

Electronic Supplementary Information

Heterobimetallic Cerium(IV) Oxo Clusters Supported by a Tripodal Oxygen Ligand

Kang-Long Wong,[‡] Yat-Ming So,[‡] Guo-Cang Wang, Herman H.-Y. Sung, Ian D. Williams
and Wa-Hung Leung**

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1. NMR and IR Spectra of **3** and **4**

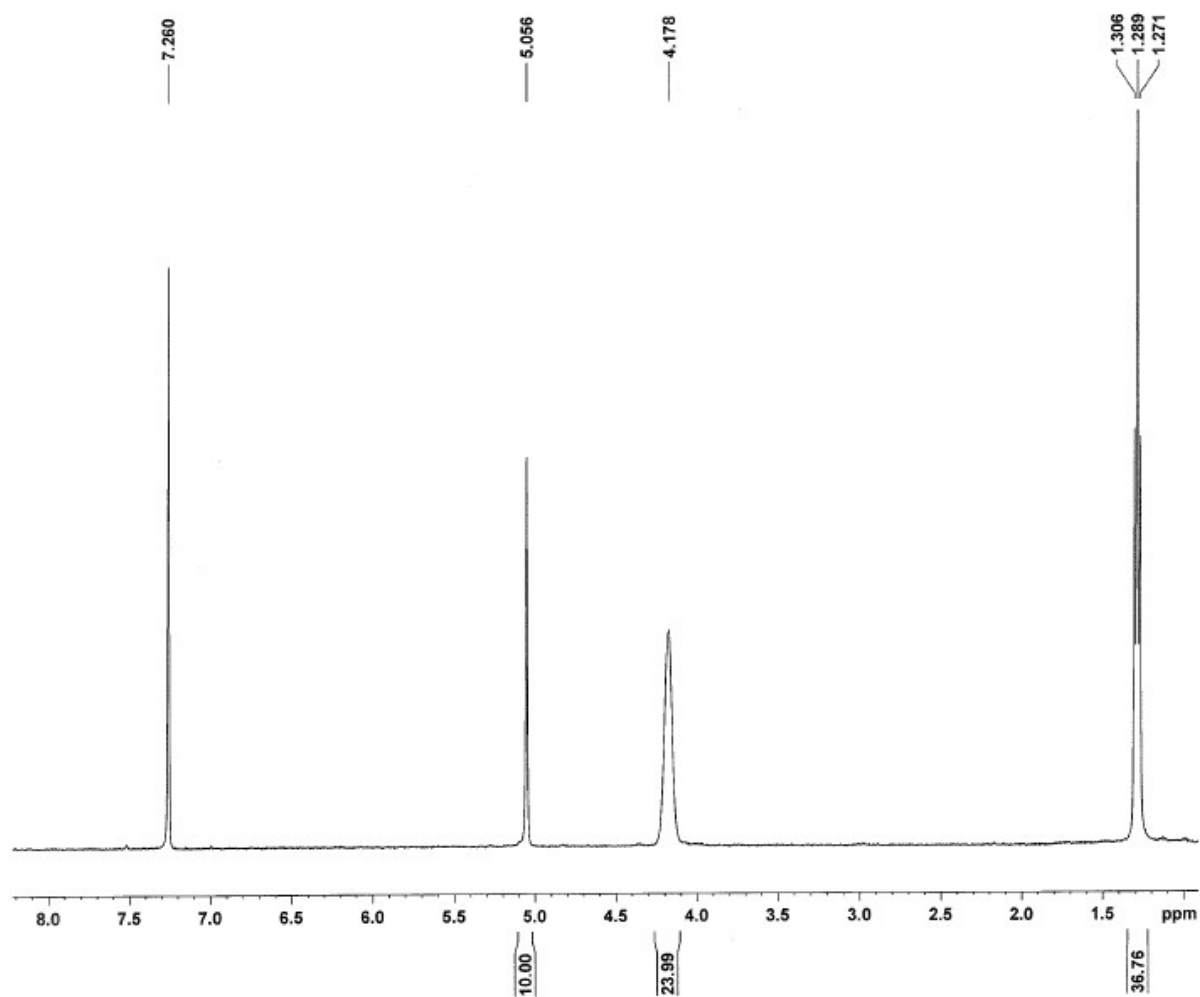


Figure S1. ^1H NMR (400 MHz, 25 $^\circ\text{C}$) spectrum of **3** in CDCl_3 .

