Supporting Information

Highly active dinuclear cobalt complexes for solvent-free cycloaddition of CO$_2$ to epoxides at ambient pressure

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1. General comments

CoCl₂·6H₂O, salicylaldehyde, 2-hydroxy-4-methoxybenzaldehyde, 2-hydroxy-1-naphthaldehyde, 3,5-di-tert-butyl salicylaldehyde, tris(hydroxymethyl)aminomethane, tertiary-butylammonium bromide, triethylamine, and methanol were purchased from Aladdin and were used without any further purification. Nuclear Magnetic Resonance (NMR) spectra were recorded at room temperature using 500 MHz Bruker Advance III-HD at 500 MHz and 125 MHz for ¹H-NMR and ¹³C-NMR, respectively. All chemical shifts are expressed in δ units (ppm). Fourier Transform Infrared (FT-IR) spectra were measured from KBr pellets using a Thermo-Nicolet 6700 spectrometer over the 4000-400 cm⁻¹ range.

2. Synthesis

2.1 Synthesis of ligands

The Schiff base ligands were synthesized according to the reported methods via amine-aldehyde condensation. To the solution of salicylaldehyde or its derivatives (10 mmol) in methanol was added tris(hydroxymethyl)aminomethane (10 mmol, 1.21 g) and the reaction mixture was refluxed overnight at room temperature. On evaporation under reduced pressure, a yellow mass of the ligand was obtained, which was then dried under vacuum at room temperature.

**Ligand H₄L¹:** Yield: 81 %. ¹H-NMR (500 MHz, DMSO-d₆): δ 14.52 [s, 1H, (O-H)phenolic], 8.57 [s, 1H, (N=C-H)imine], 7.41 [d, 1H, (Ar-H)], 7.28 [t, 1H, (Ar-H)], 6.79 [d, 2H, (Ar-H)], 4.73 [t, 3H, (O-H)alcoholic], 3.63 [d, 6H, (-CH₂-)aliphatic] ppm. ¹³C-NMR (125 MHz, DMSO- d₆) δ 164.9 (Ar-C)phenolic, 163.7 (C=N)imine, 132.8 (Ar-C), 132.6 (Ar-C), 118.9 (Ar-C), 117.8 (Ar-C), 117.6 (Ar-C), 67.5 (-C(CH₂)₃-), 61.8 (-CH₂-OH) ppm. **FT-IR Data [KBr, (cm⁻¹)]:** 3600-3200 [br, (O-H)phenolic, alcoholic], 3066 [br, (C-H)sp² and (=C-H)imine], 2819 [m, (C-H)sp³], 1635, 1611 and 1539 [s, (C=C)aromatic and (C=N)imine], 1483 (m, CH₂ bending), 1230 [s, (C-O)phenolic], 1060 [s, (C-O)alcohol], 764 (s, CH₂ bending). Anal. Calcd. for C₁₁H₁₅NO₄: C, 58.66; H, 6.71; N, 6.22%. Found: C, 58.73; H, 6.74; N, 6.17%.

**Ligand H₄L²:** Yield: 89 %. ¹H-NMR (500 MHz, DMSO- d₆) δ 14.27 [d, 1H, (O-H)phenolic], 8.27 [s, 1H, (N=C-H)imine], 7.16 [d, 1H, (Ar-H)], 6.12 [dd, 2.4 Hz, 1H, (Ar-H)], 6.04 [d, 1H, (Ar-H)], 5.98 [d, 1H, (Ar-H)], 5.72 [d, 1H, (Ar-H)].
4.93 [t, 3H, (O-H)alcoholic], 3.71 [s, 3H, (O-CH$_3$)] 3.60 [s, 6H, (-CH$_2$$_2$)-aliphatic] ppm. $^{13}$C-NMR (125 MHz, DMSO- $d_6$) $\delta$ 174.3 (Ar-C)phenolic, 165.3 (C=N)amine, 162.4 (Ar-C), 134.9 (Ar-C), 111.4 (Ar-C), 105.3 (Ar-C), 102.3 (Ar-C), 65.6 (-CH$_2$CH$_3$), 61.4 (-CH$_2$OH), 55.4 (-OCH$_3$) ppm.

