49 421 200 3229; Tel: +49 421 200 3235

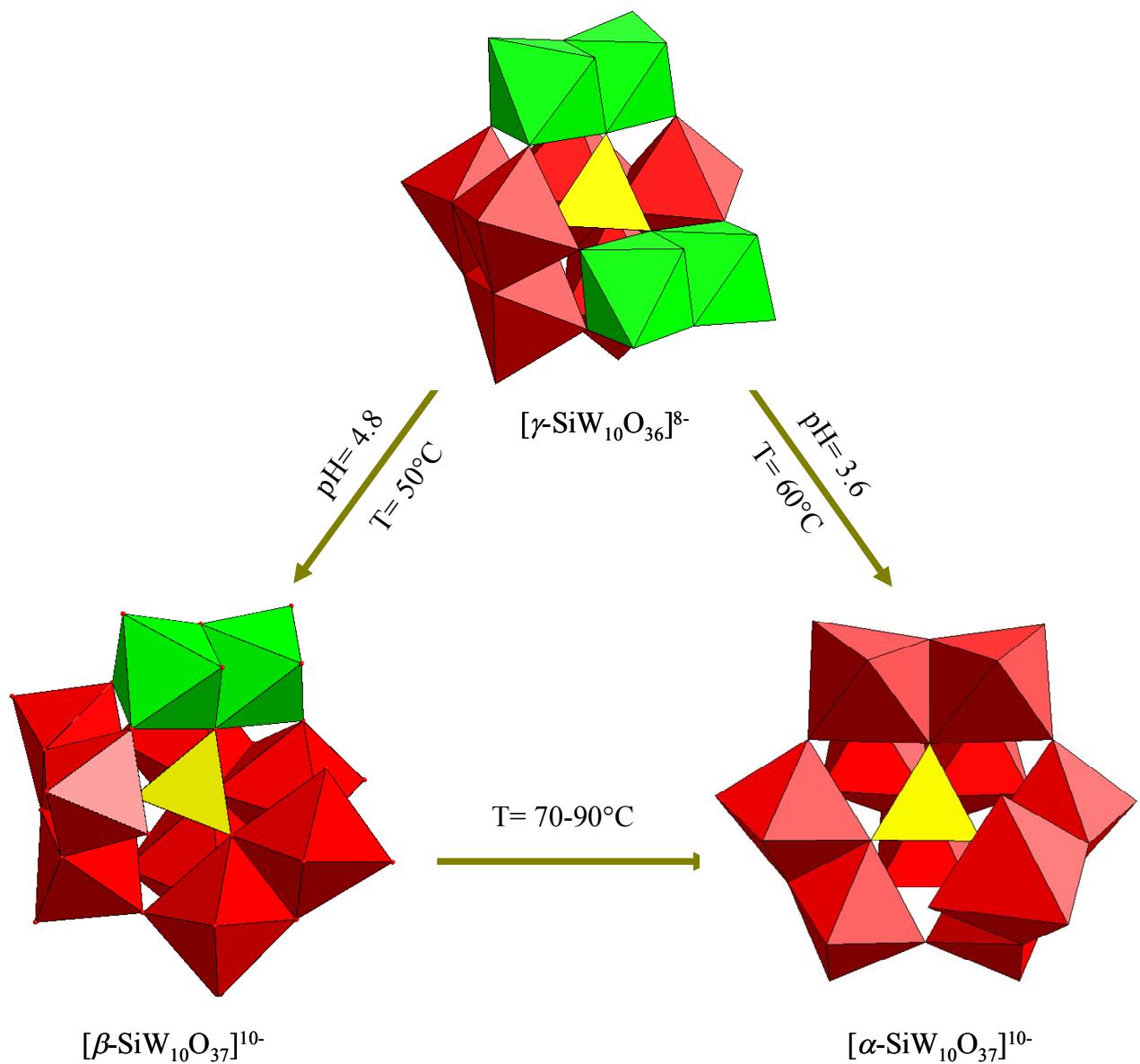


Figure S1. Representation of three dilacunary decatungstosilicate Keggin isomers and the experimental conditions for irreversible transformation. Color code: SiO_4 yellow tetrahedra, WO_6 red octahedra. The WO_6 polyhedra of the rotated triads are highlighted in green.

