Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

A Density Functional Theory Analysis of Trends in Glycerol Decomposition on Close-Packed Transition Metal Surfaces

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Table S1. Energy barriers of selected elementary steps for glycerol decomposition on Pt(111) (via dehydrogenation, C-C and C-O bond scission) calculated using the CI-NEB/dimer method in explicit DFT calculations. The same set of reactions is used to generate the BEP relationships (Fig. 4 in the main text).

Table S2. Energy barriers of elementary steps for glycerol decomposition (only reactions corresponding to the lowest transition state energies for dehydrogenation, C-C, and C-O scission in the free energy diagrams in Fig. 5 and Fig. S1 are shown) on the close-packed surfaces of Pd, Rh, Ni and Cu. The tabulated energy barriers are estimated from the BEP relationship discussed in the main text.

Figure S1. Free energy diagram for glycerol decomposition on the Cu(111) surface at 483 K and standard pressure. Black squares represent the adsorption thermochemistry of the most stable glycerol dehydrogenation intermediates, blue diamonds represent the most stable dehydrogenation transition states, red triangles represent the corresponding energetics for C-C bond breaking transition states, and purple circles represent the lowest energy transition states for C-O bond scissions at each level of dehydrogenation. All transition state free energies are estimated using the BEP relationships. Bold letters indicate the designated bonds to be broken.

Figure S2. Black squares represent the adsorption thermochemistry of the most stable glycerol dehydrogenation intermediates, blue diamonds represent the most stable dehydrogenation transition states, red triangles represent the corresponding energetics for C-C bond breaking transition states, and purple circles represent the lowest energy

transition states for C-O bond scissions at each level of dehydrogenation. All transition state free energies are estimated using the BEP relationships. Bold letters indicate the designated bonds to be broken.

Figure S3. Brønsted-Evans-Polanyi (BEP) relationship for (a) C-H/O-H and (b) C-O/C-C bond scission reactions in glycerol dehydrogenation intermediates. Final state (E_{FS}) and transition state (E_{TS}) energies are relative to initial state gas phase energies, where each corresponding surface reaction is represented in the exothermic direction. Unlabeled points are reactions on Pt(111), as given in Figure 4 of the manuscript. Selected additional calculations on Pd(111) and Rh(111) are as labeled. Bold letters indicate the bond to be broken.

Reaction		Energy Barrier (eV)
dehydrogenation	CH_2OH-$CHOH$-CH_2OH* + * → CH_2OH-$CHOH$-CH_2O* + H*	0.87
	CH_2OH-$CHOH$-CH_2OH* + * → CH_2OH-CHO-CH_2OH* + H*	0.74
	CH_2OH-$CHOH$-CH_2OH* + * → CH_2OH-COH-CH_2OH* + H*	0.71
	CH_2OH-$CHOH$-CH_2OH* + * → CH_2OH-$CHOH$-$CHOH$* +H*	0.84
	CH_2OH-COH-CH_2OH* + * → CH_2OH-COH-$CHOH$* + H*	0.54
	CH_2OH-COH-CH_2OH* + * → CH_2OH-COH-CH_2O* + H*	0.75
	CH_2OH-COH-CH_2OH* + * → CH_2OH-CO-CH_2OH* + H*	0.79
	CH_2OH-$CHOH$-$CHOH$* + * → CH_2OH-COH-$CHOH$* + H*	0.50
	CH_2OH-$CHOH$-$CHOH$* + * → CH_2OH-$CHOH$-CHO* + H*	0.60
	CH_2OH-$CHOH$-$CHOH$* + * → $CHOH$-$CHOH$-$CHOH$* + H*	0.66
	$CHOH$-$CHOH$-$CHOH$* + * → $CHOH$-$CHOH$-COH* + H*	0.68
	$CHOH$-COH-$CHOH$* + * → $CHOH$-COH-COH* + H*	0.73
	CH_2OH-COH-CHO* + * → CH_2OH-COH-CO* + H*	0.55
	$CHOH$-COH-COH* + * → COH-COH-COH* + H*	0.39
	COH-$CHOH$-COH* + * → COH-COH-COH* + H*	0.31
	COH-COH-COH* + * → COH-COH-CO* + H*	0.42
	COH-COH-CO* + * → CO-COH-CO* + H*	0.38
	CO-COH-CO* + * → CO-CO-CO* + H*	1.14
C-C scission	CH_2OH-COH-CH_2OH* + * → CH_2OH-COH* + CH_2OH*	1.58
	CH_2OH-$CHOH$-$CHOH$* + * → CH_2OH-$CHOH$* +$CHOH$*	1.38
	$CHOH$-$CHOH$-$CHOH$* + * → $CHOH$-$CHOH$* + $CHOH$*	1.30
	CH_2OH-$CHOH$-CHO* + * → CH_2OH-$CHOH$* + CHO*	1.34
	CH_2OH-$CHOH$-CO* + * → CH_2OH-$CHOH$* + CO*	0.85
	$CHOH$-$CHOH$-CHO* + * → $CHOH$-$CHOH$* + CHO*	1.26
	$CHOH$-$CHOH$-CO* + * → $CHOH$-$CHOH$* + CO*	0.88
	CH_2OH-COH-CO* + * → CH_2OH-COH* + CO*	0.41
	$CHOH$-COH-CO* + * → $CHOH$-COH* + CO*	0.53
	COH-COH-COH* + * → COH-COH* + COH*	1.32
	CH_2OH-CO-CO* + * → CH_2OH-CO* + CO*	0.03
	COH-COH-CO* + * → COH-COH* + CO*	0.41
	COH-CO-CO* + * → COH-CO* + CO*	0.20
C-O scission	CH_2OH-$CHOH$-$CHOH$* + * → CH_2OH-CH-$CHOH$* + OH*	1.21
	CH_2OH-$CHOH$-$CHOH$* + * → CH_2OH-$CHOH$-CH* + OH*	1.10
	CH_2OH-COH-CH_2OH* + * → CH_2OH-C-CH_2OH* + OH*	1.03
	CH_2OH-COH-CH_2OH* + * → CH_2OH-COH-CH_2* + OH*	1.41
	CH_2OH-COH-COH* + * → CH_2OH-COH-C* + OH*	1.36
	$CHOH$-COH-COH* + * → $CHOH$-COH-C*+ OH*	1.40

Table S1. Energy barriers of selected elementary steps for glycerol decomposition on Pt(111) (via dehydrogenation, C-C and C-O bond scission) calculated using the CI-NEB/dimer method in explicit DFT calculations. The same set of reactions is used to generate the BEP relationships (Fig. 4 in the main text).

