Modeling Photoelectron Spectra of CuO, Cu_2O, and CuO_2 Anions with Equation-of-Motion Coupled-Cluster Methods: An Adventure in Fock Space. Supplemental Information.

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1 Symmetry labels

Table S1: Correspondence between C_{2v} and $C_{\infty v}$ point groups[1]

$C_{\infty v}$	C_{2v}
Σ^+	A_1
Σ^-	A_2
$E_1 = \Pi$	B_1/B_2
$E_2 = \Delta$	A_1/A_2

Table S2: Correspondence between D_{2h} and $D_{\infty h}$ point groups[1]

$D_{\infty h}$	D_{2h}
Σ_g^+	A_g
Σ_g^-	B_{1g}
Π_g	B_{2g}/B_{3g}
Δ_g	A_g/B_{1g}
Σ_u^+	B_{1u}
Σ_u^-	A_u
Π_u	B_{2u}/B_{3u}
Δ_u	A_u/B_{1u}

2 Additional EOM-CCSD and CIS results CuO^-

Table S3: Six lowest EOM-IP-CCSD/cc-pVTZ (all-electron) detachment energies obtained from the closed-shell singlet CuO^- reference.

Orbital[a]	State	DE (eV)	$\|\|R_1\|\|^2$ [b]	Leading r_i	Dyson norm[b]
$4b_1/4b_2$	$^2B_1/^2B_2$	1.628	0.898	0.944	0.927
$10a_1$	$^2A_1$	2.167	0.923	0.958	0.947
$1a_2$	$^2A_2$	4.913	0.905	0.951	0.939
$8a_1$	$^2A_1$	4.913	0.905	0.951	0.939
$9a_1$	$^2A_1$	4.996	0.853	0.920	0.904
$3b_1/3b_2$	$^2B_1/^2B_2$	5.561	0.895	0.943	0.931

[a] See Fig. 3 for the symmetries and shapes of Hartree-Fock orbitals.
[b] Norm of the right Dyson orbital associated with the EOM-IP transition.

Table S4: Six lowest EOM-IP-CCSD/ECP10MDF/cc-pVTZ-PP detachment energies obtained from the closed-shell singlet CuO^- reference. ECP applied to copper only. All-electron cc-pVTZ basis used for oxygen.

Orbital[a]	State	DE (eV)	$\|\|R_1\|\|^2$	Leading r_i	Dyson norm[b]
$3b_1/3b_2$	$^2B_1/^2B_2$	1.674	0.901	0.942	0.932
$7a_1$	$^2A_1$	2.332	0.931	0.960	0.954
$1a_2$	$^2A_2$	4.578	0.909	0.953	0.940
$5a_1$	$^2A_1$	4.578	0.909	0.953	0.940
$6a_1$	$^2A_1$	4.869	0.864	0.919	0.908
$2b_1/2b_2$	$^2B_1/^2B_2$	5.339	0.899	0.942	0.933

[a] See Fig. 3 for the symmetries and shapes of Hartree-Fock orbitals.
[b] Norm of the right Dyson orbital associated with the EOM-IP transition.

Table S5: Six lowest excitation energies (from the closed-shell singlet reference) of CuO^- computed at the EOM-EE-CCSD/cc-pVTZ level of theory. All-electron basis used for copper and oxygen.

Transition[a]	State	E_{ex} (eV)	$\|\|R_1\|\|^2$	Leading r_i^a
$4b_1/4b_2 \rightarrow 11a_1$	$^1B_1$, $^1B_2$	0.919	0.898	0.594
	$^3B_1$, $^3B_2$	0.488	0.915	0.578
$10a_1 \rightarrow 11a_1$	$^1A_1$	2.095	0.910	0.522
	$^3A_1$	0.873	0.957	0.596
$8a_1 \rightarrow 11a_1$	$^1A_1$	2.886	0.914	0.579
	$^3A_1$	2.629	0.923	0.525
$1a_2 \rightarrow 11a_1$	$^1A_2$	2.886	0.914	0.579
	$^3A_2$	2.629	0.923	0.525
$9a_1 \rightarrow 11a_1$	$^1A_1$	4.128	0.860	0.458
	$^3A_1$	3.019	0.923	0.496

[a] See Fig. 3 for the symmetries and shapes of Hartree-Fock orbitals.

Table S6: Six lowest excitation energies (from the closed-shell singlet reference) of CuO^- computed at the EOM-EE-CCSD/ECP10MDFD/cc-pVTZ-PP level of theory. ECP applied to Cu only. All-electron cc-pVTZ basis used for O.

Transition[a]	State	E_{ex} (eV)	$\|\|R_1\|\|^2$	Leading r_i^a
$4b_1/4b_2 \rightarrow 8a_1$	$^1B_1$, $^1B_2$	0.933	0.906	0.575
	$^3B_1$, $^3B_2$	0.457	0.920	0.556
$7a_1 \rightarrow 8a_1$	$^1A_1$	2.140	0.916	0.513
	$^3A_1$	0.941	0.958	0.582
$1a_2 \rightarrow 8a_1$	$^1A_2$	2.537	0.919	0.590
	$^3A_2$	2.239	0.928	0.576
$5a_1 \rightarrow 8a_1$	$^3A_1$	2.240	0.928	0.576
$6a_1 \rightarrow 8a_1$	$^3A_1$	2.913	0.927	0.488
$2b_1/2b_2 \rightarrow 8a_1$	$^1B_1$, $^1B_2$	3.422	0.895	0.535
	$^3B_1$, $^3B_2$	3.219	0.910	0.525

[a] See Fig. 3 for the symmetries and shapes of Hartree-Fock orbitals.

