Supplementary Information

1. Correlation parameters of the specific linear energy relationships described in this paper.....2

a) Metal dependent linear energy relationships.....2
b) Reaction dependent linear energy relationships **3**

2. List of structures and energies of the species considered in the current paper.....4

1. Correlation parameters of the specific linear energy relationships described in this paper

a) Metal dependent linear energy relationships

BEP.diss

CHα	*Slope*	*Intercept*
Global	0.60±0.03	0.75±0.11
Rh	1.02±0.39	0.80±0.06
Pt	1.05±0.75	0.90±0.28
Ir	0.99±0.35	0.71±0.06
Pd	0.07±0.45	0.64±0.19
Ni	0.80±0.36	0.71±0.08
Ru	0.97±0.31	0.77±0.05
Co	0.87±0.51	0.64±0.19

OH	*Slope*	*Intercept*
Global	0.11±0.03	0.83±0.07
Rh	0.48±0.59	0.87±0.11
Pt	0.18±0.14	0.80±0.07
Ir	0.21±0.18	0.73±0.05
Pd	0.45±0.33	0.89±0.08
Ni	0.44±0.63	0.98±0.26
Ru	-0.16±0.41	0.67±0.20
Co	-0.07±0.80	0.76±0.49

TSS.diss.FS/FS

CHα	*Slope*	*Intercept*
Global	0.96±0.10	0.68±0.04
Rh	1.00±0.03	0.80±0.08
Pt	0.92±0.06	0.68±0.17
Ir	0.98±0.05	0.67±0.12
Pd	1.06±0.13	1.16±0.34
Ni	1.00±0.09	0.69±0.19
Ru	1.01±0.05	0.78±0.13
Co	0.87±0.08	0.36±0.17

OH	*Slope*	*Intercept*
Global	0.97±0.26	0.87±0.08
Rh	1.03±0.06	1.04±0.21
Pt	1.08±0.15	0.56±0.39
Ir	1.06±0.10	0.86±0.31
Pd	1.11±0.11	1.17±0.31
Ni	1.01±0.12	1.23±0.39
Ru	1.04±0.11	1.35±0.38
Co	0.95±0.15	1.23±0.51

TSS.diss.IS/FS

CHα	*Slope*	*Intercept*
Global	0.94±0.12	0.58±0.05
Rh	0.98±0.09	0.64+0.22
Pt	0.87±0.12	0.30±0.30
Ir	0.95±0.14	0.56±0.34
Pd	1.01±0.06	0.64±0.14
Ni	0.97±0.18	0.74±0.41
Ru	1.00±0.17	0.78±0.43
Co	0.82±0.21	0.47±0.50

OH	*Slope*	*Intercept*
Global	0.95±0.05	0.69±0.02
Rh	0.96±0.04	0.67±0.14
Pt	0.98±0.03	0.83±0.10
Ir	0.98±0.04	0.72±0.13
Pd	0.91±0.05	0.65±0.16
Ni	0.92±0.04	0.61±0.12
Ru	1.00±0.04	0.75±0.11
Co	0.93±0.04	0.63±0.11

b) Reaction dependent linear energy relationships

BEP.diss

CHα	*Slope*	*Intercept*
Radicals	0.57±0.10	0.78±0.02
Unsaturated	0.55±0.23	0.70±0.08

OH	*Slope*	*Intercept*
Radicals	0.06±0.06	0.87±0.03
Unsaturated	0.15±0.71	0.74±0.04

TSS.diss.FS/FS

CHα	*Slope*	*Intercept*
Radicals	0.92±0.05	0.57±0.14
Unsaturated	0.69±0.32	0.40±0.41

OH	*Slope*	*Intercept*
Radicals	0.86±0.16	0.42±0.59
Unsaturated	0.89±0.61	0.86+0.71

TSS.diss.IS/FS

CHα	*Slope*	*Intercept*
Radicals	1.09±0.07	1.02±0.21
Unsaturated	0.56±0.17	0.14±0.19

OH	*Slope*	*Intercept*
Radicals	1.01±0.03	0.90±0.12
Unsaturated	0.93±0.33	0.64±0.08

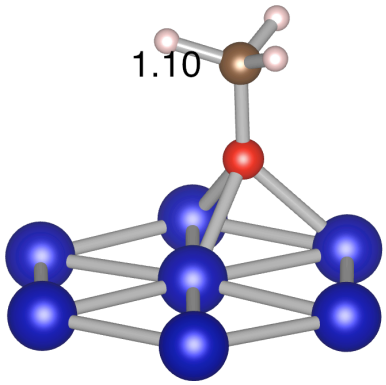
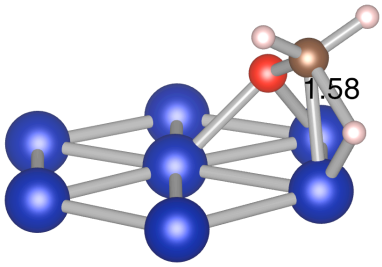
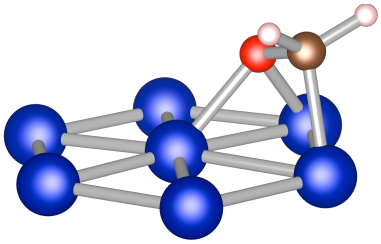
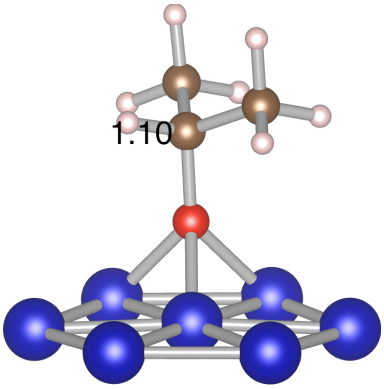
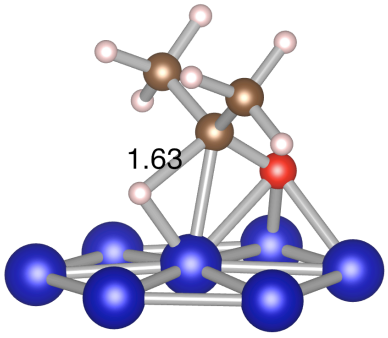
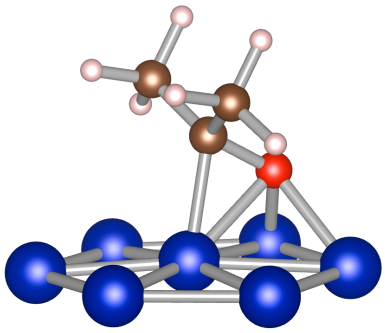
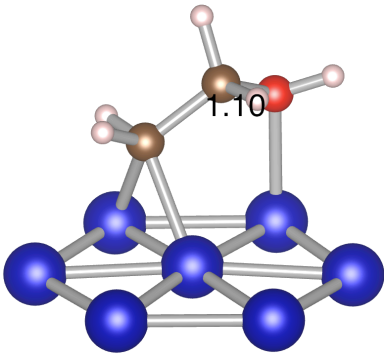
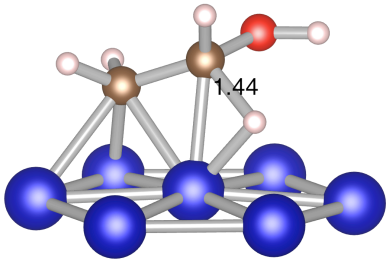
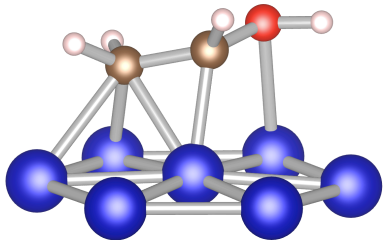
2. List of structures and energies of the species considered in the current paper

- *Energies of the various metallic slab with and without adsorbed H*

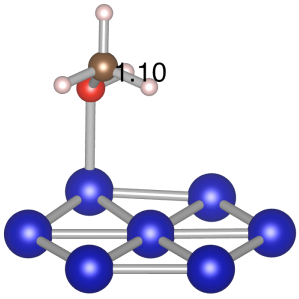
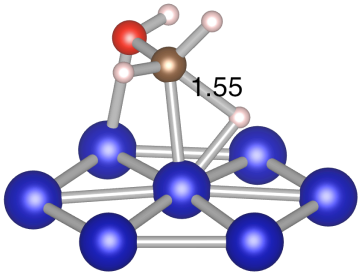
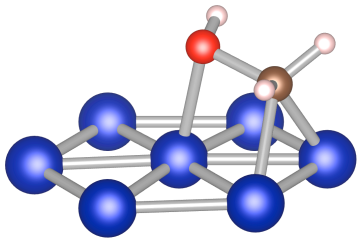
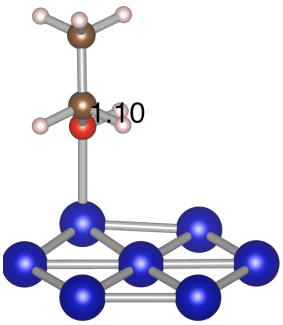
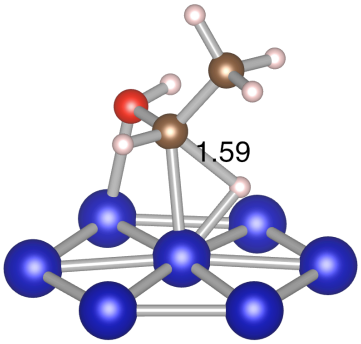
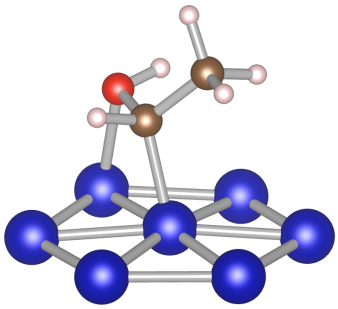
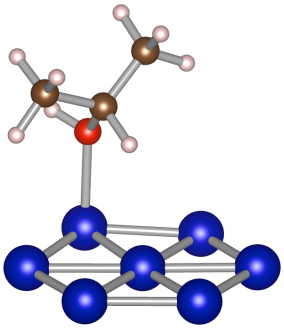
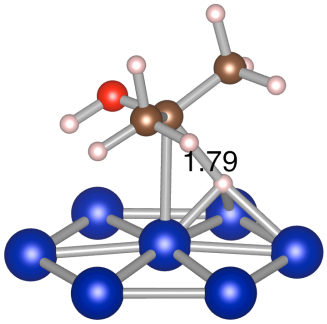
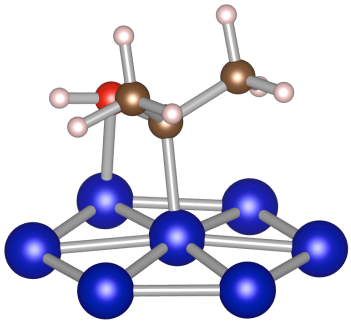
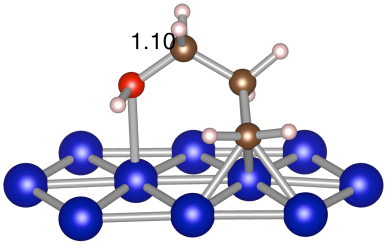
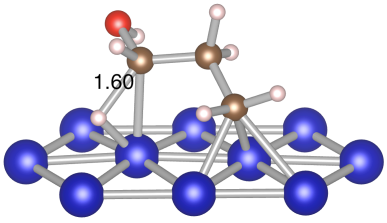
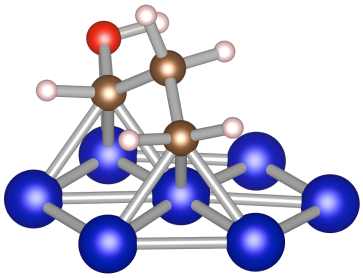
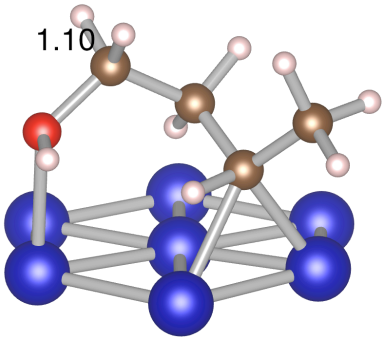
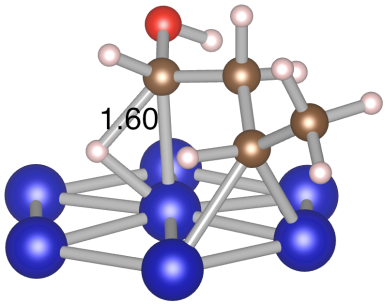
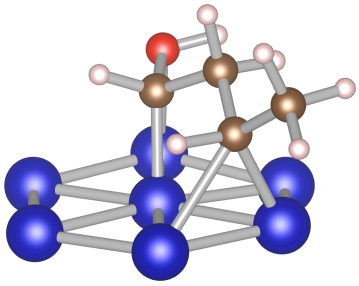
Metal	*H @ slab (hollow) (eV)*	*Bare slab (eV)*
Co	-243.67	-239.77
Ni	-189.27	-185.33
Ru	-314.93	-310.95
Rh	-249.28	-245.32
Pd	-181.35	-177.24
Ir	-304.19	-300.35
Pt	-210.68	-206.81

Monoalcohols Co

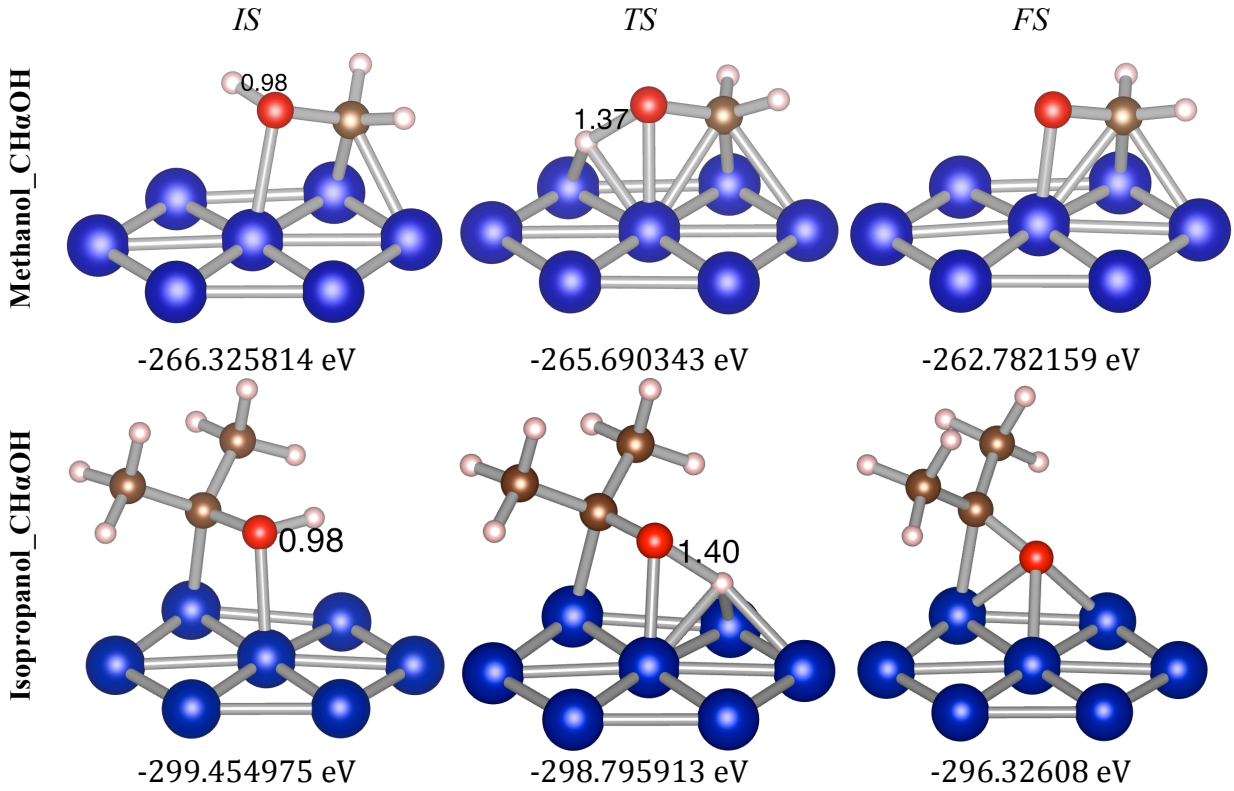
Unsaturated species formation via CHα breaking

	IS	*TS*	*FS*
Methanol_OHCHα			
	-267.171047 eV	-266.299598 eV	-262.830275 eV
Isoproanol_OHCHα			
	-300.650426 eV	-299.812393 eV	-296.32608 eV
Ethanol_CHβCHα			
	-282.910297 eV	-282.600489 eV	-279.281693 eV