Reaction Type	Metal	Reactions	Energy Barrier (eV)
1. *Glycerol*			
dehydrogenation	Pd	CH_2OH-$CHOH$-CH_2OH* → CH_2OH-COH-CH_2OH* + H*	0.80
	Rh	CH_2OH-$CHOH$-CH_2OH* → CH_2OH-COH-CH_2OH* + H*	0.76
	Ni	CH_2OH-$CHOH$-CH_2OH* → CH_2OH-COH-CH_2OH* + H*	0.71
	Cu	CH_2OH-$CHOH$-CH_2OH* → CH_2OH-CHO-CH_2OH* + H*	0.80
C-C scission	Pd	CH_2OH-$CHOH$-CH_2OH* → CH_2OH-$CHOH$* + CH_2OH*	1.48
	Rh	CH_2OH-$CHOH$-CH_2OH* → CH_2OH-$CHOH$* + CH_2OH*	1.43
	Ni	CH_2OH-$CHOH$-CH_2OH* → CH_2OH-$CHOH$* + CH_2OH*	1.57
	Cu	CH_2OH-$CHOH$-CH_2OH* → CH_2OH-$CHOH$* + CH_2OH*	1.56
C-O scission	Pd†	CH_2OH-$CHOH$-CH_2OH* → CH_2OH-$CHOH$-CH_2* + OH*	1.54
		CH_2OH-$CHOH$-CH_2OH* → CH_2OH-CH-CH_2OH* + OH*	1.54
	Rh	CH_2OH-$CHOH$-CH_2OH* → CH_2OH-CH-CH_2OH* + OH*	1.29
	Ni	CH_2OH-$CHOH$-CH_2OH* → CH_2OH-CH-CH_2OH* + OH*	0.90
	Cu	CH_2OH-$CHOH$-CH_2OH* → CH_2OH-CH-CH_2OH* + OH*	1.46
2. *Glycerol – 1H*			
dehydrogenation	Pd	CH_2OH-$CHOH$-$CHOH$* → $CHOH$-$CHOH$-$CHOH$* + H*	0.53
	Rh	CH_2OH-$CHOH$-$CHOH$* → $CHOH$-$CHOH$-$CHOH$* + H*	0.52
	Ni	CH_2OH-$CHOH$-CH_2O* → CH_2OH-COH-CH_2O* + H*	0.49
	Cu†	CH_2OH-CHO-CH_2OH* → CH_2OH-CHO-CH_2O* + H*	0.73
		CH_2OH-CHO-CH_2OH* → CH_2OH-CHO-$CHOH$* + H*	0.73
C-C scission	Pd	CH_2OH-COH-CH_2OH* → CH_2OH-COH* + CH_2OH*	1.43
	Rh	CH_2OH-$CHOH$-$CHOH$* → CH_2OH* + $CHOH$-$CHOH$*	1.36
	Ni	CH_2OH-COH-CH_2OH* → CH_2OH-COH* + CH_2OH*	1.43
	Cu	CH_2OH-COH-CH_2OH* → CH_2OH-COH* + CH_2OH*	1.44
C-O scission	Pd	CH_2OH-COH-CH_2OH* → CH_2OH-C-CH_2OH* + OH*	1.48
	Rh	CH_2OH-$CHOH$-$CHOH$* → CH_2-$CHOH$-$CHOH$* + OH*	1.09
	Ni	CH_2OH-$CHOH$-$CHOH$* → CH_2-$CHOH$-$CHOH$* + OH*	0.70
	Cu†	CH_2OH-CHO-CH_2OH* → CH_2OH-CHO-CH_2* + OH*	1.49
		CH_2OH-CHO-CH_2OH* → CH_2OH-CH-CH_2O* + O*	1.49
3. *Glycerol – 2H*			
dehydrogenation	Pd	$CHOH$-$CHOH$-$CHOH$* → $CHOH$-$CHOH$-COH* + H*	0.73
	Rh	CH_2OH-$CHOH$-COH* → CH_2OH-COH-COH* + H*	0.39
	Ni	CH_2OH-$CHOH$-COH* → CH_2OH-$CHOH$-CO* + H*	0.11
	Cu	CH_2OH-CHO-CH_2O* → CH_2O-CHO-CH_2O* + H*	0.65
C-C scission	Pd	CH_2OH-$CHOH$-COH* → CH_2OH-$CHOH$* + COH*	1.03
	Rh	CH_2OH-$CHOH$-COH* → CH_2OH-$CHOH$* + COH*	0.89
	Ni	CH_2OH-CO-CH_2OH* → CH_2OH-CO* + CH_2OH*	1.36
	Cu	CH_2OH-CHO-CH_2O* → CH_2OH* + CHO-CH_2O*	1.55
C-O scission	Pd	$CHOH$-$CHOH$-$CHOH$* → $CHOH$-$CHOH$-CH* + OH*	1.49
	Rh	CH_2OH-$CHOH$-COH* → CH_2OH-CH-COH* + OH*	0.99
	Ni	CH_2OH-COH-CH_2O* → CH_2OH-COH-CH_2* + O*	0.97
	Cu†	CH_2OH-CHO-CH_2O* → CH_2OH-CHO-CH_2* + O*	1.43
		CH_2OH-CHO-CH_2O* → CH_2OH-CH-CH_2O* + O*	1.43
4. *Glycerol – 3H*			
dehydrogenation	Pd	$CHOH$-COH-$CHOH$* → $CHOH$-COH-COH* + H*	0.66
	Rh	$CHOH$-CHO-$CHOH$* → $CHOH$-CO-$CHOH$* + H*	0.34
	Ni	CH_2OH-CHO-COH* → CH_2OH-CHO-CO* + H*	0.00
	Cu	CH_2OH-$CHOH$-CO* → CH_2OH-CHO-CO* + H*	0.74
C-C scission	Pd	CH_2OH-$CHOH$-CO* → CH_2OH-$CHOH$* + CO*	0.33
	Rh	CH_2OH-$CHOH$-CO* → CH_2OH-$CHOH$* + CO*	0.74
	Ni	CH_2OH-$CHOH$-CO* → CH_2OH-$CHOH$* + CO*	0.91
	Cu	CH_2OH-$CHOH$-CO* → CH_2OH-$CHOH$* + CO*	1.22
C-O scission	Pd	CH_2OH-COH-COH* → CH_2OH-COH-C* + OH*	1.45
	Rh	CH_2OH-$CHOH$-CO* → CH_2-$CHOH$-CO* + OH*	1.23
	Ni	CH_2OH-$CHOH$-CO* → CH_2-$CHOH$-CO* + OH*	0.92
	Cu	CH_2OH-$CHOH$-CO* → CH_2OH-$CHOH$-C* + O*	1.40
5. *Glycerol – 4H*			
dehydrogenation	Pd	COH-$CHOH$-COH* → COH-COH-COH* + H*	0.38
	Rh	CHO-$CHOH$-COH* → CO-$CHOH$-COH* + H*	0.21
	Ni	$CHOH$-CHO-COH* → $CHOH$-CHO-CO* + H*	0.05
	Cu	CH_2OH-CHO-CO* → $CHOH$-CHO-CO* + H*	0.67
C-C scission	Pd	$CHOH$-$CHOH$-CO* → $CHOH$-$CHOH$* + CO*	0.29
	Rh	$CHOH$-$CHOH$-CO* → $CHOH$-$CHOH$* + CO*	0.69
	Ni	CH_2OH-CHO-CO* → CH_2OH-CHO* + CO*	0.86
	Cu	CH_2OH-CHO-CO* → CH_2OH-CHO* + CO*	1.18

