Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Structural and bonding properties of $Cu_3O_3^-$ and $Cu_3O_4^-$ clusters: anion photoelectron spectroscopy and density functional calculations

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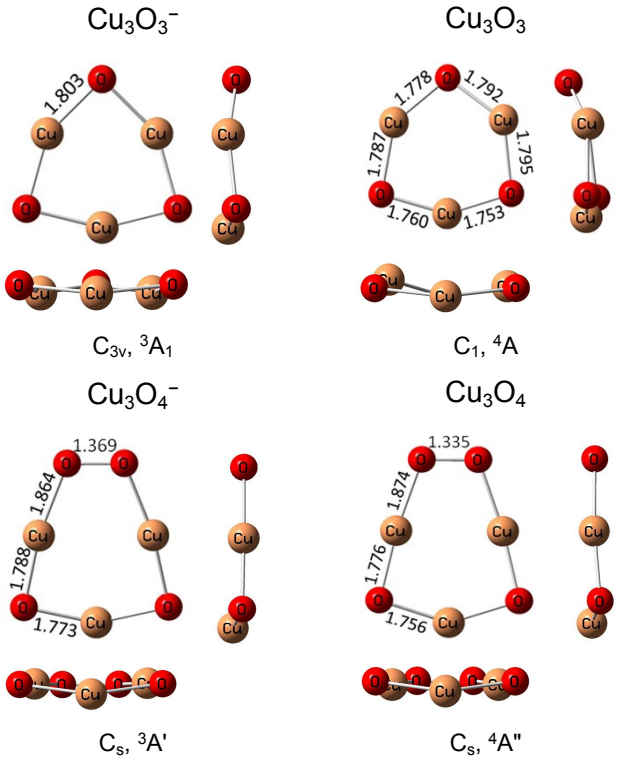

Fig. S1 The most stable structures of $Cu_3O_3^{-/0}$ and $Cu_3O_4^{-/0}$ clusters viewed from different angles. The bond lengths are in angstroms.

Table S1 The relative energies and vertical detachment energies (VDEs) of $Cu_3O_3^-$ obtained from different functionals with the aug-cc-pVTZ/O/aug-cc-pVTZ-pp/Cu basis sets.

$Cu_3O_3^-$	ΔE(eV)			VDE (eV)			
	B3LYP	PBE0	B3P86	B3LYP	PBE0	B3P86	Expt.
3A	0.00	0.00	0.00	3.52	3.42	4.02	3.48
3B	0.38	0.32	0.35	3.15	3.67	4.24	
3C	0.82	0.90	0.79	3.20	3.20	3.74	

Table S2 Cartesian coordinates for stable isomers of $Cu_3O_3^-$ and $Cu_3O_4^-$ clusters.

$Cu_3O_3^-$

3A

	X	Y	Z
O	1.73448700	1.00140700	0.14751500
O	0.00000000	-2.00281300	0.14751500
O	-1.73448700	1.00140700	0.14751500
Cu	0.00000000	1.45757800	-0.04069400
Cu	-1.26230000	-0.72878900	-0.04069400
Cu	1.26230000	-0.72878900	-0.04069400

3B

	X	Y	Z
Cu	0.00000000	0.00000000	1.46515500
Cu	0.00000000	1.15251100	-0.72436800
Cu	0.00000000	-1.15251100	-0.72436800
O	0.00000000	0.00000000	-2.13378900
O	0.00000000	1.72533700	1.03713400
O	0.00000000	-1.72533700	1.03713400

3C

O	0.00000000	0.00000000	-2.19974700
O	0.00000000	1.66442300	0.93373200
O	0.00000000	-1.66442300	0.93373200
Cu	0.00000000	-1.10845400	-0.75292700
Cu	0.00000000	0.00000000	1.59751900
Cu	0.00000000	1.10845400	-0.75292700

$Cu_3O_4^-$

4A

	X	Y	Z
Cu	0.06677700	-0.53921400	1.33504900
Cu	-0.18866100	1.67164000	0.00000000
Cu	0.06677700	-0.53921400	-1.33504900
O	0.03310300	1.21094700	1.69791500
O	0.03310300	1.21094700	-1.69791500
O	0.06677700	-2.28614200	-0.68442100
O	0.06677700	-2.28614200	0.68442100

4B

	X	Y	Z
Cu	0.00000000	0.00000000	-3.45225100
O	0.00000000	0.00000000	-5.12159100
O	0.00000000	0.00000000	-1.75939300
O	0.00000000	0.00000000	1.75939600
O	0.00000000	0.00000000	5.12158900
Cu	0.00000000	0.00000000	3.45224800
Cu	0.00000000	0.00000000	0.00000200

4C

O	-0.76526400	1.40289100	0.34156600
O	-0.37415600	-1.57546700	0.26780800
O	2.41916700	0.26701500	-0.01874200
Cu	0.92501800	1.27626200	-0.04537000
Cu	1.27180500	-1.11801700	-0.06394200
Cu	-1.63345300	-0.24609800	0.03400600
O	-3.32196400	0.22402900	-0.31764900