

Theoretical Study on the Structures and Stabilities of $\text{Cu}_n\text{Zn}_3\text{O}_3$ ($n = 1 - 4$) Clusters: Sequential Doping of Zn_3O_3 Cluster with Cu Atoms

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Supplementary Materials

Table S1 Calculated results at B3LYP/BS level for the bond lengths (d), binding energies (E_b), vibrational frequencies (ω_e) and dipole moments (μ) of ZnO and CuO along with the corresponding available experimental data.

Table S2 Relative energies of $\text{Cu}_n\text{Zn}_3\text{O}_3$ ($n = 1-4$) clusters at the B3LYP/BS level ($\Delta E < 0.50$ eV) and those in the CCSD(T) single-point calculations.

Table S3 The calculated d-band centers for the spin up (α), spin down (β) and both spin modes (*total*).

Figure S1 Alternative optimized structures for CuZn_3O_3 at the B3LYP/BS level. The bond lengths are in angstroms.

Figure S2 Alternative optimized structures for $\text{Cu}_2\text{Zn}_3\text{O}_3$ at the B3LYP/BS level. The bond lengths are in angstroms.

Figure S3 Alternative optimized structures for $\text{Cu}_3\text{Zn}_3\text{O}_3$ at the B3LYP/BS level. The bond lengths are in angstroms.

Figure S4 Alternative optimized structures for $\text{Cu}_4\text{Zn}_3\text{O}_3$ at the B3LYP/BS level. The bond lengths are in angstroms.

Table S4 Cartesian coordinates for the optimized $\text{Cu}_n\text{Zn}_3\text{O}_3$ ($n = 0-4$) clusters.

Table S1 Calculated results at B3LYP/BS level for the bond lengths (d), binding energies (E_b), vibrational frequencies (ω_e) and dipole moments (μ) of ZnO and CuO along with the corresponding available experimental data.

Molecule	Method	d (Å)	E_b (eV)	ω_e (cm ⁻¹)	μ (Debyes)
ZnO	B3LYP/BS	1.700	1.24	741	5.61
	Experiment	1.705 ^a	1.61 ± 0.04^b	738 ^a	/
CuO	B3LYP/BS	1.719	2.98	639	4.53
	Experiment	1.724 ^c	2.85 ± 0.15^b	640 ^c	4.45 ± 0.30^d

^a Zack, L.N.; Pulliam, R.L.; Ziurys, L.M. *Journal of Molecular Spectroscopy*, 2009, 256, 186-191.

^b Clemmer, D.E.; Dalleska, N.F.; Armentrout, P.B. *The Journal of Chemical Physics*, 1991, 95, 7263-7268.

^c Huber, K.P.; Herzberg, G. Constants of diatomic molecules. In *Molecular Spectra and Molecular Structure: IV. Constants of Diatomic Molecules*, Huber, K.P., Herzberg, G., Eds.; Springer US: Boston, MA, 1979; pp. 8-689.

^d Steimle, T.C.; Nachman, D.F.; Fletcher, D.A. *The Journal of Chemical Physics*, 1987, 87, 5670-5673.

Table S2 Relative energies of Cu_nZn₃O₃ ($n = 1-4$) clusters at the B3LYP/BS level ($\Delta E \leq 0.50$ eV) and those in the CCSD(T) single-point calculations.

Cluster	B3LYP/BS ^a	CCSD(T) ^{a,b}
CuZn ₃ O ₃ (C_s ² A')	0.00	0.00
(C_1 ² A)	0.50	0.16
Cu ₂ Zn ₃ O ₃ (C_s ¹ A')	0.00	0.00
(C_1 ¹ A)	0.39	0.03
Cu ₃ Zn ₃ O ₃ (C_1 ² A)	0.00	0.00
(C_1 ² A)	0.20	0.69
(C_1 ² A)	0.20	0.45
(C_1 ² A)	0.22	0.42
(C_1 ² A)	0.30	0.54
(C_1 ² A)	0.31	0.65
(C_1 ² A)	0.33	0.57
(C_1 ² A)	0.44	0.68
(C_1 ² A)	0.45	0.72
(C_1 ² A)	0.47	0.76
Cu ₄ Zn ₃ O ₃ (C_1 ¹ A)	0.00	0.00
(C_1 ¹ A)	0.10	0.28
(C_1 ¹ A)	0.41	0.04
(C_1 ¹ A)	0.43	0.63

^a All energies are in eV.

^b CCSD(T) single-point calculations at the B3LYP/BS geometries.