C-O scission	Pd	COH-CHOH-COH* → COH-CH-COH* + OH*	1.32
	Rh	COH-CHOH-COH* → COH-CH-COH* + OH*	0.81
	Ni	CH_2OH-COH-CO* → CH_2-COH-CO* + OH*	0.81
	Cu	CH_2O-CHOH-CO* → CH_2O-CHOH-C* + O*	1.32
6. *Glycerol – 5H*			
dehydrogenation	Pd	COH-CHOH-CO* → COH-CHO-CO* + H*	0.49
	Rh	COH-CHOH-CO* → CO-CHOH-CO* + H*	0.71
	Ni	COH-CHOH-CO* → CO-CHOH-CO* + H*	0.06
	Cu	CHOH-CHO-CO* → COH-CHO-CO* + H*	0.58
C-C scission	Pd	COH-CHOH-CO* → COH-CHOH* + CO*	0.30
	Rh	COH-CHOH-CO* → COH-CHOH* + CO*	0.71
	Ni	CH_2OH-CO-CO* → CH_2OH-CO* + CO*	0.61
	Cu	CH_2OH-CO-CO* → CH_2OH-CO* + CO*	0.95
C-O scission	Pd	COH-COH-COH* → COH-COH-C* + OH*	1.47
		COH-COH-COH* → COH-C-COH* + OH*	1.47
	Rh	COH-CHO-COH* → COH-CH-COH* + O*	0.67
	Ni	CH_2OH-CO-CO* → CH_2-CO-CO* + OH*	0.88
	Cu	CH_2O-CHO-CO* → CH_2O-CHO-C* + O*	1.29
7. *Glycerol – 6H*			
dehydrogenation	Pd	CO-CHOH-CO* → CO-CHO-CO* + H*	0.59
	Rh	COH-CHO-CO* → CO-CHO-CO* + H*	0.04
	Ni	CHO-CHO-CO* → CO-CHO-CO* + H*	0.07
	Cu	CO-CHOH-CO* → CO-CHO-CO* + H*	0.67
C-C scission	Pd	COH-COH-CO* → COH-COH* + CO*	0.35
	Rh	CO-CHOH-CO* → CO-CHOH* + CO*	0.94
	Ni	CH_2O-CO-CO* → CH_2O-CO* + CO*	0.52
	Cu	CH_2O-CO-CO* → CH_2O-CO* + CO*	0.87
C-O scission	Pd	CO-CHOH-CO* → CO-CHOH-C* + O*	1.39
	Rh	CO-CHOH-CO* → CO-CHOH-C* + O*	1.36
	Ni	CO-CHOH-CO* → CO-CH-CO* + OH*	1.09
	Cu	CO-CHOH-CO* → CO-CHOH-C* + O*	1.43
8. *Glycerol – 7H*			
dehydrogenation	Pd	CO-COH-CO* → CO-CO-CO* + H*	0.74
	Rh	CO-COH-CO* → CO-CO-CO* + H*	0.70
	Ni	CO-CHO-CO* → CO-CO-CO* + H*	0.68
	Cu	CO-CHO-CO* → CO-CO-CO* + H*	0.83
C-C scission	Pd	CO-COH-CO* → CO-COH* + CO*	0.29
	Rh	COH-CO-CO* → COH-CO* + CO*	0.32
	Ni	CO-CHO-CO* → CO-CHO* + CO*	1.00
	Cu	CO-CHO-CO* → CO-CHO* + CO*	1.37
C-O scission	Pd	CO-COH-CO* → CO-COH-C* + O*	1.42
	Rh	CO-CHO-CO* → CO-CH-CO* + O*	1.32
	Ni	CO-CHO-CO* → CO-CH-CO* + O*	1.16
	Cu	CO-CHO-CO* → CO-CHO-C* + O*	1.43
9. *Glycerol – 8H*			
C-C scission	Pd	CO-CO-CO* → CO-CO* + CO*	0.02
	Rh	CO-CO-CO* → CO-CO* + CO*	0.40
	Ni	CO-CO-CO* → CO-CO* + CO*	0.56
	Cu	CO-CO-CO* → CO-CO* + CO*	1.35
C-O scission	Pd	CO-CO-CO* → CO-CO-C* + O*	1.40
	Rh	CO-CO-CO* → CO-CO-C* + O*	1.37
	Ni	CO-CO-CO* → CO-C-CO* + O*	1.22
	Cu	CO-CO-CO* → CO-CO-C* + O*	1.45

[†]If the transition state energies are the same, all the corresponding reactions are listed.

Table S2. Energy barriers of elementary steps for glycerol decomposition (only reactions corresponding to the lowest transition state energies for dehydrogenation, C-C, and C-O scission in the free energy diagrams in Fig. 5 and Fig. S1 are shown) on the close-packed surfaces of Pd, Rh, Ni and Cu. The tabulated energy barriers are estimated from the BEP relationship discussed in the main text.

