SUPPORTING INFORMATION

A novel method for measuring the Tc L_3-edge of technetium compounds

Peter E. R. Blanchard, Emily Reynolds, Brendan J. Kennedy* Chris D. Ling

School of Chemistry, The University of Sydney, Sydney, NSW 2006, Australia

Zhaoming Zhang, Gordon Thorogood

Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW 2234, Australia

Bruce C. C. Cowie, Lars Thomsen

Australian Synchrotron, 800 Blackburn Road, Clayton, Victoria 3168, Australia

Experimental Section

Ru L_3-edge XANES

Ru L_3-edge XANES spectra were collected on beamline 16A1 at the National Synchrotron Radiation Research Center (NSRRC) in Hsinchu, Taiwan.[1] Finely ground samples were dispersed onto Kapton tape and placed in the X-ray beam at a 45° angle. Spectra were collected from ~50 eV below to ~200 eV in fluorescence yield mode using a Lytle detector. An energy step-size of 0.2 eV was used near the absorption edge. The Ru L_3-edge spectra were calibrated against Ru reference foil with the maximum in the first derivative of the L_3-edge set to 2838 eV.

Results

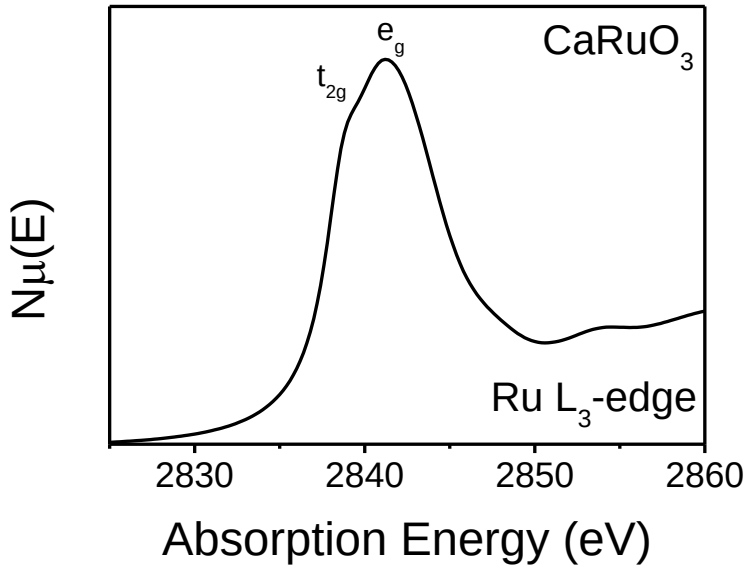

Figure S1. Ru L_3-edge XANES spectrum of $CaRuO_3$ collected on the BL16A beamline at NSRRC.