Table S3 The calculated d-band centers for the spin up (α), spin down (β) and both spin modes (*total*)

ε_d (eV)	Zn ₃ O ₃	CuZn ₃ O ₃	Cu ₂ Zn ₃ O ₃	Cu ₃ Zn ₃ O ₃	Cu ₄ Zn ₃ O ₃
α	-6.16	-5.84	-4.83	-5.31	-4.09
β	-6.16	-5.09	-4.83	-4.66	-4.09
<i>total</i>	-6.16	-5.72	-4.83	-5.25	-4.09

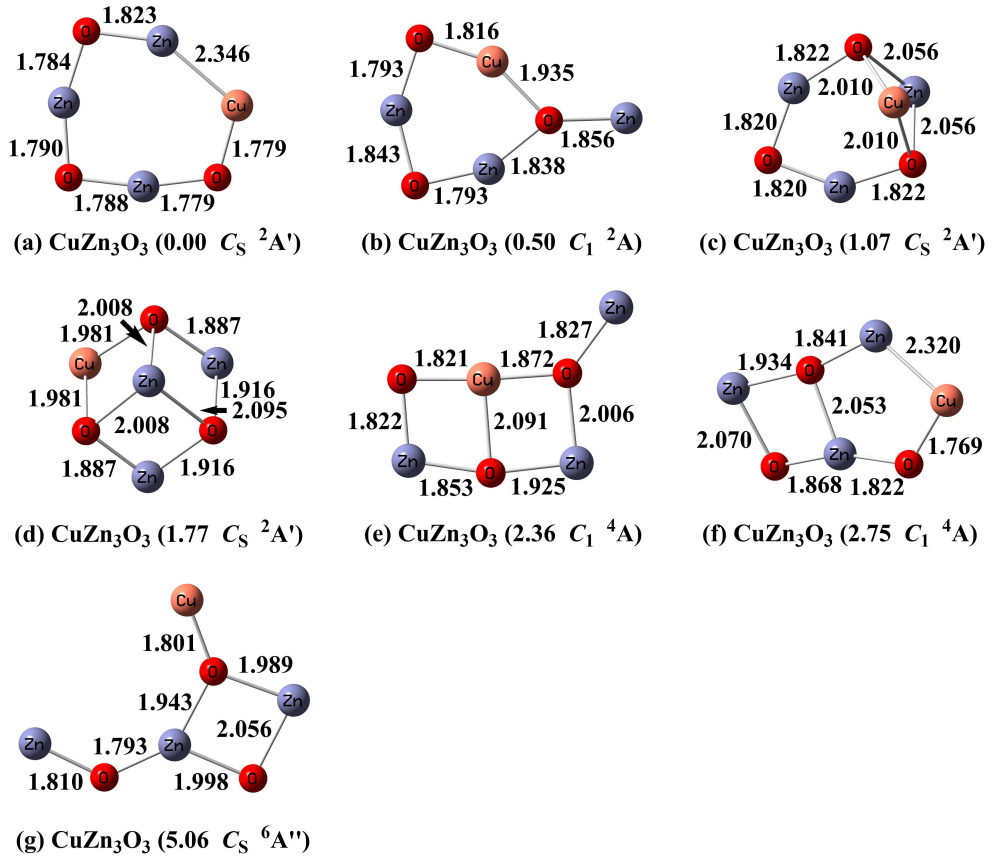


Figure S1 Alternative optimized structures for CuZn₃O₃ at the B3LYP/BS level. The bond lengths are in angstroms.

