

Supplementary Materials: Oxidative Thermal Sintering and Redispersion of Rh Nanoparticles on Supports with High Oxygen Ion Lability

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Table S1. H₂-uptake values obtained by the isothermal H₂-chemisorption experiments and corresponding Rh dispersion values D (%)

Catalyst	H ₂ uptake in H ₂ -chemisorption experiments (cc/g _{cat})			Rh Dispersion, D (%)		
	Fresh	Sinter #1	Sinter #2	Fresh	Sinter #1	Sinter #2
Rh/γ-Al ₂ O ₃	1.05	0.816	0.490	88	69	41
Rh/ACZ	0.735	0.898	0.772	77	91	81
Rh/CZ	0.260	0.621	0.595	27	65	62

CALCULATIONS:

(i) Dispersion, D (%):

$$D (\%) = \frac{(H_2 - \text{uptake}) \cdot F_s \cdot AW_{\text{Metal}} \cdot 100}{V_{\text{mol}} \cdot (\text{metal loading}/100)}$$

(ii) Specific metal surface area, S_{SP} , (in m²/g of catalyst):

$$S_{SP} \left(\text{in } \frac{\text{m}^2}{\text{g}_{\text{cat}}} \right) = \frac{(H_2 - \text{uptake}) \cdot N_{AV} \cdot F_s \cdot S_{\text{atom}} \cdot 10^{-20}}{V_{\text{mol}}}$$

(iii) Average metal particle size diameter, d_{Metal} (nm):

$$d_{\text{Metal}} (\text{nm}) = \frac{6 \cdot (\text{metal loading}/100) \cdot 10^3}{S_{SP} \cdot \rho_{\text{met}}}$$

OR

$$d_{\text{Metal}} (\text{nm}) = \frac{6 \cdot V_{\text{mol}} \cdot (\text{metal loading}) \cdot 10^{21}}{(H_2 - \text{uptake}) \cdot N_{AV} \cdot F_s \cdot S_{\text{atom}} \cdot \rho_{\text{met}}}$$

where

AW_{Metal} : relative atomic mass of a metal (e.g. Rh=102.9)

V_{mol} : molar volume of an ideal gas at room temperature and 1 atmosphere of pressure (~24450 cc/mol)

metal loading: wt% of metal on catalysts (for the present catalysts: 1, 0.8 and 0.8 wt% on Rh/γ-Al₂O₃, Rh/ACZ and Rh/CZ, respectively).

N_{AV} : Avogadro number (=6.023x10²³ atoms/mol)

F_s : hydrogen to metal correlation factor (=2 in case of one-to-one correlation of adsorbed H atoms with metal sites, i.e. H-Rh)

S_{atom} = cross sectional surface area of a metal atom (for Rh: 7.6 Å²/atom = 0.076 nm²/atom)

10^{-20} : unit conversion factor ($\text{m}^2/\text{\AA}^2$)

10^3 : unit conversion factor ($\text{m}^2\cdot\text{nm}/\text{cm}^3$)

ρ_{met} = metal density (for Rh: $12.4\text{ g}/\text{cm}^3$)