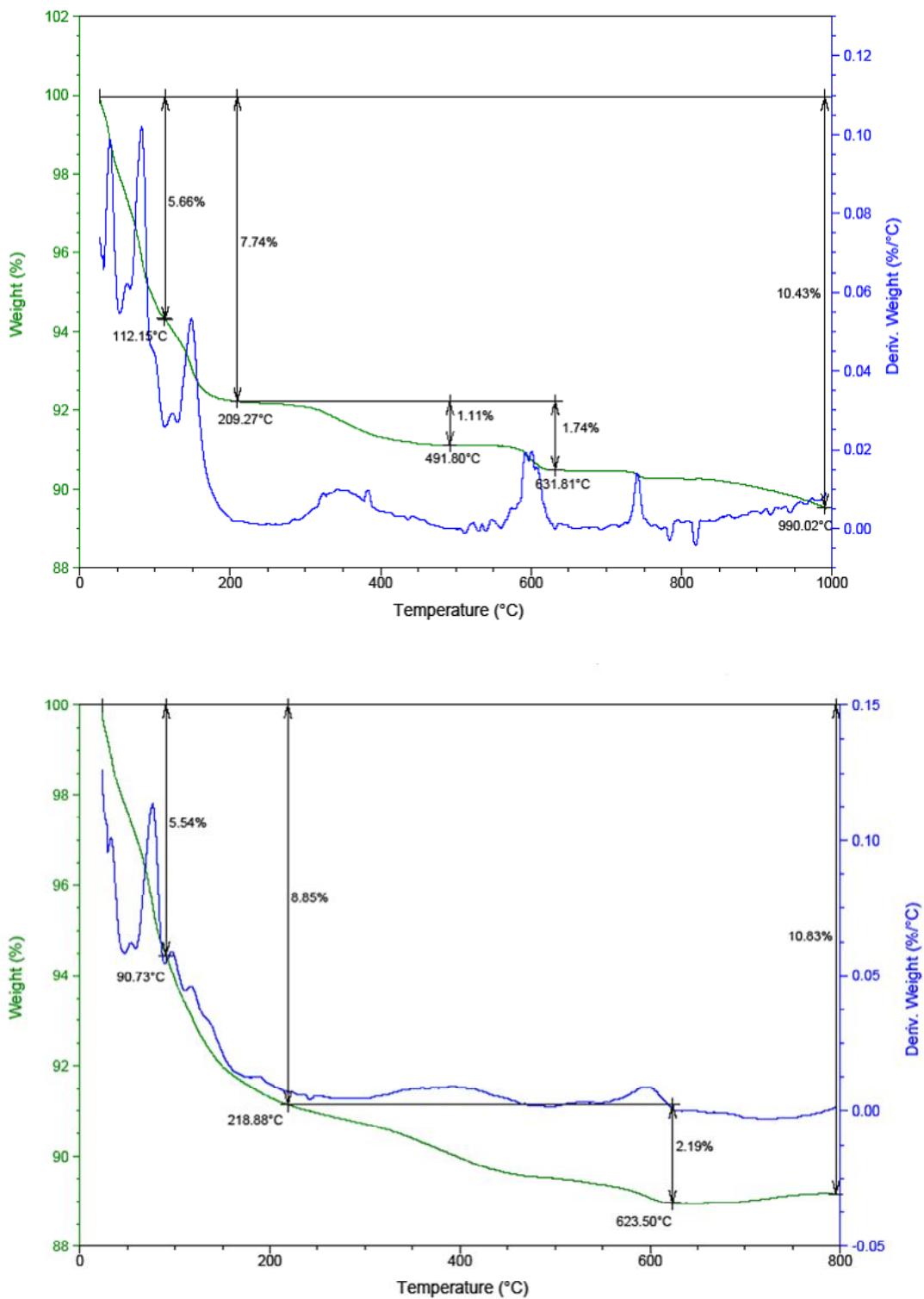


Figure S2. Thermogram of **K-1** (top) and **K-2** (bottom).

Colour legend: TGA, green line; DTA, blue line.