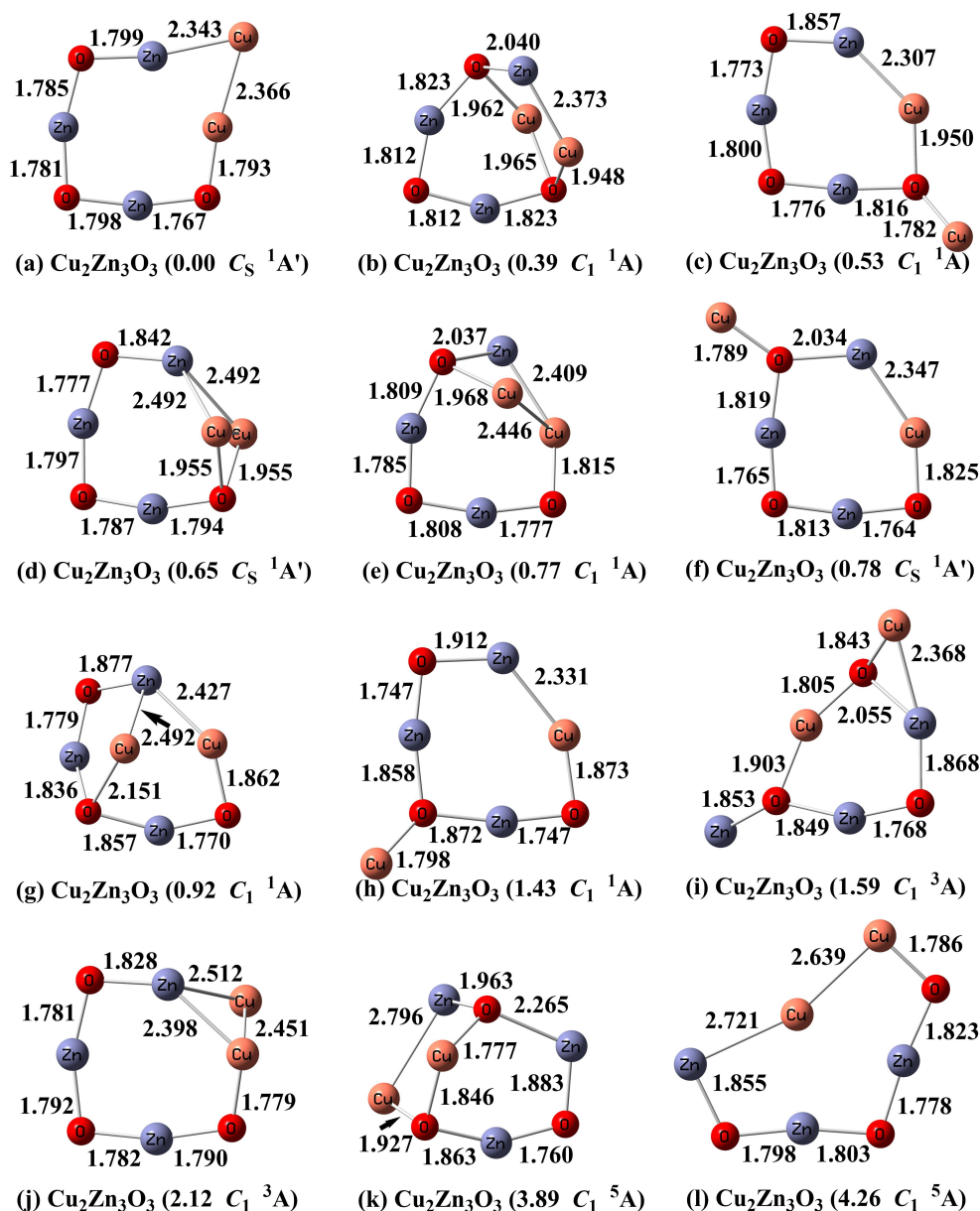


Figure S2 Alternative optimized structures for $\text{Cu}_2\text{Zn}_3\text{O}_3$ at the B3LYP/BS level. The bond lengths are in angstroms.

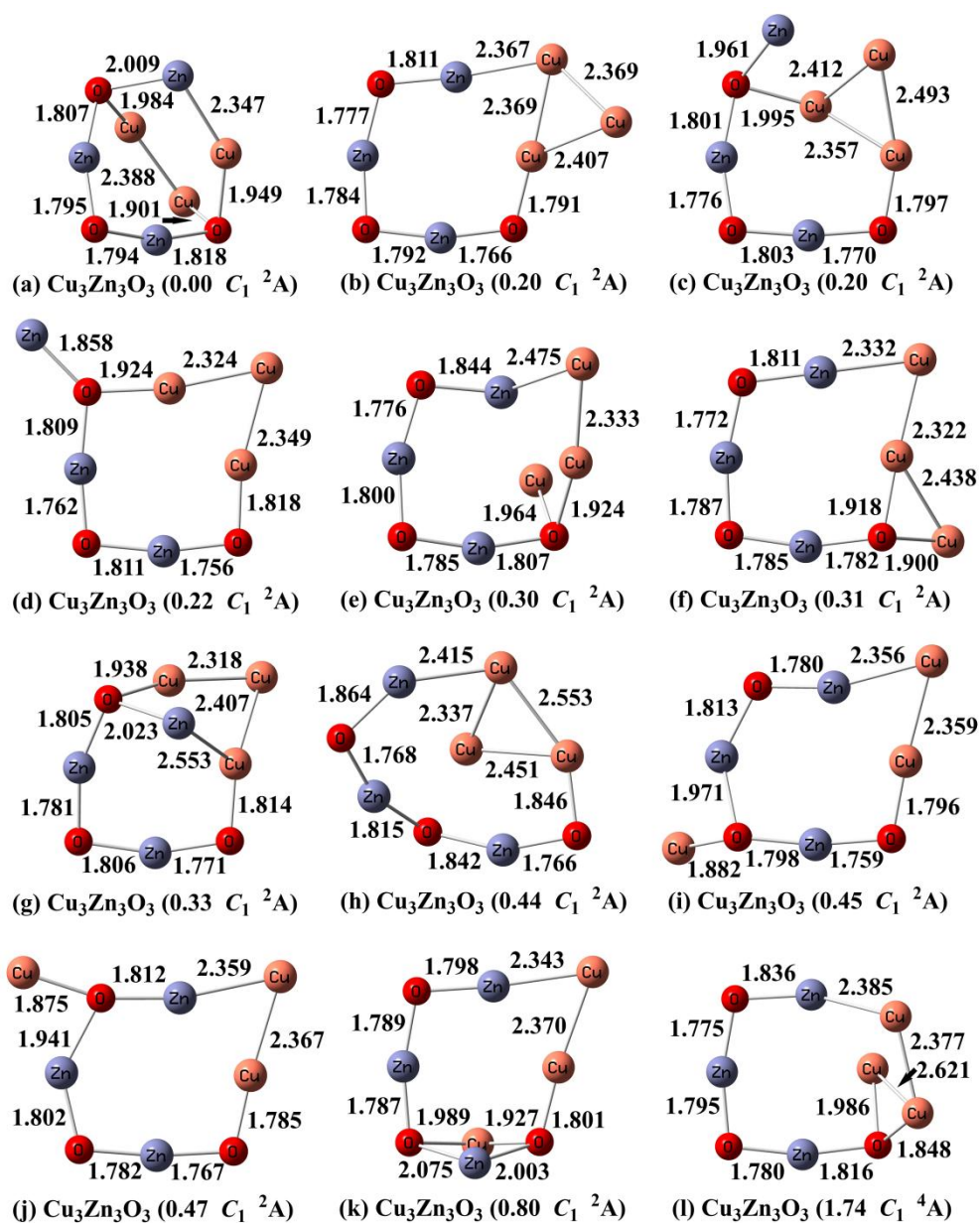


Figure S3 Alternative optimized structures for $\text{Cu}_3\text{Zn}_3\text{O}_3$ at the B3LYP/BS level. The bond lengths are in angstroms. (Continued)

