Table S1. Calculated adsorption energies of the reactants (CH_3CO, CH_3CN, and CH_3CH_2) and the products (CH_3, CO, CN, and CH_2) on Ni, Cu/Ni and Pt/Ni surfaces respectively.

		Ni	Cu/Ni	Pt/Ni
	site	adsorption energy /eV		
Reactant				
CH_3CO	$\eta^2\eta^1$(C,O)	-3.29	-3.52	-4.27
CH_3CN	$\eta^1\eta^3$(C,N)	-1.15	-1.57	-2.33
CH_3CH_2	Top-η1(C)	-1.82	-1.92	-2.18
Products				
CH_3	top	-2.17	-2.24	-2.49
CO	fcc	-1.91	-2.23	-2.45
CN	fcc	-4.46	-4.70	-5.21
CH_2	bridge	-5.34	-5.45	-5.90