Electronic Supplementary Material (ESI) for Catalysis Science & Technology.


# Phenol hydrodeoxygenation: Effect of support and Re promoter on the reactivity of Co catalysts

I.T. Ghampson[a,*], C. Sepúlveda[b], A.B. Dongil[b], G. Pecchi[b], R. García[b], J.L.G. Fierro[c], N. Escalona[a,d**]

[a]*Departamento de Ingeniería Química y Bioprocesos, Escuela de Ingeniería, Pontificia Universidad Católica de Chile, Avenida Vicuña Mackenna 4860, Macul, Santiago, 7820436, Chile.*

[b]*Universidad de Concepción, Facultad de Ciencias Químicas, Casilla 160c, Concepción, Chile*

[c]*Instituto de Catálisis y Petroleoquímica, CSIC, Cantoblanco, 28049 Madrid, Spain*

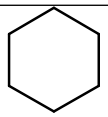
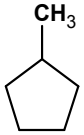
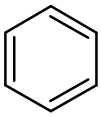
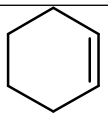
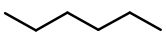
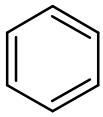
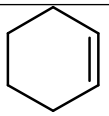
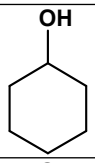
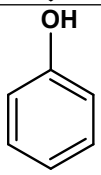
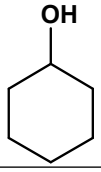
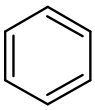
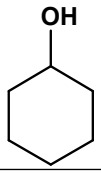
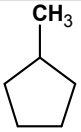
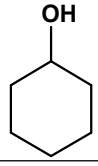
[d]*Departamento de Fisicoquímica, Facultad de Químicas, Pontificia Universidad Católica de Chile, Santiago, 7820436, Chile*

*Corresponding authors:

[*] *Dr. I. Tyrone Ghampson, e-mail*: isghampson@uc.cl

[**] *Dr. Nestor Escalona, e-mail:* neescalona@ing.puc.cl

**Table S1** Conversion of phenol intermediates over $Co/Al_2O_3$ catalyst at 300 °C, 3 MPa $H_2$, 4 h

| Substrate(s) | Conv. (%) | Products distribution (%) | | | | | |
|---|---|---|---|---|---|---|---|
| | |  |  |  |  |  | Alkylation products |
|  | 10 | 100 | - | - | - | - | - |
|  * | 100 | 44 | 1 | 48 | - | 1 | - |
|  | 100 | 93 | | 7 | | | |
|  | 100 | 76 | 1 | 9 | 5 | - | 9 |
|  | 33 | | | | | | |
|  | 3.3 | 95 | 5 | - | - | - | - |
|  | 100 | | | | | | |
|  | 26.1 | 51 | - | - | - | 3 | 46 |
|  | 89.2 | | | | | | |

* Products from hydrocracking of cyclohexane accounted for 5% of the products.