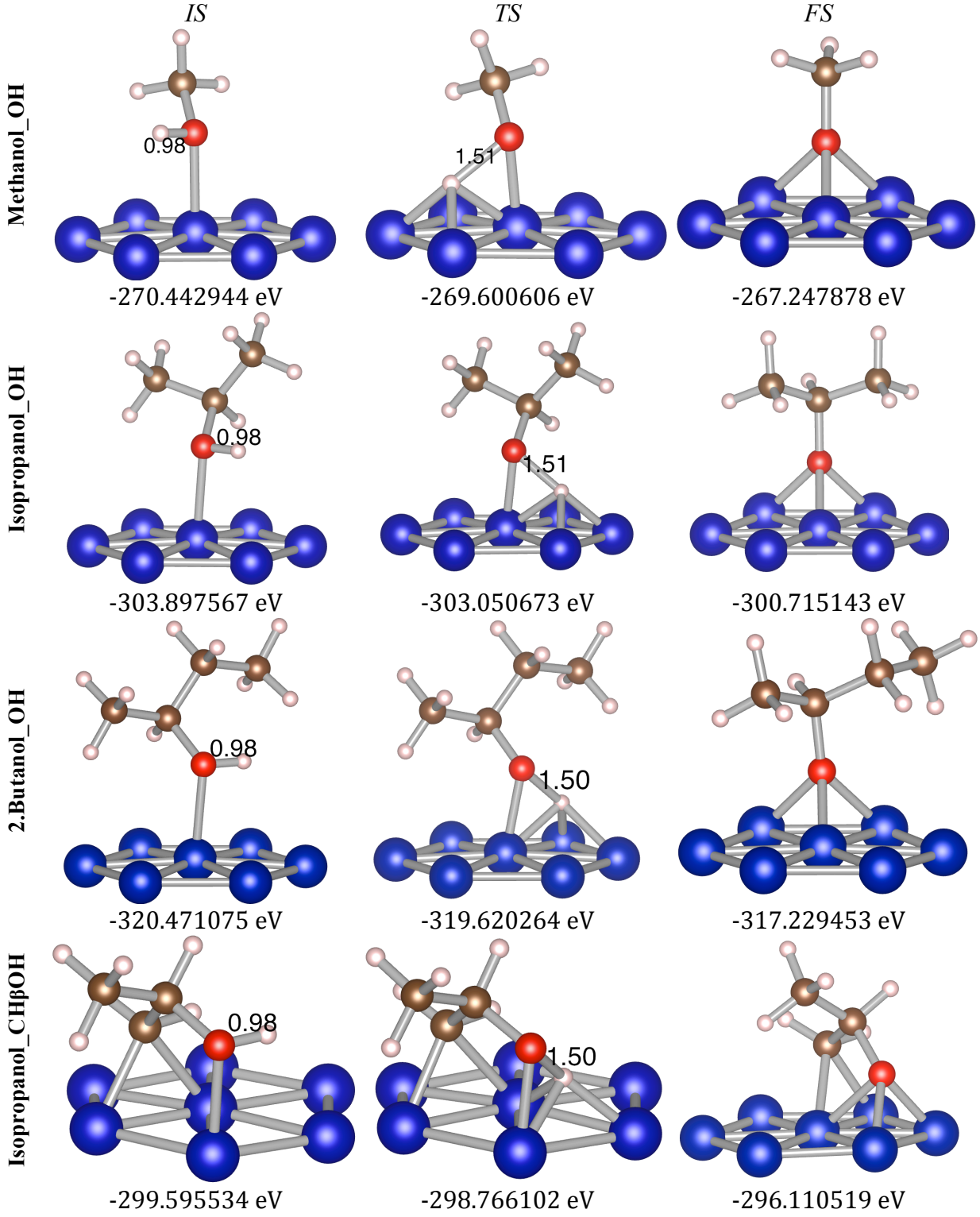
Radical formation via CHα breaking

	IS	*TS*	*FS*
Methanol_CHα	 -270.442944 eV	 -269.513627 eV	 -266.325814 eV
Ethanol_CHα	 -287.182413 eV	 -286.234611 eV	 -282.872209 eV
Isopropanol_CHα	 -303.889627 eV	 -302.708119 eV	 -299.454975 eV
Propanol_CHγCHα	 -299.419516 eV	 -298.369241 eV	 -295.242677 eV
1-butanol_CHγCHα	 -315.673737 eV	 -314.779076 eV	 -311.584882 eV

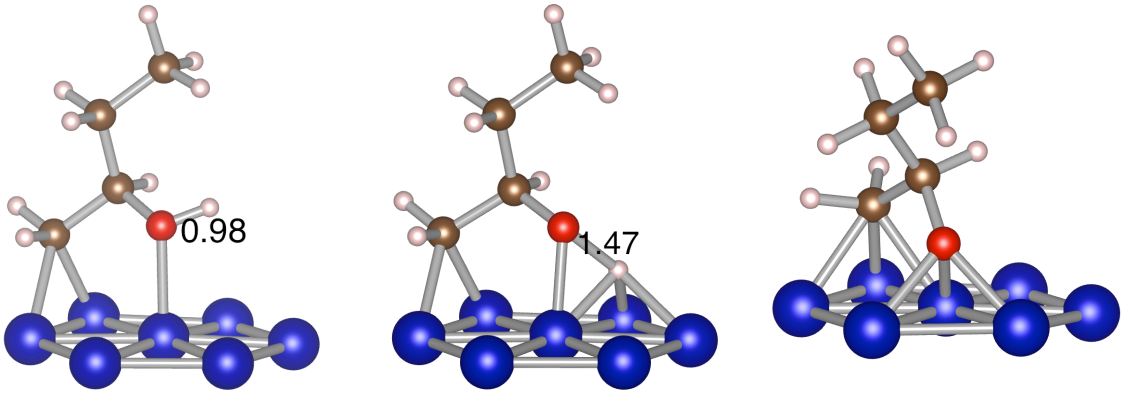
Unsaturated species formation via OH breaking



Radical formation via OH breaking



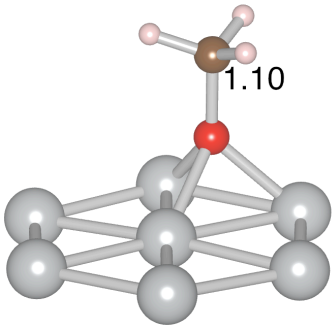
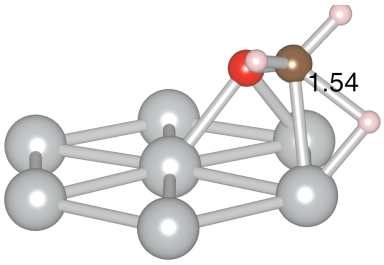
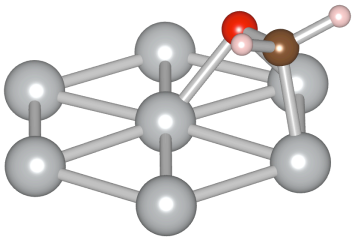
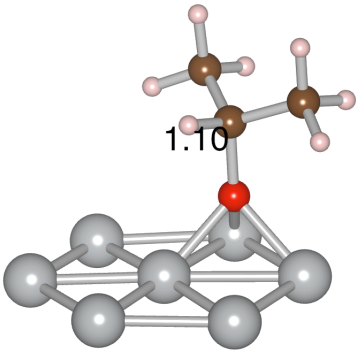
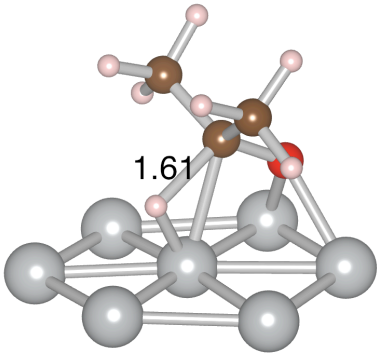
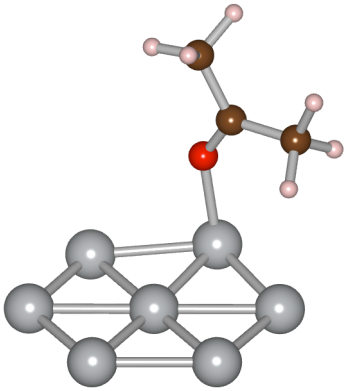
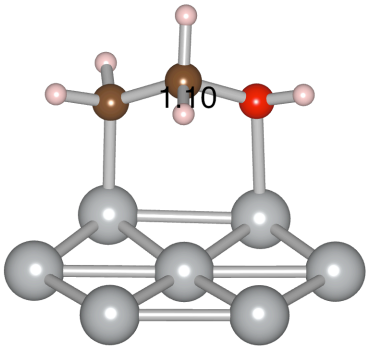
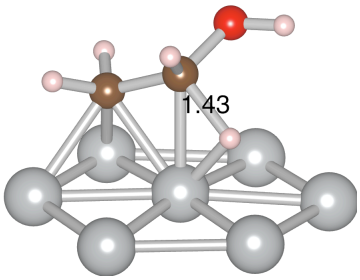
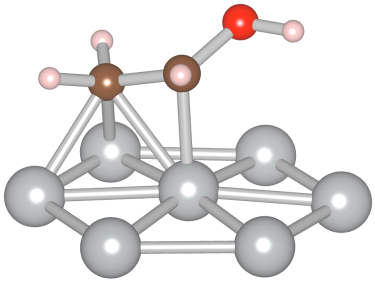
2-Butanol_CHβOH



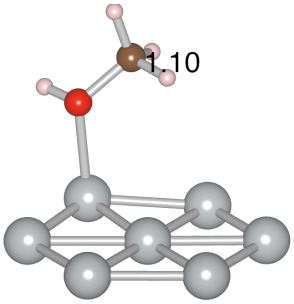
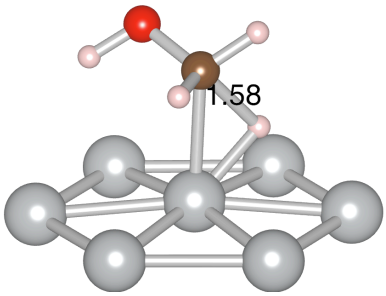
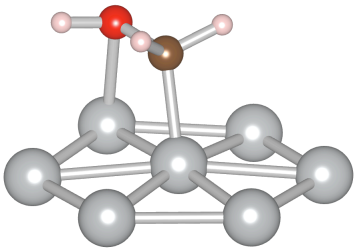
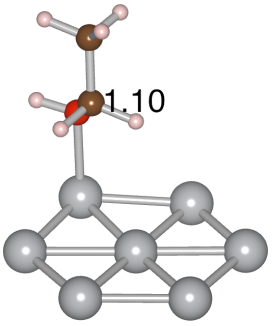
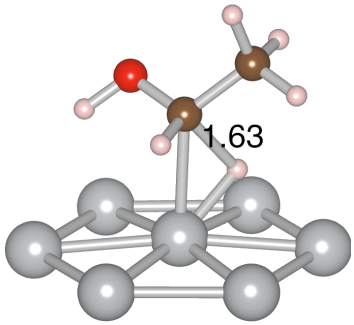
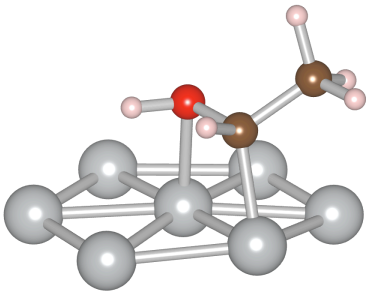
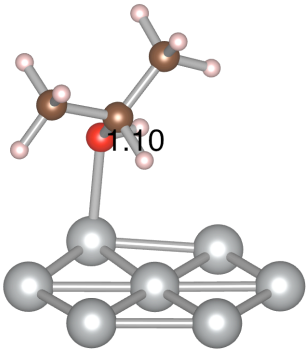
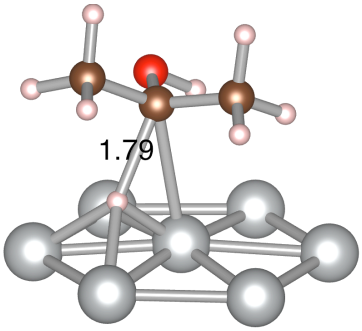
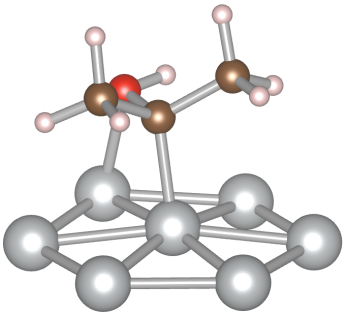
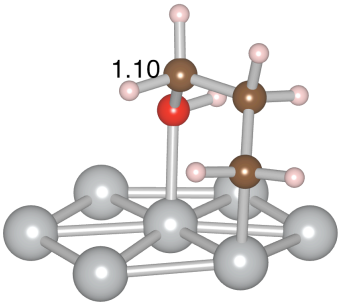
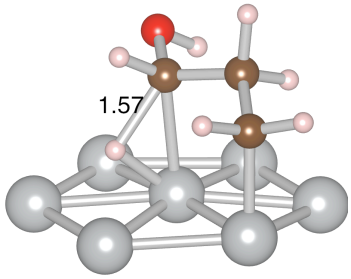
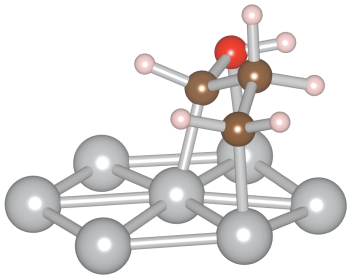
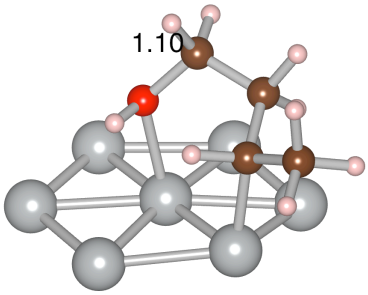
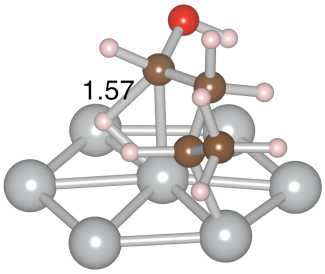
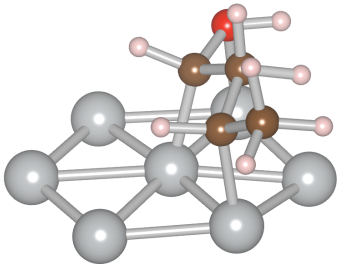
-316.210511 eV -315.413030 eV -312.826337 eV

Monoalcohols Ni

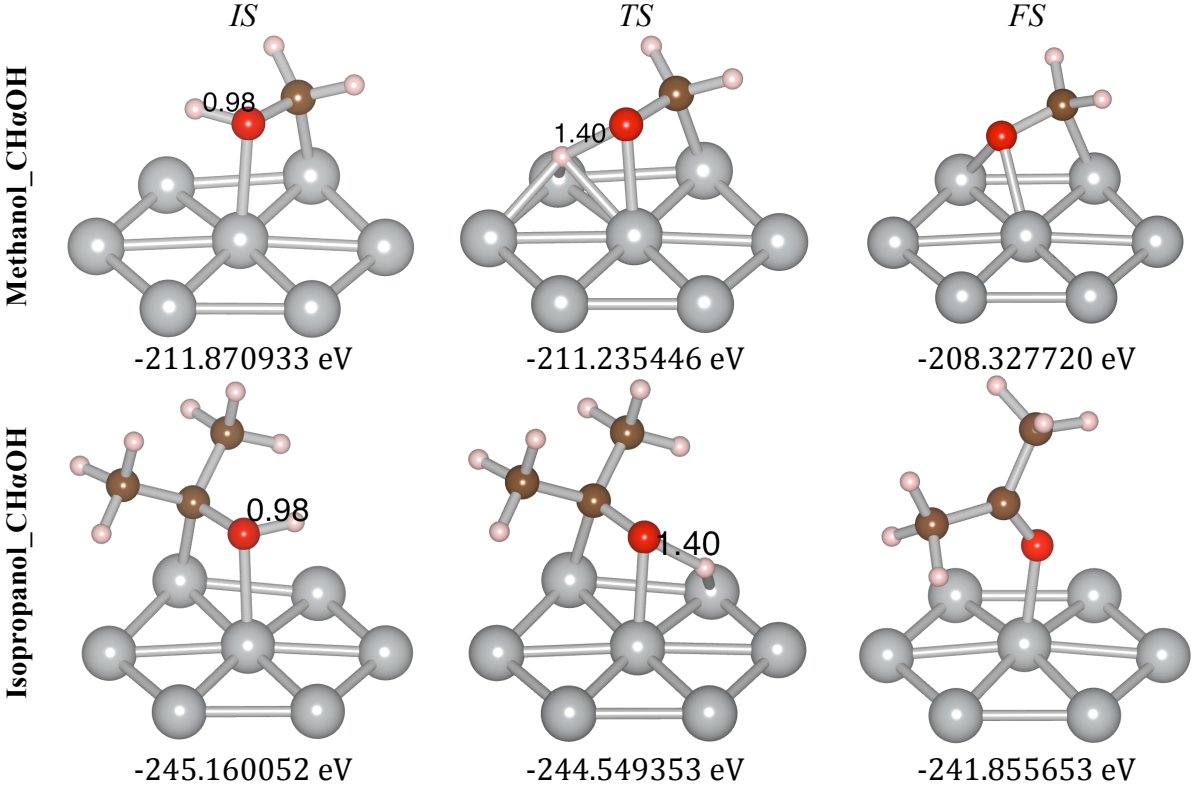
Unsaturated species formation via CHα breaking