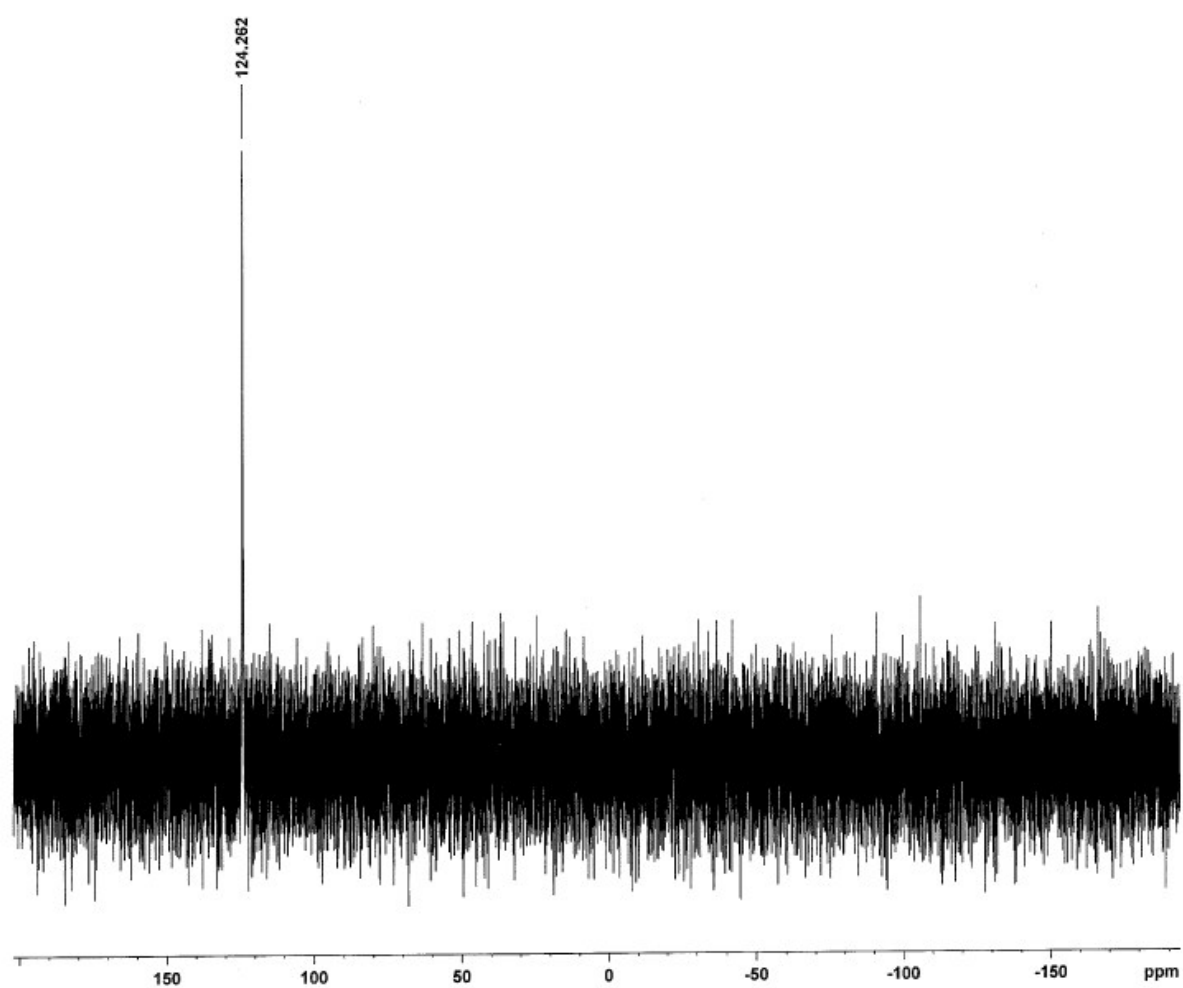


Figure S2. ^{31}P $\{^1\text{H}\}$ NMR (162 MHz, 25 °C) spectrum of **3** in CDCl_3 .