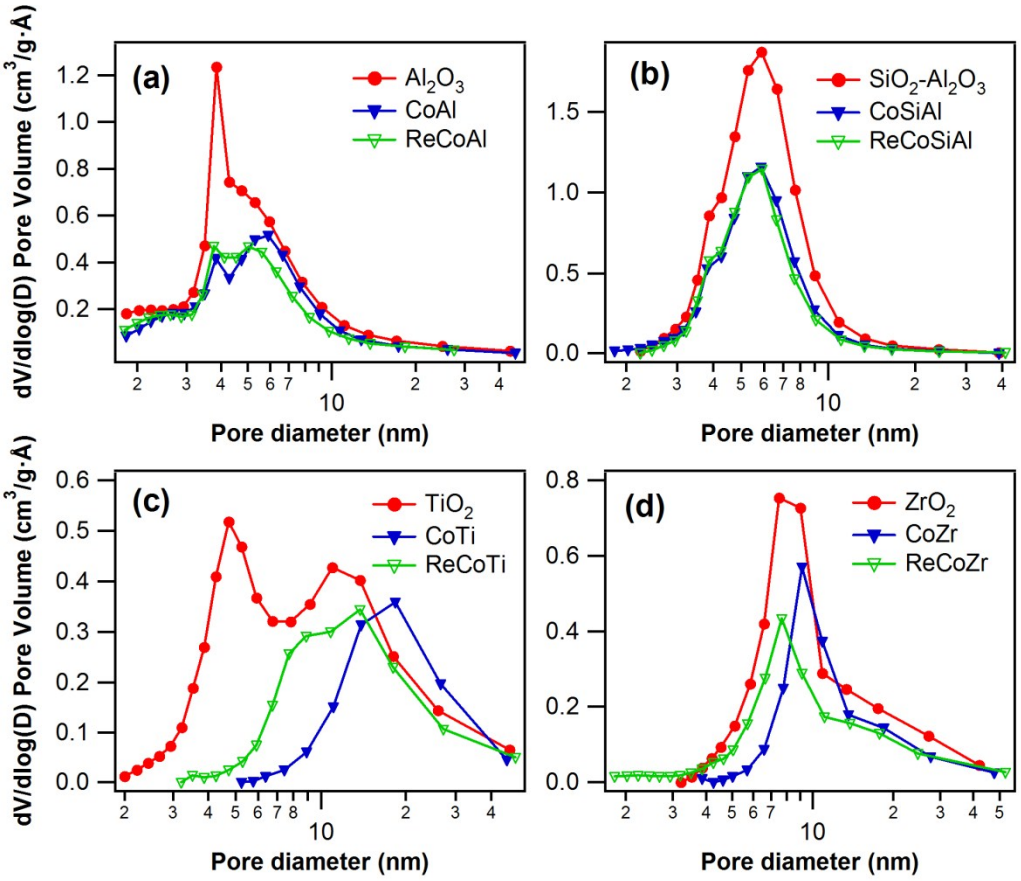



**Figure S1**. BJH pore size distributions of calcined (a) $Al_2O_3$-supported, (b) $SiO_2$-$Al_2O_3$-supported, (c) $TiO_2$-supported, and (d) $ZrO_2$-supported catalysts

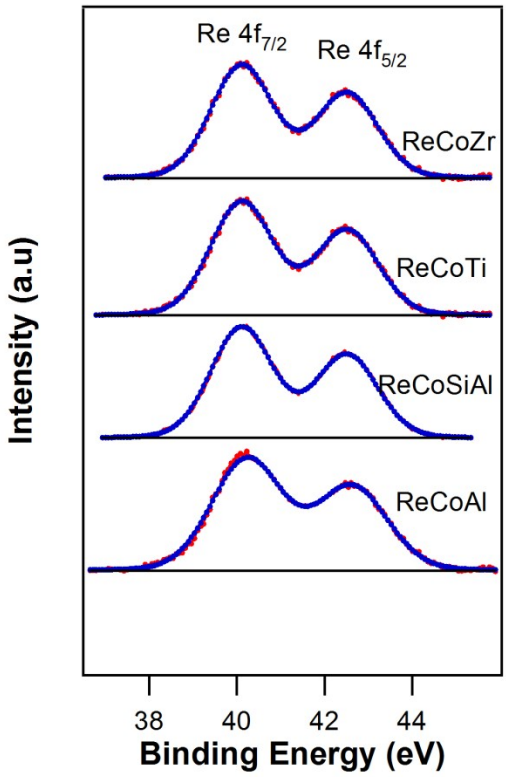



**Figure S2.** Re 4f core level spectra of reduced-passivated supported Re-Co catalysts. Reduction conditions to remove the passivation layer: 50 mL $min^{-1}$ $H_2$, 300 °C, 1 h