	IS	*TS*	*FS*
Methanol_OHCHα			
	-212.448403 eV	-211.591881 eV	-208.331885 eV
Isoproanol_OHCHα			
	-246.002494 eV	-245.035938 eV	-241.855653 eV
Ethanol_CHβCHα			
	-228.468440 eV	-228.016201 eV	-224.790414 eV

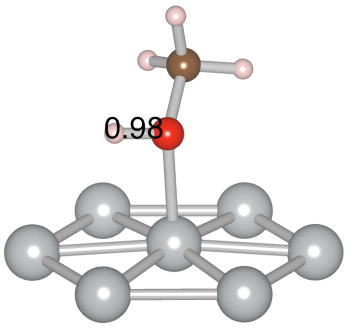
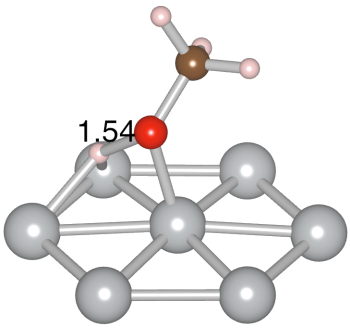
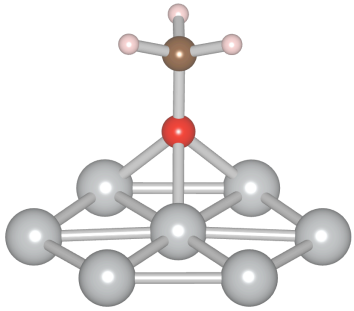
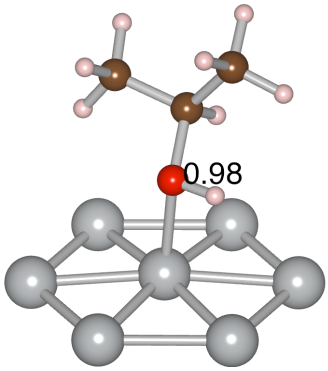
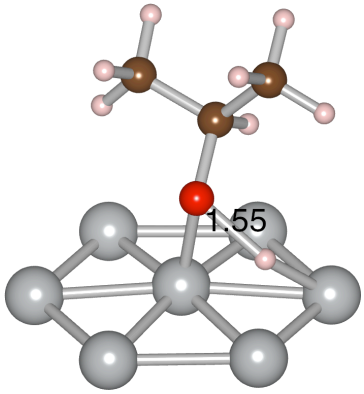
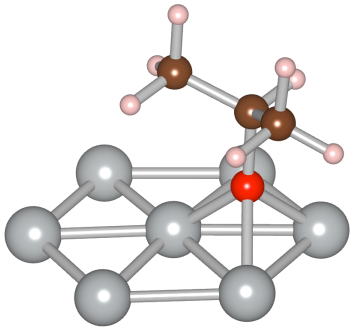
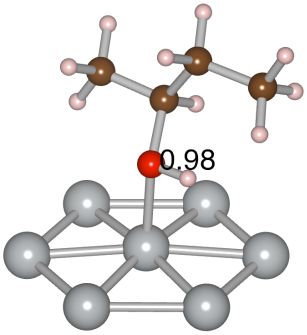
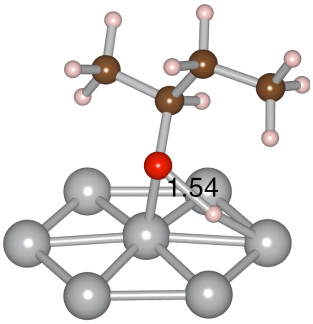
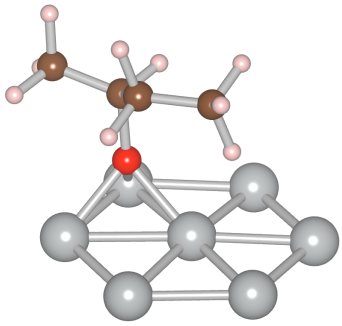
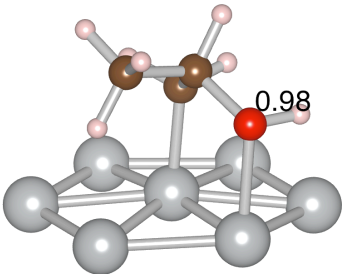
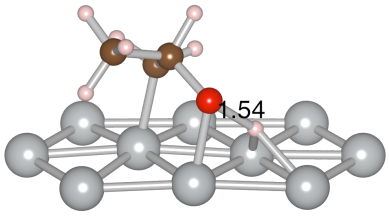
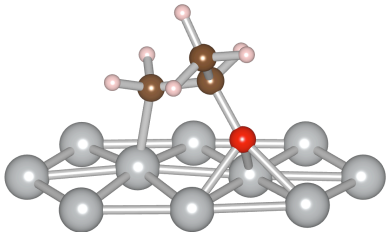
Radical formation via CHα breaking

	IS	*TS*	*FS*
Methanol_CHα	 -215.996647 eV	 -215.171742 eV	 -211.870749 eV
Ethanol_CHα	 -232.734171 eV	 -231.917758 eV	 -228.528521 eV
Isopropanol_CHα	 -249.455466 eV	 -248.426644 eV	 -245.156238 eV
Propanol_CHγCHα	 -244.881255 eV	 -244.088216 eV	 -240.802808 eV
1-butanol_CHγCHα	 -261.245373 eV	 -260.470369 eV	 -257.345895 eV

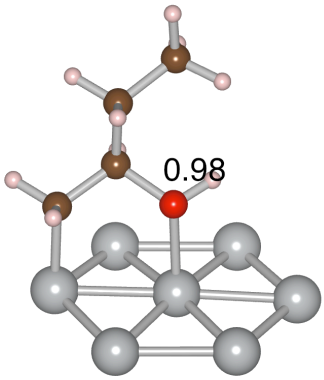
Unsaturated species formation via OH breaking



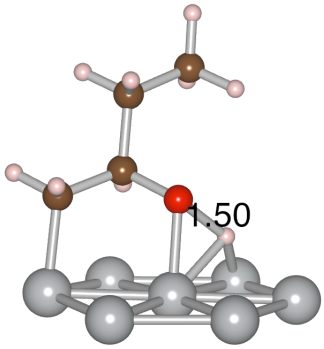
Radical formation via OH breaking

	IS	*TS*	*FS*
Methanol_OH	 -215.996647 eV	 -215.120611 eV	 -212.448403 eV
Isopropanol_OH	 -249.458336 eV	 -248.574612 eV	 -246.002494 eV
2.Butanol_OH	 -266.031658 eV	 -265.142066 eV	 -262.453984 eV
Isopropanol_CHβOH	 -245.109106 eV	 -244.241239 eV	 -241.466077 eV

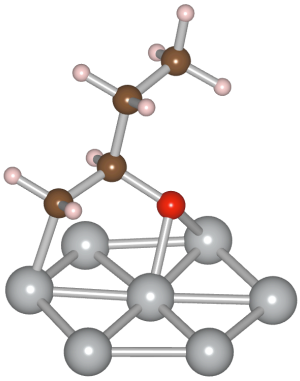
2-Butanol_CHβOH



-261.773478 eV



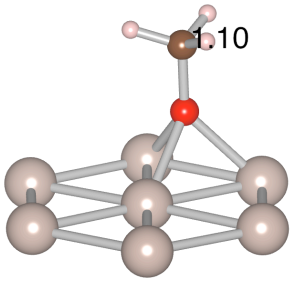
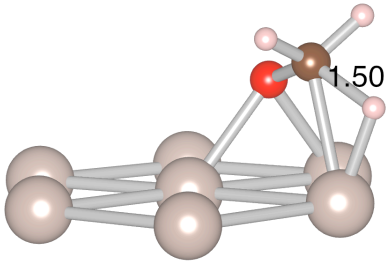
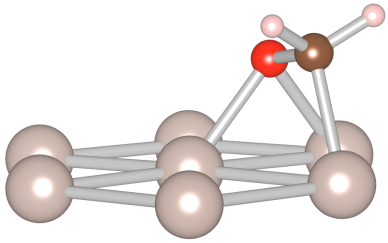
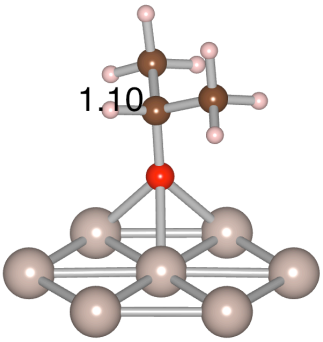
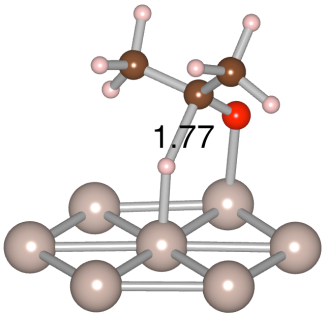
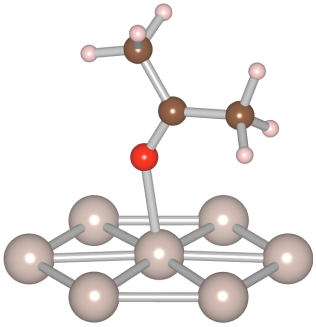
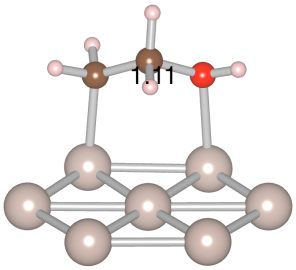
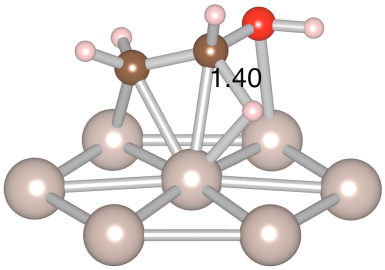
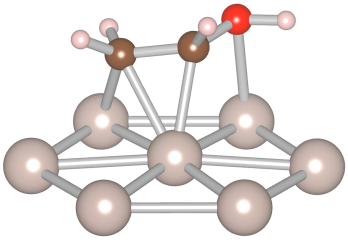
-260.857046 eV



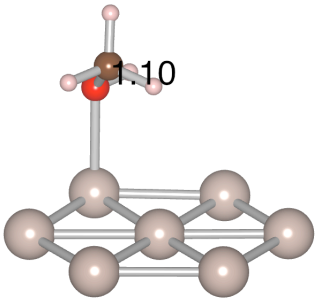
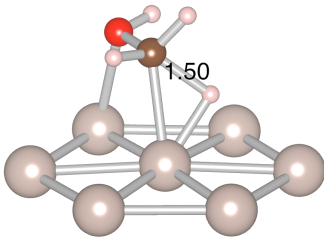
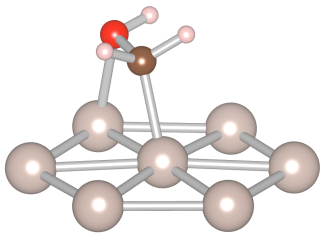
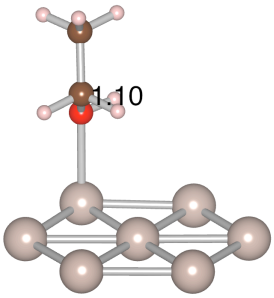
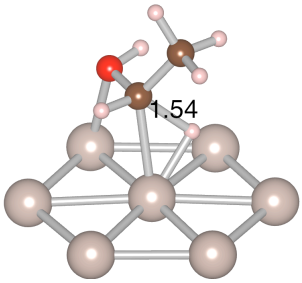
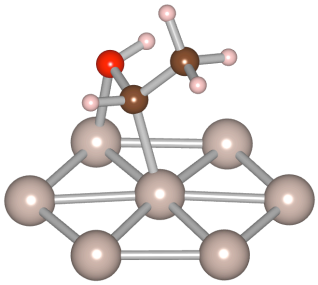
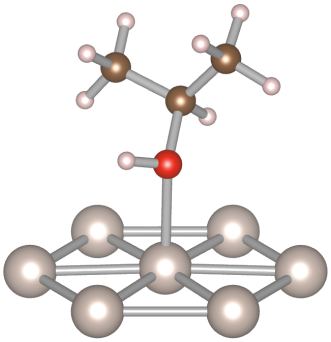
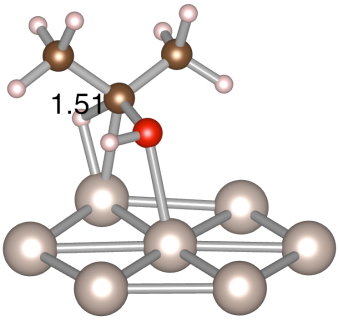
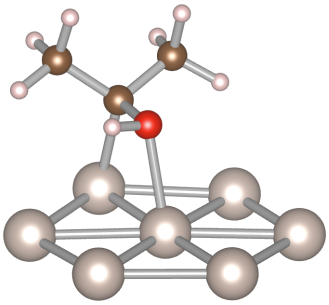
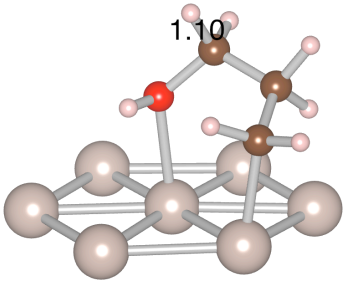
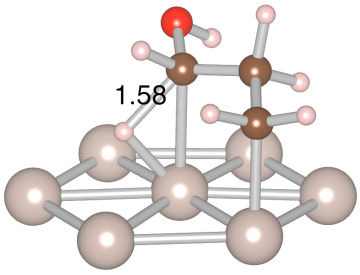
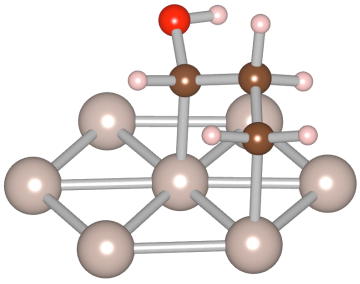
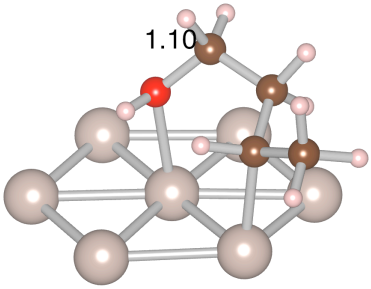
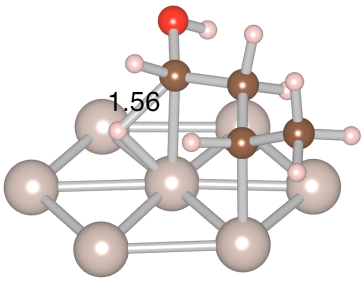
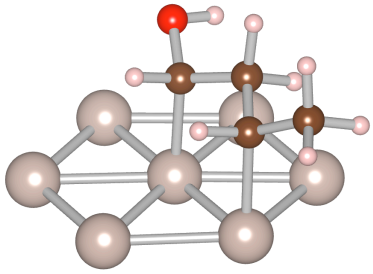
-257.865194 eV

Monoalcohols Ru

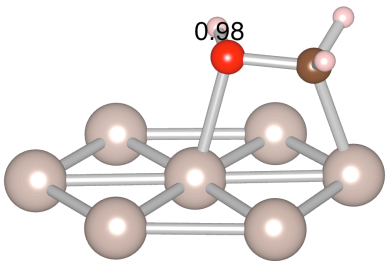
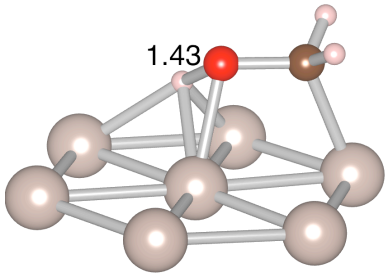
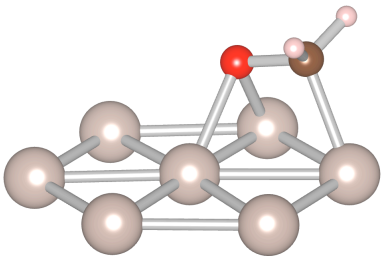
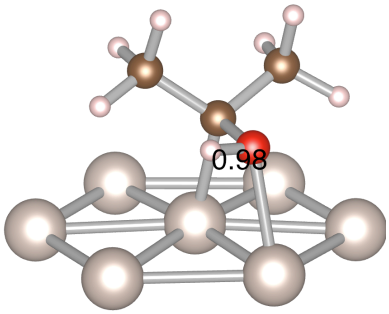
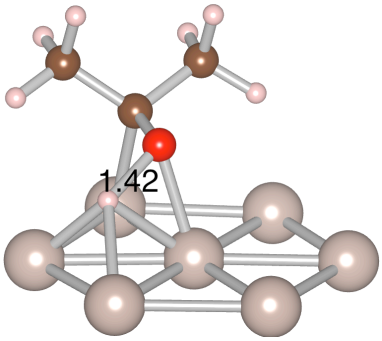
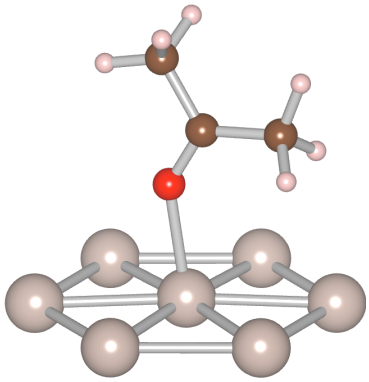
Unsaturated species formation via CHα breaking