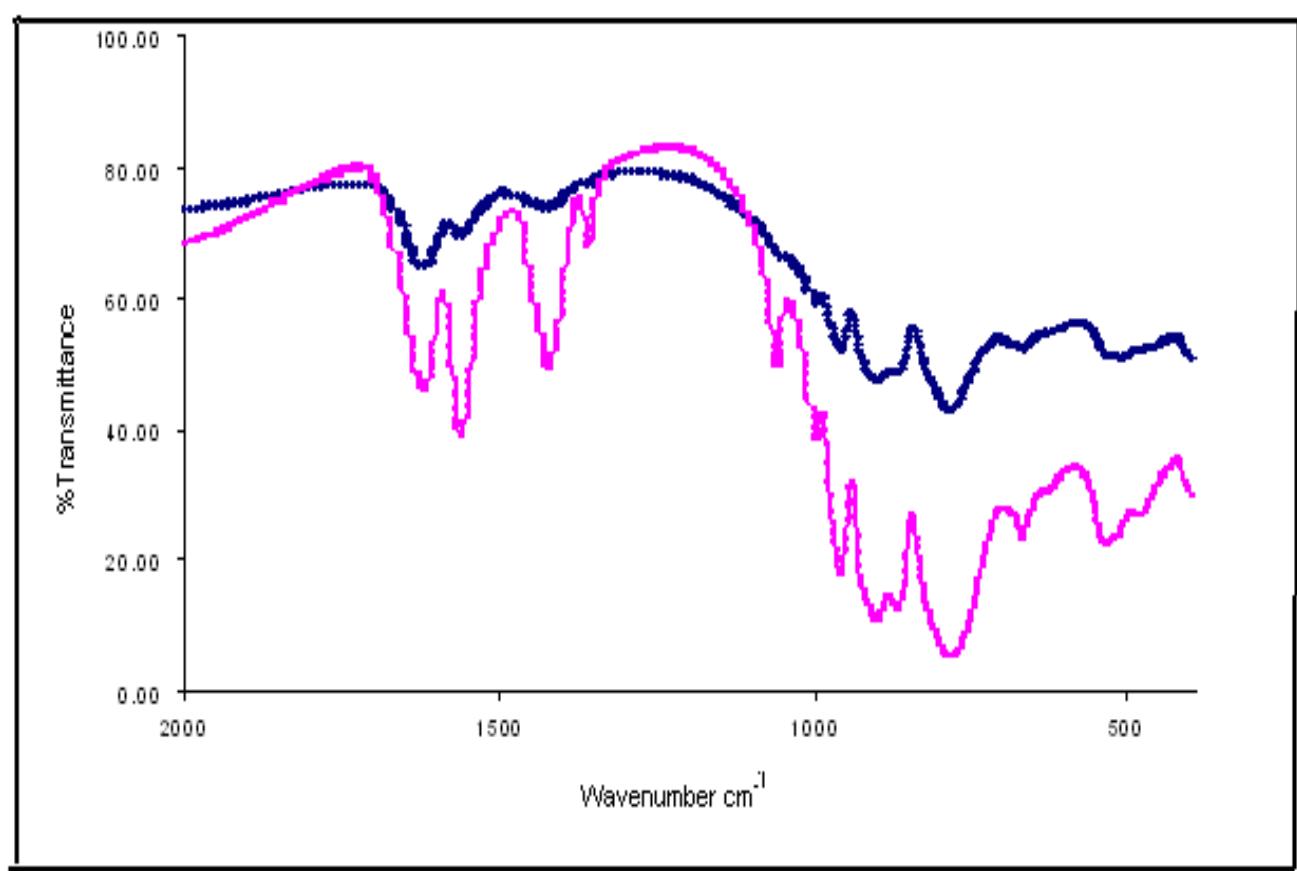


Figure S3. IR spectra of **K-1** (blue) and **K-2** (pink).