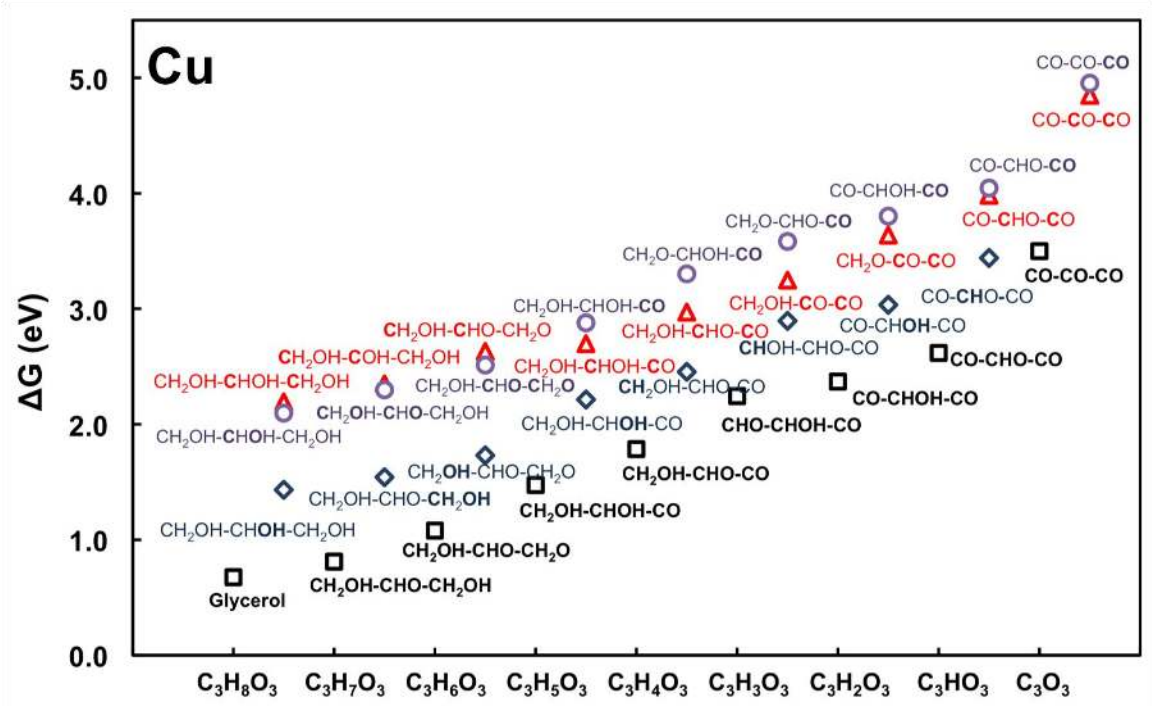

Figure S1. **Liu and Greeley**

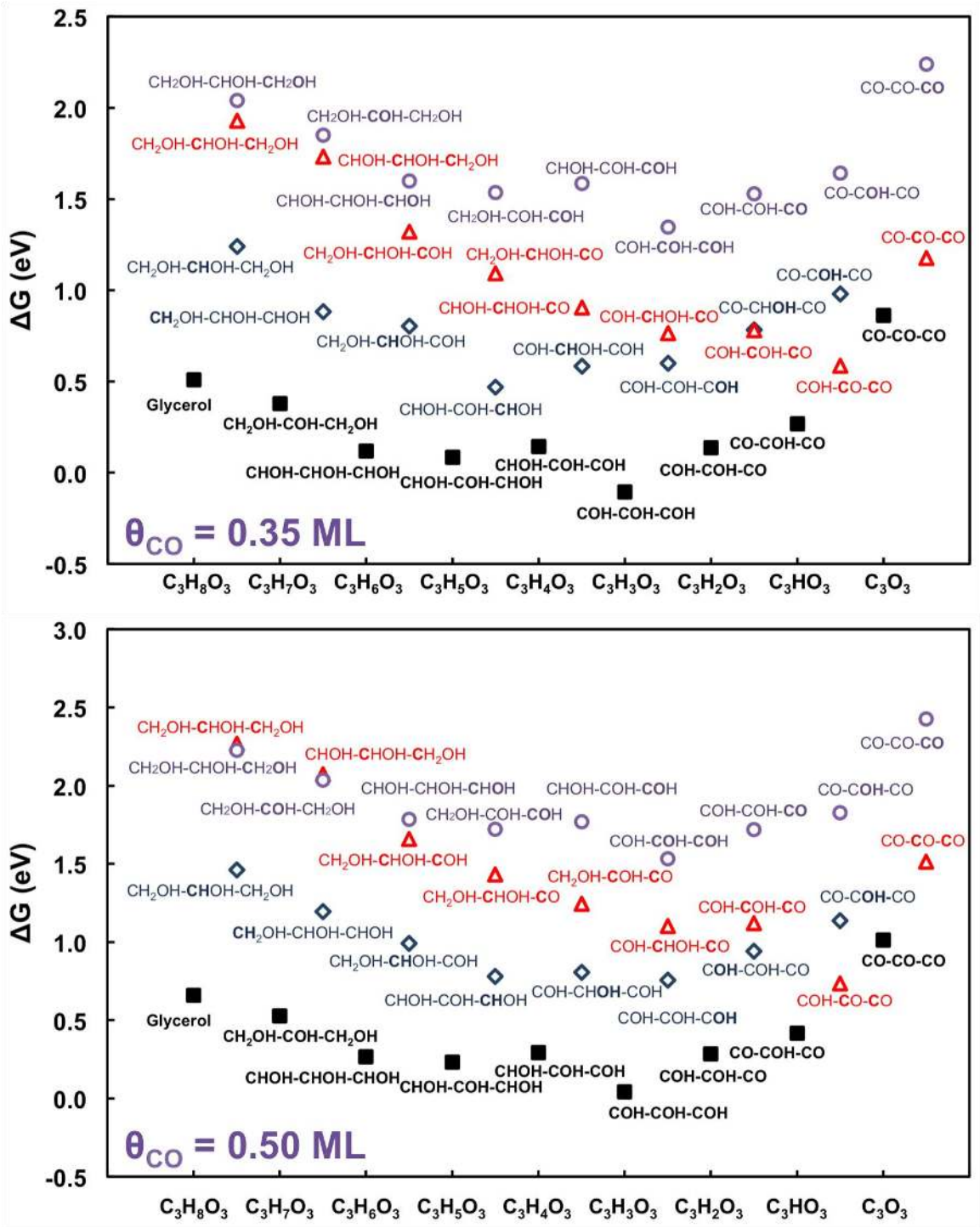

Figure S2. **Liu and Greeley**

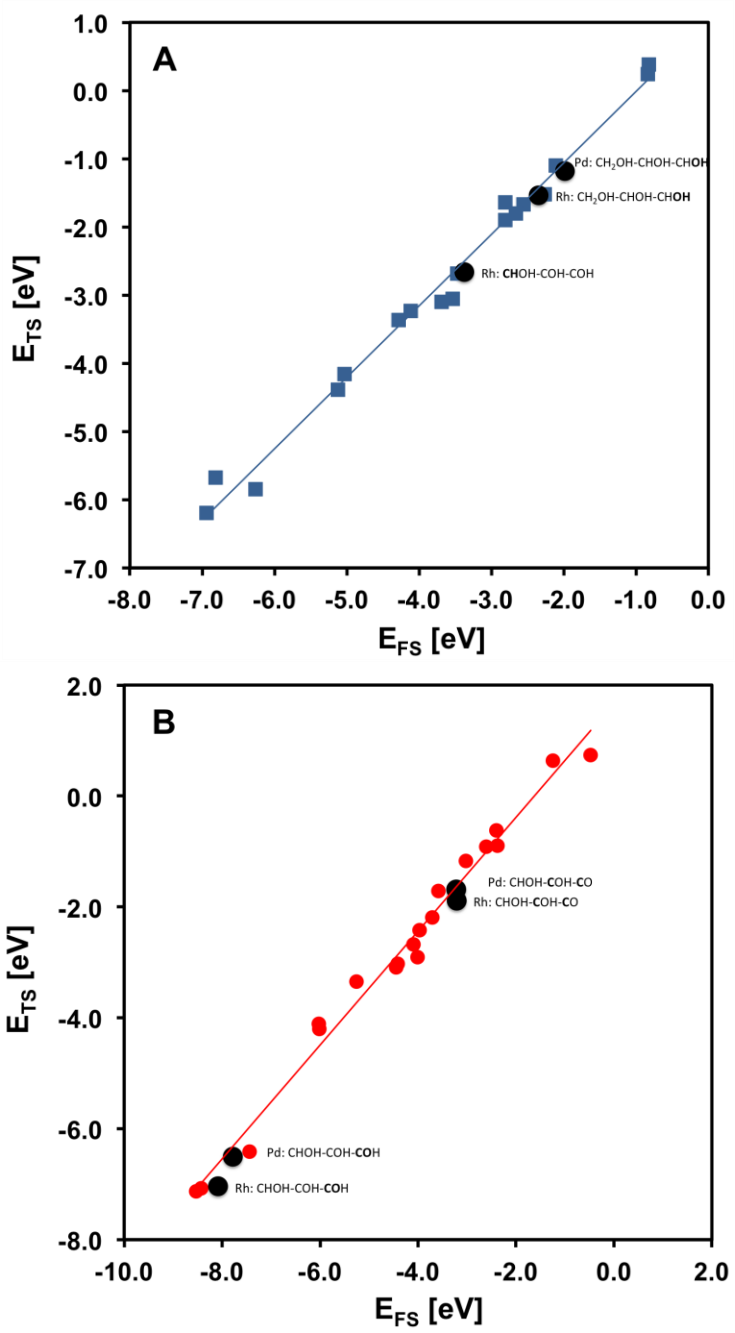

Figure S3. **Liu and Greeley**

CO surface coverage corrections for transition state energies

This section describes the estimation method, where Pt is used as an example, to correct the transition state energies. It has been reported that CO is the most abundant surface species under experimental conditions.[1] The coverage dependent binding energy of CO was calculated using Eq. (S1), similar to ref. 2.[2]

$$BE_{CO}(\ _{CO}) = BE_{CO}(\ _{CO} = 0) + 0.0065e^{4.79\ _{CO}} + 0.031135\ _{CO}e^{4.79\ _{CO}}, \qquad \text{(S1)}$$

where $BE_{CO}(\theta_{CO})$ is the differential binding energy at coverage θ_{CO}, $BE_{CO}(\theta_{CO} = 0)$ is the CO binding energy on clean Pt (111) surface. The binding energies of other surface intermediates are assumed to be a function of θ_{CO}, and are corrected using the second and third terms of eqn (S1) as well.

Cartesian coordinates of the geometries reported in Figure 1 of the main text. Only the coordinates of the adsorbates are shown. All coordinates are reported in Å.

Cell parameters for the surface (corresponding to a *p*(4×4) cell):

(2√3a, 2a, 0)
(0, 4a, 0)
(0, 0, 20.0)

where "a" is the nearest-neighbor atom-atom distance (2.821, 2.793, 2.715 and 2.574 Å for Pt, Pd, Rh and Cu, respectively).

1. $CH_2OH-CHOH-CH_2OH$

Pt:

C	4.49	5.15	7.82
C	3.86	6.35	8.51
C	3.54	3.96	7.70
H	4.77	5.46	6.76
H	6.25	4.28	7.97
