Supporting Information

Supplemental Table 1. Fit Diagnostic Parameters for the EXAFS models

		Sample calcined at 120 °C			Sample calcined at 300 °C		
	Model[b]	I	II	III	I	II	III
Δk (Å^{-1})		4.40–14.10			4.43–14.72		
Δr (Å)		1.14–4.22			1.14–4.19		
ε_ν^2		23.9	25.4	23.0	20.1	30.3	18.8
k^0	Chi Variance	6.76	7.20	6.49	4.29	6.58	5.26
	FT Im Part	0.09	0.12	0.11	0.15	0.29	0.23
	FT Re Part	0.04	0.07	0.05	0.06	0.15	0.14
k^1	Chi Variance	7.27	8.46	7.45	4.21	6.33	4.54
	FT Im Part	0.16	0.21	0.21	0.66	0.27	0.31
	FT Re Part	0.06	0.10	0.08	0.34	0.17	0.17
k^2	Chi Variance	8.15	10.12	8.67	4.75	6.96	4.64
	FT Im Part	0.42	0.48	0.43	0.66	0.46	0.58
	FT Re Part	0.15	0.22	0.17	0.34	0.27	0.35
k^3	Chi Variance	9.64	11.92	9.68	6.12	8.23	5.65
	FT Im Part	1.00	1.02	0.81	1.35	0.85	1.03
	FT Re Part	0.31	0.41	0.41	0.55	0.34	0.62

[a]Standard deviations of the data were used as error estimates for $Rh^+(CO)_2$ in the zeolite calcined at 300 °C, and a conservative error estimate of 0.002 was used for the Fourier-filtered (Δk: 2.36–15.69 Å^{-1}, Δr: 0.325–6.25 Å) data file used for $Rh^+(CO)_2$ in the zeolite calcined at 120 °C.

[b]Each model was fitted with 20 free parameters; the maximum number of statistically justified parameters[15] was found to be 22 and 21 for the zeolite supported samples calcined at 300 and 120 °C, respectively.

Supplemental Table 2. Crystallographic Data Characterizing the Reference Compounds and Fourier Transform Ranges Used in the EXAFS Analysis

		Crystallographic Data			Fourier Transform		
Reference compound	shell	*N*	*R* (Å)	Ref.	Δk ($Å^{-1}$)	Δr (Å)	n[a]
Rh foil	Rh–Rh	12	2.687	59	2.86–19.60	1.60–3.12	3
Rh_2O_3	Rh–O	6	2.050	60	2.67–15.69	0.00–2.10	2
$[Ru_3(CO)_{12}]$	Ru–C[b]	4	1.910	61	3.71–14.80	0.95–1.87	1
	Ru–O*[c]	4	3.050	61	3.75–14.80	1.90–3.11	2
Rh-Al alloy	Rh–Al	8	2.570	55	0.00–20.00	0.00–8.00	0

[a]A k^n-weighting was used when taking the Fourier transform of the data for purposes of extracting the reference phase and amplitude functions of the absorber–backscatterer pair.

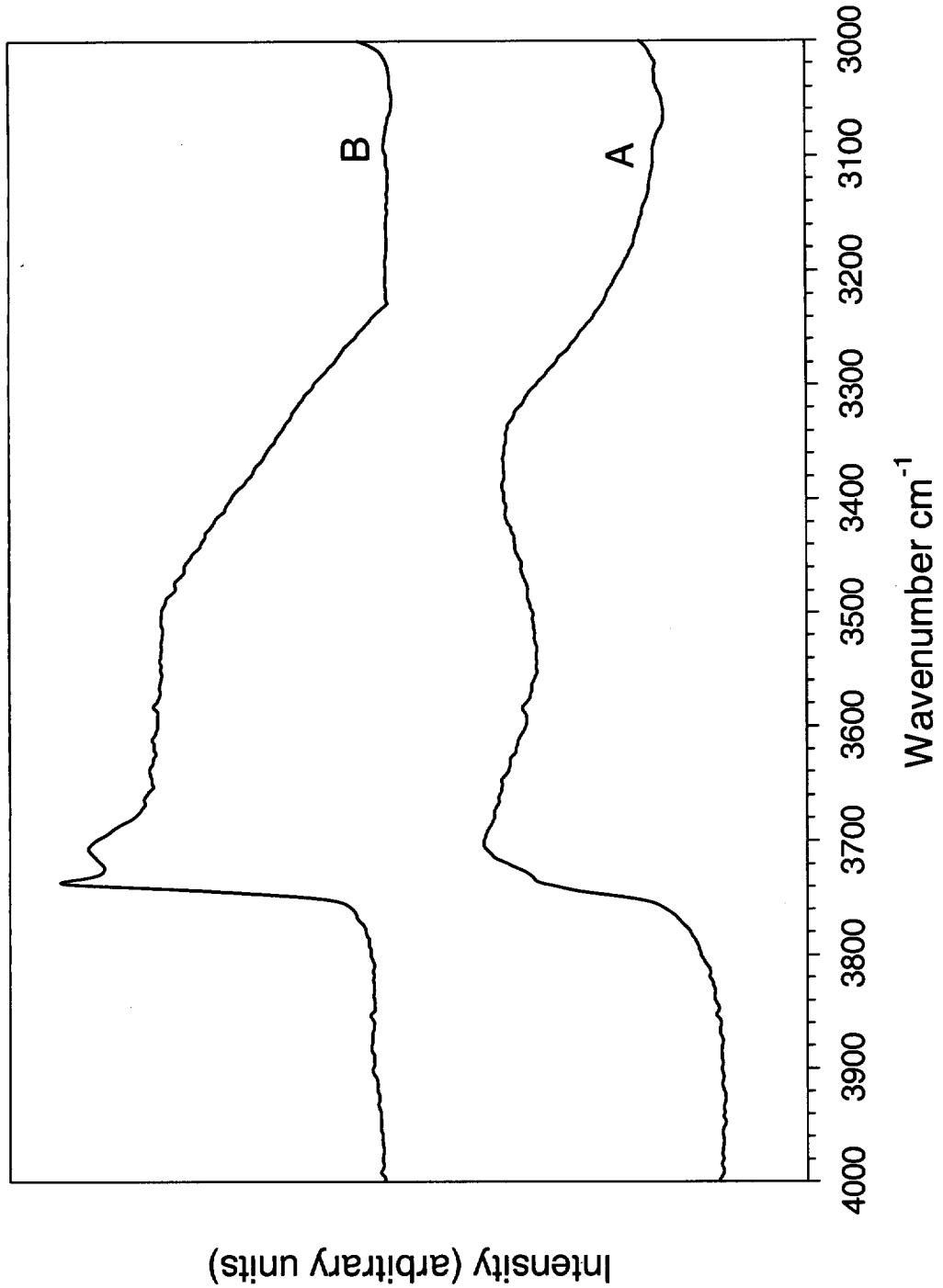
[b]Used as the reference phase shift and backscattering amplitude for the Rh–C shell.