	IS	*TS*	*FS*
Methanol_OHCHα	 -338.288992 eV	 -337.501290 eV	 -334.221456 eV
Isoproanol_OHCHα	 -371.788612 eV	 -370.794092 eV	 -367.561910 eV
Ethanol_CHβCHα	 -354.425980 eV	 -353.950776 eV	 -350.752833 eV

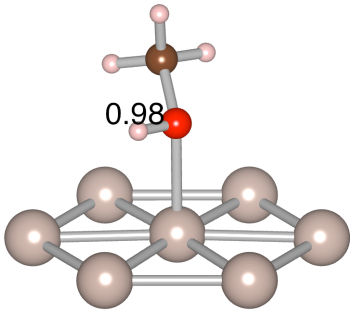
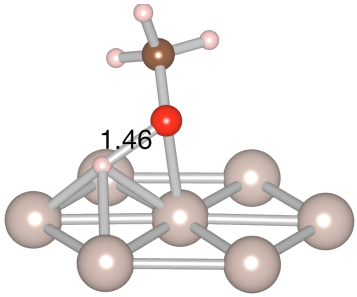
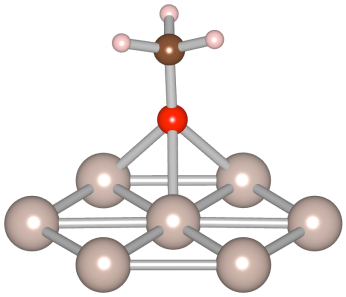
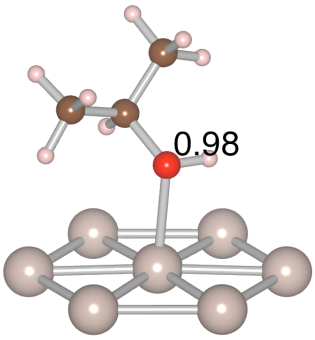
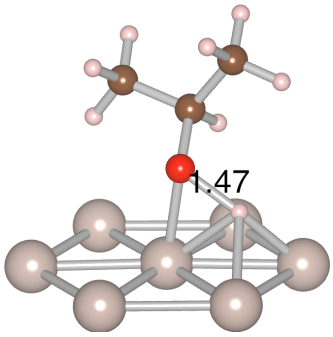
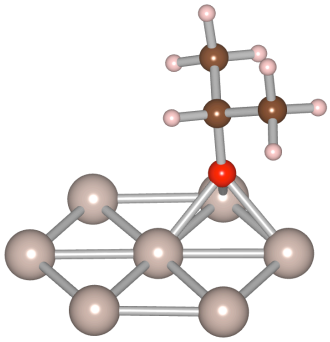
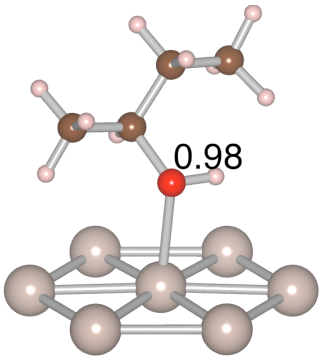
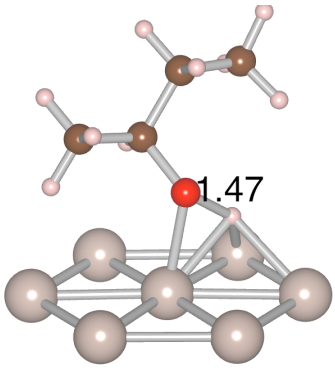
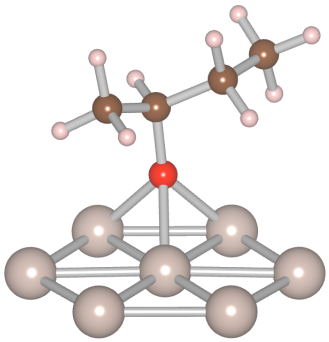
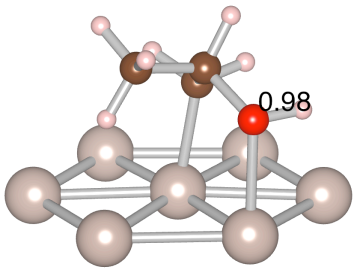
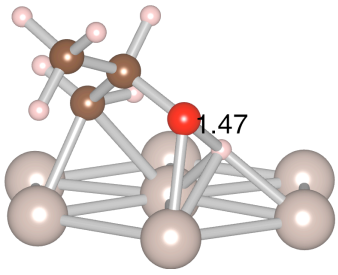
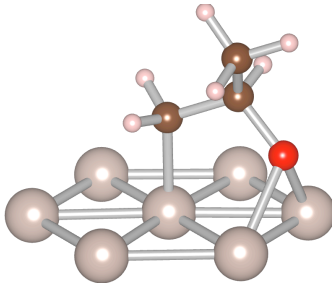
Radical formation via CHα breaking

	IS	*TS*	*FS*
Methanol_CHα	 -341.714454 eV	 -340.930442 eV	 -337.757669 eV
Ethanol_CHα	 -358.456223 eV	 -357.648503 eV	 -354.437197 eV
Isopropanol_CHα	 -375.147328 eV	 -374.151798 eV	 -371.032118 eV
Propanol_CHγCHα	 -370.724993 eV	 -369.968813 eV	 -366.711134 eV
1-butanol_CHγCHα	 -387.191453 eV	 -386.443420 eV	 -383.214885 eV

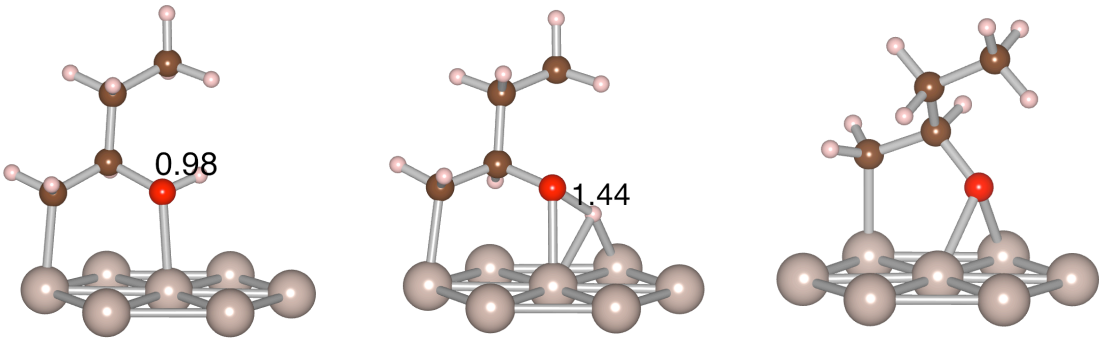
Unsaturated species formation via OH breaking

	IS	*TS*	*FS*
Methanol_CHαOH			
	-337.757669 eV	-337.016001 eV	-334.221456 eV
Isopropanol_CHαOH			
	-371.032118 eV	-370.307606 eV	-367.561910 eV

Radical formation via OH breaking

	IS	*TS*	*FS*
Methanol_OH	 -341.714454 eV	 -340.939588 eV	 -338.288992 eV
Isopropanol_OH	 -375.163441 eV	 -374.373565 eV	 -371.761665 eV
2.Butanol_OH	 -391.732618 eV	 -390.927380 eV	 -388.310684 eV
Isopropanol_CHβOH	 -371.027454 eV	 -370.358128 eV	 -367.437849 eV

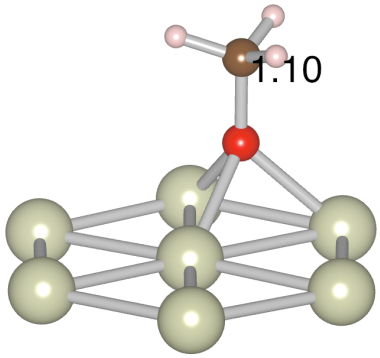
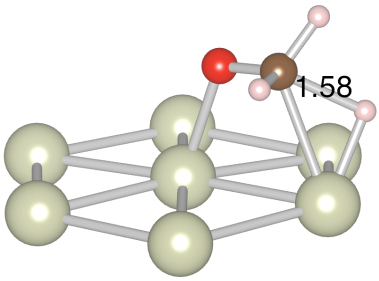
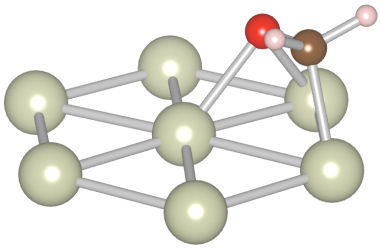
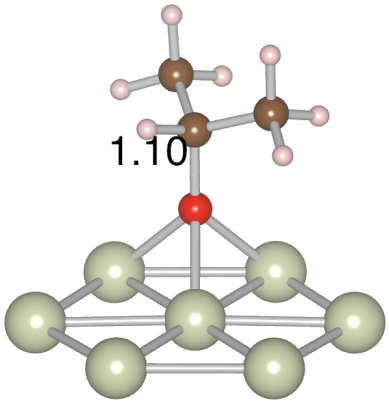
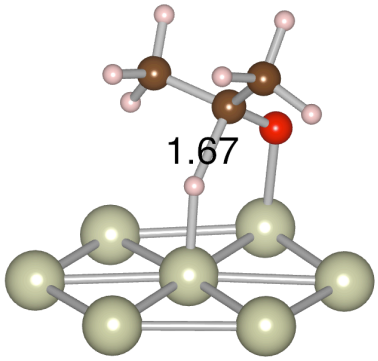
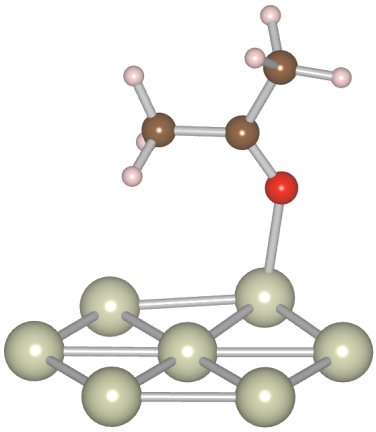
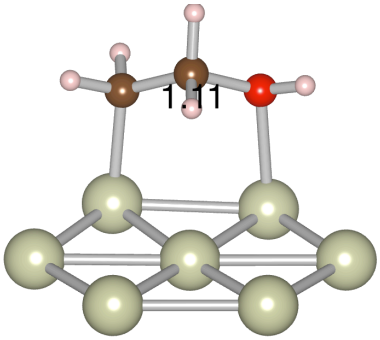
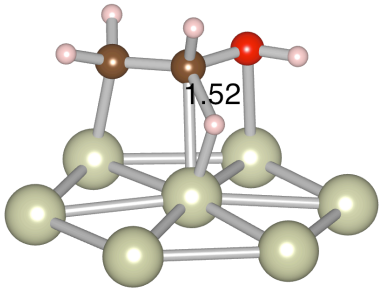
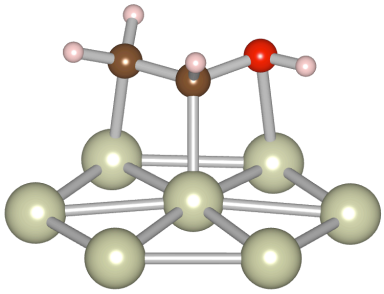
2-Butanol_CHβOH



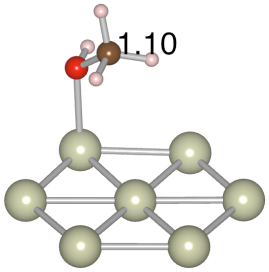
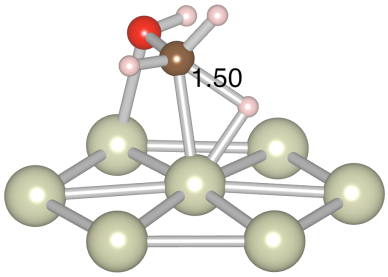
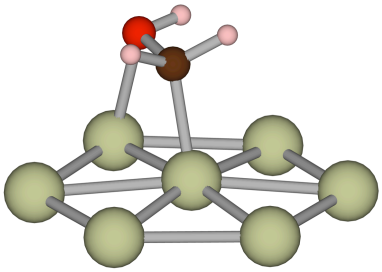
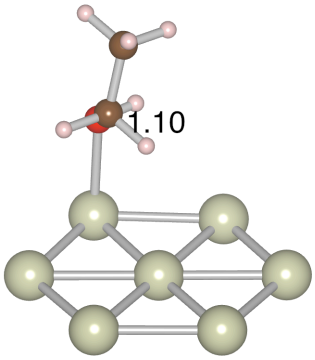
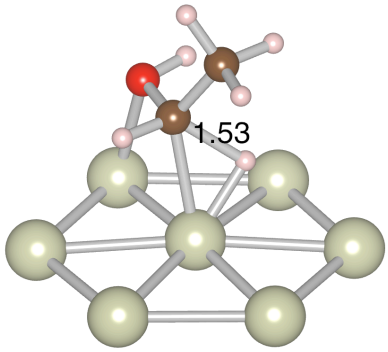
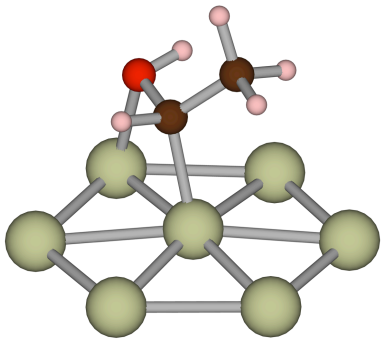
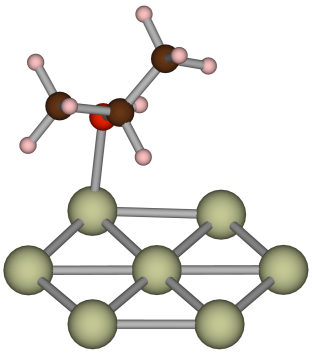
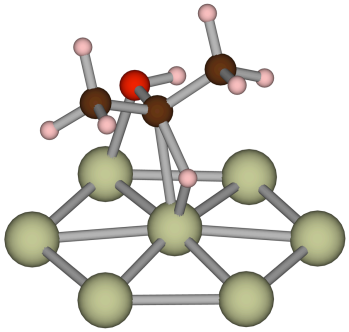
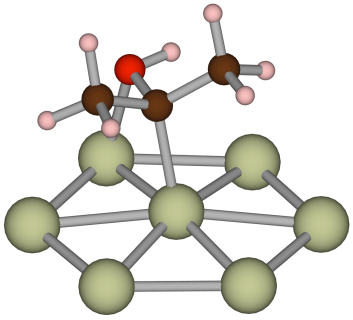
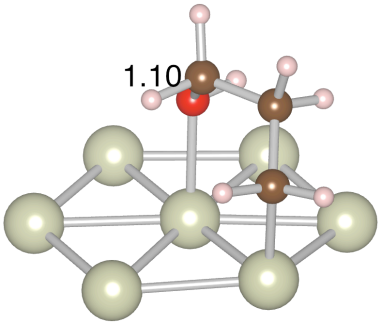
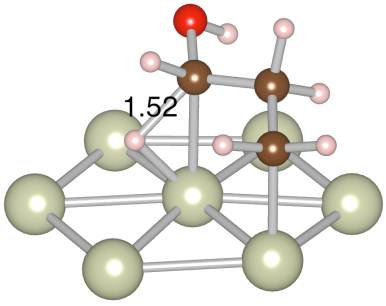
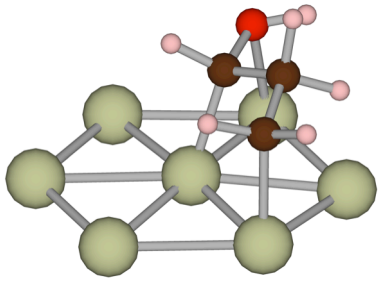
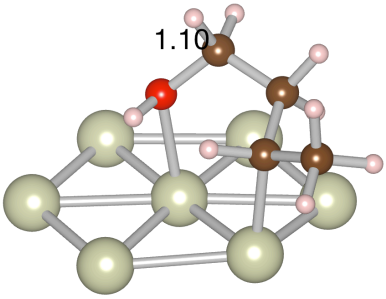
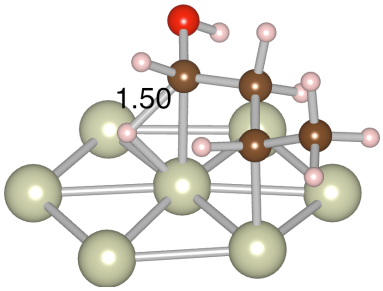
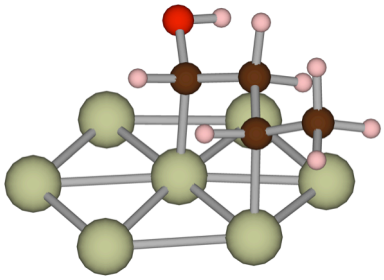
-387.729473 eV -386.965864 eV -384.010706 eV