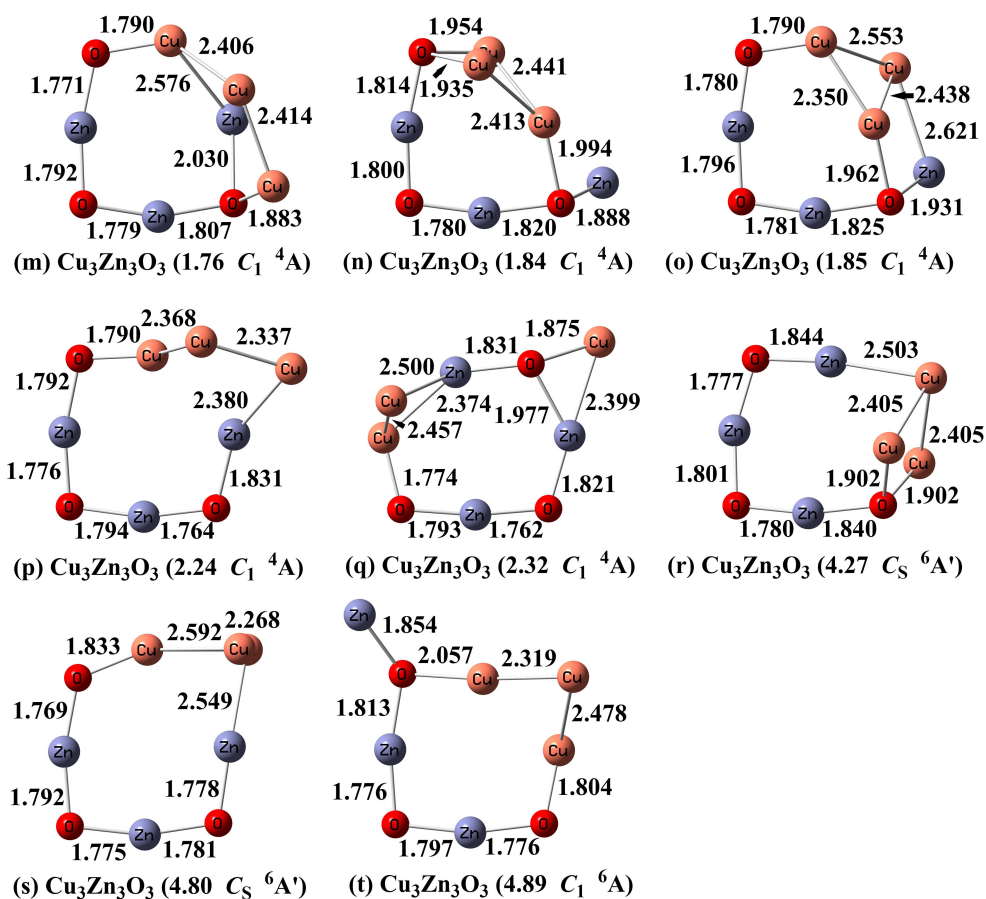


Figure S3 Alternative optimized structures for $\text{Cu}_3\text{Zn}_3\text{O}_3$ at the B3LYP/BS level. The bond lengths are in angstroms.

