

**Effect of Atomicity on Oxidation of Cationic Copper Clusters Studied Using Thermal
Desorption Spectrometry**

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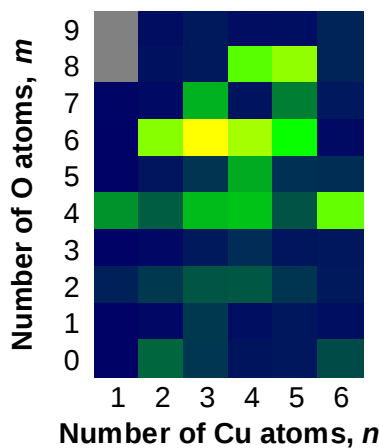


Figure S1. Relative abundances of Cu_nO_m^+ formed by introducing O_2 from the second pulsed valve located downstream of the laser ablation region for different numbers of Cu and O atoms at room temperature.

Table S1. Cartesian coordinates (in Angstrom) of Cu_2O_2^+ clusters shown in Figure 5.

Cu_2^+	Cu	-0.000000	-0.000000	1.223456
	Cu	0.000000	0.000000	-1.223456
IM1	Cu	0.000000	0.497937	0.000000
	Cu	-1.011756	-1.732127	-0.000000
	O	1.237031	2.170398	0.000000
	O	2.430586	2.303540	0.000000
TS1	Cu	-0.919585	1.097333	-0.000000
	Cu	-0.000000	-1.164007	0.000000
	O	1.217494	0.567485	0.000000
	O	2.116001	-0.325791	-0.000000
IM2	Cu	1.963394	-0.297773	0.000012
	Cu	-1.963395	-0.297773	-0.000016
	O	-0.646915	1.079426	0.000004
	O	0.646916	1.079428	0.000013
TS2	Cu	-1.424334	-1.688630	0.000000
	Cu	-1.172076	0.204922	0.000000
	O	0.000000	0.752423	0.000000
	O	1.747665	1.424535	0.000000
P1	Cu	-2.269273	-0.025737	0.000000
	Cu	2.269275	0.025722	0.000001
	O	0.422254	-0.501218	0.000002
	O	-0.422262	0.501268	-0.000007

Table S2. Cartesian coordinates (in Angstrom) of Cu_4O_2^+ clusters shown in Figure 5.

Cu_4^+	Cu	0.000137	1.179702	0.001436
	Cu	2.155528	0.000087	-0.001436

	Cu	-0.000200	-1.179692	0.001436
	Cu	2.155591	-0.000097	-0.001436
IM3	Cu	1.232916	-0.001705	1.197168
	Cu	-0.561967	-1.259008	-0.005087
	Cu	1.242819	0.001667	-1.190259
	Cu	-0.561839	1.258984	-0.002149
	O	-2.450353	0.656080	0.001494
	O	-2.450387	-0.655856	-0.000313
TS3	Cu	0.922533	-1.565534	0.019710
	Cu	-0.983394	-0.551958	1.250918
	Cu	-0.986042	-0.540131	-1.149113
	Cu	0.733350	0.889553	0.002055
	O	-1.015438	1.925782	0.097809
	O	-1.971094	1.038964	0.299629
IM4	Cu	0.939143	-1.540241	-0.037124
	Cu	-0.948497	-0.572475	1.241908
	Cu	-1.018082	-0.513930	-1.151507
	Cu	0.733138	0.908884	0.030586
	O	-1.043791	1.909945	0.106204
	O	-1.988452	0.985445	0.100129
TS4	Cu	-0.937991	-0.197942	1.557096
	Cu	1.416449	-0.305793	2.006187
	Cu	-1.194271	-0.595375	-1.488224
	Cu	0.590508	1.188287	0.318943
	O	-1.182734	1.297881	-0.758729
	O	-2.066263	0.513802	-0.038570
IM5	Cu	-0.713572	-0.716235	0.928080
	Cu	1.565282	-1.033794	1.655525
	Cu	-2.333653	1.177103	-2.102763
	Cu	1.013783	0.266383	-0.297516
	O	-0.576980	0.812436	-1.261708
	O	-1.646855	0.171186	-0.516775
TS5	Cu	-0.483554	-0.725236	1.331815
	Cu	1.826811	-1.240414	1.872619
	Cu	-1.930739	1.673715	-1.038504
	Cu	1.228694	0.424586	0.240457
	O	-0.128592	1.337140	-0.672264
	O	-1.517194	0.348778	0.260283
IM6	Cu	-0.712404	-0.414312	1.191002
	Cu	1.421024	-1.545214	0.985005
	Cu	-1.595748	1.012148	-1.316469

	Cu	1.081587	0.577829	-0.231739
	O	0.096806	1.428691	-1.495909
	O	-1.975284	-0.181342	-0.051503
P2	Cu	-2.990964	0.000651	-0.076232
	Cu	2.991557	0.000472	0.074608
	Cu	0.000106	1.227619	0.000596
	Cu	-0.000546	-1.228820	0.000687
	O	1.312804	-0.000228	-0.622195
	O	-1.313358	0.000511	0.623427