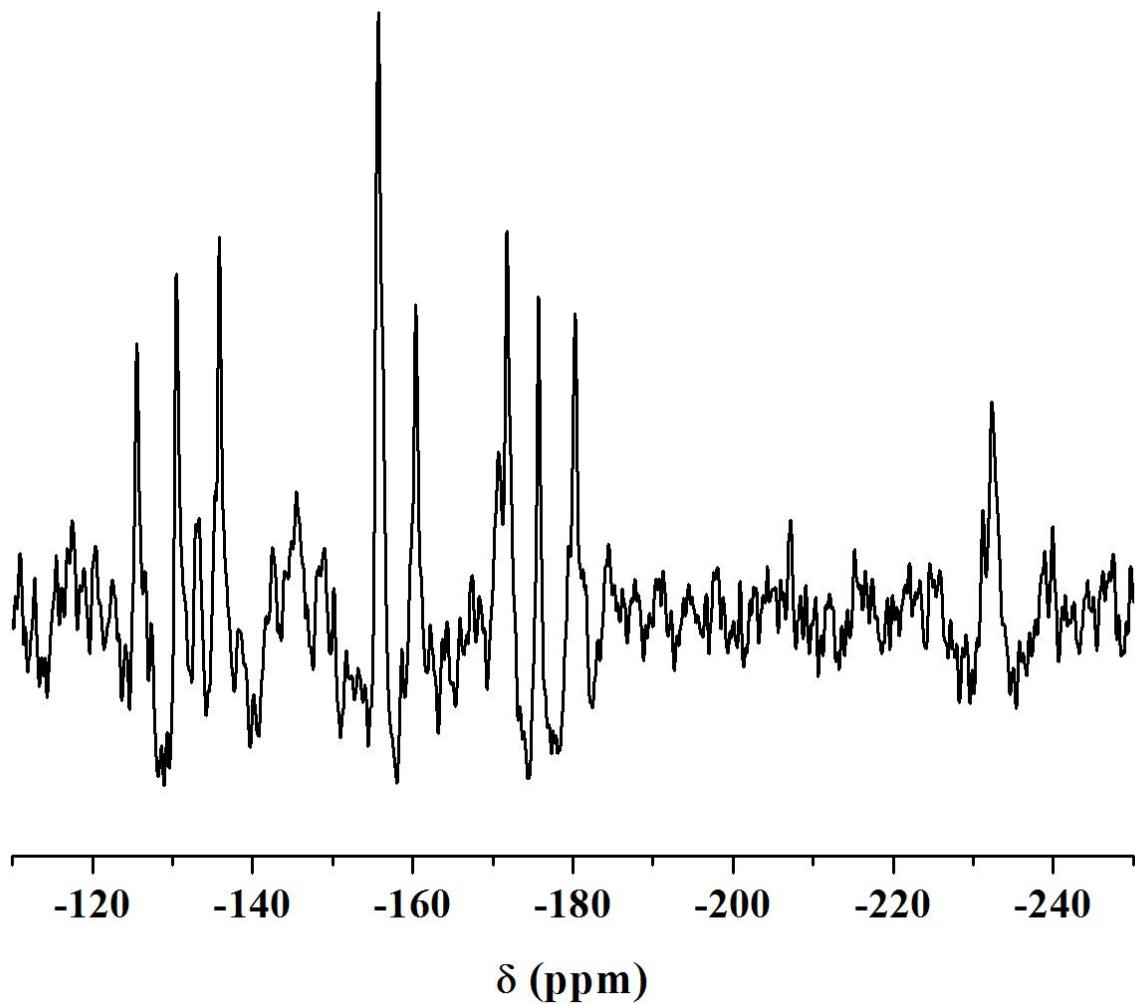


Figure S4. Room temperature ^{183}W NMR spectrum of **K-2** redissolved in 1M CH_3COOLi buffer (pH = 5).