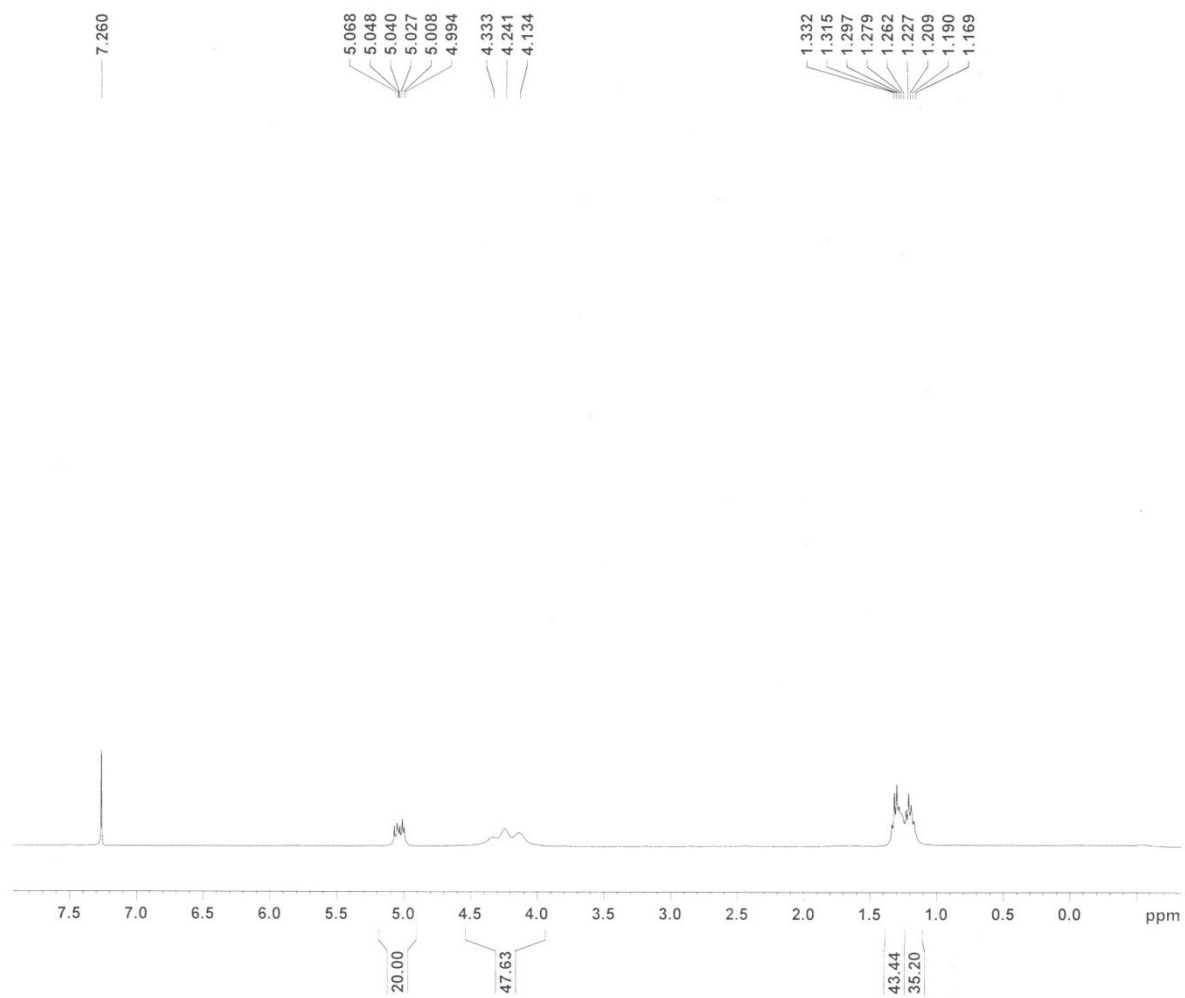


Figure S3. ¹H NMR (400 MHz, 25 °C) spectrum of **4** in CDCl₃.