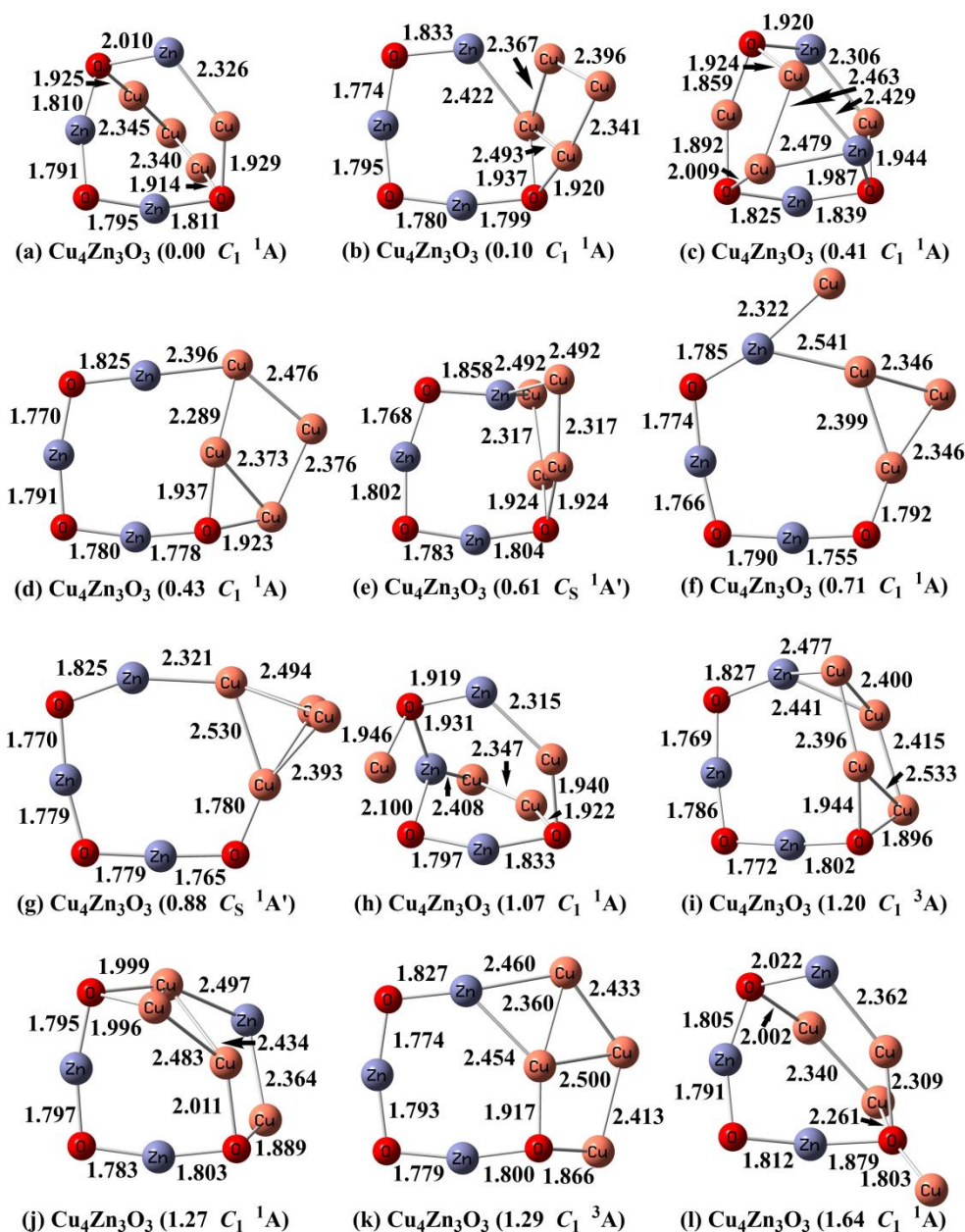


Figure S4 Alternative optimized structures for $\text{Cu}_4\text{Zn}_3\text{O}_3$ at the B3LYP/BS level. The bond lengths are in angstroms. (Continued)