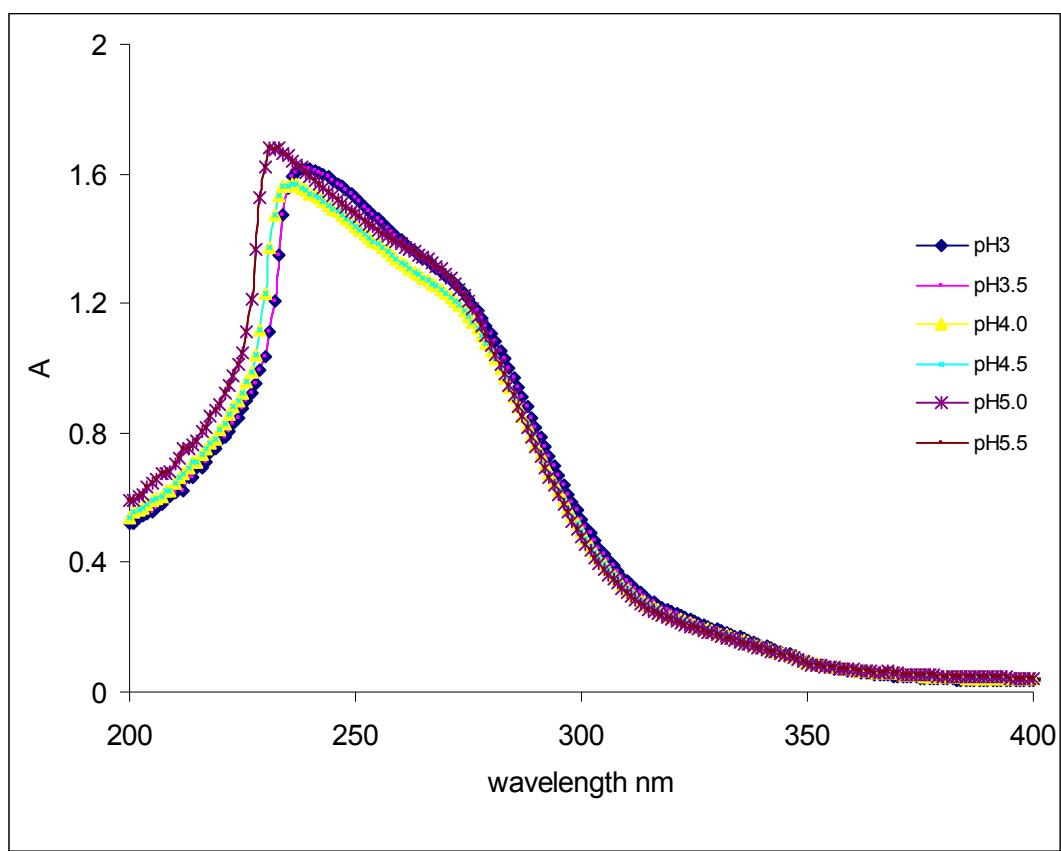


Figure S5. UV-vis spectrum of **K-1** (3×10^{-5} M) in 1 M CH₃COOLi solutions at different pH.