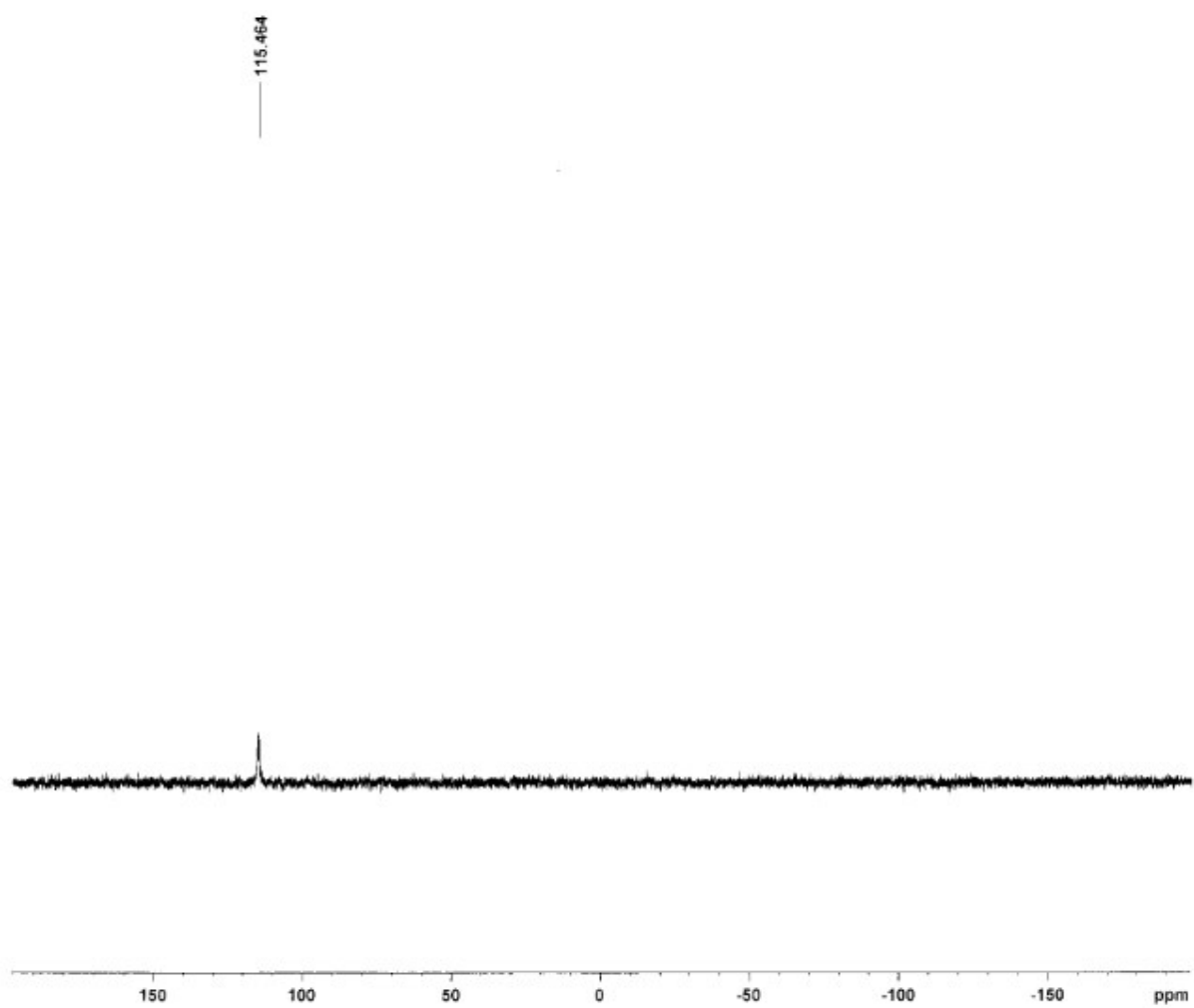


Figure S4. ^{31}P $\{^1\text{H}\}$ NMR (162 MHz, 25 °C) spectrum of **4** in CDCl_3 .

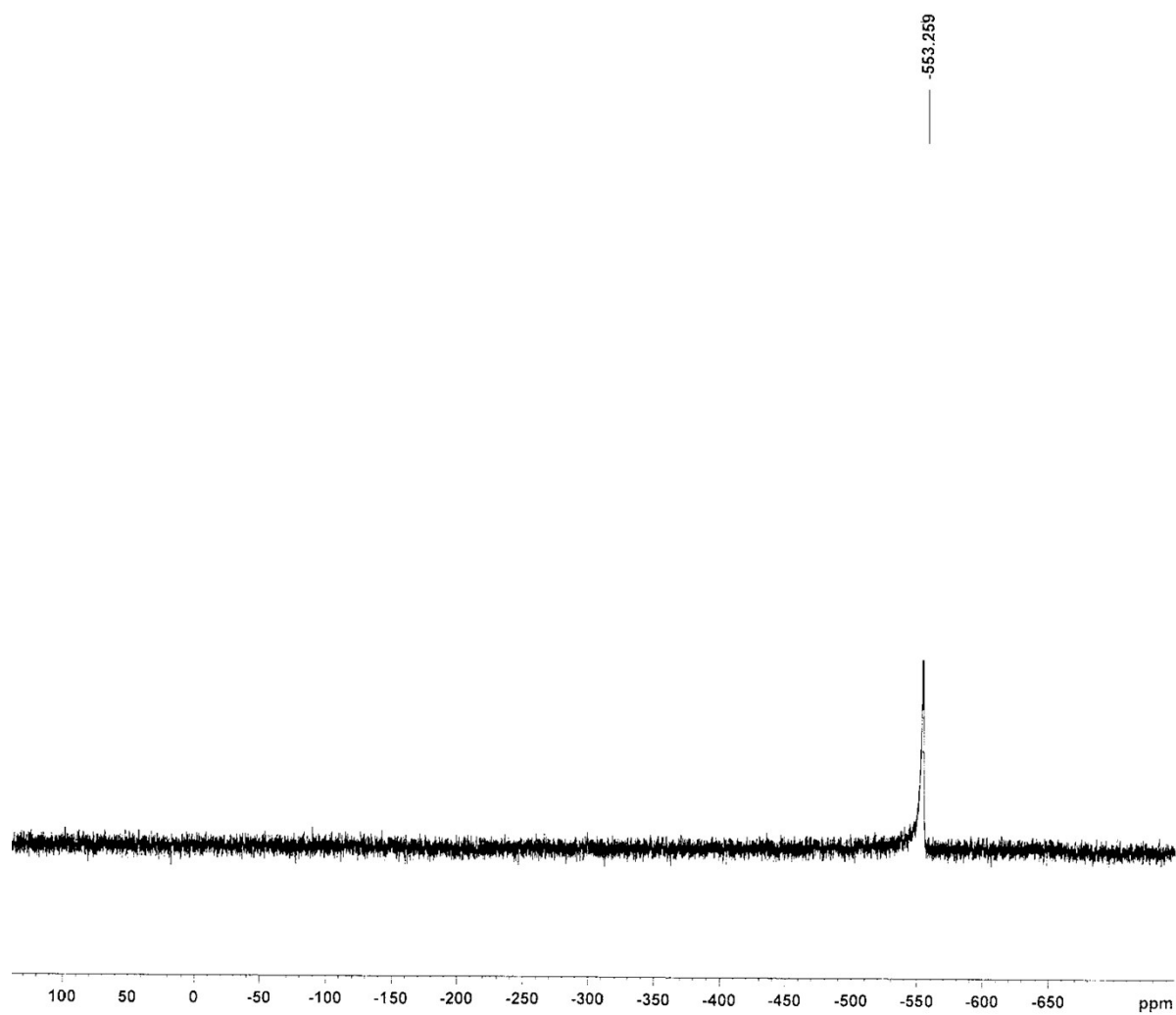


Figure S5. ^{51}V $\{^1\text{H}\}$ NMR (105 MHz, 25 °C) spectrum of **4** in CDCl_3 .

