Supplementary Information

Three rare-earth incorporating 6-peroxotantalo-4-selenate and catalytic activities for imidation reaction

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<table>
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<th>STD-Eu</th>
<th>STD-Gd</th>
<th>STD-Lu</th>
</tr>
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<tr>
<td><strong>Empirical formula</strong></td>
<td>CsKEuSe$_4$Ta$<em>6$O$</em>{53}$H$_4$</td>
<td>CsKGdSe$_4$Ta$<em>6$O$</em>{53}$H$_4$</td>
<td>CsKLuSe$_4$Ta$<em>6$O$</em>{51}$H$_3$</td>
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<td><strong>Formula weight</strong></td>
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<td>2622.09</td>
<td>2603.78</td>
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<td><strong>Temperature/K</strong></td>
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<td><strong>$a$/Å</strong></td>
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<td>12.3307(5)</td>
<td>12.2537(9)</td>
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<td><strong>$b$/Å</strong></td>
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<td>27.2604(11)</td>
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<td><strong>$c$/Å</strong></td>
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<td><strong>$\beta$/°</strong></td>
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<td><strong>Z</strong></td>
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<td><strong>$D_c$/ g cm$^{-3}$</strong></td>
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<td><strong>$\mu$/ mm$^{-1}$</strong></td>
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<td><strong>F(000)</strong></td>
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<td>4448.0</td>
<td>4476.0</td>
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<td><strong>Crystal size / mm$^3$</strong></td>
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<td>$0.34 \times 0.17 \times 0.13$</td>
<td>$0.21 \times 0.16 \times 0.13$</td>
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<td><strong>$2\theta$ range for data collection /°</strong></td>
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<td>3.51 to 50.198</td>
<td>2.982 to 50.196</td>
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<td>$R_{int} = 0.0422$,</td>
<td>$R_{int} = 0.0578$,</td>
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<td>$R_1 = 0.0421$, $wR_2 = 0.0920$</td>
<td>$R_1 = 0.0388$, $wR_2 = 0.0910$</td>
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<tr>
<td>$^aR_1, ^bW_2$ [all data]</td>
<td>$R_1 = 0.0606$, $wR_2 = 0.1007$</td>
<td>$R_1 = 0.0493$, $wR_2 = 0.0963$</td>
<td>$R_1 = 0.0633$, $wR_2 = 0.1059$</td>
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</tbody>
</table>

$aR_1 = \sum |F_o| - |F_c| / \sum |F_o|$.  $^bW_2 = \{\sum [w(F_o^2 - F_c^2)]^2 / \sum [w(F_o^2)]^2\}^{1/2}$. 
Figure S1. Composition of compounds STD-Eu, STD-Gd and STD-Lu.

Figure S2. Representation of Ln coordination environment. Ln, lavender; O, red.

Figure S3. Connection mode of Ta atoms. Ta, teal; Se, lime; O, red; peroxo bond, red.

Figure S4. Ball-and-stick representation of polyanion cis-\(\text{Se}_4\text{(TaO}_2\text{)}_6\)^−. Ta, teal; Se, lime; O, red; peroxo bond, red.
Table S2. $O_{\text{axial}}$−Ta−$O_{\text{axial}}$ angles in polyanions STD-Eu, STD-Gd and STD-Lu.

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<th>STD-Gd</th>
<th>STD-Lu</th>
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<td>170.60°</td>
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<td>O26-Ta2-O27</td>
<td>169.27°</td>
<td>168.72°</td>
<td>168.66°</td>
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<td>O19-Ta3-O20</td>
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<td>173.88°</td>
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<td>O23-Ta5-O26</td>
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<td>Bond</td>
<td>Length</td>
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Figure S5. Se–O, Ta–O (left) bond lengths and the average Ln–O (right) bond length in STD-Eu, STD-Gd and STD-Lu.
Table S5. BVS calculation results.

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#, ‡ and ψ represent peroxy oxygen atoms, H₂O and OH ligands.
Figure S6. Ball-and-stick representation of polyanion **STD-Eu**, highlighting the protonated oxygen atoms. Ta, teal; Se, lime; Eu, lavender; H$_2$O, turquoise; OH, pink; O, red; peroxo bond, red.

Figure S7. TG curves of compounds **STD-Eu**, **STD-Gd** and **STD-Lu**.