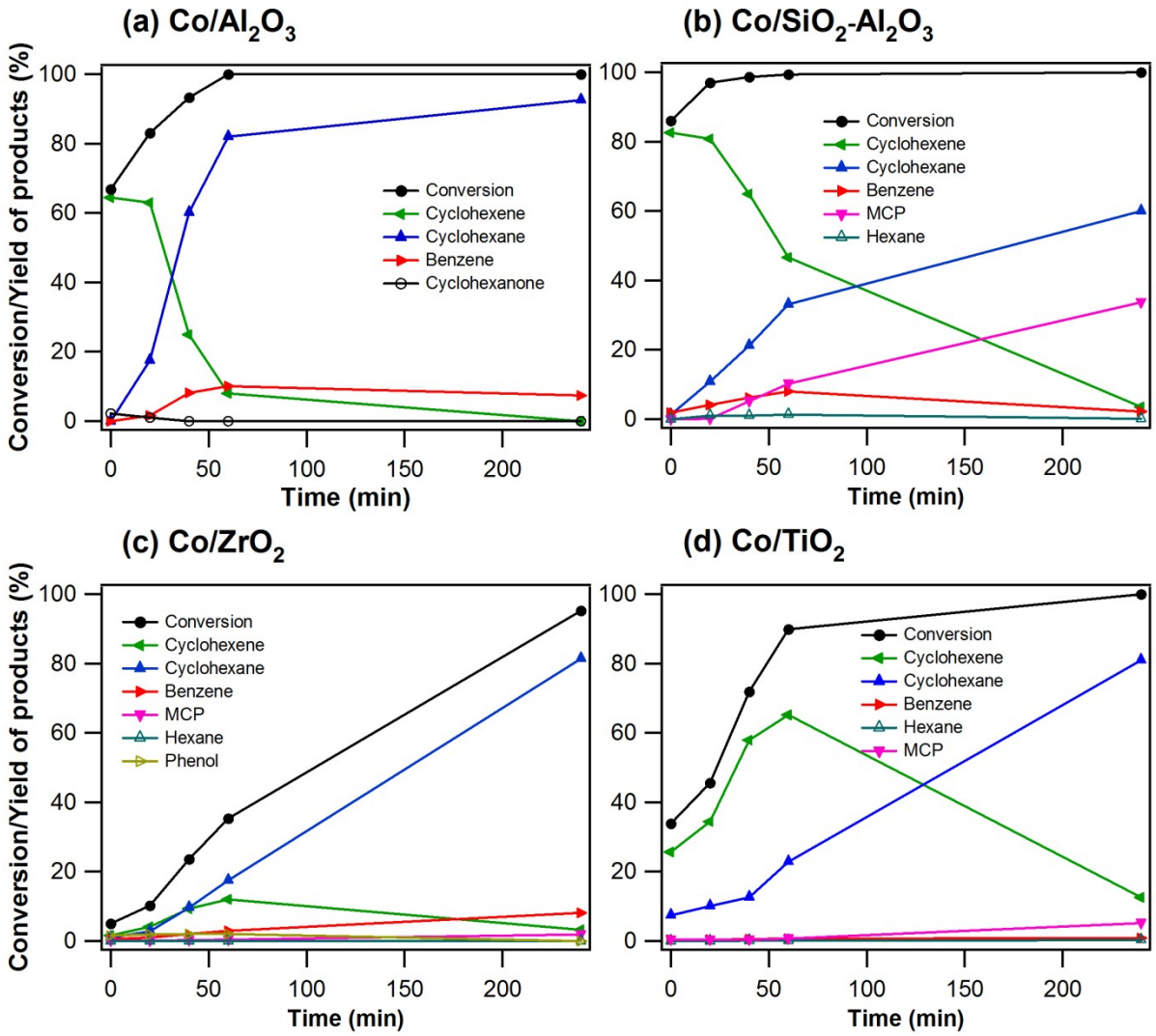



**Figure S3.** Variation of the conversion of cyclohexanol and the yield of products with time over $Co/Al_2O_3$ catalyst. Reaction conditions: cyclohexanol (1.98 mL, 19 mmol), catalyst (100 mg), dodecane (80 mL), 300 °C, 3 MPa $H_2$.

