Supplementary information

Density Functional Theory Study of the Hydrogenation of Carbon Monoxide over the Co (001) Surface: Implications for the Fischer-Tropsch Process

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Table S1: The structural details of the preferred adsorption geometries for all intermediates on the Co (001) surface.

Species	Site	bond length (Å)
CO	Hollow	Co–C, 2.03 Co–O, 2.865
COH	Hollow	Co–C, 1.960 Co–O, 2.863 Co–H, 2.822
HCO	Hollow	Co–C, 1.917 Co–H, 2.619 Co–O, 1.928
Cis-HCOH	Hollow	Co–H, 2.747 Co–C, 1.970 Co–O, 2.365 Co–H, 3.144
Trans-HCOH	Bridge	Co–H, 2.685 Co–C, 1.930 Co–O, 2.854 Co–H, 2.597
CH	Hollow	Co–C, 1.942 Co–H, 2.627
CH_2	Hollow	Co–C, 2.091 Co–H, 1.841 Co–H, 2.554
CH_3	Hollow	Co–C, 1.967 Co–H, 1.923

		Co–H, 1.929
		Co–H, 2.266
CH_4	Hollow	Co–C, 3.645
		Co–H, 2.841
		Co–H, 2.928
		Co–H, 4.046
		Co–H, 4.041
H_2O	Top	Co–O, 2.141
		Co–H, 2.218
		Co–H, 2.631
CH_2OH	Hollow	Co–C, 1.941
		Co–H, 1.802
		Co–H, 2.502
		Co–O, 2.110
		Co–H, 2.510
CH_3OH	Top	Co–C, 3.101
		Co–H, 2.933
		Co–H, 3.127
		Co–H, 4.061
		Co–O, 2.117
		Co–H, 2.488
C_2H_2	Hollow	Co–C, 1.843
		Co–H, 2.487
		Co–C, 1.843
		Co–H, 2.487

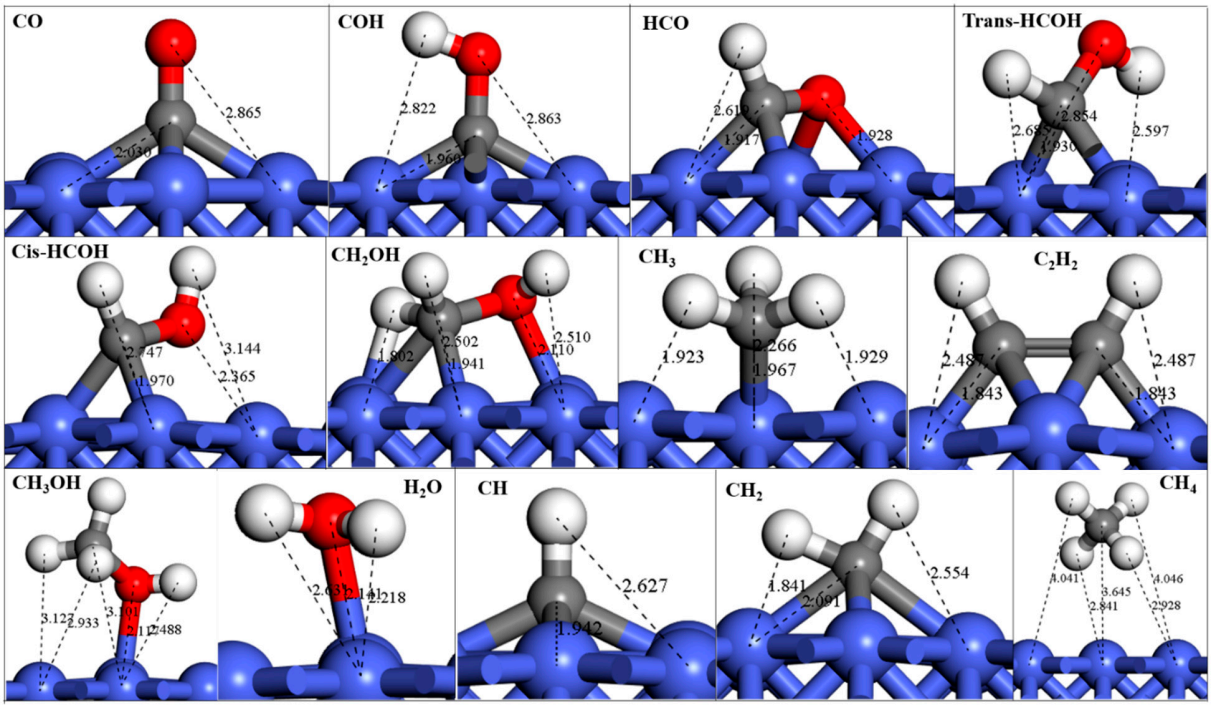

Figure S1: Side views of the lowest-energy adsorption configurations of each intermediate on the Co (001) surface. The bond lengths are shown in Å; the gray, white, red, and blue balls represent carbon, hydrogen, oxygen, and cobalt atoms, respectively.