Monoalcohols Rh

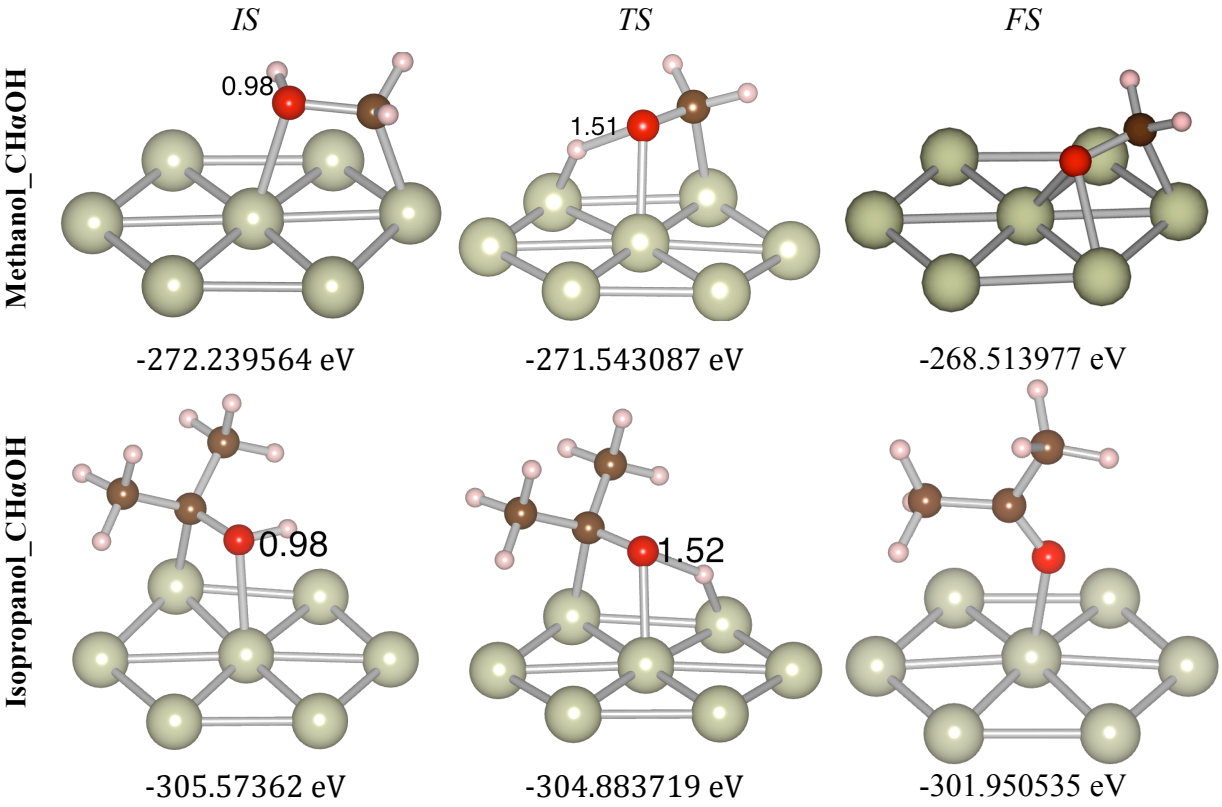
Unsaturated species formation via CHα breaking

	IS	*TS*	*FS*
Methanol_OHCHα			
	-272.30421 eV	-271.662282 eV	-268.513977 eV
Isoproanol_OHCHα			
	-305.812811 eV	-305.167493 eV	-301.950535 eV
Ethanol_CHβCHα			
	-288.829064 eV	-288.275622 eV	-285.153061 eV

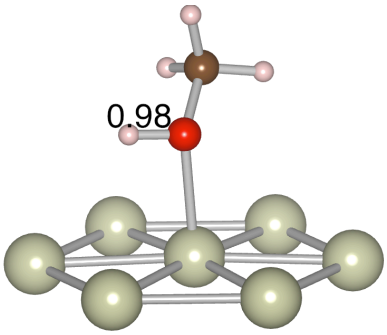
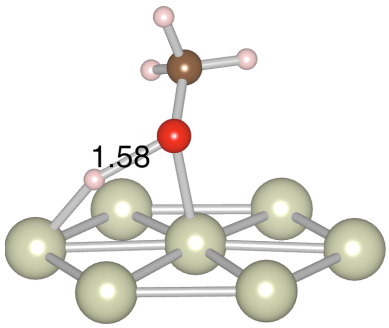
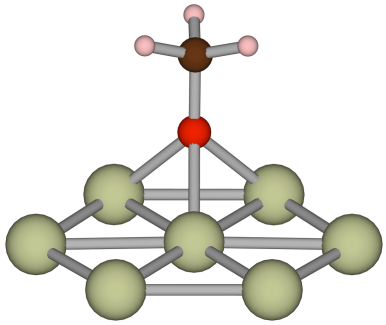
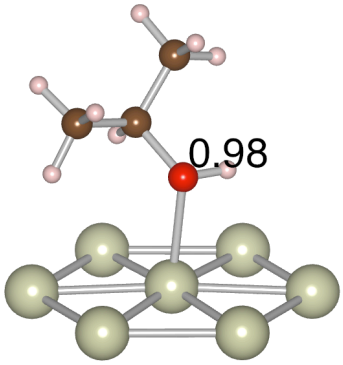
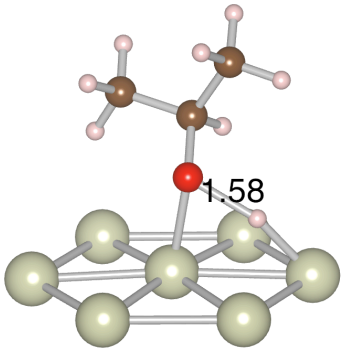
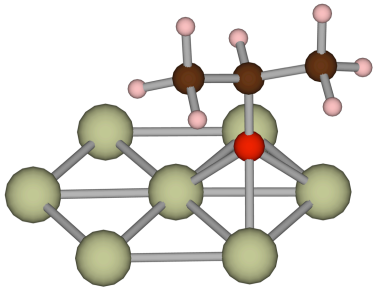
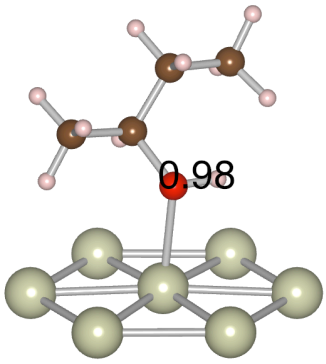
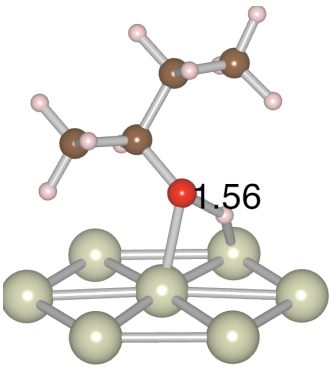
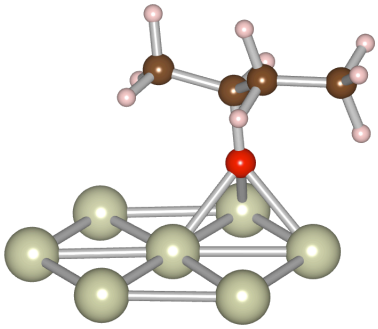
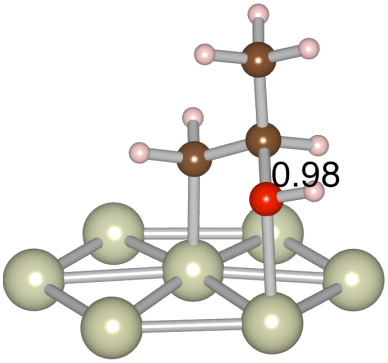
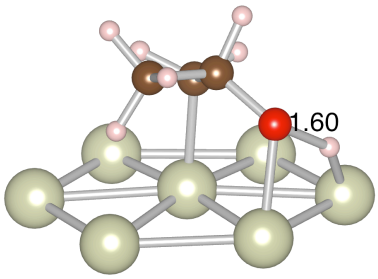
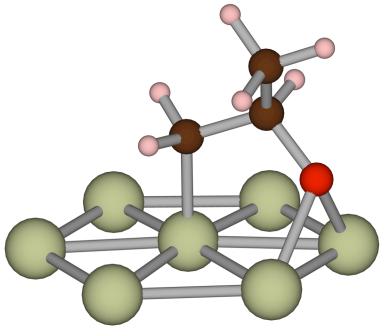
Radical formation via CHα breaking

	IS	*TS*	*FS*
Methanol_CHα	 -276.088221 eV	 -275.406309 eV	 -272.246692 eV
Ethanol_CHα	 -292.833404 eV	 -292.108156 eV	 -288.941227 eV
Isopropanol_CHα	 -309.555802 eV	 -308.667107 eV	 -305.566593 eV
Propanol_CHγCHα	 -305.258345 eV	 -304.590306 eV	 -301.426408 eV
1-butanol_CHγCHα	 -321.755037 eV	 -321.123101 eV	 -317.943754 eV

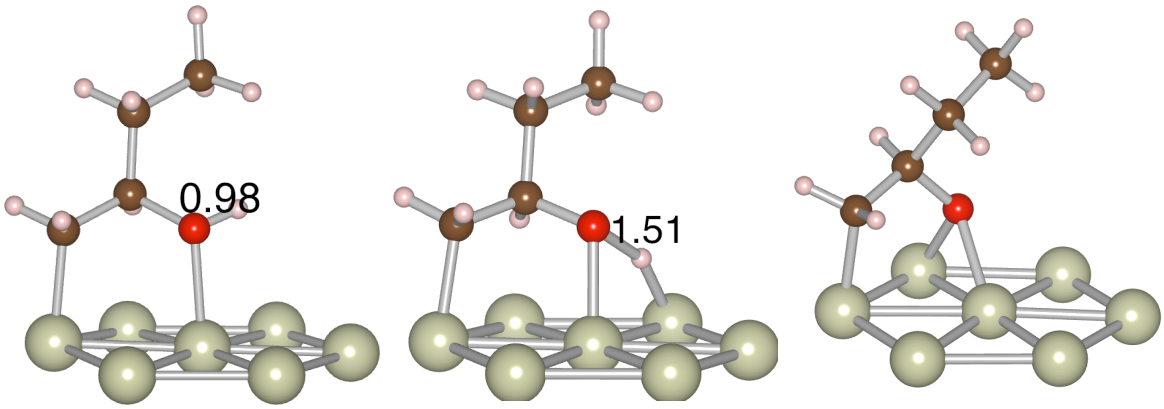
Unsaturated species formation via OH breaking



Radical formation via OH breaking

	IS	*TS*	*FS*
Methanol_OH	 -276.088221 eV	 -275.267718 eV	 -272.30421 eV
Isopropanol_OH	 -309.559483 eV	 -308.722177 eV	 -305.812811 eV
2.Butanol_OH	 -326.131711 eV	 -325.284134 eV	 -322.231639
Isopropanol_CHβOH	 -305.546327 eV	 -304.614375 eV	 -301.608649 eV

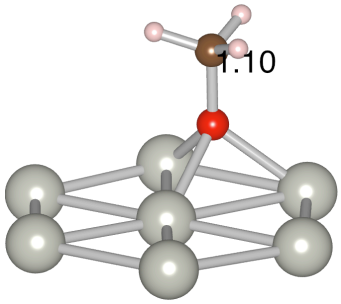
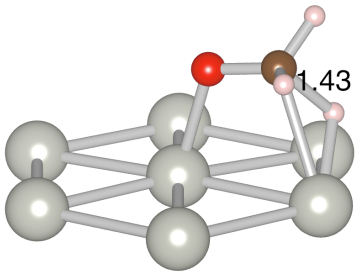
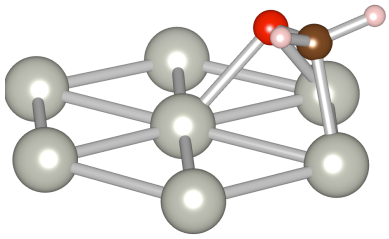
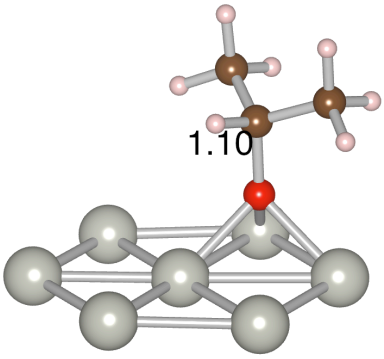
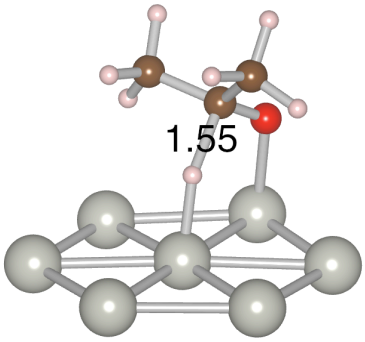
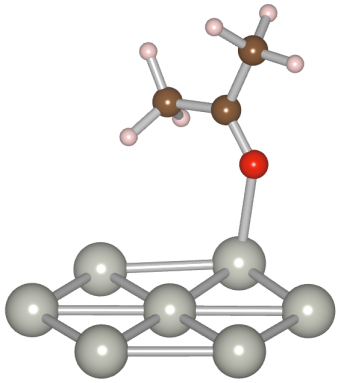
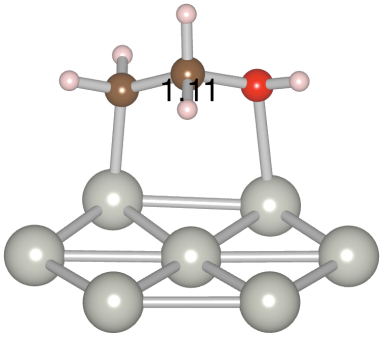
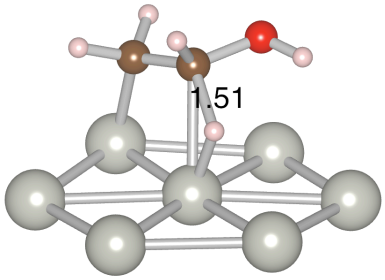
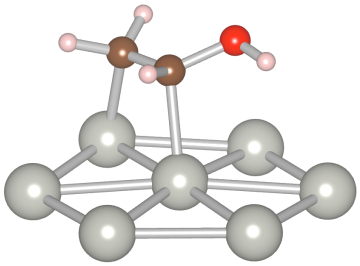
2-Butanol_CHβOH



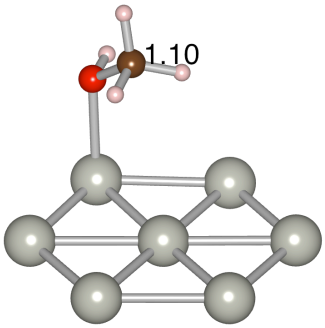
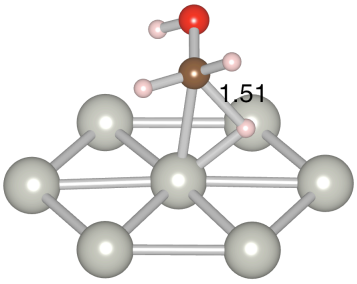
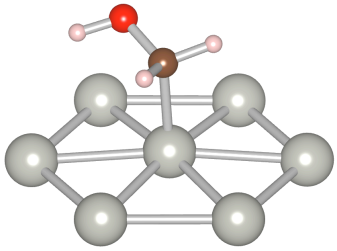
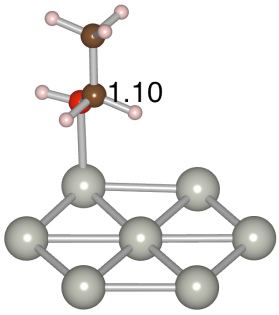
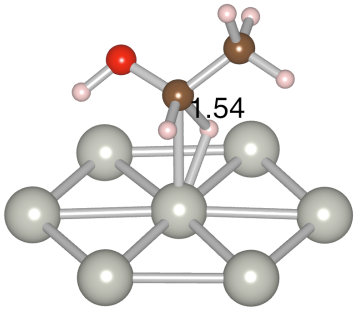
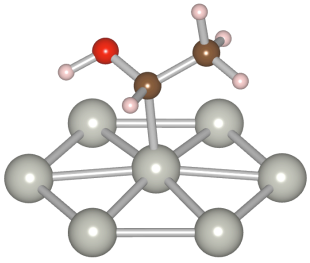
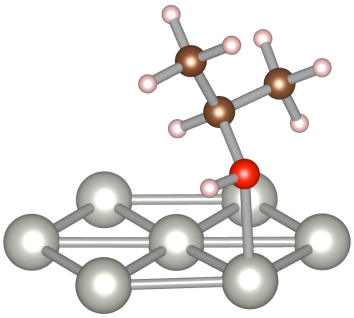
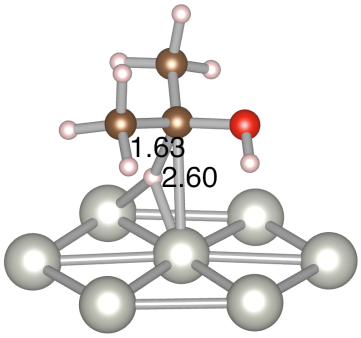
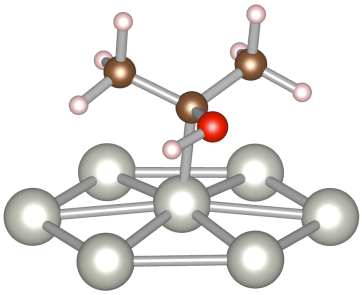
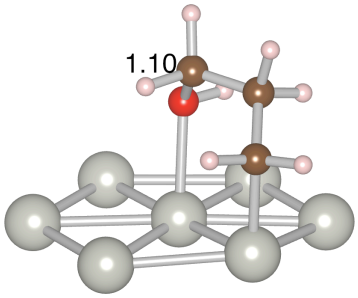
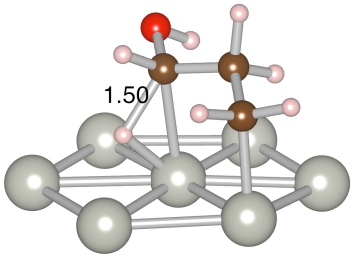
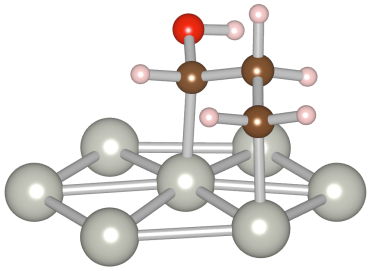
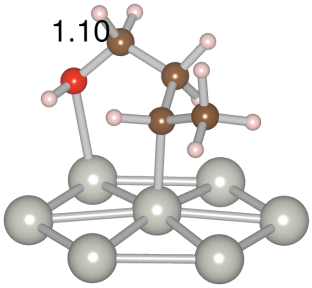
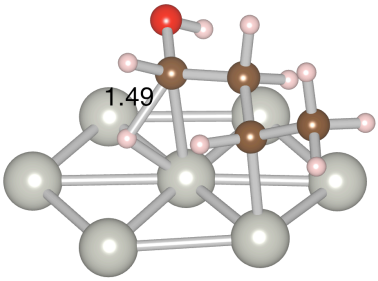
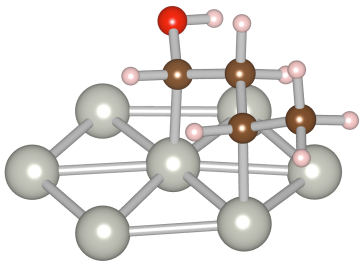
-322.134 eV -321.359922 eV -318.18462 eV