[c]Used as the reference phase shift and backscattering amplitude for the Rh–O* shell.

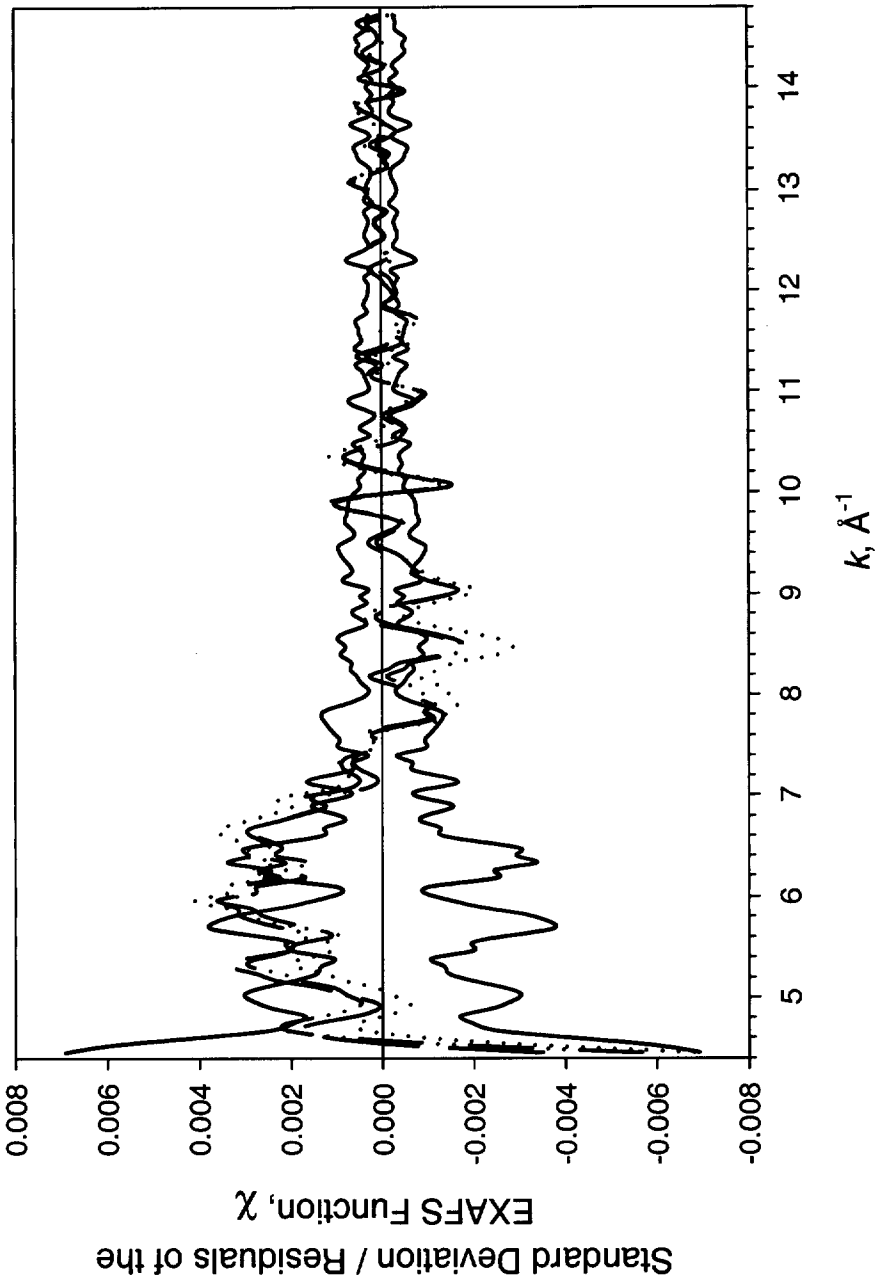
Supplemental Figure Captions

Supplemental Figure 1. Infrared spectra in the OH stretching region of $Rh^{+}(CO)_2$ supported on dealuminated Y zeolite. (A) zeolite calcined at 120 °C; (B) zeolite calcined at 300 °C.

Supplemental Figure 2. Standard deviations in the EXAFS χ function and the residuals of the model fits from the data for $Rh^{+}(CO)_2$ supported on dealuminated Y zeolite calcined at 300 °C. Solid lines, standard deviations; dashed line, residuals of Model I; dotted line – residuals of Model II; dashed-dotted line, residuals of Model III.



Supplemental Figure 1.



Supplemental Figure 2.