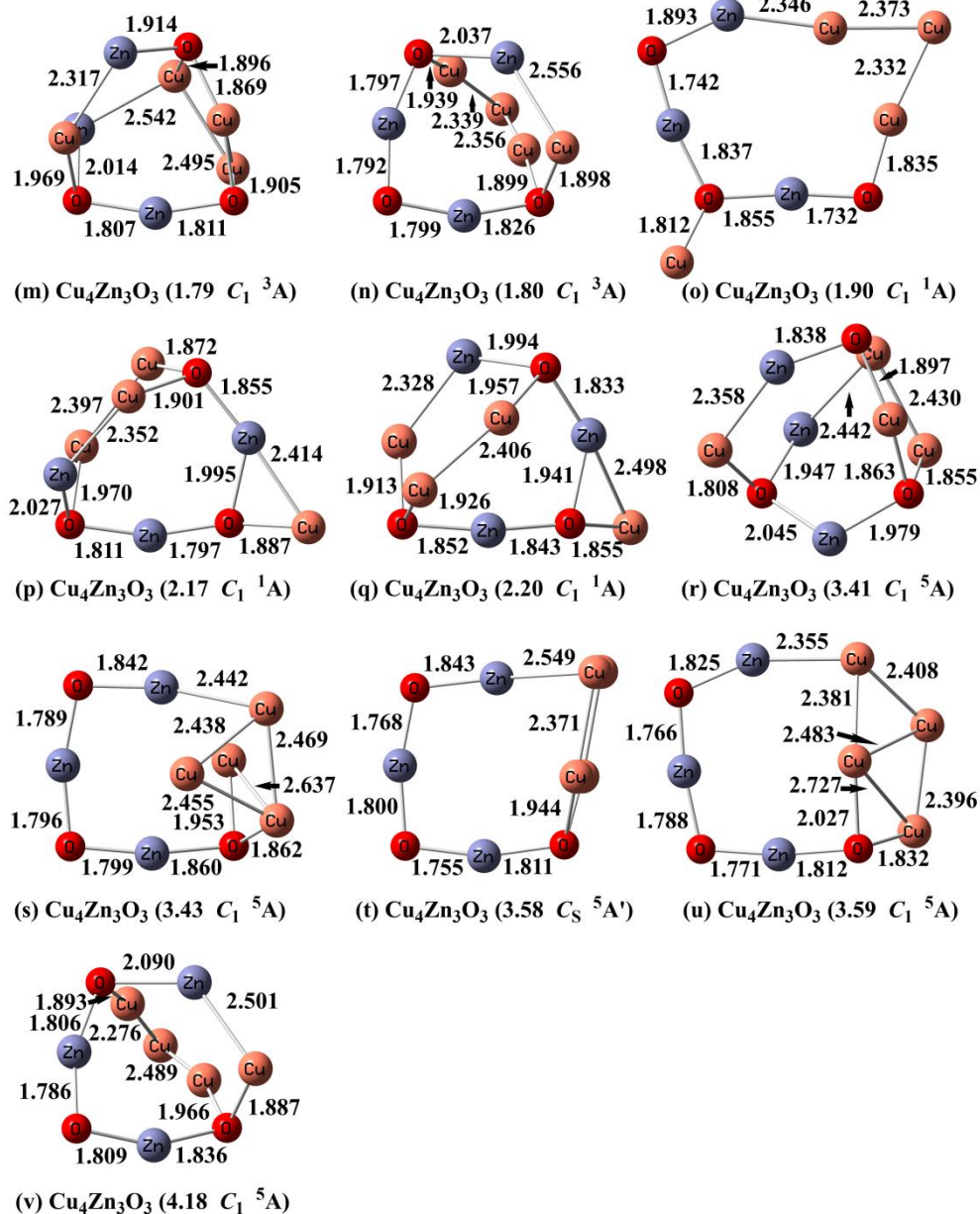


Figure S4 Alternative optimized structures for $\text{Cu}_4\text{Zn}_3\text{O}_3$ at the B3LYP/BS level. The bond lengths are in angstroms.

Table S4 Cartesian coordinates for the optimized $\text{Cu}_n\text{Zn}_3\text{O}_3$ ($n = 0-4$) clusters.

Zn_3O_3			
Zn_3O_3 (D_{3h} $^1A_1'$)			
O	-1.003335000	-1.737755000	0.000000000
O	-1.003335000	1.737755000	0.000000000
O	2.006738000	0.000000000	0.000000000
Zn	-1.532402000	0.000000000	0.000000000
Zn	0.766192000	-1.327119000	0.000000000
Zn	0.766192000	1.327119000	0.000000000

CuZn_3O_3			
CuZn_3O_3 (0.00 eV C_s $^2A'$)			
O	1.986864000	-1.139782000	0.000000000
O	-1.464987000	-1.932363000	0.000000000
O	-1.814022000	1.563489000	0.000000000
Zn	0.312282000	-1.740960000	0.000000000
Zn	0.000000000	1.741676000	0.000000000
Zn	-1.968793000	-0.214245000	0.000000000
Cu	2.070086000	0.637072000	0.000000000

CuZn_3O_3 (0.50 eV C_1 2A)			
O	-1.842215000	-1.756624000	0.014823000
O	-1.819712000	1.738781000	0.032881000
O	1.296203000	0.075163000	-0.119825000
Zn	-2.331722000	-0.031894000	0.043845000
Zn	3.140818000	-0.038838000	0.050956000
Zn	-0.087704000	1.282425000	-0.038579000
Cu	-0.093653000	-1.269288000	-0.038265000

CuZn_3O_3 (1.07 eV C_s $^2A'$)			
O	0.002265000	-0.726328000	1.529987000
O	0.002265000	-0.726328000	-1.529987000
O	-0.015248000	2.360546000	0.000000000
Zn	-1.216429000	-1.359674000	0.000000000
Zn	0.002265000	1.080573000	1.293891000
Zn	0.002265000	1.080573000	-1.293891000
Cu	1.256646000	-1.079562000	0.000000000

CuZn_3O_3 (1.77 eV C_s $^2A'$)			
O	0.876888000	-1.462564000	0.000000000
O	-0.088964000	0.873388000	1.562932000
O	-0.088964000	0.873388000	-1.562932000

Zn	-0.088964000	-1.013560000	1.592311000
Zn	-0.088964000	-1.013560000	-1.592311000
Zn	1.145569000	0.615037000	0.000000000
Cu	-1.193825000	1.382371000	0.000000000

CuZn₃O₃ (2.36 eV C₁ ⁴A)

O	1.336664000	0.011675000	-0.000100000
O	-1.893514000	-1.772054000	-0.000022000
O	-1.267916000	1.034646000	0.000032000
Zn	3.024325000	-0.688099000	0.000042000
Zn	0.485649000	1.828228000	-0.000012000
Zn	-2.702061000	-0.139010000	0.000037000
Cu	-0.332388000	-0.835438000	-0.000044000

CuZn₃O₃ (2.75 eV C₁ ⁴A)

O	1.504591000	1.541126000	-0.153627000
O	-0.818549000	-0.769423000	0.031267000
O	-2.100353000	1.430843000	0.369035000
Zn	0.890387000	-1.450749000	0.101919000
Zn	-0.278530000	1.211622000	0.019771000
Zn	-2.724211000	-0.479494000	-0.126939000
Cu	2.575348000	0.135802000	-0.062619000

CuZn₃O₃ (5.06 eV C_s ⁶A'')

O	-0.871512000	-0.808319000	0.000000000
O	-1.838220000	1.711487000	0.000000000
O	1.618171000	1.701187000	0.000000000
Zn	-2.742814000	-0.134516000	0.000000000
Zn	3.250168000	0.917770000	0.000000000
Zn	0.000000000	0.928320000	0.000000000
Cu	-0.223728000	-2.489037000	0.000000000