Monoalcohols Pd

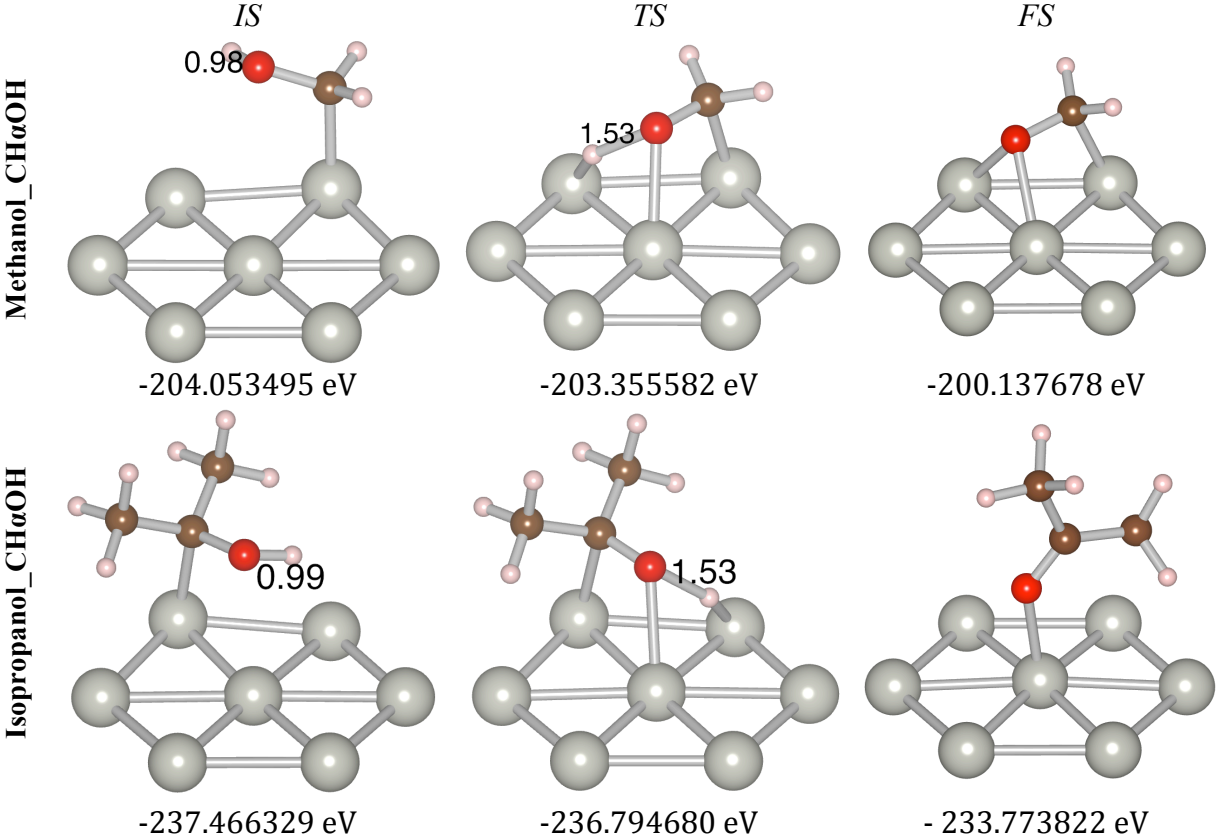
Unsaturated species formation via CHα breaking

	IS	*TS*	*FS*
Methanol_OHCHα			
	-203.853375 eV	-203.227149 eV	-200.137678 eV
Isoproanol_OHCHα			
	-237.326776 eV	-236.724203 eV	- 233.773822 eV
Ethanol_CHβCHα			
	-220.540843 eV	-219.890862 eV	-217.090980 eV

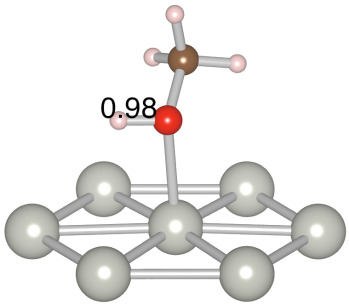
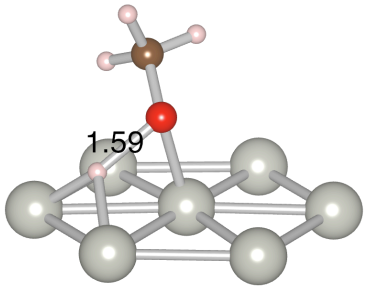
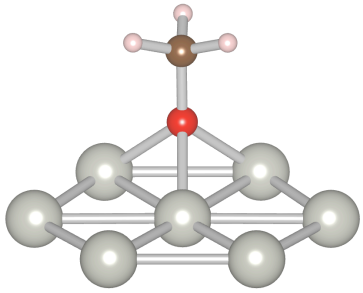
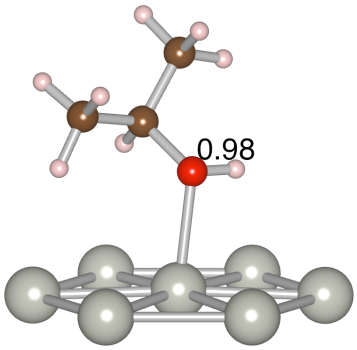
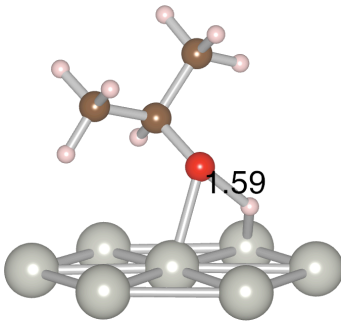
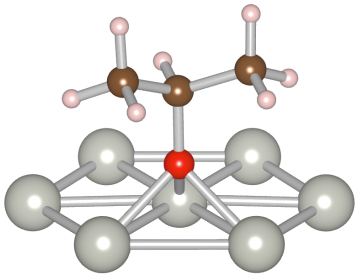
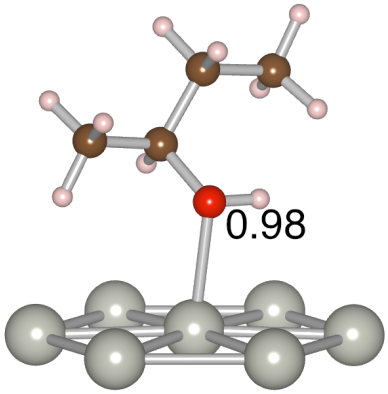
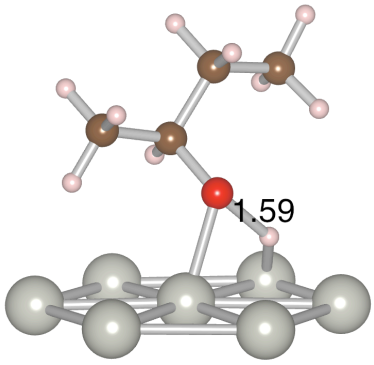
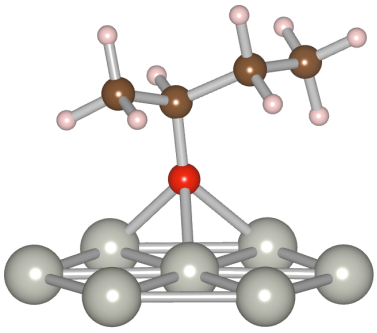
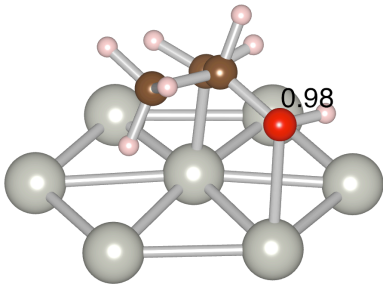
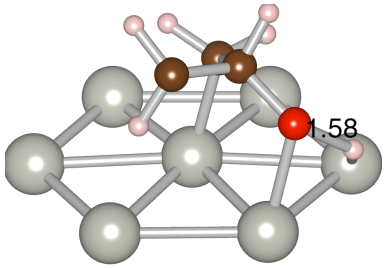
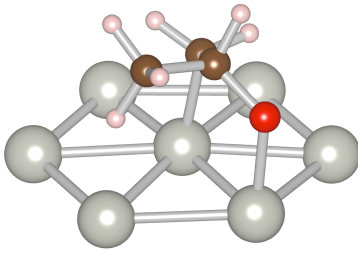
Radical formation via CHα breaking

	IS	*TS*	*FS*
Methanol_CHα	 -207.904837 eV	 -207.346007 eV	 -204.064301 eV
Ethanol_CHα	 -224.642341 eV	 -224.104511 eV	 -220.829129 eV
Isopropanol_CHα	 -241.392006 eV	 -240.628223 eV	 -237.469869 eV
Propanol_CHγCHα	 -237.056809 eV	 -236.437140 eV	 -233.314503 eV
1-butanol_CHγCHα	 -253.588323 eV	 -253.022599 eV	 -249.921308 eV

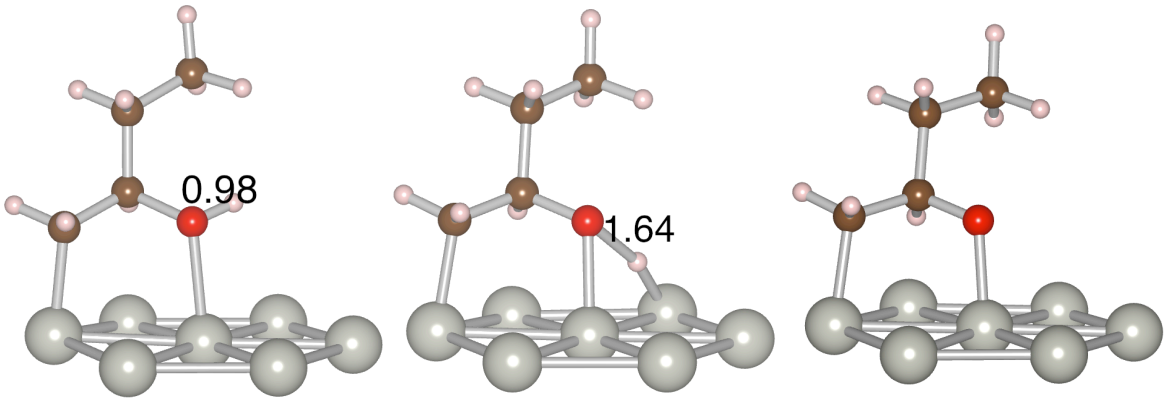
Unsaturated species formation via OH breaking



Radical formation via OH breaking

	IS	*TS*	*FS*
Methanol_OH	 -207.904837 eV	 -206.955860 eV	 -203.853272 eV
Isopropanol_OH	 -241.393403 eV	 -240.419159 eV	 -237.326776 eV
2.Butanol_OH	 -257.965407 eV	 -256.986880 eV	 -253.745430 eV
Isopropanol_CHβOH	 -237.221123 eV	 -236.235583 eV	 -232.767382 eV

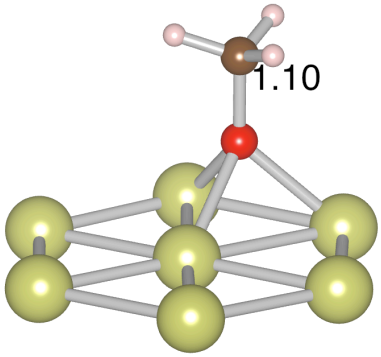
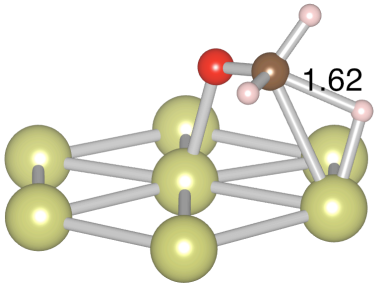
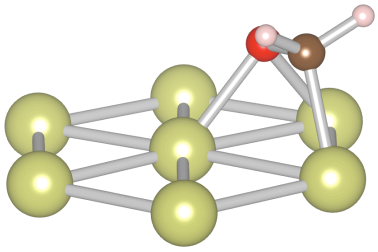
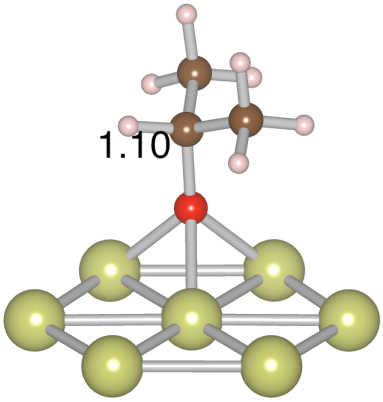
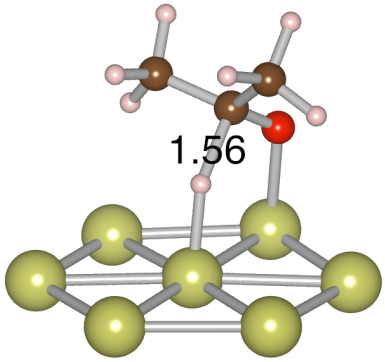
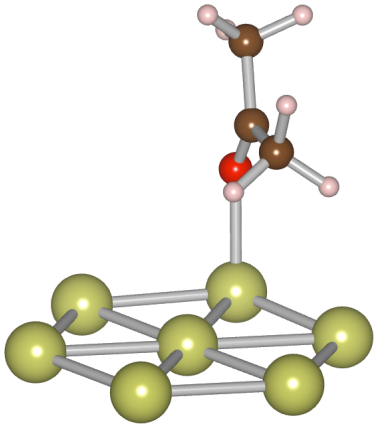
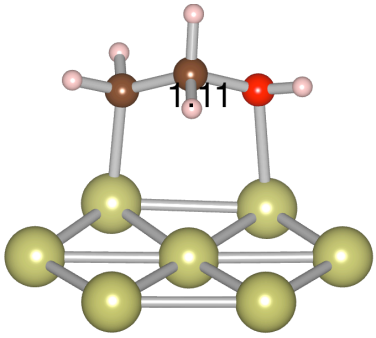
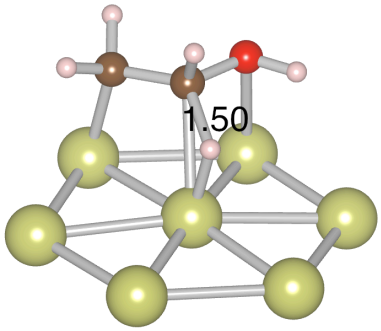
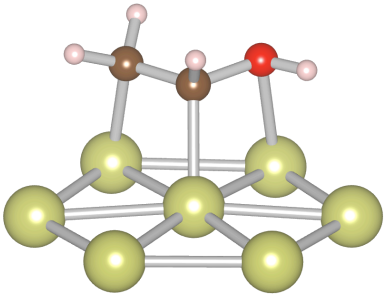
2-Butanol_CHβOH