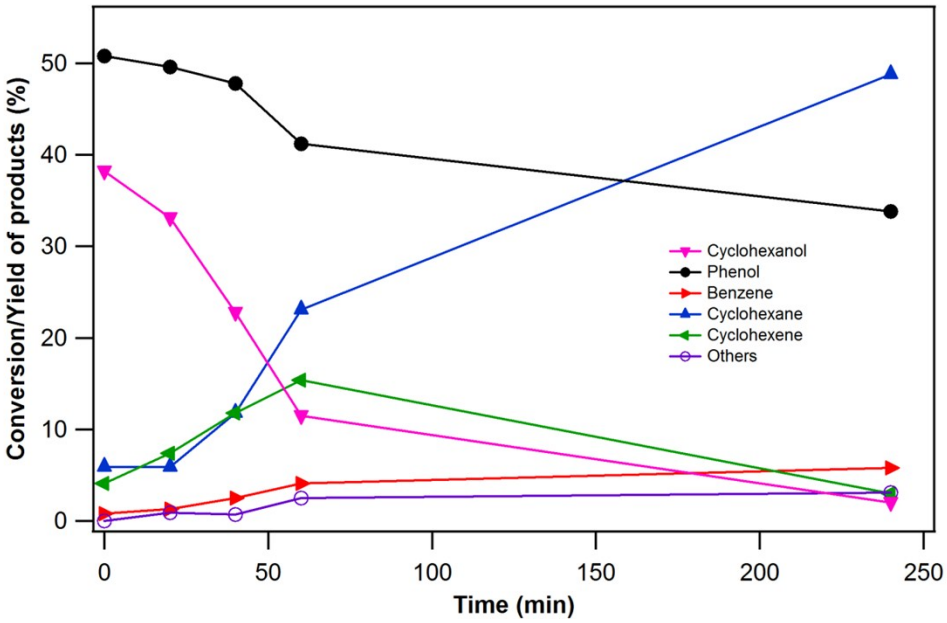



**Figure S4.** Variation of the conversion of phenol and cyclohexanol, and the yield of products with time over $Co/Al_2O_3$ catalyst. Reaction conditions: phenol (1.8 g, 19.1 mmol), catalyst (200 mg), dodecane (80 mL), 300 °C, 3 MPa $H_2$.

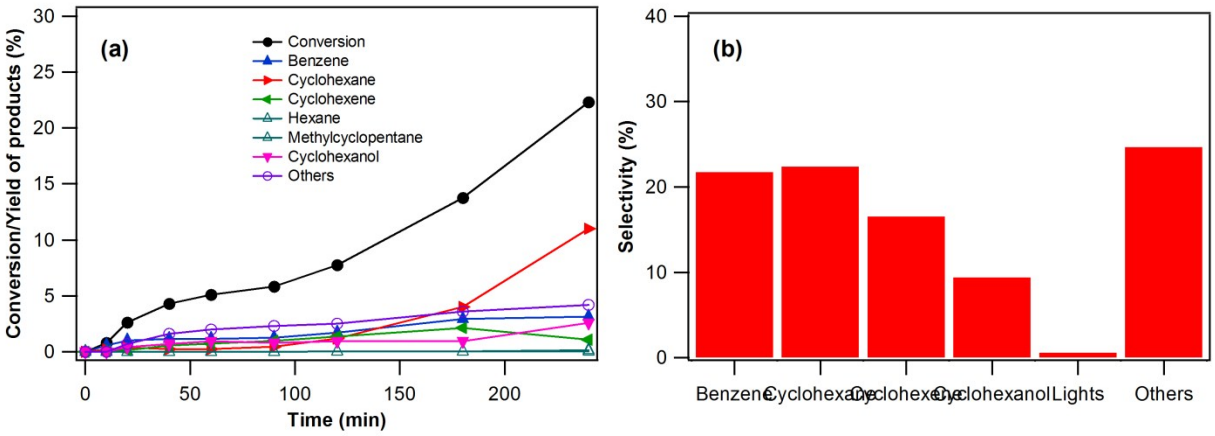



**Figure S5.** (a) Time-course of the conversion of phenol, and (b) Products selectivity calculated at 10% phenol conversion over unpassivated $Co/Al_2O_3$ catalyst. Reaction conditions: phenol (1.8 g, 19.1 mmol), catalyst (200 mg), dodecane (80 mL), 300 °C, 3 MPa $H_2$.