Cu₂Zn₃O₃

Cu₂Zn₃O₃ (0.00 eV C_s ¹A')

O	-1.176162000	-2.117461000	0.000000000
O	2.360354000	-1.904257000	0.000000000
O	1.798270000	1.576879000	0.000000000
Zn	0.588499000	-2.210679000	0.000000000
Zn	0.000000000	1.526329000	0.000000000
Zn	2.340962000	-0.123374000	0.000000000
Cu	-1.536078000	-0.361421000	0.000000000
Cu	-2.317148000	1.871436000	0.000000000

Cu₂Zn₃O₃ (0.39 eV C₁ ¹A)

O	0.160095000	-1.890211000	0.618540000
O	2.439513000	0.341744000	-0.852010000
O	-0.369673000	1.758668000	0.686445000
Zn	-1.849379000	0.974459000	-0.479159000
Zn	1.209557000	1.493007000	-0.185232000
Zn	1.556765000	-1.132334000	-0.275218000
Cu	-0.203256000	-0.091055000	1.319330000
Cu	-1.360459000	-1.348103000	-0.472280000

Cu₂Zn₃O₃ (0.53 eV C₁ ¹A)

O	1.871751000	-0.086793000	0.354055000
O	-0.783633000	2.298503000	0.027691000
O	-3.174911000	-0.290921000	-0.165335000
Zn	0.608518000	1.203655000	0.162651000
Zn	-1.790103000	-1.521618000	-0.044730000
Zn	-2.191627000	1.182498000	-0.086711000
Cu	0.509554000	-1.462986000	0.123563000
Cu	3.555643000	0.038767000	-0.215548000

Cu₂Zn₃O₃ (0.65 eV C_s ¹A')

O	-1.492951000	1.478193000	0.000000000
O	-1.659937000	-2.056780000	0.000000000
O	1.850702000	-1.736714000	0.000000000
Zn	-1.850843000	-0.280024000	0.000000000
Zn	1.809206000	0.104371000	0.000000000
Zn	0.132575000	-2.188814000	0.000000000
Cu	0.132575000	1.542352000	1.154761000
Cu	0.132575000	1.542352000	-1.154761000

Cu₂Zn₃O₃ (0.77 eV C₁ ¹A)

O	1.212996000	2.143136000	0.189634000
O	2.316304000	-1.180200000	-0.384226000
O	-1.123172000	-1.667803000	0.172862000
Zn	1.998694000	0.579241000	-0.115387000
Zn	-1.992572000	-0.108107000	-0.806763000
Zn	0.643485000	-1.775608000	-0.202367000
Cu	-0.496412000	1.684268000	-0.211737000
Cu	-0.839355000	-0.140367000	1.381026000

Cu₂Zn₃O₃ (0.78 eV C_s ¹A')

O	-2.782502000	-1.625798000	0.000000000
O	-1.720029000	1.762392000	0.000000000
O	1.666572000	0.635034000	0.000000000

Zn	-2.463275000	0.108860000	0.000000000
Zn	1.220690000	-1.349990000	0.000000000
Zn	0.000000000	1.364946000	0.000000000
Cu	-1.013141000	-2.071000000	0.000000000
Cu	3.080907000	1.730051000	0.000000000

Cu₂Zn₃O₃ (0.92 eV C₁ ¹A)

O	2.501010000	0.389621000	-0.786039000
O	0.146831000	-1.922628000	0.435202000
O	-2.481858000	0.027656000	-0.778101000
Zn	1.600827000	-1.068903000	-0.342275000
Zn	-1.333689000	1.379467000	-0.164908000
Zn	-1.401323000	-1.317584000	-0.345609000
Cu	1.091996000	1.457270000	-0.200796000
Cu	0.035510000	-0.000257000	1.394426000

Cu₂Zn₃O₃ (1.43 eV C₁ ¹A)

O	0.695474000	2.647692000	-0.006364000
O	-1.639243000	-0.071270000	0.323399000
O	1.024116000	-2.451057000	0.031152000
Zn	-0.575703000	1.460498000	0.155549000
Zn	2.330267000	-1.061735000	-0.114689000
Zn	-0.395646000	-1.443139000	0.172801000
Cu	1.919696000	1.232469000	-0.091692000
Cu	-3.347638000	-0.186663000	-0.225388000

Cu₂Zn₃O₃ (1.59 eV C₁ ³A)

O	1.406630000	-1.061532000	0.576809000
O	0.630569000	2.328017000	0.073317000
O	-1.928902000	-0.074779000	-0.378540000
Zn	-3.635212000	-0.658251000	0.049076000
Zn	-0.873883000	1.427687000	-0.155748000
Zn	1.841173000	0.911059000	0.199674000
Cu	-0.326157000	-0.994842000	0.074371000
Cu	3.056201000	-1.072348000	-0.245501000

Cu₂Zn₃O₃ (2.12 eV C₁ ³A)

O	0.419279000	2.264625000	-0.206282000
O	-2.654230000	0.647971000	0.507044000
O	-0.909108000	-2.302173000	-0.300905000
Zn	-1.212052000	1.645390000	0.190992000
Zn	0.623260000	-1.349018000	-0.593881000
Zn	-2.031657000	-0.993883000	0.147396000
Cu	1.386745000	0.911045000	-0.835823000