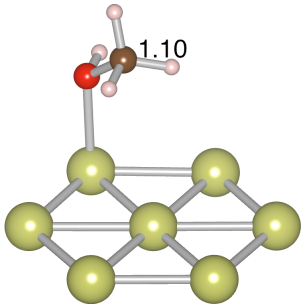
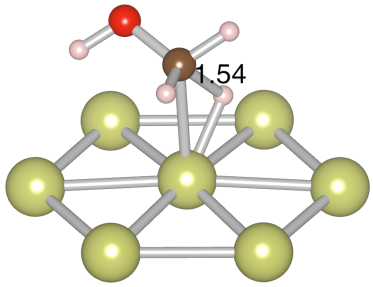
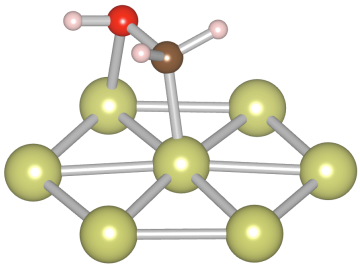
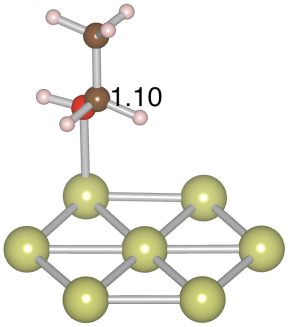
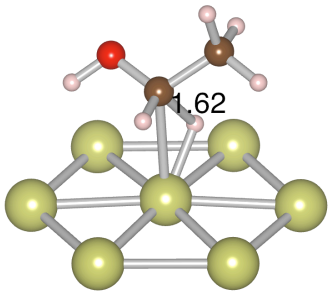
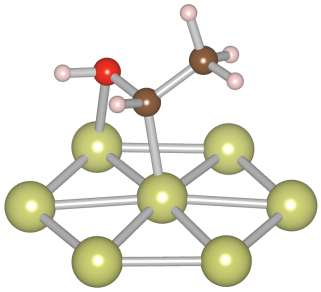
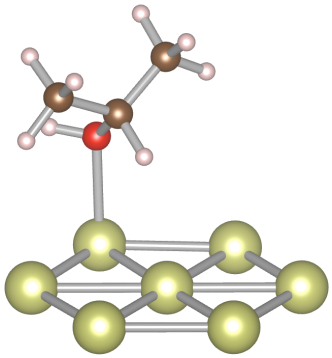
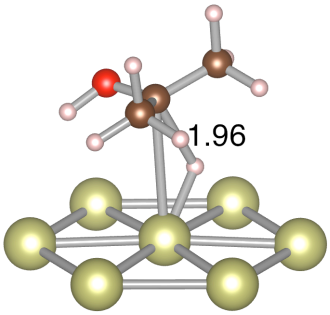
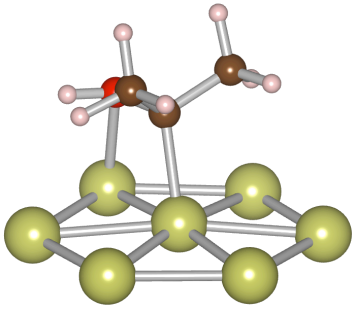
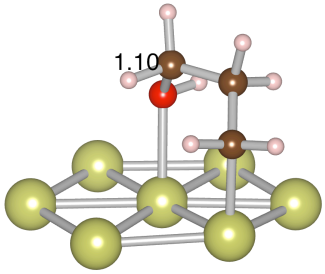
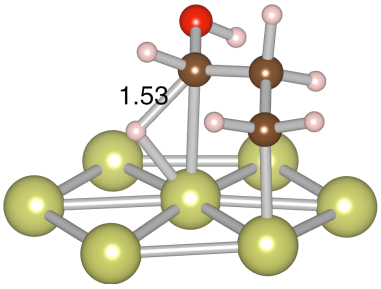
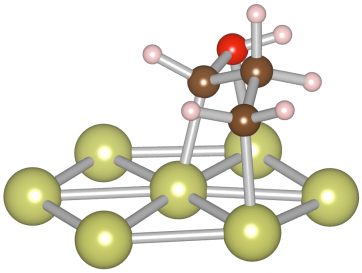
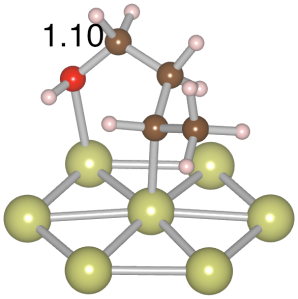
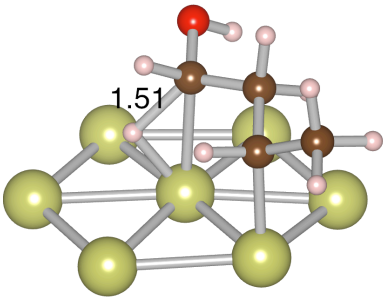
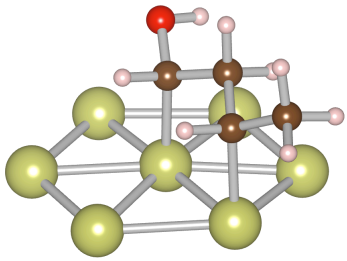
-253.839903 eV -252.851738 eV -249.464247 eV

Monoalcohols Ir

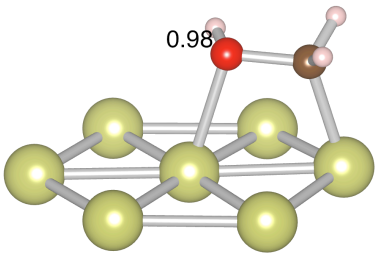
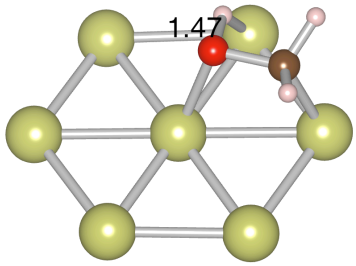
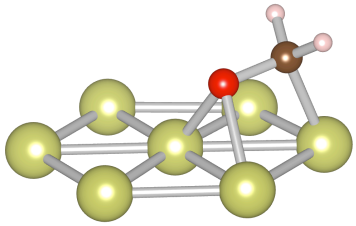
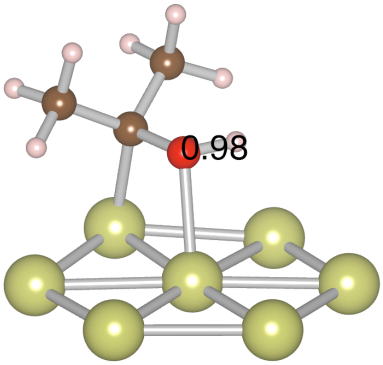
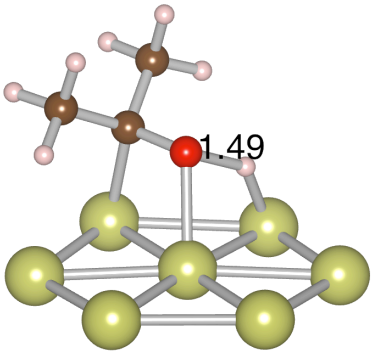
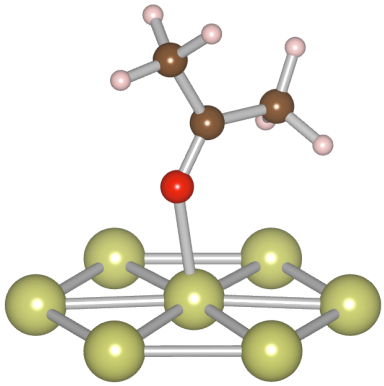
Unsaturated species formation via CHα breaking

	IS	*TS*	*FS*
Methanol_OHCHα	 -326.886189 eV	 -326.359756 eV	 -323.222752 eV
Isoproanol_OHCHα	 -360.385909 eV	 -360.028068 eV	 -356.814976 eV
Ethanol_CHβCHα	 -343.807987 eV	 -343.048130 eV	 -340.003066 eV

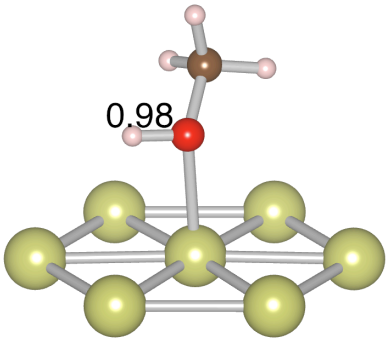
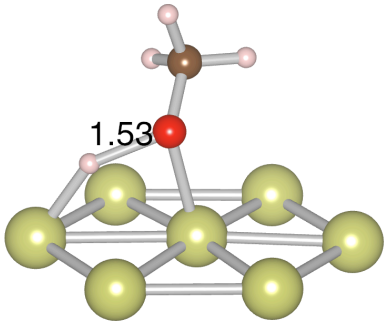
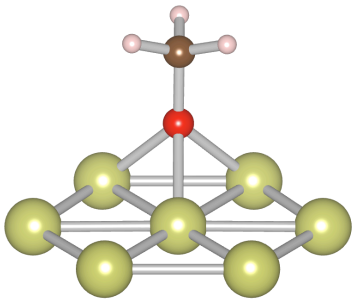
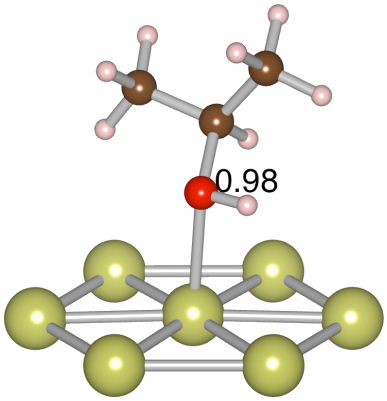
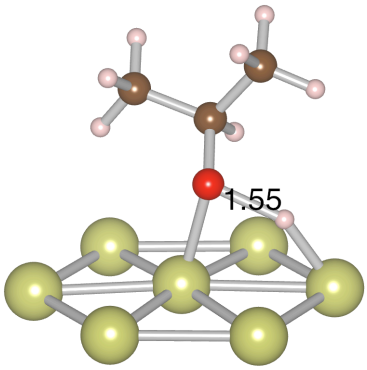
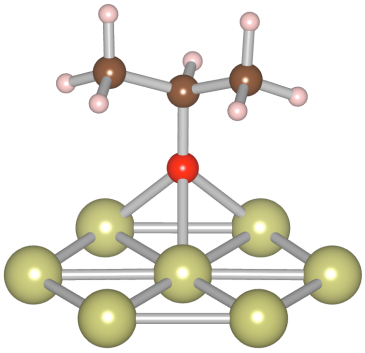
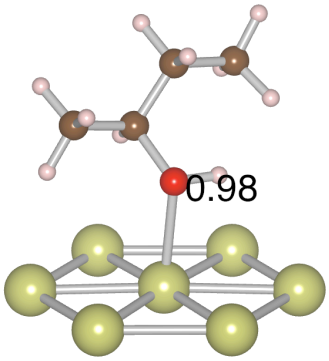
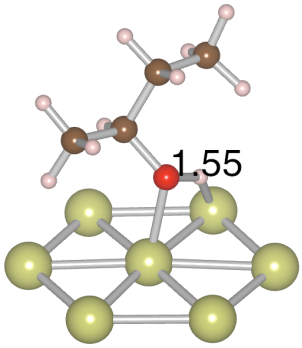
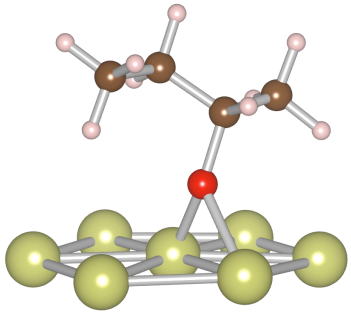
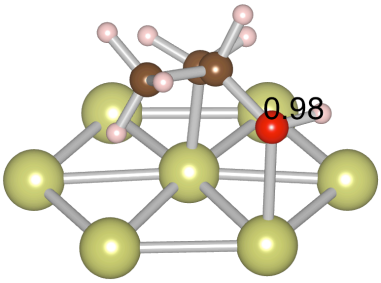
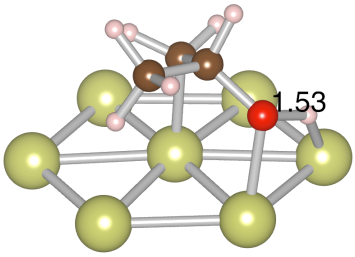
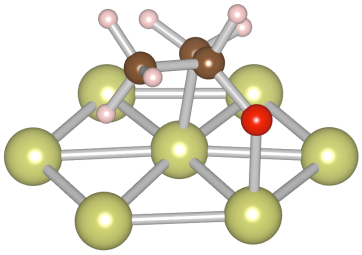
Radical formation via CHα breaking

	IS	*TS*	*FS*
Methanol_CHα	 -331.036677 eV	 -330.258627 eV	 -327.145084 eV
Ethanol_CHα	 -347.775667 eV	 -347.006956 eV	 -343.804695 eV
Isopropanol_CHα	 -364.467600 eV	 -363.541364 eV	 -364.493856 eV
Propanol_CHγCHα	 -360.151138 eV	 -359.492364 eV	 -356.367658 eV
1-butanol_CHγCHα	 -376.583046 eV	 -375.996455 eV	 -372.942528 eV

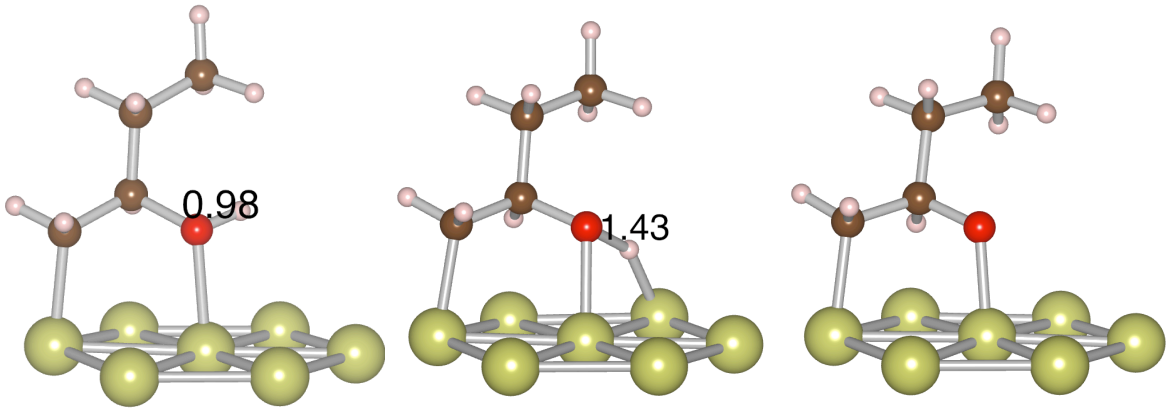
Unsaturated species formation via OH breaking

	IS	*TS*	*FS*
Methanol_CHαOH			
	-327.145263 eV	-326.449696 eV	-323.222752 eV
Isopropanol_CHαOH			
	-360.417012 eV	-359.709233 eV	-356.814976 eV

Radical formation via OH breaking

	IS	*TS*	*FS*
Methanol_OH	 -331.036677 eV	 -330.255178 eV	 -326.886189 eV
Isopropanol_OH	 -364.494878 eV	 -363.667166 eV	 -360.385909 eV
2.Butanol_OH	 -381.063092 eV	 -380.199849 eV	 -376.741586 eV
Isopropanol_CHβOH	 -360.402588 eV	 -359.633202 eV	 -356.253120 eV