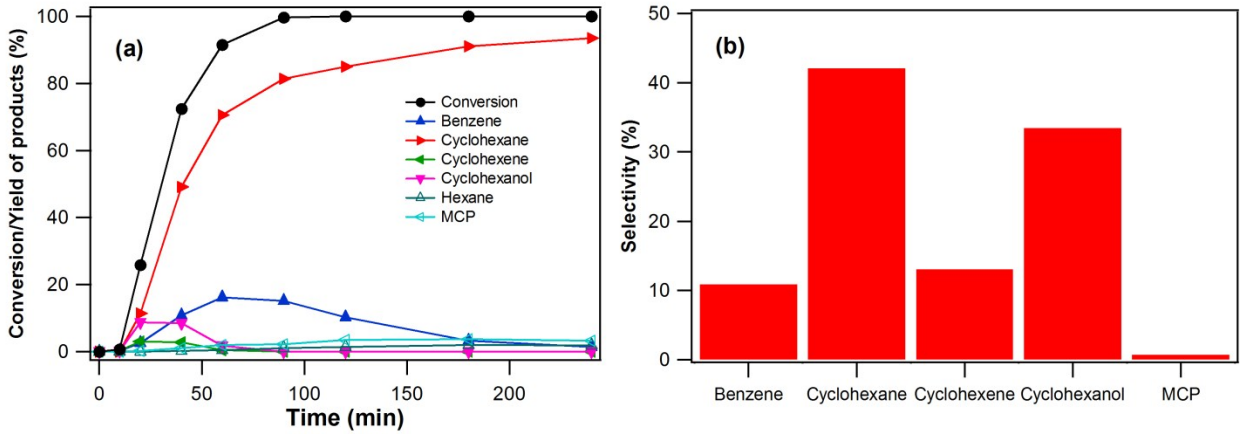



**Figure S6.** (a) Time-course of the conversion of phenol, and (b) products selectivity calculated at 10% phenol conversion over $Co/SiO_2$ catalyst. Reaction conditions: phenol (1.8 g, 19.1 mmol), catalyst (200 mg), dodecane (80 mL), 300 °C, 3 MPa $H_2$.

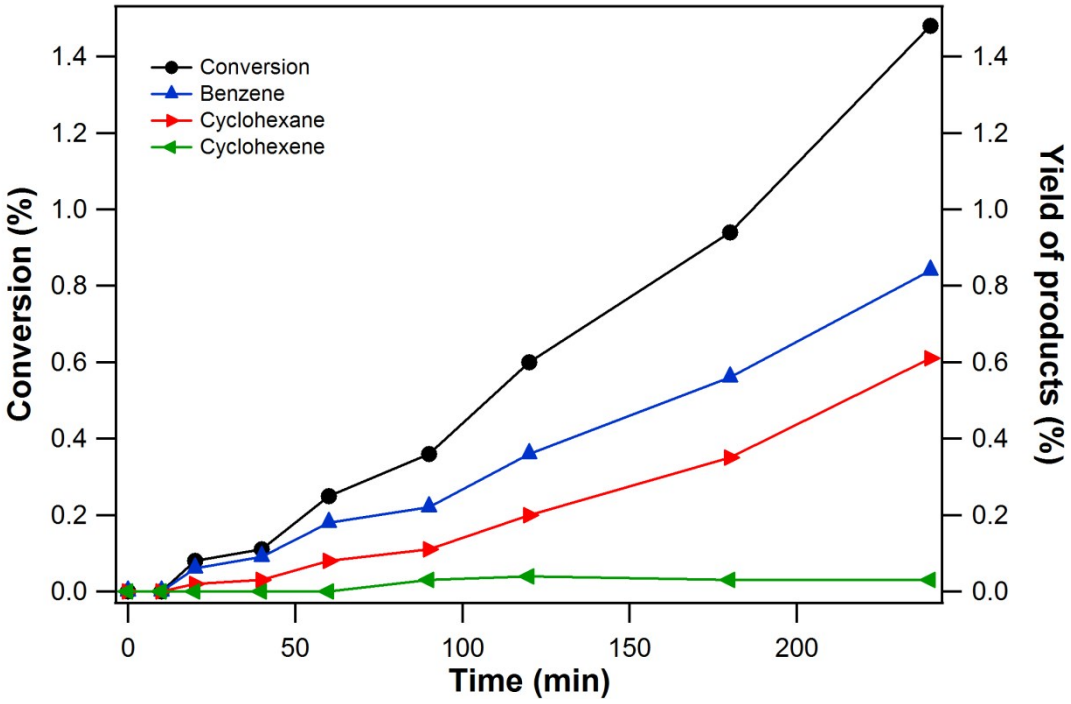



**Figure S7.** Variation of the conversion of phenol and the yield of products with time over $Re/SiO_2$-$Al_2O_3$ catalyst. Reaction conditions: phenol (1.8 g, 19.1 mmol), catalyst (200 mg), dodecane (80 mL), 300 °C, 3 MPa $H_2$.