FT-IR Data [KBr, (cm$^{-1}$)]: 3500-3000 [m, br, (O-H)phenolic, alcoholic, (C-H)$_3$sp2 and (N=C-H)amine], 2838 [m, (C-H)$_3$sp3], 1638, 1619 and 1525 [s, (C=C)aromatic and (C=N)amine], 1481 (s, CH$_2$ bending), 1358 (m, CH$_3$ bending), 1323 [s, (C-O)methoxy], 1227 [s, (C-O)phenolic], 1042 [s, (C-O)alcoholic], 788 (s, CH$_2$ bending). Anal. Calcd. for C$_{12}$H$_{17}$NO$_5$: C, 56.46; H, 6.71; N, 5.49%. Found: C, 56.59; H, 6.79; N, 5.51%.

Ligand H$_4$L$_3$: Yield: 90 %. $^1$H-NMR (500 MHz, DMSO- $d_6$) $\delta$ 14.04 [d, 1H, (O-H)phenolic], 8.91 [s, 1H, (Ar-H)], 7.68 [d, 1H, (Ar-H)], 7.60 [d, 1H, (Ar-H)], 7.41 [t, 1H, (Ar-H)], 7.16 [t, 1H, (Ar-H)], 6.64 [d, 1H, (Ar-H)], 5.13 [t, 3H, (O-H)alcoholic], 3.66 [d, 6H, (-CH$_2$$_2$)-aliphatic] ppm. $^{13}$C-NMR (125 MHz, DMSO- $d_6$) $\delta$ 179.7 (Ar-C)phenolic, 156.1 (C=N)imine, 137.7 (Ar-C), 135.3 (Ar-C), 129.3 (Ar-C), 128.3 (Ar-C), 127.2 (Ar-C), 125.3 (Ar-C), 122.4 (Ar-C), 118.5 (Ar-C), 105.6 (Ar-C), 64.9 (-CH$_2$CH$_3$), 61.3 (-CH$_2$OH) ppm. FT-IR Data [KBr, (cm$^{-1}$)]: 3600-3000 [m, br, (O-H)phenolic, alcoholic, (C-H)$_3$sp2 and (N=C-H)amine], 2924 [m, (C-H)$_3$sp3], 1635 and 1542 [s, (C=C)aromatic and (C=N)amine], 1490 (m, CH$_2$ bending), 1171 [w, (C-O)aromatic], 1023 [s, (C-O)alcoholic], 750 (s, CH$_2$ bending). Anal. Calcd. for C$_{15}$H$_{17}$NO$_4$: C, 65.44; H, 6.22; N, 5.09%. Found: C, 65.48; H, 6.31; N, 5.15%.

2.2 Synthesis of cobalt complexes (1-3)

Cobalt-Schiff base complexes were synthesized by the dropwise addition of CoCl$_2$·6H$_2$O solution (1 mmol, 0.23 g in 10 mL methanol) to the solution of the ligand (1 mmol) in 10 mL methanol. The solution was then stirred for 24 hours at room temperature. The dark brown solution was filtered, and the precipitate obtained was washed with acetone and dried under vacuum at room temperature.

Complex 1, [Co(HL$_1$)]$_2$: Yield: 73%. FT-IR Data [KBr, (cm$^{-1}$)]: 3600-3000 [m, br, (O-H)alcoholic, (C-H)$_3$sp2 and (N=C-H)amine], 2866 [w, (C-H)$_3$sp3], 1633, 1595 and 1547 [s, (C=C)aromatic and (C=N)amine], 1446 (m, CH$_2$ bending), 1275 [m, (C-O)phenolic], 1031 [s, (C-O)alcoholic], 756 (s, CH$_2$ bending). Anal. Calcd. for C$_{22}$H$_{26}$ClCo$_2$N$_2$O$_9$: C, 42.91; H, 5.76; N, 4.55%. Found: C, 43.01; H, 5.83; N, 4.46%. ESI-MS (negative mode): m/z = 597.9931 [(Co$_2$(H$_2$L$_1$)(HL$_1$))]$^-$ (calc. 

4
597.9969); m/z = 505.0993 [(Co(H₂L¹)₂]− (calc. 505.1027); m/z = 328.1166 [(Co(H₂L¹)(C₂H₅OH)]
(calc. 328.0595).