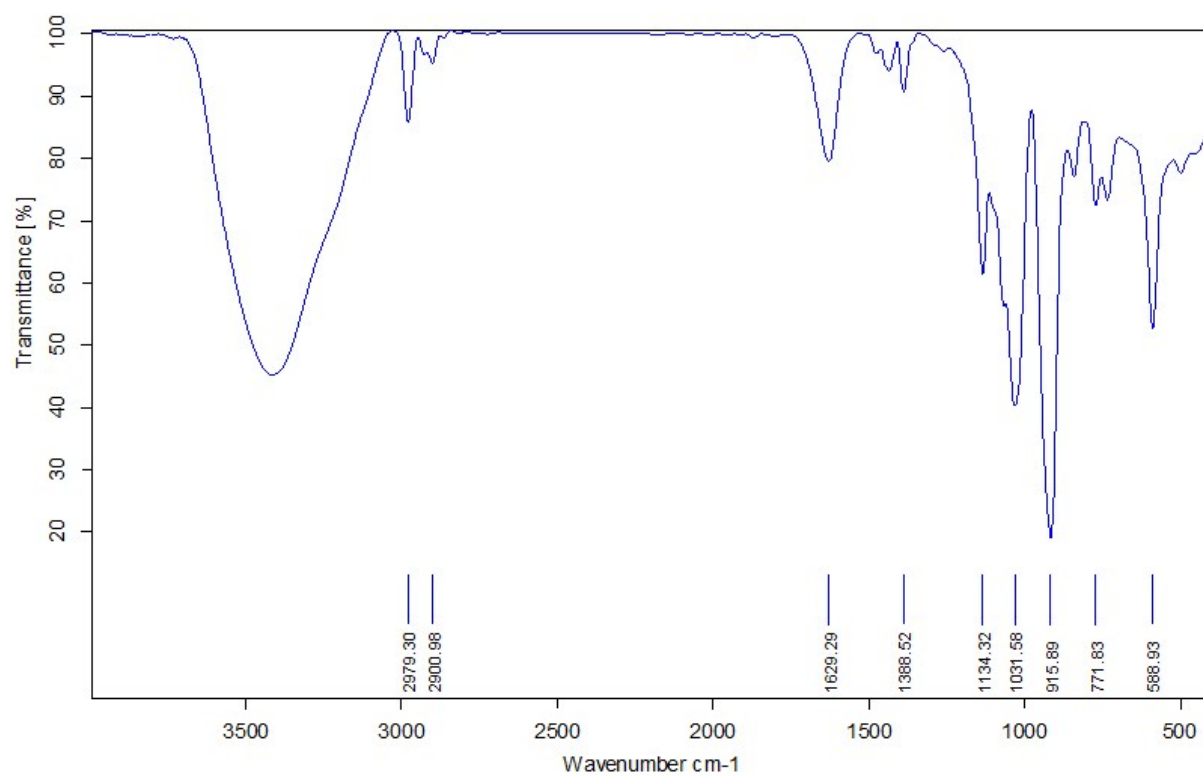


Figure S6. IR (KBr) spectrum (400-4000 cm^{-1} region) of **3**.