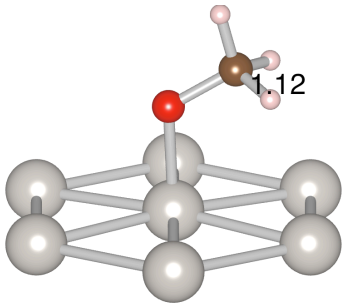
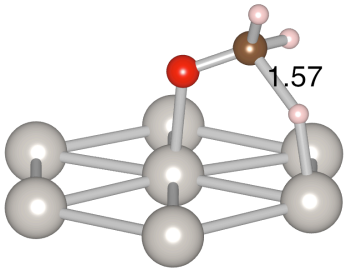
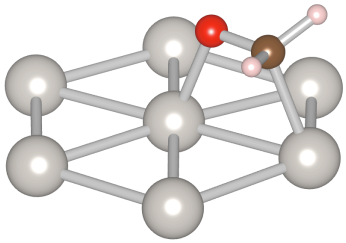
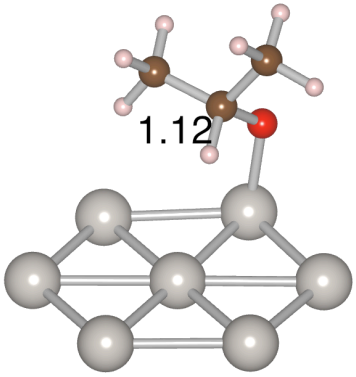
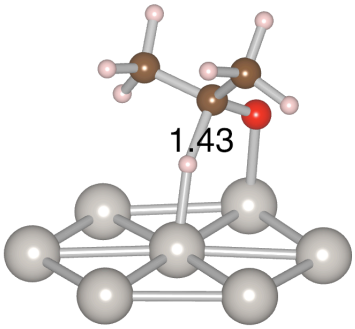
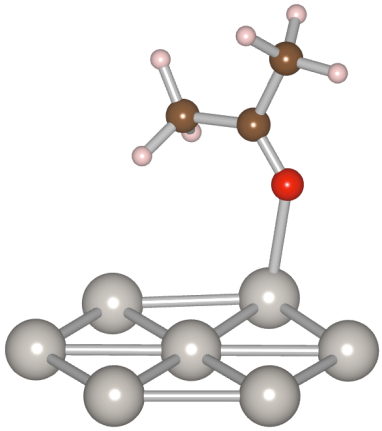
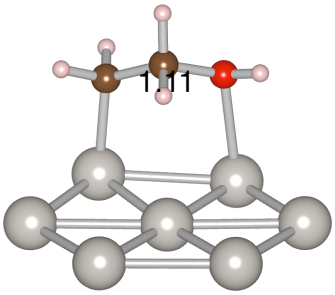
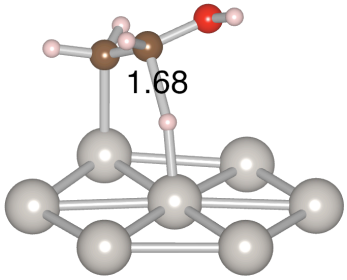
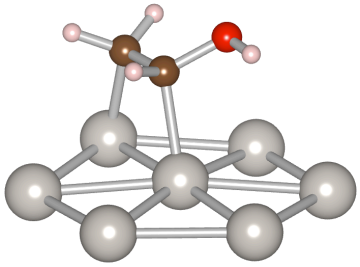
2-Butanol_CHβOH



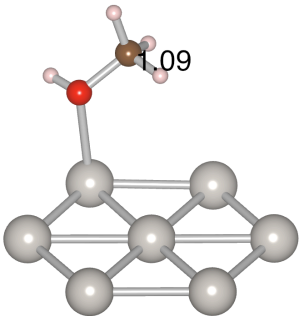
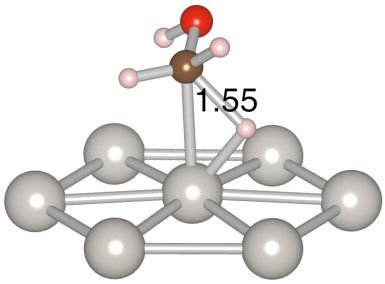
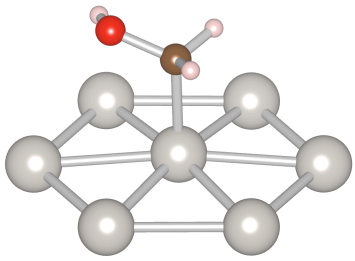
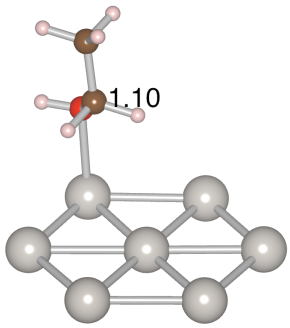
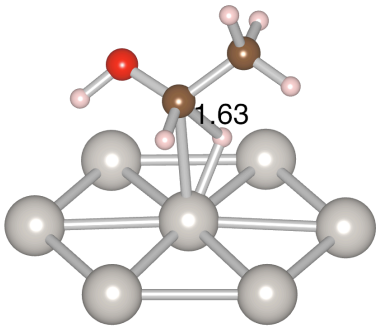
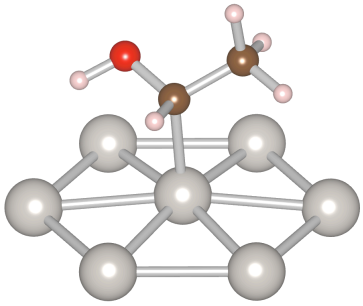
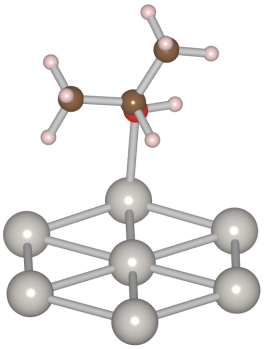
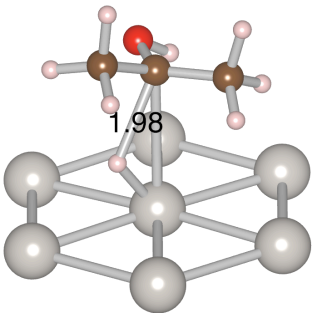
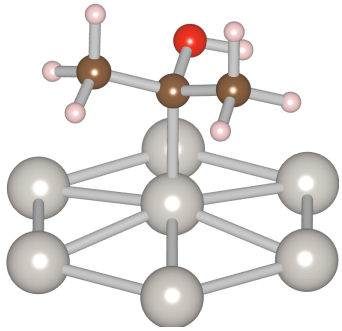
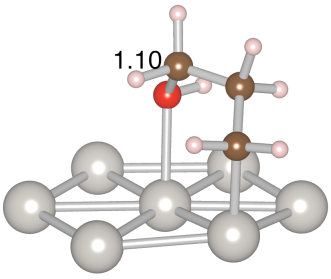
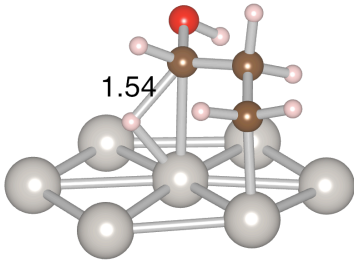
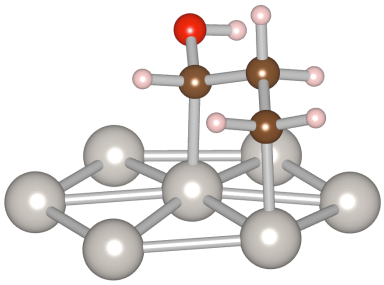
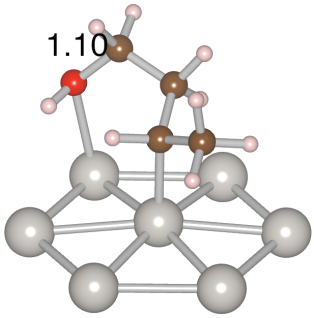
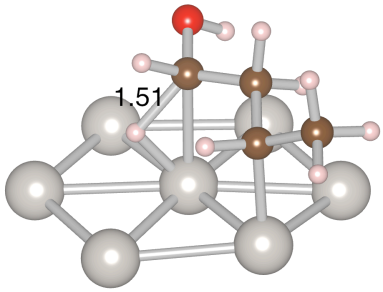
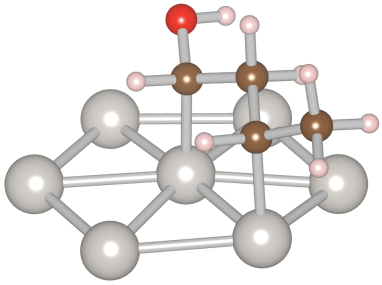
-377.111998 eV -376.349905 eV -373.026823 eV

Monoalcohols Pt

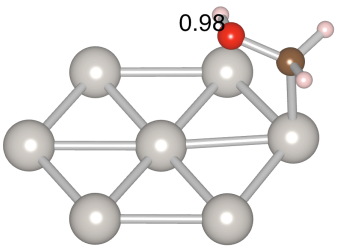
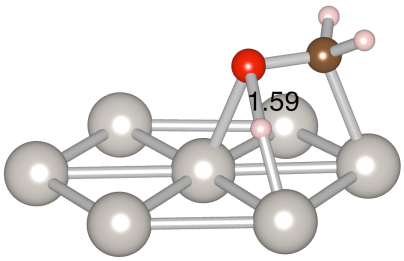
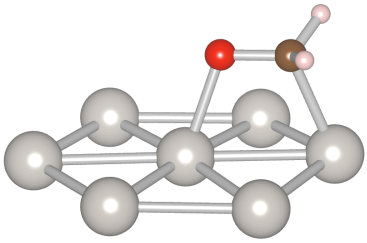
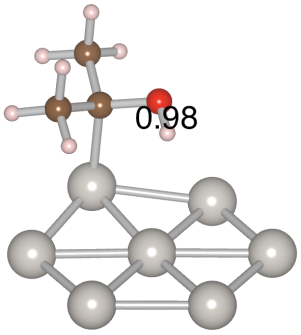
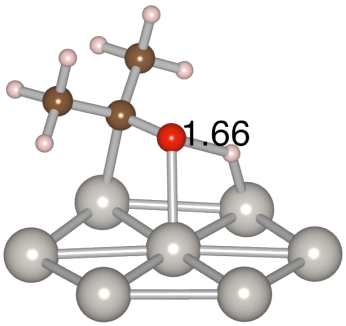
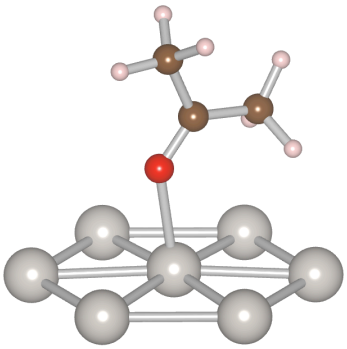
Unsaturated species formation via CHα breaking

	IS	*TS*	*FS*
Methanol_OHCHα			
	-232.966949 eV	-232.728653 eV	-229.453890 eV
Isoproanol_OHCHα			
	-266.393520 eV	-266.318966 eV	-263.262361 eV
Ethanol_CHβCHα			
	-250.269863 eV	-249.624705 eV	-246.704394 eV

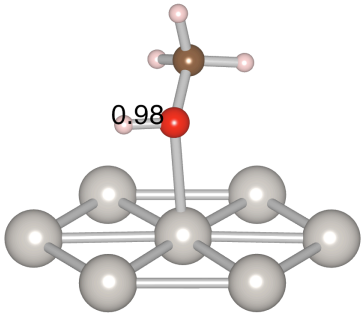
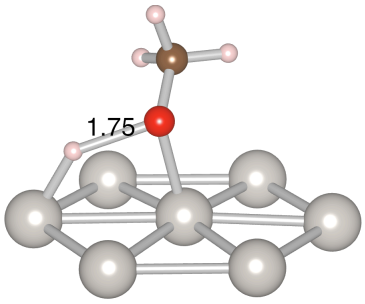
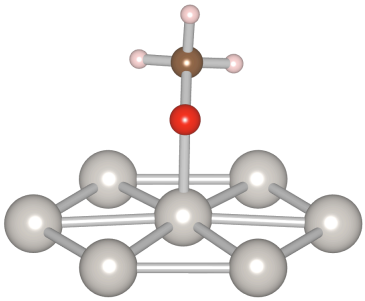
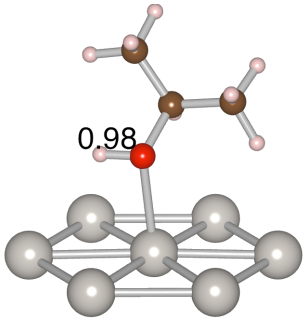
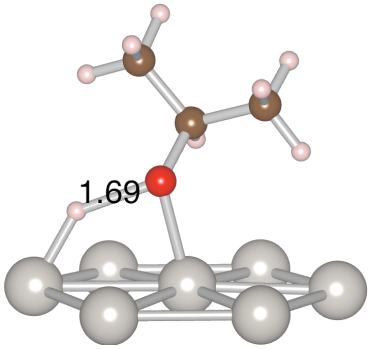
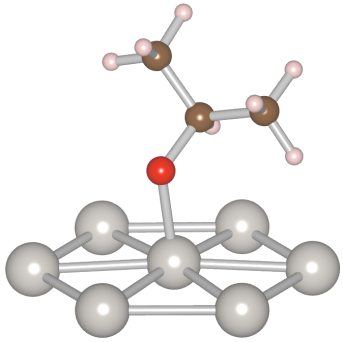
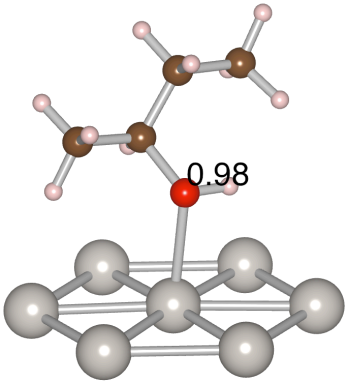
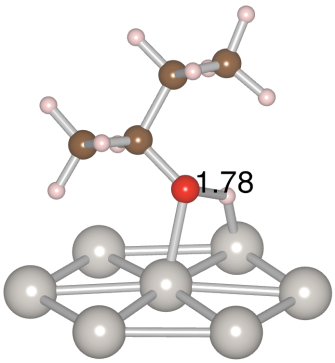
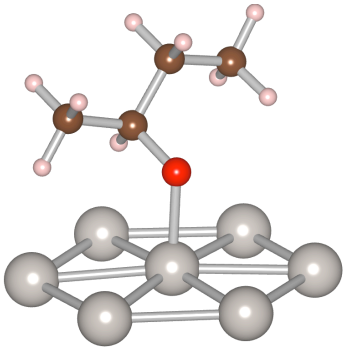
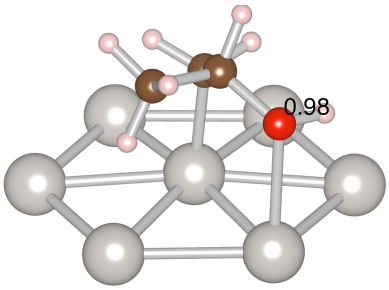
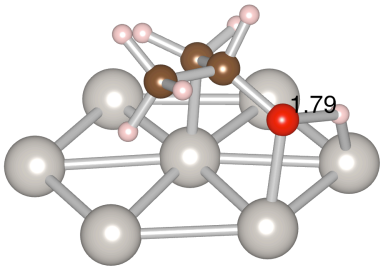
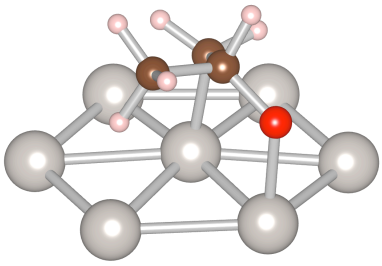
Radical formation via CHα breaking

	IS	*TS*	*FS*
Methanol_CHα	 -237.445615 eV	 -236.746239 eV	 -233.790532 eV
Ethanol_CHα	 -254.186908 eV	 -253.518752 eV	 -250.517355 eV
Isopropanol_CHα	 -270.922080 eV	 -270.119551	 -267.113866
Propanol_CHγCHα	 -266.751175 eV	 -266.062430 eV	 -263.216629 eV
1-butanol_CHγCHα	 -283.239910 eV	 -282.629121 eV	 -279.814530 eV

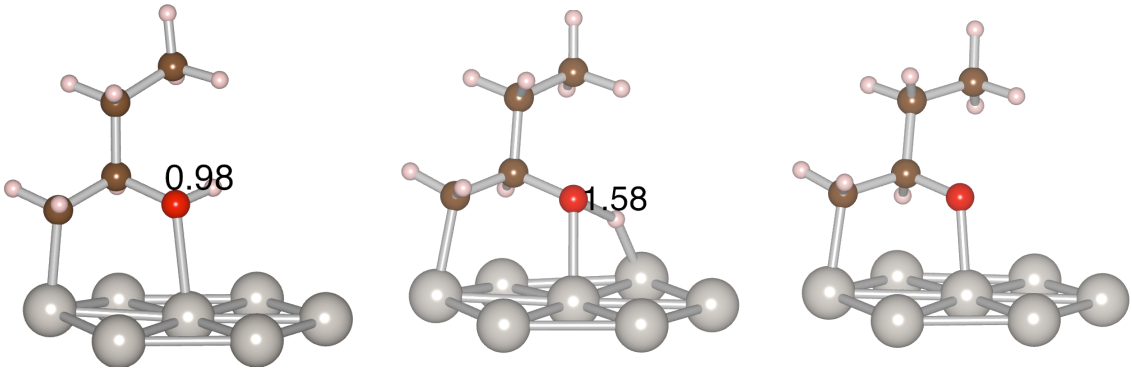
Unsaturated species formation via OH breaking

	IS	*TS*	*FS*
Methanol_CHαOH			
	-233.790552 eV	-232.951594 eV	-229.453890 eV
Isopropanol_CHαOH			
	-267.113866 eV	-266.306334 eV	-263.262361 eV

Radical formation via OH breaking

	IS	*TS*	*FS*
Methanol_OH	 -237.445615 eV	 -236.563554 eV	 -232.966949 eV
Isopropanol_OH	 -270.922080 eV	 -269.995990 eV	 -266.393520 eV
2-Butanol_OH	 -287.497821 eV	 -286.540085 eV	 -282.978855 eV
Isopropanol_CHβOH	 -266.918178 eV	 -266.001726 eV	 -262.427095 eV

2-Butanol_CHβOH



-283.571084 eV -282.685143 eV -279.198254 eV