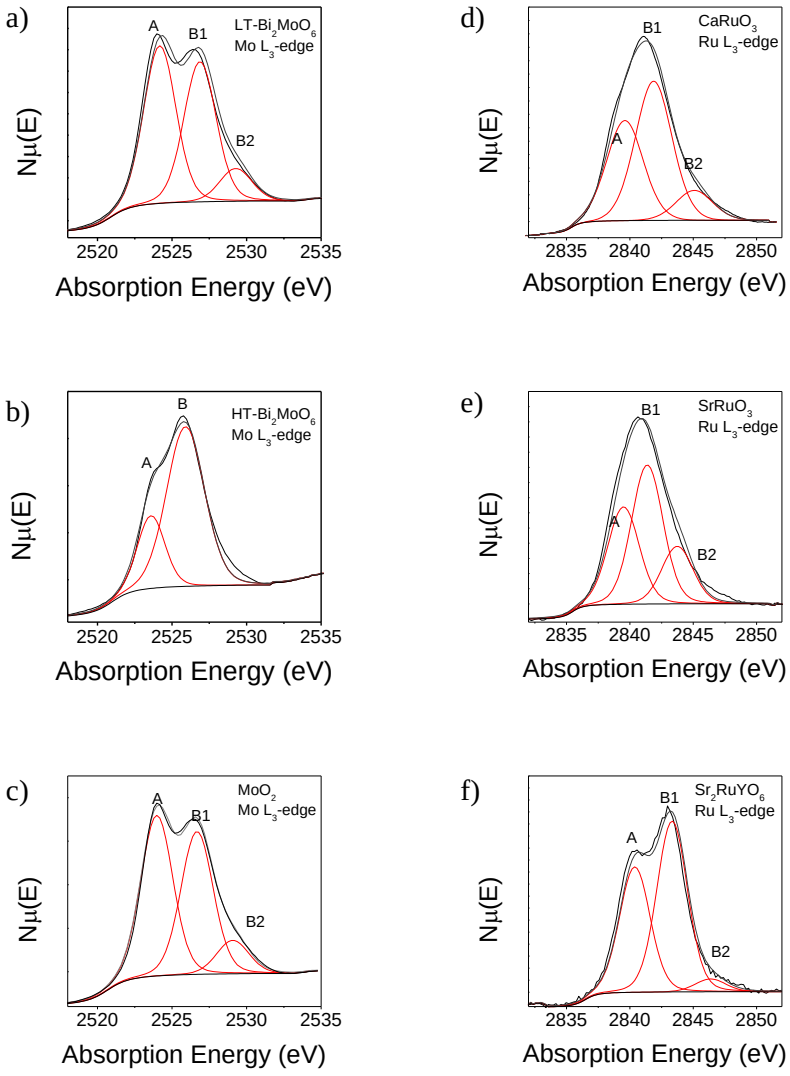

Figure S2. Fitted XANES spectra of a) LT-Bi_2MoO_6, b) HT-Bi_2MoO_6, c) MoO_2, d) $CaRuO_3$, e) $SrRuO_3$, and f) Sr_2RuYO_6.

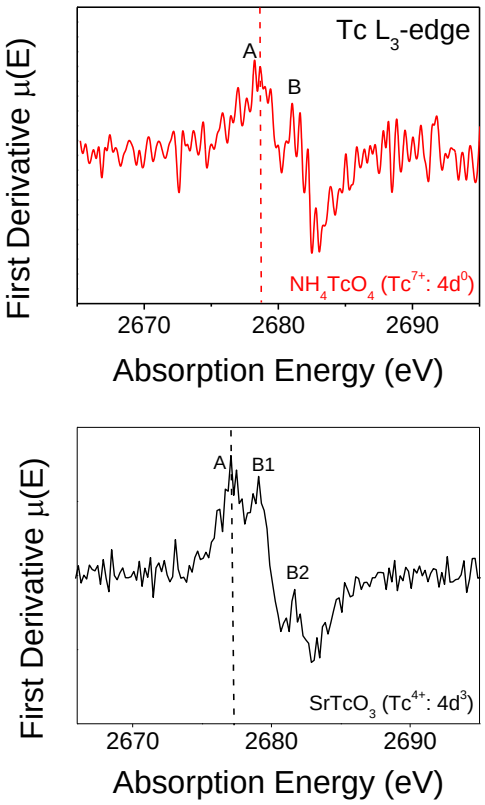

Figure S3. First derivative Tc L_3-edge XANES spectra of NH_4TcO_4 (top) and $SrTcO_3$ (bottom). Dashlines corresponds to the respective absorption edge energy of each spectrum. A and B (B1 and B2) correspond to the peak maxima.

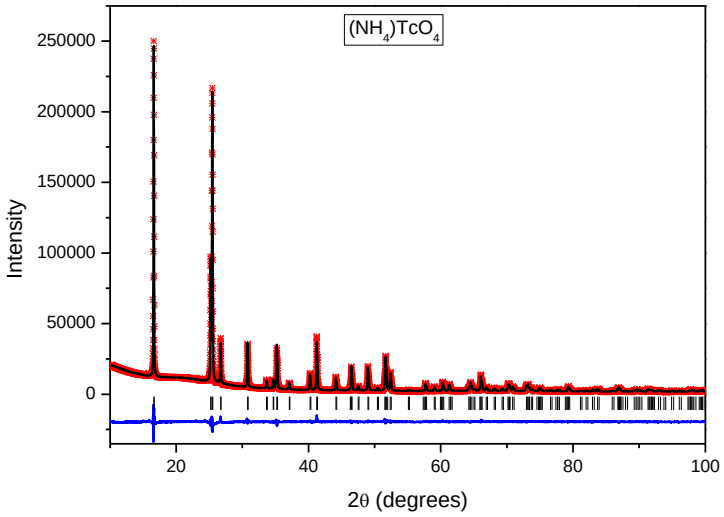

Figure S4. Observed, calculated and difference X-ray diffraction profiles for $(NH_4)TcO_4$. The structure was refined in space group $I4_1/a$ with a = 5.79094(5) and c = 13.30513(13) Å.

ATOM	x	y	z	Biso
Tc	0	0.25	0.125	1.18(1)
N	0	0.25	0.625	-0.06(7)
O	0.1009(2)	0.4741(3)	0.1979(1)	2.05(5)
H	0.109	0.244	0.593	0.6

References

1. T. E. Dann, S. C. Chung, L. J. Huang, J. M. Juang, C. I. Chen and K. L. Tsang, *J. Synchrotron Rad.* 1998, **5**, 664-666.