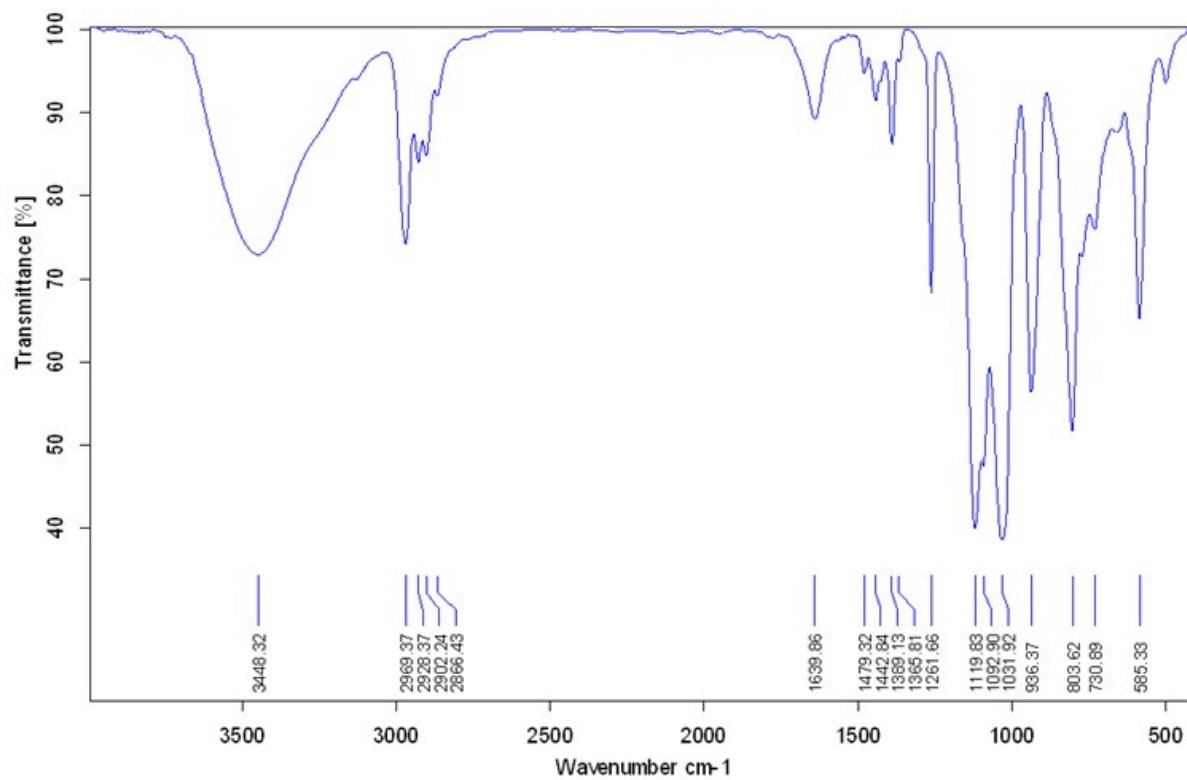


Figure S7. IR (KBr) spectrum (400-4000 cm^{-1} region) of **4**.

2. Mass Spectra of 4

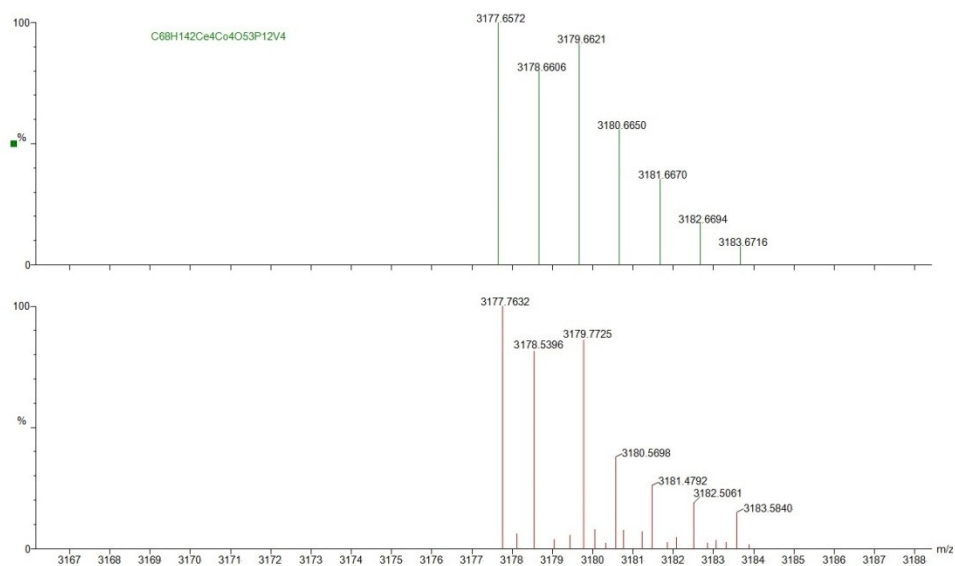


Figure S8. The $[M]^+$ signal in the MALDI mass spectrum of **4** (bottom) and the simulated spectrum (top).

