

Supplementary information for

Heterogeneous Selective Cross-coupling of Alcohols Mediated by O/ Au(111)

Table 1 Signature mass fragments (unique in most cases) monitored for molecules introduced or produced in the reactions

Molecule	m/z	Molecule	m/z
H ₂ O	18	Methylacetate-d ₃ (CD ₃ OC(=O)CH ₃)	77
CO ₂	44	Methylacetate-d ₃ (CH ₃ OC(=O)CD ₃)	77
Methanol (CH ₃ OH)	32	Ethylformate (HC(=O)OC ₂ H ₅)	74
Ethanol (C ₂ H ₅ OH)	46	Ethylformate-d ₁ (DC(=O)OC ₂ H ₅)	75
Butanol (C ₄ H ₉ OH)	74	Ethylformate-d ₅ (HC(=O)OC ₂ D ₅)	79
Formaldehyde (HC(=O)H)	30	Ethylacetate (CH ₃ C(=O)OC ₂ H ₅)	88
Acetaldehyde (CH ₃ C(=O)H)	44	Ethylacetate-d ₈ (CD ₃ C(=O)OC ₂ D ₅)	96
Butanal (C ₃ H ₇ C(=O)H)	72	Methylbutyrate (CH ₃ OC(=O)C ₃ H ₇)	87, 102
Formic acid (HC(=O)OH)	46	Methylbutyrate-d ₃ (CD ₃ OC(=O)C ₃ H ₇)	105
Acetic acid (CH ₃ OC(=O)H)	60	Butylformate (HC(=O)OC ₄ H ₉)	102
Butanoic acid (C ₃ H ₇ C(=O)OH)	73, 88	Butylformate-d ₁ (DC(=O)OC ₄ H ₉)	103
Methylformate (CH ₃ OC(=O)H)	60	Butylbutyrate (C ₄ H ₉ OC(=O)C ₃ H ₇)	89, 116
Methylacetate (CH ₃ OC(=O)CH ₃)	59, 74		

Table 2 Quantitative analysis of mass fragmentation pattern of products from coupling reactions

Molecule	Selected signature masses	Ratio for authentic samples	Ratio measured in reaction
Methylformate	32amu:60amu	2.2 ^a	No parent ion detected
Methylacetate	59amu:74amu	0.62 ^a	0.59
Methylbutyrate	87amu:102amu	6.1 ^a	6.2
Ethylformate	56amu:74amu	0.74 ^b	No parent ion detected
Ethylacetate	73amu:88amu	1.2 ^a	1.2
Butylformate	73amu:102amu	51 ^b	No parent ion detected
Butylbutyrate	89amu:116amu	46 ^a	49

^aThe fragmentation patterns were measured for the molecular desorption peaks from the clean Au(111) surface using authentic samples.

^bThe fragmentation patterns were taken from NIST database.