

Supporting Information for

**Structural Study of Complexes Formed by Acidic and Neutral Organophosphorus Reagents**

**Alexander D. Braatz<sup>1,2</sup>, Mark R. Antonio<sup>3</sup>, and Mikael Nilsson<sup>1,4</sup>**

<sup>1</sup> Department of Chemical Engineering and Materials Science, University of California Irvine, 916 Engineering Tower, Irvine, California 92697-2575 United States

<sup>2</sup> Nuclear Security and Isotope Technology Division, Oak Ridge National Laboratory, 1 Bethel Valley Road, Oak Ridge, TN 37831-6243 United States

<sup>3</sup> Chemical Sciences & Engineering Division, Argonne National Laboratory, 9700 South Cass Avenue, Lemont, Illinois 60439-4831 United States

<sup>4</sup> Department of Chemistry, University of California Irvine, 1102 Natural Sciences 2, Irvine, CA 92697-2025, United States.

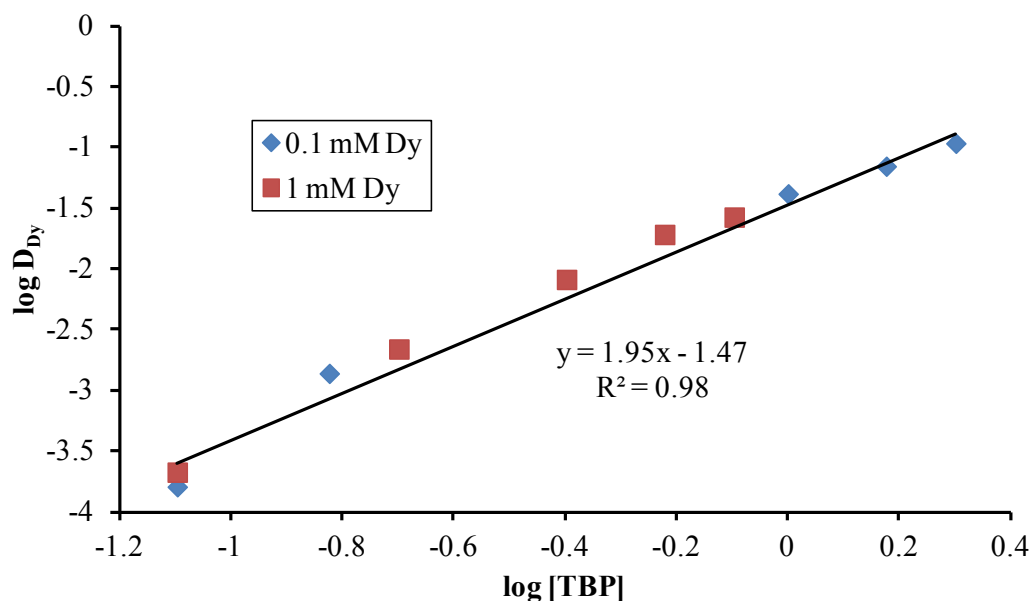


Figure S1. Slope analysis for dysprosium extraction by TBP from 2 M HNO<sub>3</sub>. Two separate experiments were carried out at different dates, one using 10<sup>-3</sup> M Dy<sup>3+</sup> and one with 10<sup>-4</sup> M Dy<sup>3+</sup>. The dysprosium concentration in each phase was determined by neutron activation analysis as outlined in the manuscript.