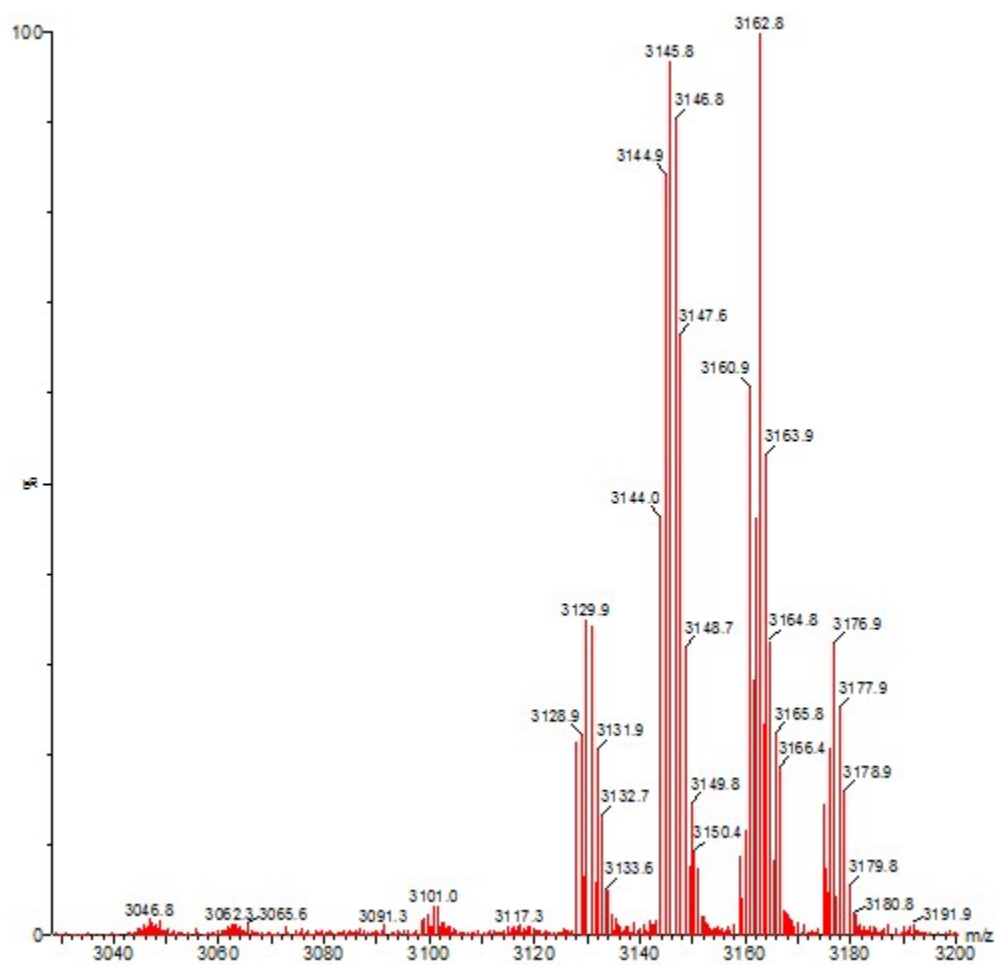


Figure S9. MALDI mass spectrum ($m/z = 3020 - 3200$) of the reaction mixture after the catalytic oxidation of methyl *p*-tolylsulfide with **4** and TBHP in CH_2Cl_2 .