The TG curves of compounds **STD-Eu**, **STD-Gd** and **STD-Lu** show similar two-step weight loss behaviors in the temperature range of 25-1000 °C. The total weight loss of 32.62% (calcd 32.79%) for **STD-Eu** and 32.67% (calcd 32.73%) for **STD-Gd** can be attributed to 14 lattice water molecules, 9 coordinated water molecules and four SeO$_2$ molecules. However, the slightly smaller total weight loss of 31.86% (calcd 31.57%) for **STD-Lu** corresponds to 12 lattice water molecules, 9 coordinated water molecules and four SeO$_2$ molecules.
Figure S8. IR spectra for STD-Eu, STD-Gd, STD-Lu, Na$_2$SeO$_3$ and Ta$_6$ in the region from 4000 to 450 cm$^{-1}$.

Figure S9. PXRD patterns (black) and simulated (red) of STD-Eu.

Figure S10. PXRD patterns (black) and simulated (red) of STD-Gd.
Figure S11. PXRD patterns (black) and simulated (red) of STD-Lu.

Figure S12. Excitation spectrum for STD-Eu ($\lambda_{em} = 613$ nm).

Figure S13. Corresponding color coordinates of STD-Eu.
Experimental section

Catalysis. The products were isolated by column chromatography on silica gel (200-300 mesh) using petroleum ether (60-90 °C) and ethyl acetate. All compounds were characterized by $^1$H NMR, $^{13}$C NMR and mass spectrometry, which were consistent with those reported in related literatures. NMR spectra were determined on Brucker ADVANCE III spectrometer at 500 MHz and 126 MHz. $^1$H NMR peaks were labeled as singlet (s), doublet (d), triplet (t), and multiplet (m). The coupling constants, $J$, are reported in Hertz (Hz). GC analysis was performed on Agilent 7890B equipped with a capillary column (HP-5, 30 m × 0.25 μm) using a flame ionization detector.

Characterization of substrates and products

![Structure of 2-phenylisoindoline-1,3-dione (3a)]

2-phenylisoindoline-1,3-dione (3a)$^{51}$

$^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.94 (dt, $J = 6.7$, 3.4 Hz, 2H), 7.78 (dd, $J = 5.3$, 3.1 Hz, 2H), 7.51 (t, $J = 7.7$ Hz, 2H), 7.47-7.37 (m, 3H);

$^{13}$C NMR (126 MHz, CDCl$_3$) $\delta$ 167.34, 134.47, 131.76, 129.18, 128.17, 126.63, 123.80, 100.00.

![Structure of 2-(m-tolyl)isoindoline-1,3-dione (3b)]

2-(m-tolyl)isoindoline-1,3-dione (3b)$^{51}$

$^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 166.85, 134.67, 134.59, 132.82, 131.51, 130.08, 128.21, 126.66, 124.62, 123.92;

$^{13}$C NMR (126 MHz, CDCl$_3$) $\delta$ 176.50, 139.29, 131.86, 129.57, 129.06, 127.17, 123.65, 28.44, 21.38.
2-(3-methoxyphenyl)isoindoline-1,3-dione (3c)\textsuperscript{52}

\textbf{\textsuperscript{1}H NMR} (500 MHz, CDCl\textsubscript{3}) \(\delta\) 7.92 (dd, \(J = 5.4, 3.1\) Hz, 2H), 7.78-7.74 (m, 2H), 7.39 (t, \(J = 7.7\) Hz, 1H), 7.25-7.19 (m, 3H), 2.41 (s, 3H);

\textbf{\textsuperscript{13}C NMR} (126 MHz, CDCl\textsubscript{3}) \(\delta\) 167.42, 139.16, 134.42, 131.78, 129.09, 128.99, 127.32, 123.81, 123.74, 21.47.

\hrule

2-(3-chlorophenyl)isoindoline-1,3-dione (3d)\textsuperscript{52}

\textbf{\textsuperscript{1}H NMR} (500 MHz, CDCl\textsubscript{3}) \(\delta\) 7.95 (dd, \(J = 5.3, 3.0\) Hz, 2H), 7.79 (dd, \(J = 5.3, 3.0\) Hz, 2H), 7.41 (t, \(J = 8.1\) Hz, 1H), 7.03 (d, \(J = 7.9\) Hz, 1H), 7.00-6.93 (m, 2H), 3.84 (s, 3H);

\textbf{\textsuperscript{13}C NMR} (126 MHz, CDCl\textsubscript{3}) \(\delta\) 167.27, 160.05, 134.46, 132.65, 131.73, 129.85, 123.79, 118.91, 114.14, 112.37, 55.46.