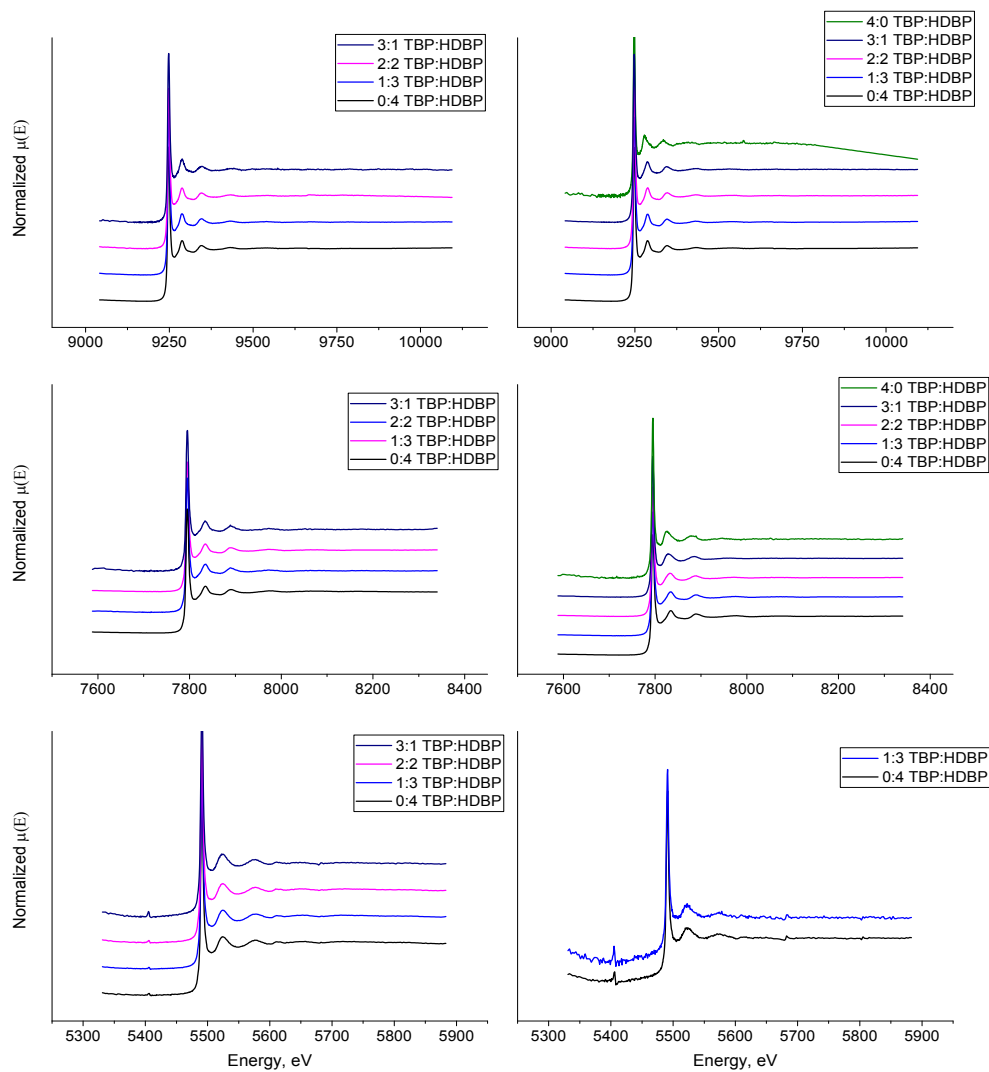


Figure S2. The normalized primary X-ray absorption spectra,  $I_f/I_0$  vs. energy for Lu in 0.2 M  $\text{HNO}_3$  (top left), Lu in 2 M  $\text{HNO}_3$  (top right), Dy in 0.2 M (middle left), Dy in 2 M  $\text{HNO}_3$  (middle right), La in 0.2 M  $\text{HNO}_3$  (bottom left), and La in 2 M  $\text{HNO}_3$  (bottom right).

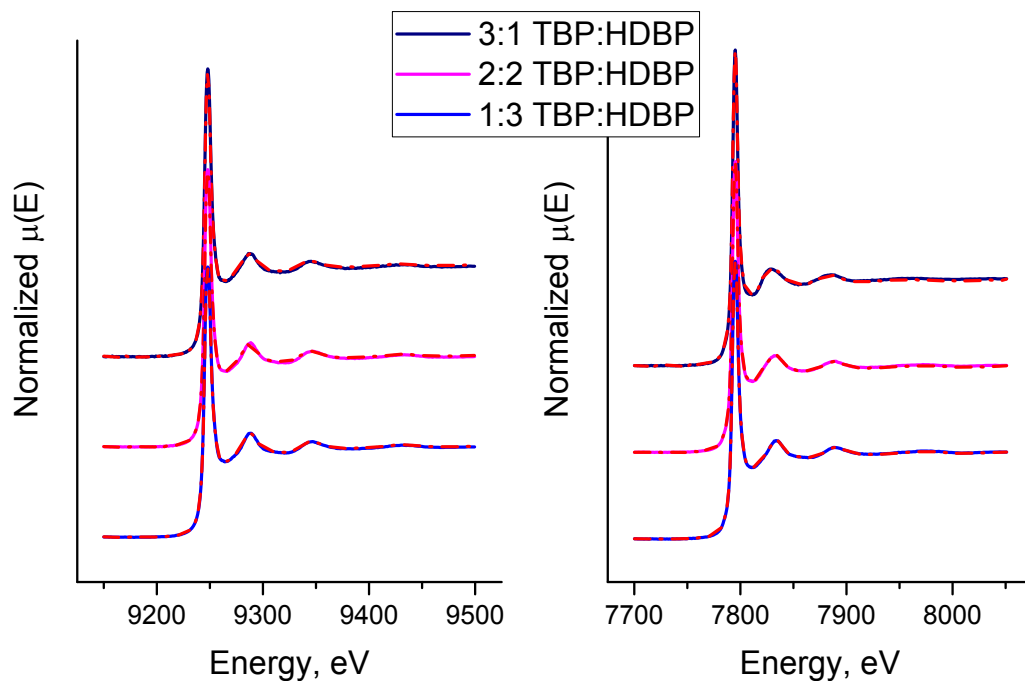


Figure S3: The normalized primary X-ray absorption spectra and linear combination fits (shown in red) for Lu in 2 M HNO<sub>3</sub> (left) and Dy in 2 M HNO<sub>3</sub> (right).

Table S1. Linear combination (LC) fitting results showing the percentage weight of each end member species giving rise to the final LC fits shown in Figure S2.

<b>Organic Phase Composition</b>	<b>Dy-TBP %</b>	<b>Dy-HDBP %</b>	<b>Lu-TBP %</b>	<b>Lu-HDBP %</b>
<b>0.75 M TBP/0.25 M HDBP</b>	56.9	43.1	23.4	76.6
<b>0.5 M TBP/0.5 M HDBP</b>	26.7	73.3	11.9	88.1
<b>0.25 M TBP/0.75 M HDBP</b>	9.5	90.5	5.5	94.5