**Complex 2**, [Co(HL²)]₂: Yield: 65%. **FT-IR Data [KBr, (cm⁻¹)]:** 3600-3000 [m, br, (O-H)alcoholic, (N=C-H)imine], 2857 [m, (C-H)sp³], 1630, 1601 and 1543 [s, (C=C)aromatic and (C=N)imine], 1485 (m, CH₂ bending), 1360 (m, CH₃ bending), 1288 [s, (O-H)methoxy], 1227 [s, (O-H)phenolic], 1025 [s, (O-H)alcoholic], 799 (w, CH₂ bending). Anal. Calcd. for C₃₂H₃₀ClCo₂N₂O₁₁: C, 42.65; H, 4.47; N, 4.15%. Found: C, 42.74; H, 4.58; N, 4.06%. **ESI-MS (negative mode):** m/z = 658.0127 [(Co₂(H₂L²)(HL²)]⁻ (calc. 658.0180); m/z = 565.1194 [(Co(H₂L²)]⁻ (calc. 565.1238); m/z = 346.9943 [(Co(H₂L²)Cl] (calc. 346.9971).

**Complex 3**, [Co(HL³)]₂: Yield: 66%. **FT-IR Data [KBr, (cm⁻¹)]:** 3600-3000 [m, br, (O-H)alcoholic, (N=C-H)imine], 2834 [m, br, (C-H)sp³], 1626 (s) and 1539 (w) [(C=C)aromatic and (C=N)imine], 1460 (m, CH₂ bending), 1178 [s, (C-O)aromatic], 1040 [s, (C-O)alcoholic], 742 (s, CH₂ bending). Anal. Calcd. for C₃₀H₃₀ClCo₂N₂O₉: C, 50.33; H, 4.22; N, 3.91%. Found: C, 50.46; H, 4.31; N, 3.87 **ESI-MS (negative mode):** m/z = 698.0222 [(Co₂(H₂L³)(HL³)]⁻ (calc. 698.0282); m/z = 605.1292 [(Co(H₂L³)]⁻ (calc. 605.1340); m/z = 402.9758 [(Co(HL³)Cl₂] (calc. 402.9794); m/z = 366.9994 [(Co(HL³)Cl] (calc. 367.0022).

### 3. General catalytic procedure

In a typical coupling reaction of epoxides and CO₂, a 30 mL stainless steel autoclave with a magnetic stirrer was charged with an appropriate ratio of catalyst, cocatalyst, and substrate and connected to CO₂ cylinder. After purging the autoclave at gentle pressure of CO₂ the outlet was closed and the pressure was set to 1 bar from CO₂ cylinder once the temperature of the autoclave (reactor) reached to the appropriate temperature of the oil bath. After the allotted reaction time, the autoclave was cooled to room temperature. After carefully removing the excess of CO₂, a small amount of the reaction mixture was taken from the autoclave for ¹H-NMR analysis in CDCl₃ to quantitatively give the conversion rate of the substrate used. The different substrates (epoxides) used in this study are: epichlorohydrin (10 mmol, 0.93 g), allyl glycidyl ether (10 mmol, 1.14 g), butyl glycidyl ether (10 mmol, 1.3 g), benzyl glycidyl ether (10 mmol, 1.6 g), glycidyl isopropyl ether (10 mmol, 1.2 g), vinyl oxirane (10 mmol, 0.70 g), styrene oxide (10 mmol, 1.2 g), propylene oxide (10 mmol, 0.58 g), 1,2-epoxyhexane (10 mmol, 1.0 g), isobutylene oxide (10 mmol, 0.7 g),
3,6-Dioxabicyclo [3.1.0] hexane (10 mmol, 0.98 g), cyclopentene oxide (10 mmol, 0.98 g), and cyclohexene oxide (10 mmol, 0.98 g).