\hrule

2-(3-bromophenyl)isoindoline-1,3-dione (3e)\textsuperscript{52}

\textbf{\textsuperscript{1}H NMR} (500 MHz, CDCl\textsubscript{3}) \(\delta\) 7.93 (dd, \(J = 4.9, 3.3\) Hz, 2H), 7.79 (dd, \(J = 5.1, 3.1\) Hz, 2H), 7.64 (s, 1H), 7.52 (d, \(J = 7.8\) Hz, 1H), 7.42 (d, \(J = 7.9\) Hz, 1H), 7.37 (t, \(J = 7.9\) Hz, 1H);

\textbf{\textsuperscript{13}C NMR} (126 MHz, CDCl\textsubscript{3}) \(\delta\) 166.84, 134.68, 132.94, 131.49, 131.12, 130.35, 129.48, 125.12, 123.93, 122.41.

\hrule

2-(3-(trifluoromethyl)phenyl)isoindoline-1,3-dione (3f)\textsuperscript{52}
$^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 7.92 (dd, $J$ = 5.3, 3.1 Hz, 2H), 7.78 (dd, $J$ = 5.5, 2.8 Hz, 3H), 7.68 (d, $J$ = 7.2 Hz, 1H), 7.66-7.60 (m, 2H);

$^{13}$C NMR (126 MHz, CDCl$_3$) $\delta$ 166.80 (s), 134.73 (s), 132.36 (s), 131.65-131.19 (m), 129.70 (s), 129.66 (s), 124.75 (s), 124.62 (d, $J$ = 3.7 Hz), 123.91 (s), 123.33 (q, $J$ = 3.8 Hz), 122.58 (s).

5-methyl-2-phenylisoindoline-1,3-dione (3g)$^{52}$

$^1$H NMR (500 MHz, (CD$_3$)$_2$SO) $\delta$ 7.85 (d, $J$ = 7.6 Hz, 1H), 7.79 (s, 1H), 7.71 (d, $J$ = 7.6 Hz, 1H), 7.55-7.50 (m, 2H), 7.47-7.41 (m, 3H), 2.52 (s, 3H);

$^{13}$C NMR (126 MHz, (CD$_3$)$_2$SO) $\delta$ 167.55, 167.45, 146.18, 135.55, 132.41, 132.33, 129.36, 129.31, 128.45, 127.81, 124.29, 123.83, 21.88.

5-chloro-2-phenylisoindoline-1,3-dione (3h)$^{52}$

$^1$H NMR (500 MHz, (CD$_3$)$_2$SO) $\delta$ 8.05 (s, 1H), 8.00-7.94 (m, 2H), 7.56-7.52 (m, 2H), 7.46 (t, $J$ = 7.1 Hz, 3H);

$^{13}$C NMR (126 MHz, (CD$_3$)$_2$SO) $\delta$ 166.64, 166.28, 139.91, 134.92, 134.09, 132.19, 130.63, 129.37, 128.68, 127.80, 125.64, 123.96.

5-bromo-2-phenylisoindoline-1,3-dione (3i)$^{52}$

$^1$H NMR (500 MHz, (CD$_3$)$_2$SO) $\delta$ 8.18 (d, $J$ = 1.2 Hz, 1H), 8.11 (dd, $J$ = 7.9, 1.2 Hz, 1H), 7.90 (d, $J$ = 7.9 Hz, 1H), 7.54 (t, $J$ = 7.8 Hz, 2H), 7.45 (t, $J$ = 7.4 Hz, 3H);

$^{13}$C NMR (126 MHz, (CD$_3$)$_2$SO) $\delta$ 166.83, 166.25, 137.85, 134.08, 132.18, 131.03, 129.37, 128.69, 128.66, 127.81, 126.76, 125.75.
4-chloro-2-phenylisoindoline-1,3-dione (3j)\(^{52}\)

\(^1\)H NMR (500 MHz, (CD\(_3\))\(_2\)SO) \(\delta\) 7.89 (dt, \(J = 22.3, 7.4\) Hz, 3H), 7.58-7.51 (m, 2H), 7.46 (dd, \(J = 7.3, 4.8\) Hz, 3H);

\(^{13}\)C NMR (126 MHz, (CD\(_3\))\(_2\)SO) \(\delta\) 166.17, 165.18, 136.53, 136.30, 134.43, 132.14, 130.25, 129.36, 128.74, 127.99, 127.76, 122.78.

1-(3-methoxyphenyl)pyrrolidine-2,5-dione (3k)\(^{53}\)

\(^1\)H NMR (500 MHz, (CD\(_3\))\(_2\)SO) \(\delta\) 7.39 (t, \(J = 8.3\) Hz, 1H), 7.03-6.95 (m, 1H), 6.83 (d, \(J = 7.3\) Hz, 2H), 3.75 (s, 3H), 2.76 (s, 4H);

\(^{13}\)C NMR (126 MHz, (CD\(_3\))\(_2\)SO) \(\delta\) 177.34, 159.90, 134.32, 130.06, 119.84, 114.19, 113.49, 55.76, 28.93.
NMR Spectra
References