H	3.67	6.10	9.57
H	4.54	7.21	8.47
H	3.18	3.66	8.71
H	4.04	3.10	7.23
H	2.71	7.24	7.14
H	2.14	5.22	7.18
O	5.66	4.79	8.55
O	2.58	6.67	7.93
O	2.36	4.28	6.91

Pd:

C	5.37	6.48	7.67
C	4.83	7.73	8.36
C	4.37	5.32	7.67
H	5.58	6.75	6.59
H	7.09	5.54	7.75
H	4.67	7.53	9.43
H	5.57	8.55	8.27
H	4.07	5.07	8.70
H	4.83	4.42	7.21
H	3.70	8.65	6.99
H	2.94	6.55	7.15
O	6.56	6.11	8.34
O	3.55	8.13	7.83
O	3.18	5.62	6.90

Rh:

C	4.46	5.01	7.59
C	3.89	6.23	8.31
C	3.47	3.84	7.51

H	4.71	5.33	6.53
H	6.17	4.05	7.70
H	3.70	5.97	9.37
H	4.61	7.06	8.28
H	3.13	3.57	8.52
H	3.95	2.96	7.05
H	2.76	7.23	7.00
H	2.07	5.09	6.96
O	5.63	4.63	8.28
O	2.61	6.62	7.76
O	2.31	4.16	6.69

Cu:

C	4.17	4.73	7.39
C	3.58	5.95	8.11
C	3.21	3.55	7.31
H	4.42	5.04	6.34
H	5.93	3.86	7.51
H	3.40	5.70	9.16
H	4.29	6.79	8.06
H	2.86	3.26	8.32
H	3.73	2.68	6.86
H	2.44	6.91	6.78
H	1.77	4.74	6.76
O	5.36	4.38	8.10
O	2.30	6.32	7.55

2 CH_2OH-CHOH-CHOH

Pt:

C	5.06	8.45	6.89
C	5.86	7.29	7.47
C	6.20	7.49	8.96
H	5.17	10.42	6.91
H	4.01	8.35	7.21
H	5.29	6.36	7.31
H	6.52	6.53	9.40
H	5.31	7.85	9.51
H	6.99	9.27	8.81
H	7.78	7.69	7.31
O	5.63	9.66	7.36
O	7.16	7.08	6.85
O	7.31	8.38	9.09

Pd:

C	3.25	8.53	6.75
C	4.64	8.48	7.37
C	4.59	8.69	8.90
H	1.72	9.76	6.71
H	2.67	7.63	7.01
H	5.08	7.50	7.13
H	5.55	8.40	9.34
H	3.79	8.07	9.35
H	3.53	10.34	8.86

H	5.38	10.29	7.41
O	2.61	9.72	7.15
O	5.54	9.49	6.86
O	4.42	10.08	9.19

Rh:

C	5.24	8.38	6.54
C	5.74	7.14	7.25
C	6.13	7.37	8.72
H	5.87	10.28	6.50
H	4.32	8.74	7.03
H	4.95	6.37	7.18
H	6.18	6.40	9.24
H	5.37	7.99	9.23
H	7.39	8.83	8.42
H	7.69	6.99	7.11
O	6.28	9.40	6.69
O	6.93	6.59	6.62
O	7.44	7.94	8.82

Cu:

C	4.56	7.77	6.35
C	5.26	6.58	6.97
C	5.55	6.76	8.48
H	4.78	9.74	6.44
H	3.51	7.77	6.69
H	4.63	5.69	6.81
H	5.78	5.78	8.93
H	4.66	7.18	8.99
H	6.46	8.46	8.32
H	7.21	6.78	6.92
O	5.23	8.95	6.81
O	6.55	6.29	6.36
O	6.71	7.57	8.67

3 $CH_2OH-COH-CH_2OH$

Pt:

C	2.50	6.95	6.98
C	3.03	8.22	7.67
C	3.34	5.73	7.38
H	2.88	4.79	7.02
H	3.41	5.69	8.49
H	2.75	8.15	8.73
H	2.57	9.12	7.23
H	0.73	6.10	6.96
H	4.73	8.84	6.84
H	4.99	6.70	7.12
O	1.19	6.81	7.47
O	4.70	5.77	6.87
O	4.47	8.31	7.64

Pd:

C	2.24	7.13	6.80

C	3.08	8.31	7.29
C	2.63	5.81	7.50
H	2.08	4.96	7.05
H	2.32	5.91	8.56
H	3.01	8.37	8.39
H	2.68	9.25	6.87
H	0.33	6.70	6.80
H	4.72	7.28	7.15
H	4.28	5.11	6.67
O	0.90	7.45	7.08
O	4.04	5.57	7.52
O	4.47	8.21	6.91

Rh:

C	2.32	6.83	6.62
C	3.02	8.07	7.16
C	2.95	5.57	7.19
H	2.83	5.55	8.30
H	4.02	5.51	6.94
H	4.08	8.11	6.83
H	2.98	8.09	8.27
H	0.33	6.70	6.41
H	1.43	9.17	6.89
H	1.39	4.37	6.90
O	0.97	6.93	7.14
O	2.35	4.34	6.69
O	2.39	9.28	6.68

Cu:

C	4.33	7.75	6.39
C	5.01	8.98	6.95
C	4.94	6.49	6.97
H	4.78	6.47	8.07
H	6.02	6.43	6.76
H	6.08	9.01	6.69
H	4.91	9.01	8.05
H	2.32	7.68	6.14
H	3.46	10.12	6.63
H	3.40	5.29	6.64
O	2.96	7.83	6.89
O	4.36	5.27	6.43
O	4.42	10.20	6.43

4 $CH_2OH-CHOH-CH_2O$

Pt:

C	4.38	4.90	7.62
C	2.85	4.79	7.61
C	2.14	6.13	7.72
H	4.71	5.20	8.63
H	4.84	3.91	7.39
H	2.55	4.33	6.59
H	1.07	6.04	7.51
H	2.28	6.54	8.74

H	2.67	3.06	8.53
H	3.76	6.79	6.76
O	4.85	5.90	6.72
O	2.36	3.98	8.66
O	2.72	7.10	6.80

Pd:

C	5.03	6.43	7.76
C	3.51	6.43	7.82
C	2.87	7.82	7.64
H	5.42	6.75	8.75
H	5.40	5.41	7.56
H	1.79	7.70	7.42
H	2.95	8.35	8.61
H	4.79	8.07	6.70
H	3.21	6.05	8.82
H	2.04	5.43	6.87
O	5.57	7.33	6.78
O	3.51	8.63	6.67
O	3.02	5.46	6.85

Rh:

C	4.17	4.85	7.59
C	2.65	4.81	7.65
C	2.00	6.20	7.51
H	4.55	5.19	8.57
H	4.57	3.83	7.40
H	0.91	6.09	7.31
H	2.11	6.72	8.48
H	3.85	6.50	6.54
H	2.35	4.39	8.63
H	1.20	3.80	6.68
O	4.67	5.75	6.59
O	2.61	7.01	6.51
O	2.18	3.87	6.65

Cu:

C	3.58	5.03	7.71
C	3.87	3.75	6.94
C	2.17	5.62	7.44
H	3.64	4.77	8.78
H	4.96	5.94	6.60
H	4.90	3.42	7.18
H	3.18	2.96	7.29
H	1.77	6.07	8.37
H	1.47	4.86	7.07
H	3.10	7.12	6.63
O	4.56	6.05	7.50
O	3.74	3.89	5.52
O	2.24	6.66	6.44

5 CH_2OH-CHO-CH_2OH

Pt:

C	3.77	6.40	7.39
C	3.58	4.90	7.56
C	2.65	7.22	8.04
H	4.72	6.67	7.89
H	2.76	7.14	9.14
H	2.75	8.28	7.76
H	3.49	4.66	8.64
H	4.43	4.34	7.13
H	1.01	7.16	6.92
H	1.67	5.07	7.13
O	3.91	6.77	6.01
O	1.34	6.72	7.74
O	2.38	4.40	6.91

Pd:

C	3.79	6.35	7.40
C	3.63	4.83	7.54
C	2.64	7.12	8.06
H	4.72	6.62	7.94
H	2.69	6.96	9.15
H	2.77	8.20	7.85
H	3.60	4.57	8.61
H	4.48	4.32	7.07
H	1.12	7.08	6.77
H	1.72	4.96	7.14
O	3.94	6.75	6.04
O	1.34	6.68	7.65
O	2.44	4.32	6.90

Rh:

C	3.68	6.24	7.31
C	3.50	4.72	7.42
C	2.53	7.02	7.95
H	4.61	6.50	7.86
H	2.56	6.88	9.04
H	2.66	8.10	7.74
H	3.40	4.44	8.49
H	4.37	4.21	6.99
H	1.02	6.98	6.65
H	1.61	4.86	6.94
O	3.85	6.63	5.94
O	1.23	6.57	7.53
O	2.34	4.23	6.71

Cu:

C	3.61	6.06	6.91
C	3.42	4.56	7.14
C	2.52	6.90	7.57
H	4.58	6.34	7.37
H	2.63	6.83	8.67
H	2.63	7.96	7.27
H	3.34	4.35	8.22
H	4.28	4.00	6.73
H	0.89	6.83	6.42

H	1.52	4.66	6.72
O	3.68	6.33	5.50
O	1.19	6.43	7.28
O	2.25	4.04	6.47

6 CH_2OH-CHOH-COH

Pt:

C	4.82	8.57	6.71
C	4.75	7.44	7.72
C	3.29	7.19	8.16
H	5.29	7.80	8.61
H	2.81	8.14	8.43
H	3.33	6.54	9.05
H	2.83	5.67	6.97
H	6.13	6.32	6.82
H	4.82	10.48	6.64
O	5.27	6.19	7.29
O	2.48	6.57	7.16
O	4.82	9.72	7.34

Pd:

C	5.97	7.74	6.33
C	5.34	6.77	7.35
C	3.94	7.20	7.82
H	6.01	6.80	8.23
H	3.87	8.30	7.84
H	3.79	6.82	8.85
H	2.94	5.75	6.94
H	6.10	5.07	6.65
H	6.83	9.47	6.53
O	5.21	5.42	6.89
O	2.87	6.73	7.00
O	6.47	8.74	7.12