Table S7: Six lowest CIS/cc-pVTZ excitation energies from the closed-shell singlet reference of CuO^-. All-electron basis used for copper and oxygen.

Transition	State	ΔE (eV)
$4b_1/4b_2 \rightarrow 11a_1$	$^1B_1$, $^1B_2$	1.208
	$^3B_1$, $^3B_2$	0.539
$10a_1 \rightarrow 11a_1$	$^1A_1$	1.842
	$^3A_1$	-0.371
$8a_1 \rightarrow 11a_1$	$^1A_1$	3.884
	$^3A_1$	3.375
$1a_2 \rightarrow 11a_1$	$^1A_2$	3.884
	$^3A_2$	3.375
$9a_1 \rightarrow 11a_1$	$^1A_1$	4.494
	$^3A_1$	2.229

[a] See Fig. 3 for the symmetries and shapes of Hartree-Fock orbitals.

3 Additional EOM-CCSD results for Cu_2O^-

Table S8: Six lowest EOM-EE-CCSD/cc-pVTZ excitation energies of closed-shell singlet Cu_2O. All-electron basis used for Cu and O.

Orbital[a]	State	E_{ex} (eV)	$\|\|R_1\|\|^2$	Leading r_i^a
$5b_2 \rightarrow 14a_1$	$^1B_2$	1.696	0.920	0.552
	$^3B_2$	1.283	0.928	0.537
$11b_1 \rightarrow 14a_1$	$^1B_1$	1.774	0.926	0.546
	$^3B_1$	1.379	0.938	0.528
$5b_2 \rightarrow 12b_1$	$^1A_2$	2.274	0.926	0.449
	$^3A_2$	1.905	0.932	0.427
$11b_1 \rightarrow 12b_1$	$^1A_1$	2.374	0.928	0.415
	$^3A_1$	1.896	0.937	0.418
$13a_1 \rightarrow 14a_1$	$^1A_1$	2.517	0.932	0.407
	$^3A_1$	1.675	0.947	0.481
$10b_1 \rightarrow 14a_1$	$^1B_1$	2.517	0.932	0.388
	$^3B_1$	2.088	0.941	0.410

[a] See Fig. 7 for the symmetries and shapes of Hartree-Fock orbitals.

Table S9: Six lowest EOM-EE-CCSD/ECP10MDF/cc-pVTZ-PP excitation energies of closed-shell singlet Cu_2O. ECP applied to copper only. All-electron basis used for oxygen.

Orbital[a]	State	E_{ex} (eV)	$\|\|R_1\|\|^2$	Leading r_i^a
$4b_2 \rightarrow 10a_1$	$^1B_2$	1.604	0.920	0.537
	$^3B_2$	1.158	0.928	0.522
$7b_1 \rightarrow 10a_1$	$^1B_1$	1.678	0.925	0.536
	$^3B_1$	1.225	0.938	0.522
$4b_2 \rightarrow 8b_1$	$^1A_2$	2.069	0.926	0.423
	$^3A_2$	1.656	0.932	0.402
$7b_1 \rightarrow 8b_1$	$^1A_1$	2.182	0.927	0.391
	$^3A_1$	1.662	0.936	0.363
$6b_1 \rightarrow 10a_1$	$^1B_1$	2.323	0.930	0.409
	$^3B_1$	1.821	0.940	0.434
$9a_1 \rightarrow 10a_1$	$^1A_1$	2.377	0.930	0.384
	$^3A_1$	1.571	0.948	0.407

[a] See Fig. 7 for the symmetries and shapes of Hartree-Fock orbitals.

References

[1] Chen, J.-Q.; Ping, J.; Wang, F. *Group representation theory for physicists;* World Scientific, 2nd ed., 2002.

Cartesian coordinates of relevant structures

Closed-shell singlet geometry of CuO- anion optimized at the
wB97X-D/cc-pVTZ level of theory.

1	Cu	0.0000000000	0.0000000000	-0.3616121081
2	O	0.0000000000	0.0000000000	1.3108438919

Nuclear Repulsion Energy: 73.4065 hartrees

Closed-shell doublet geometry of the (Cu2O)- anion optimized at the
wB97X-D/cc-pVTZ level of theory.

1	Cu	1.2492124637	0.0000000000	0.1565252450
2	O	0.0000000000	0.0000000000	-1.1348080259
3	Cu	-1.2492124637	0.0000000000	0.1565252450

Nuclear Repulsion Energy: 314.7893 hartrees

Triplet geometry of (CuO2)- anion optimized at the
wB97X-D/cc-pVTZ level of theory.

1	Cu	0.0000000000	0.0000000000	0.0000000000
2	O	0.0000000000	0.0000000000	1.7367260000
3	O	0.0000000000	0.0000000000	-1.7367260000

Nuclear Repulsion Energy: 151.1303 hartrees