4. Stability and recycling of the catalyst

The recyclability and hence stability of the catalysts were carried out using epichlorohydrin as a substrate. 1 mol% of the catalyst (0.05 mmol) and epichlorohydrin (5 mmol, 0.463 g) was taken in an autoclave with a stirrer and connected to CO$_2$ cylinder. After purging with CO$_2$ for a few seconds at room temperature the pressure was set to 1 bar when the reactor temperature reach to 120 °C in an oil bath. After the given reaction time, the conversion of the substrate into the product was analyzed by $^1$H-NMR in CDCl$_3$ and the catalyst was recovered from the reaction mixture by adding acetone, which helps in the precipitation of the catalyst, and doing centrifugation. The catalyst was washed with acetone and dried in vacuum at 60 °C before using for the next cycle. The catalyst was characterized by FT-IR after each cycle.

5. Optimization Table of the catalytic activity of Co-complexes

Table S1. Optimizing conditions for the cycloaddition of CO$_2$ and epichlorohydrin at 1 bar

<table>
<thead>
<tr>
<th>Entry</th>
<th>Catalyst</th>
<th>Cat. : Cocat. : Substrate</th>
<th>T (°C)</th>
<th>Time (h)</th>
<th>Conversion (%)</th>
<th>TON</th>
<th>TOF (h$^{-1}$)</th>
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<td>1</td>
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<td>6</td>
<td>6.5</td>
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<td>11</td>
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<td>2</td>
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<td>9</td>
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<td>15</td>
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<tr>
<td>3</td>
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<td>4</td>
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<td>6</td>
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<td>6</td>
<td>66</td>
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<td>110</td>
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<td>9$^b$</td>
<td>-</td>
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<td>120</td>
<td>6</td>
<td>61</td>
<td>610</td>
<td>102</td>
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<tr>
<td>10$^{a, c}$</td>
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<td>120</td>
<td>5</td>
<td>100</td>
<td>1000</td>
<td>200</td>
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</table>

$^a$ DMAP was used as cocatalyst, $^b$ TBAB was used as cocatalyst, $^c$ carried out at 10 bar pressure of CO$_2$. TON and TOF values are calculated per mole of complex.
6. Comparison of the catalytic activity with reported complexes

Table S2. Comparison of TON and TOF values for cycloaddition of CO₂ to epoxides of this study with the reported literature.

<table>
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<tr>
<th>Entry</th>
<th>Catalyst a</th>
<th>Cocatalyst</th>
<th>Temp. (°C)</th>
<th>P (bar)</th>
<th>TON</th>
<th>TOF (h⁻¹)</th>
<th>Reference</th>
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<tr>
<td>1 b</td>
<td>Cobalt, (2)</td>
<td>TBAB</td>
<td>120</td>
<td>1</td>
<td>168,600</td>
<td>3333</td>
<td>This work</td>
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<td>2 c</td>
<td>Cobalt</td>
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<td>2,930</td>
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<td>2</td>
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<td>3 c</td>
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<td>TBAB</td>
<td>20</td>
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<td>119</td>
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<td>9</td>
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<tr>
<td>12 e</td>
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<td>PPNBr</td>
<td>90</td>
<td>10</td>
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<td>17</td>
<td>240,000</td>
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<td>16</td>
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a Only the metal centre is mentioned here instead of the whole complex. b epichlorohydrin substrate; c propylene oxide substrate; d Styrene epoxide substrate, e 1,2-epoxyhexane substrate, (TBAB = tetrabutylammonium bromide, DMAP = 4-dimethylamino pyridine, TPPB = tetraphenyl phosphonium bromide, PPNBr = bis(triphenylphosphoranylidene)ammonium bromide, PPNCl = bis(triphenylphosphoranylidene)ammonium chloride).

7. NMR Spectra of Ligands
Fig. S1: $^1\text{H}$-NMR Spectrum of Ligand, $\text{H}_4\text{L}^1$

Fig. S2: $^{13}\text{C}$-NMR Spectrum of Ligand, $\text{H}_4\text{L}^1$
Fig. S3: $^1$H-NMR Spectrum of Ligand, $\text{H}_4\text{L}^2$

Fig. S4: $^{13}$C-NMR Spectrum of Ligand, $\text{H}_4\text{L}^2$
Fig. S5: $^1$H-NMR Spectrum of Ligand, $H_4L^3$

Fig. S6: $^{13}$C-NMR Spectrum of Ligand, $H_4L^3$
8. Powder XRD of complex 2

Fig. S7 Diffractograms of the Co-complex (2), simulated standard pattern of CCDC 1027789\textsuperscript{1b} (Blue) and that of the as-synthesized compound in this study (Red).