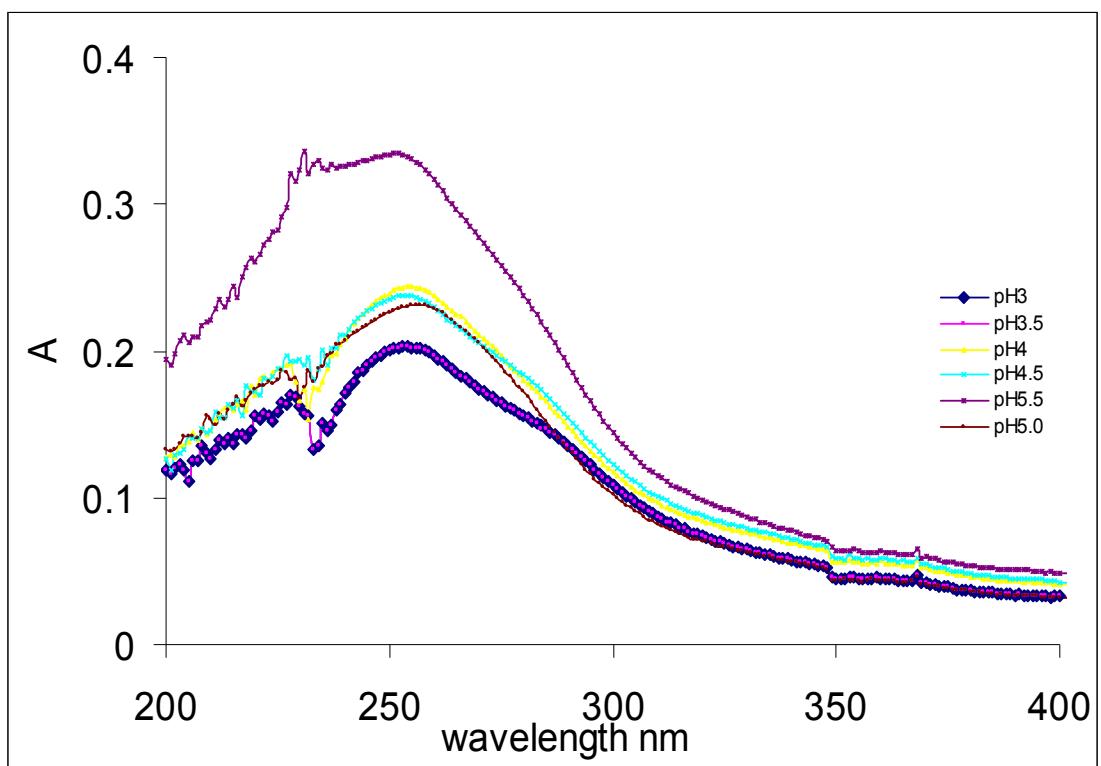


Figure S6. UV-vis spectrum of **K-2** (3×10^{-6} M) in 1 M CH₃COOLi solutions at different pH.

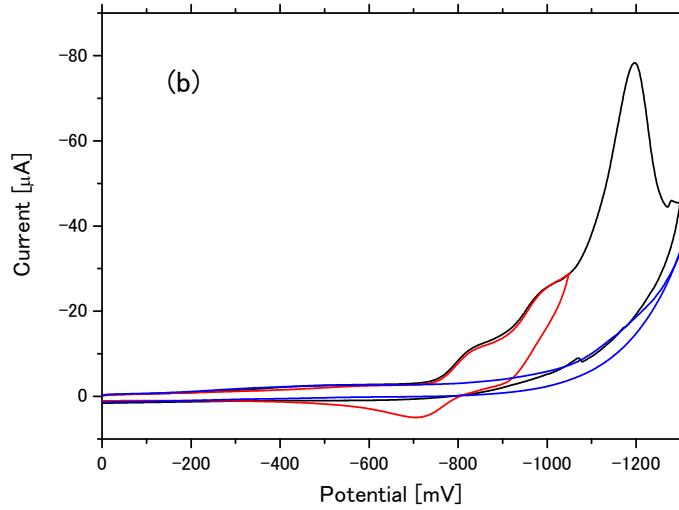
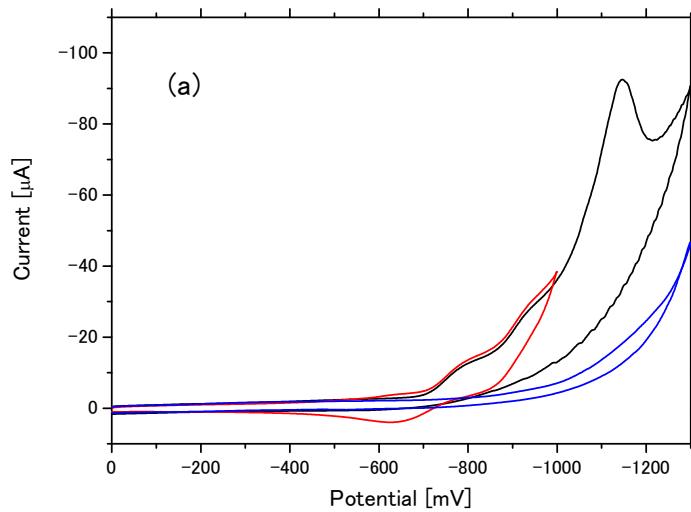


Figure S7. Cyclic voltammogram of **1** in 0.5 M LiOAc (pH 4.0) (a) and **2** in 0.5 M LiOAc (pH 4.8). Scan rate: 25 mV/s. The color code is Black line: scan until -1300 mV, red line: scan until -1000 mV, blue line: scan until -1300 mV without polyoxometalates (blank only electrolyte).