Rh:

C	4.80	8.15	6.45
C	4.59	6.96	7.37
C	3.13	6.86	7.82
H	5.07	10.02	6.60
H	5.20	7.14	8.29
H	5.92	5.70	6.60
H	3.06	6.15	8.66
H	2.79	7.85	8.16
H	2.32	5.47	6.65
O	4.98	9.23	7.21
O	4.95	5.70	6.80
O	2.23	6.44	6.78

Cu:

C	4.47	7.72	6.20
C	4.44	6.55	7.15
C	3.04	6.35	7.77
H	4.45	9.62	6.31

H 5.13 6.77 7.99
H 5.75 5.30 6.31
H 3.13 5.60 8.58
H 2.71 7.31 8.21
H 2.21 5.03 6.56
O 4.46 8.83 6.93
O 4.79 5.30 6.54
O 2.05 5.96 6.83

7 $CH_2OH-COH-CHOH$

Pt:
C 4.74 7.83 6.91
C 5.79 8.52 7.78
C 4.82 6.30 6.87
H 3.87 5.82 7.17
H 5.51 8.32 8.83
H 5.75 9.61 7.62
H 2.78 7.92 6.82
H 7.49 8.34 6.77
H 6.62 6.38 7.57
O 3.51 8.29 7.39
O 5.86 5.72 7.55
O 7.11 8.01 7.62

Pd:
C 3.02 6.82 6.75
C 3.35 8.20 7.29
C 4.16 5.87 6.67
H 4.33 8.53 6.90
H 3.39 8.14 8.39
H 1.95 5.35 7.36
H 1.51 8.93 7.09
H 5.12 6.28 7.03
H 4.34 3.93 6.84
O 1.88 6.33 7.38
O 2.42 9.25 6.92
O 3.80 4.65 7.25

Rh:
C 4.98 5.76 6.49
C 4.18 6.91 7.05
C 6.47 5.98 6.41
H 4.04 4.05 6.78
H 6.93 6.72 7.10
H 4.25 6.93 8.15
H 4.57 7.88 6.65
H 6.38 4.14 6.98
H 2.27 7.51 7.06
O 4.72 4.57 7.26
O 7.11 4.70 6.57
O 2.78 6.75 6.69

Cu:

C	2.53	6.83	7.45
C	2.88	8.27	7.45
C	3.40	5.83	7.16
H	3.92	8.42	7.14
H	2.74	8.71	8.46
H	1.08	5.62	7.75
H	1.12	8.85	6.71
H	4.44	6.03	6.88
H	3.40	3.96	6.65
O	1.23	6.59	7.83
O	2.07	9.04	6.52
O	2.99	4.53	7.34

8 CH_2OH-CHOH-CHO

Pt:

C	5.64	8.86	6.70
C	6.04	7.60	7.45
C	6.49	7.94	8.88
H	4.74	9.33	7.16
H	5.21	6.87	7.44
H	6.58	7.02	9.47
H	5.75	8.60	9.36
H	7.72	9.35	8.31
H	7.97	7.40	7.25
O	6.69	9.75	6.61
O	7.19	6.94	6.84
O	7.79	8.52	8.84

Pd:

C	5.54	8.21	6.60
C	4.84	7.13	7.41
C	5.50	7.05	8.80
H	5.24	9.23	6.93
H	3.77	7.36	7.48
H	4.89	6.42	9.47
H	5.57	8.06	9.25
H	7.31	6.98	8.08
H	5.81	5.45	7.18
O	6.87	8.07	6.44
O	4.95	5.80	6.85
O	6.77	6.42	8.69

Rh:

C	5.39	8.10	6.39
C	4.85	6.97	7.26
C	5.65	6.83	8.57
H	5.09	9.07	6.85
H	3.79	7.18	7.47
H	5.12	6.17	9.27
H	5.77	7.82	9.04
H	7.39	6.82	7.70
H	5.78	5.29	6.90
O	6.77	8.06	6.18

```
O     4.90  5.65  6.64
O     6.91  6.21  8.30

Cu:
C     5.01  7.76  6.11
C     4.52  6.63  7.00
C     5.36  6.58  8.30
H     4.71  8.73  6.55
H     3.46  6.80  7.24
H     4.86  5.93  9.04
H     5.46  7.59  8.72
H     7.08  6.57  7.37
H     5.51  4.98  6.69
O     6.36  7.71  5.79
O     4.63  5.32  6.40
O     6.63  5.98  8.02

9     COH-COH-CO

Pt:
C     3.22  9.73  6.42
C     3.94  8.49  6.72
C     3.10  7.22  6.59
H     2.81  11.48 7.00
H     4.74  7.63  8.23
O     3.22  10.65 7.37
O     3.03  6.44  7.52
O     4.76  8.52  7.82

Pd:
C     3.79  9.40  6.15
C     3.36  8.36  7.05
C     2.74  7.20  6.54
H     4.03  9.37  8.51
H     1.98  5.52  6.96
O     4.38  10.45 6.60
O     2.37  6.28  7.44
O     3.57  8.51  8.38

Rh:
C     3.21  9.36  6.27
C     3.86  8.15  6.70
C     3.64  6.90  6.01
H     2.91  11.17 6.76
H     4.89  7.23  7.98
O     3.28  10.36 7.18
O     4.24  5.84  6.48
O     4.57  8.15  7.86

Cu:
C     3.51  8.68  5.78
C     3.02  7.69  6.68
C     2.39  6.54  6.19
H     3.65  8.70  8.15
```

H	2.19	5.95	8.00
O	4.11	9.72	6.26
O	1.97	5.64	7.09
O	3.18	7.85	8.03

10 CO-CO-CO

Pt:

C	4.96	8.38	6.80
C	4.30	7.06	7.33
C	4.95	5.73	6.80
O	3.36	7.06	8.09
O	5.41	4.93	7.57
O	5.42	9.18	7.57

Pd:

C	3.70	9.60	6.21
C	3.40	8.38	7.09
C	3.70	7.17	6.21
O	3.09	8.38	8.26
O	4.30	6.15	6.64
O	4.29	10.61	6.64

Rh:

C	3.65	9.36	6.07
C	3.48	8.15	6.99
C	3.65	6.96	6.07
O	3.42	8.15	8.20
O	4.25	5.88	6.45
O	4.24	10.43	6.45

Cu:

C	3.49	8.90	5.82
C	3.22	7.72	6.72
C	3.49	6.53	5.82
O	3.08	7.72	7.93
O	3.88	5.41	6.23
O	3.88	10.02	6.23

11 CH_2OH-CHOH-CH_3

Pt:

C	5.86	8.49	7.79
C	6.27	7.02	7.96
C	5.45	9.17	9.09
H	6.84	6.88	8.89
H	6.90	6.71	7.10
H	5.07	5.61	7.24
H	4.25	7.65	7.12
H	6.66	9.06	7.28
H	5.10	10.19	8.90
H	6.31	9.22	9.77
H	4.64	8.61	9.59
O	4.70	8.52	6.89

O 5.07 6.23 8.00

Pd:
C 4.26 8.40 7.72
C 4.77 6.96 7.77
C 3.90 8.98 9.08
H 5.49 6.82 8.59
H 5.28 6.71 6.81
H 3.62 5.43 7.22
H 2.61 7.59 7.09
H 5.01 9.03 7.21
H 3.48 9.99 8.96
H 4.80 9.04 9.71
H 3.16 8.34 9.59
O 3.08 8.43 6.87
O 3.64 6.09 7.96

Rh:
C 5.67 8.23 7.62
C 6.39 6.88 7.66
C 5.14 8.68 8.97
H 7.09 6.84 8.51
H 6.98 6.74 6.73
H 5.56 5.18 7.08
H 4.21 7.19 6.85
H 6.34 8.99 7.18
H 4.58 9.62 8.87
H 5.98 8.84 9.66
H 4.48 7.91 9.41
O 4.55 8.11 6.69
O 5.40 5.85 7.77

Cu:
C 5.35 7.76 7.42
C 5.80 6.31 7.55
C 4.89 8.39 8.72
H 6.43 6.18 8.45
H 6.39 6.02 6.66
H 4.68 4.77 7.00
H 3.73 6.99 6.67
H 6.16 8.35 6.96
H 4.53 9.42 8.55
H 5.73 8.44 9.43
H 4.08 7.80 9.18
O 4.25 7.80 6.45
O 4.62 5.48 7.66

12 $CH_2OH-COH-CH_3$

Pt:
C 2.30 7.23 6.96
C 2.99 8.51 7.43
C 2.90 6.00 7.64
H 2.37 5.09 7.33

H	2.79	6.11	8.73
H	4.04	8.54	7.12
H	2.92	8.57	8.53
H	0.40	6.69	6.94
H	1.38	9.58	7.05
H	3.96	5.89	7.38
O	0.94	7.42	7.33
O	2.35	9.70	6.90

Pd:

C	2.27	7.16	6.84
C	2.96	8.41	7.35
C	2.85	5.90	7.45
H	2.34	5.00	7.10
H	2.74	5.95	8.56
H	4.02	8.44	7.04
H	2.91	8.41	8.46
H	0.38	6.59	6.76
H	1.39	9.55	7.04
H	3.92	5.80	7.21
O	0.90	7.34	7.14
O	2.35	9.63	6.88

Rh:

C	1.90	7.09	6.59
C	2.69	8.22	7.21
C	2.09	5.82	7.40
H	1.51	4.98	6.99
H	1.78	5.98	8.46
H	3.78	8.07	7.07
H	2.48	8.29	8.30
H	-0.08	6.77	6.61
H	1.43	9.70	6.83
H	3.15	5.52	7.39
O	0.52	7.55	6.68
O	2.37	9.52	6.64

Cu:

C	2.09	6.57	6.45
C	2.78	7.81	6.98
C	2.63	5.33	7.14
H	2.12	4.41	6.81
H	2.50	5.41	8.24
H	3.86	7.80	6.73
H	2.66	7.86	8.08
H	0.18	6.02	6.50
H	1.28	9.03	6.64
H	3.71	5.20	6.93
O	0.71	6.79	6.79
O	2.24	9.03	6.42

13 CH_3-COH-CHOH

Pt:

C	4.87	6.31	6.94
C	3.61	5.78	7.60
C	4.97	7.82	6.81
H	6.71	6.37	7.45
H	4.09	8.34	7.22
H	3.64	6.04	8.67
H	2.71	6.24	7.15
H	6.45	9.10	7.01
H	3.54	4.69	7.50
O	5.97	5.73	7.53
O	6.17	8.24	7.40

Pd:

C	4.84	6.26	6.83
C	3.57	5.69	7.42
C	4.95	7.73	6.68
H	6.69	6.30	7.31
H	4.05	8.28	7.03
H	3.56	5.89	8.50
H	2.68	6.15	6.96
H	6.43	9.02	6.81
H	3.51	4.60	7.27
O	5.95	5.64	7.36
O	6.15	8.18	7.25

Rh:

C	5.26	7.45	6.66
C	4.36	6.48	7.35
C	5.06	8.86	6.67
H	7.17	7.84	6.82
H	4.14	9.28	7.10
H	4.66	6.40	8.41
H	3.31	6.80	7.28
H	6.13	10.52	6.55
H	4.44	5.46	6.91
O	6.62	7.03	6.69
O	6.23	9.60	6.92

Cu:

C	4.56	6.92	7.34
C	3.41	6.01	7.56
C	4.47	8.23	6.98
H	6.44	7.08	7.48
H	3.51	8.75	6.89
H	3.36	5.73	8.63
H	2.46	6.49	7.27
H	5.68	9.66	6.38
H	3.53	5.08	6.98
O	5.77	6.37	7.60
O	5.63	8.99	7.10

14 CH_3-CHOH-CHO

Pt:

C	5.57	7.99	6.70
C	4.61	7.02	7.39
C	4.79	7.00	8.90
H	5.59	9.00	7.17
H	3.56	7.22	7.12
H	5.84	6.80	9.18
H	4.14	6.24	9.36
H	5.89	5.61	6.95
H	4.52	7.99	9.31
O	6.83	7.43	6.63
O	4.90	5.68	6.87

Pd:

C	6.34	9.35	6.70
C	5.38	8.35	7.34
C	5.49	8.40	8.86
H	6.21	10.40	7.02
H	4.33	8.52	7.02
H	6.53	8.20	9.17
H	4.83	7.64	9.31
H	6.70	6.99	6.93
H	5.20	9.39	9.24
O	7.58	8.91	6.61
O	5.72	7.02	6.87

Rh:

C	5.40	8.11	6.40
C	4.84	6.98	7.25
C	5.41	6.96	8.66
H	5.10	9.08	6.83
H	3.74	7.10	7.28
H	6.50	6.82	8.65
H	4.95	6.15	9.25
H	5.98	5.43	6.70
H	5.20	7.91	9.16
O	6.77	8.06	6.17
O	5.02	5.65	6.65

Cu:

C	5.41	6.69	8.18
C	4.22	6.23	7.37
C	3.02	5.89	8.24
H	5.25	7.55	8.87
H	3.96	7.07	6.69
H	3.25	5.07	8.93
H	2.17	5.60	7.61
H	5.58	4.98	6.78
H	2.71	6.77	8.83
O	6.50	6.14	8.07
O	4.62	5.10	6.58

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