9. FTIR spectra of ligands and complexes

Fig. S8: FT-IR Spectrum of Ligand (H\textsubscript{4}L\textsuperscript{1}) and Co-complex, [Co(HL\textsuperscript{1})\textsubscript{2}]
Fig. S9: FT-IR Spectrum of Ligand (H₄L²) and Co-complex, [Co(HL²)]₂

Fig. S10: FT-IR Spectrum of Ligand (H₄L³) and Co-complex, [Co(HL³)]₂
10. Mass spectra of dinuclear cobalt complexes

**Fig. S11:** Mass Spectrum complex 1, $[\text{Co}(\text{H}_2\text{L}^1)]_2$

**Fig. S12:** Mass Spectrum complex 2, $[\text{Co}(\text{H}_2\text{L}^2)]_2$
11. NMR spectra of carbon dioxide fixation reactions

Fig. S14: $^1$H-NMR spectrum in CDCl$_3$ of the crude product [4-(chloromethyl)-1,3-dioxolan-2-one] obtained from the conversion of epichlorohydrin using complex 2 as a catalyst.
Fig. S15: $^1$H-NMR spectrum in CDCl$_3$ of the crude product [4-((allyloxy)methyl)-1,3-dioxolan-2-one] obtained from the conversion of allyl glycidyl ether using complex 2 as a catalyst.

Fig. S16: $^1$H-NMR spectrum in CDCl$_3$ of the crude product [4-(butoxymethyl)-1,3-dioxolan-2-one] obtained from the conversion of butyl glycidyl ether using complex 2 as a catalyst.
Fig. S17: $^1$H-NMR spectrum in CDCl$_3$ of the crude product [4-(isopropoxymethyl)-1,3-dioxolan-2-one] obtained from the conversion of glycidyl isopropyl ether using complex 2 as a catalyst.

Fig. S18: $^1$H-NMR spectrum in CDCl$_3$ of the product [4-(bromomethyl)-1,3-dioxolan-2-one] obtained from the conversion of epibromohydrin using complex 2 as a catalyst.
Fig. S19: $^1$H-NMR spectrum in CDCl$_3$ of the crude product [4-phenyl-1,3-dioxolan-2-one] obtained from the conversion of styrene oxide using complex 2 as a catalyst. The small peaks in the range of 2.6 to 3.3 ppm are due to the presence of trace amount of unreacted styrene oxide.

Fig. S20: $^1$H-NMR spectrum in CDCl$_3$ of the crude product [4-methyl-1,3-dioxolan-2-one] obtained from the conversion of propylene oxide using complex 2 as a catalyst. The small peaks in the range of 2.5-3.5 and at 1.28 ppm are due to the unreacted propylene oxide (substrate).
Fig. S21: $^1$H-NMR spectrum in CDCl$_3$ of the crude product [4-butyl-1,3-dioxolan-2-one] obtained from the conversion of 1,2-epoxyhexane using complex 2 as a catalyst. The small peaks in the range of 2.4 to 2.8 ppm are due to the unreacted 1,2-epoxyhexane (substrate).

Fig. S22: $^1$H-NMR spectrum in CDCl$_3$ of the crude product (tetrahydrofuro[3,4-d][1,3]dioxol-2-one) obtained from the conversion of 3,6-dioxabicyclo[3.1.0]hexane using complex 2 as a catalyst.
**Fig. S23:** $^1$H-NMR spectrum in CDCl$_3$ of the crude product (tetrahydro-4H-cyclopenta[d][1,3]dioxol-2-one) obtained from the conversion of cyclopentene oxide using complex 2 as a catalyst.

**Fig. S24:** $^1$H-NMR spectrum in CDCl$_3$ of the crude product (hexahydrobenzo[d][1,3]dioxol-2-one) obtained from the conversion of cyclohexene oxide using complex 2 as a catalyst.
12. FTIR of the recycled complex

Fig. S25: FT-IR Spectra of fresh and recycled catalyst, 2, (till five catalytic cycles).

13. References


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