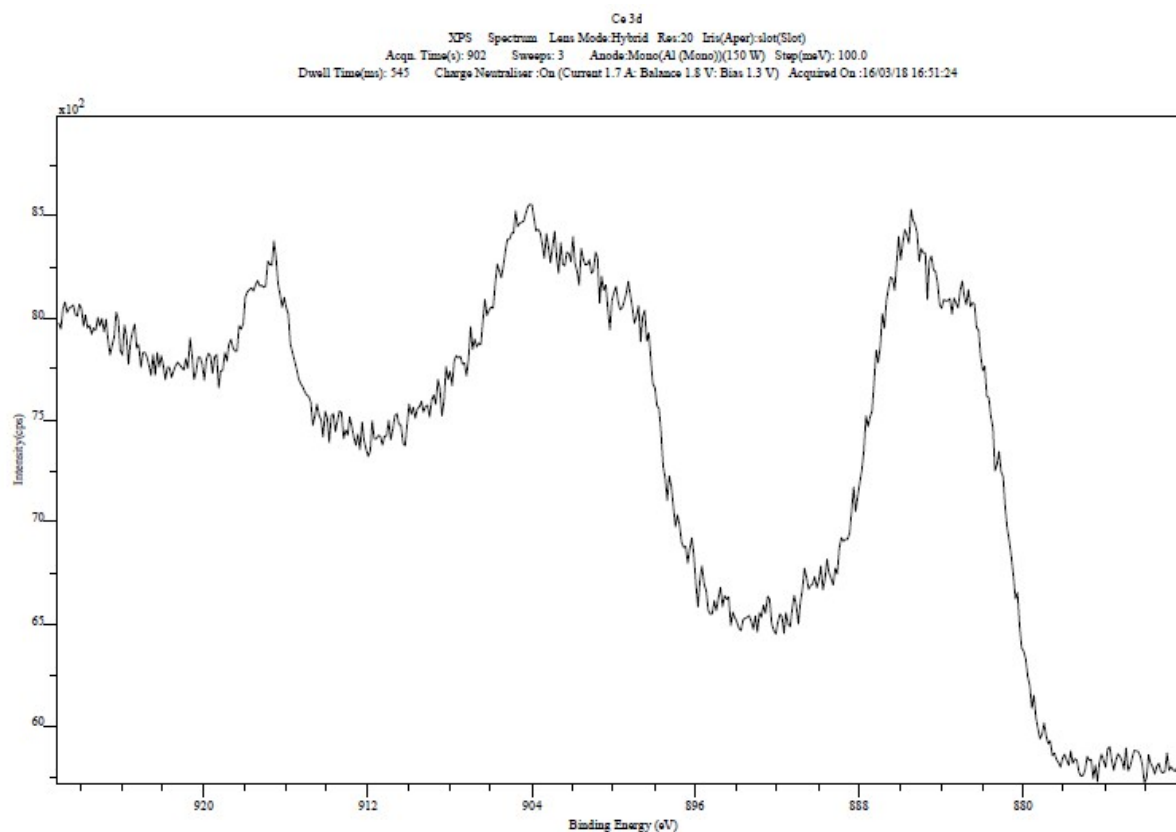


Figure S11. Ce region of the XPS spectrum of **4**

The observed signal at ca. 916 eV is characteristic of Ce(IV) (cf. lit. 917 eV^a). The absence of signal at ca. 880 eV indicates the absence of Ce(III) in **4**.

^aBeche *et al.*, *Surf. Interface Anal.* 2008, **40**, 264–267.

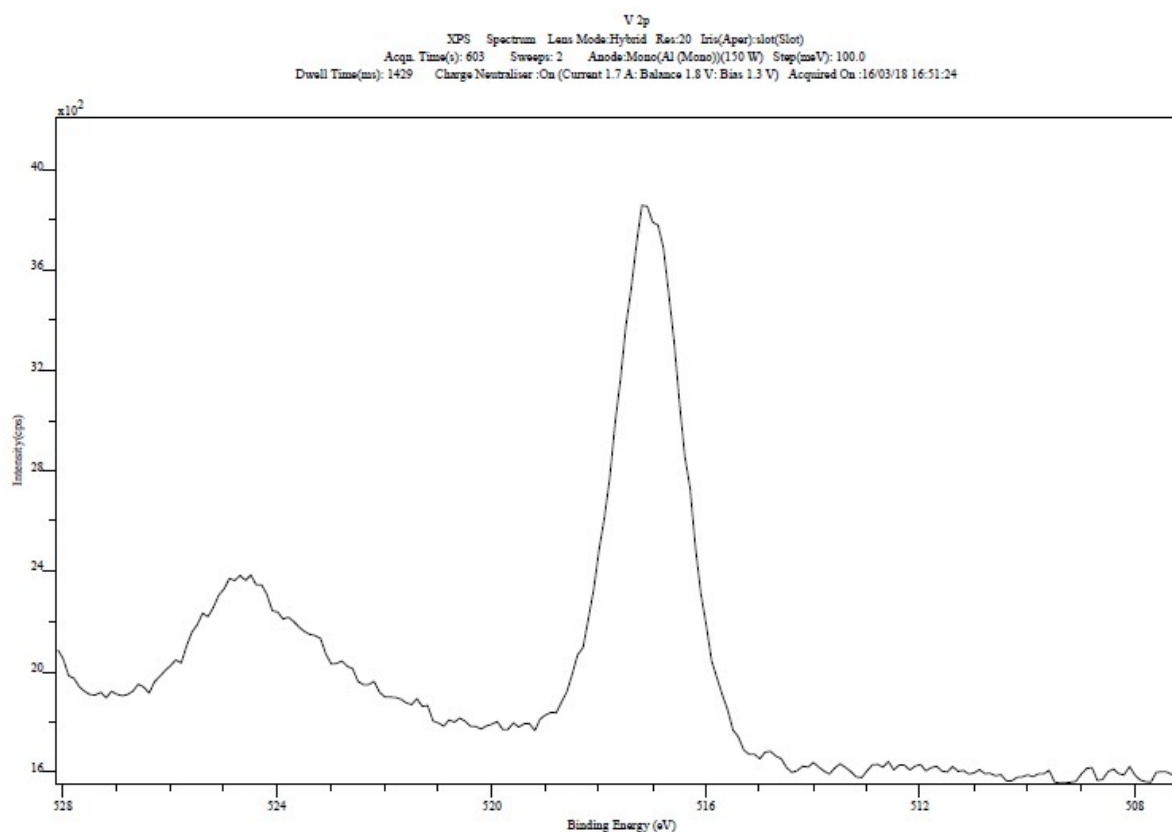


Figure S12. V region of the XPS spectrum of **4**

The peaks at ca. 516.5 (V 2p_{3/2}) and 524.5 (V 2p_{1/2}) eV are characteristic of V(V) (cf. lit. 517 and 525 eV,^{b,c} respectively).

^b C. D. Wagner, A. V. Naumkin, A. Kraut-Vass, J. W. Allison, C. J. Powell, J. R. Jr. Rumble, *NIST Standard Reference Database 20*, Version 3.4 (<http://srdata.nist.gov/xps/>) 2003.

^c M. C. Biesinger, L. W. M. Lau, A. R. Gerson, R. St. C. Smart, Resolving Surface Chemical States in XPS Analysis of First Row Transition Metals, Oxides and Hydroxides: Sc, Ti, V, Cu and Zn, *Applied Surface Science*, 2010, **257**, 887–898.