ESI For

Design and preparation of polymer resin-supported organoselenium catalyst with industrial potential

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1. Detailed Table

Table S1 Test of catalyst loadings.\textsuperscript{a}

\[
\text{SeOxH} \quad \text{(cat.)}
\]

\[
\text{1.0 equiv. water, 85 }^\circ\text{C}
\]

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<th>t (h)</th>
<th>3/(%^c)</th>
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\(^a\) 1 mmol of 1, 1 mmol of H\(_2\)O\(_2\) (30 w/w \%) and 5 mL of solvent were heat at 85 °C. \(^b\) Catalyst loadings based on 1. \(^c\) GC yield of 3 based on 1.

Table S2 Detailed XPS analysis result of the catalysts

<table>
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<th>Figure text</th>
<th>in</th>
<th>Se(^{6+})3d (BE 60 ev), %</th>
<th>Se(^{4+})3d (BE 59.5 ev), %</th>
<th>Se(^{2+})3d (BE 56 ev), %</th>
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<td>65±1</td>
<td>35±1</td>
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<td>Fig. 5</td>
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<td>79±1</td>
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2. Spectra

FT-IR Spectra of Polymer 2

FT-IR Spectra of Polymer 7
FT-IR Spectra of Polymer 6
EDS Spectra of Catalyst

EDS Spectra of Polymer 2
Characterization Spectra of Product 3

$^1$H NMR

$^{13}$C NMR
IR

GC-MS (EI): m/z 116 [M+]

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GC-MS of the by-products 8-10

2-Methoxycyclohexanol 3. GC-MS (EI): m/z 130 [M⁺]. Known compound (2979-24-0).

2- Ethoxycyclohexanol 4. GC-MS (EI): m/z 144 [M⁺]. Known compound (2979-26-2).

Solid state $^{13}$C NMR spectra of resin 2, 6 and 7
Solid state $^{77}$Se NMR spectra of resin 2

3. Detailed GC-yield Calculation Procedures

Internal standard curve
Example (Reaction in Table 1, entry 1 in text)

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<th>Peak</th>
<th>Ret. Time</th>
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<tr>
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<td>1967077</td>
<td>45818465</td>
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<td>2</td>
<td>11.298</td>
<td>962755</td>
<td>25664853</td>
<td>35.903%</td>
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</table>

\[ X = \frac{45818465}{25664853}, \text{ Thus, } Y = 81\% \text{ according to internal standard curve.} \]

4. Oxidation of other olefins by using polymer 2 as catalyst

Table S3 Oxidation of olefins catalyzed by polymer 2

\[
\begin{align*}
\text{olefin} & \\
\hline
\text{Entry} & \text{Olefin} & \text{Cat. amount (mol %)} & \text{H}_2\text{O}_2 \text{ amount (equiv.)} & \text{Diol yield (%)}^b \\
\hline
1 & \text{ } & 5 & 1.0 & 94^b \\
2 & \text{ } & 5 & 4.0 & 92^b \\
3 & \text{ } & 5 & 1.0 & 95^b \\
\end{align*}
\]
Product spectra and characterization data.

1,2-Cyclooctanediol. Known compound (4277-32-1). 92% yield. White solid. Melting point 31.1 - 32.0 °C. $^1$H NMR (500 MHz, CDCl$_3$) δ (ppm): 3.98 (s, 2H), 3.50 (d, $J$ = 2.2 Hz, 2H), 1.82 - 1.72 (m, 2H), 1.61 (d, $J$ = 3.5 Hz, 4H), 1.48 (s, 4H), 1.39 (s, 2H). $^{13}$C NMR (150 MHz, CDCl$_3$) δ (ppm): 76.06, 31.82, 26.12, 23.70. GC-MS (EI): m/z 144 [M$^+$]. IR $\nu_{max}$ (KBr): 3390, 2924, 2856, 2697, 1465, 1448, 1403, 1354, 1335, 1282, 1212, 1115, 1085, 1036, 984, 962, 902, 741, 576 cm$^{-1}$.

$^1$H NMR

$^{13}$C NMR
FT-IR
GC-MS (EI)
By-product:

1,2-Octanediol. Known compound (1117-86-8). 95% yield. White solid. Melting point 36.1 – 37.9 °C. $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ (ppm): 3.71 - 3.59 (m, 2H), 3.41 (dd, $J = 11.3$, 7.9 Hz, 1H), 3.33 (s, 2H), 1.47 - 1.37 (m, 3H), 1.34 - 1.24 (m, 7H), 0.88 (t, $J = 6.9$ Hz, 3H). $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ (ppm): 72.38, 66.76, 33.12, 31.74, 29.31, 25.54, 22.57, 14.01. GC-MS (EI): \textit{m/z} 145 [M$^+$]. IR $\nu_{\text{max}}$ (KBr): 3381, 2957, 2928, 2857, 1650, 1467, 1378, 1133, 1072, 860, 724, 668, 578 cm$^{-1}$.

$^1$H NMR

$^{13}$C NMR
FT-IR

GC-MS (EI)
5-Cyclooctene-1,2-diol. Known compound (55519-21-6). 9% yield. GC-MS (EI): m/z 142 [M⁺].
By-product:

1-Phenyl-1,2-ethanediol. Known compound (93-56-1). 18% yield. GC-MS (EI): \( m/z \) 138 \([M^+\]).