Cu	2.191390000	-0.357874000	1.100166000
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Cu₂Zn₃O₃ (3.89 eV C₁ ⁵A)

O	-1.037501000	-1.522956000	0.539003000
O	2.193416000	-1.108403000	-0.797654000
O	0.429383000	1.290940000	0.856905000
Zn	-0.765327000	1.925368000	-0.565373000
Zn	2.373958000	0.630209000	-0.098532000
Zn	0.590754000	-1.684943000	-0.352328000
Cu	-0.545093000	-0.038470000	1.519988000
Cu	-2.167456000	-0.492415000	-0.633748000

Cu₂Zn₃O₃ (4.26 eV C₁ ⁵A)

O	3.005857000	0.324552000	-0.000052000
O	0.106546000	2.449753000	0.000023000
O	-2.929863000	0.538165000	0.000047000
Zn	1.475310000	1.314426000	-0.000021000
Zn	-2.695724000	-1.301948000	-0.000002000
Zn	-1.332984000	1.363672000	0.000022000
Cu	2.592325000	-1.413262000	0.000053000
Cu	-0.001235000	-0.924127000	-0.000057000

Cu₃Zn₃O₃

Cu₃Zn₃O₃ (0.00 eV C₁ ²A)

O	2.092453000	-0.040345000	-0.856668000
O	-0.186096000	2.662376000	-0.311489000
O	-2.120014000	-0.061891000	0.838432000
Zn	1.127524000	1.485811000	-0.642573000
Zn	-1.800075000	-1.278689000	-0.728101000
Zn	-1.411119000	1.524188000	0.339741000
Cu	0.501956000	-1.126464000	-1.157487000
Cu	-0.315124000	-0.674197000	1.389112000
Cu	2.027629000	-0.696595000	0.925815000

Cu₃Zn₃O₃ (0.20 eV C₁ ²A)

O	-0.169662000	-2.171768000	-0.512469000
O	-3.379422000	-0.938970000	0.293117000
O	-1.800834000	2.205426000	0.085855000
Zn	-1.828767000	-1.763157000	-0.066175000
Zn	-0.078500000	1.699171000	-0.151404000
Zn	-2.811317000	0.751059000	0.226627000
Cu	0.908167000	-0.763274000	-0.262307000
Cu	3.215288000	-0.893096000	0.412064000

Cu	2.233677000	1.195347000	-0.122291000
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Cu₃Zn₃O₃ (0.20 eV C₁ ²A)

O	-2.028538000	2.059257000	-0.096119000
O	-2.619891000	-1.438262000	-0.446527000
O	0.714893000	-1.954520000	0.568543000
Zn	-2.441820000	0.349448000	-0.292880000
Zn	2.234034000	-1.196862000	-0.412689000
Zn	-0.992759000	-1.992356000	-0.000992000
Cu	-0.243778000	2.057564000	0.112335000
Cu	2.071352000	1.259124000	-0.352280000
Cu	0.499483000	-0.011125000	0.963726000

Cu₃Zn₃O₃ (0.22 eV C₁ ²A)

O	-2.967103000	-1.010137000	-0.020470000
O	-0.009170000	-2.966903000	0.004350000
O	1.912069000	0.027353000	0.038477000
Zn	-1.616234000	-2.131326000	-0.009346000
Zn	3.723947000	0.432518000	-0.023203000
Zn	1.066380000	-1.571492000	0.019394000
Cu	-2.030756000	0.547795000	-0.007798000
Cu	-1.303450000	2.781779000	0.003493000
Cu	0.344236000	1.143064000	0.011746000

Cu₃Zn₃O₃ (0.30 eV C₁ ²A)

O	0.407130000	-2.122847000	-0.202424000
O	2.871816000	0.343604000	-0.869447000
O	0.392050000	2.385118000	0.585127000
Zn	1.803428000	-1.071352000	-0.658873000
Zn	-0.823823000	1.004044000	0.710753000
Zn	1.809588000	1.603183000	-0.144557000
Cu	-1.156180000	-1.074255000	-0.598517000
Cu	-2.813132000	0.565783000	-0.694342000
Cu	0.071252000	-1.247502000	1.523005000

Cu₃Zn₃O₃ (0.31 eV C₁ ²A)

O	0.905547000	-1.755479000	0.582900000
O	-2.554381000	-1.865867000	-0.130576000
O	-2.407163000	1.661690000	-0.157110000
Zn	-0.807052000	-2.048390000	0.186796000
Zn	-0.630809000	1.973310000	0.012121000
Zn	-2.698347000	-0.085670000	-0.174354000
Cu	1.190964000	0.122548000	0.314885000
Cu	1.667519000	2.367892000	-0.035663000

Cu	2.539249000	-1.783551000	-0.386071000
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Cu₃Zn₃O₃ (0.33 eV C₁ ²A)

O	0.591144000	2.328505000	0.593775000
O	2.962918000	0.145163000	-0.854349000
O	0.364993000	-2.058812000	0.039367000
Zn	1.936538000	1.461873000	-0.164959000
Zn	-0.137690000	-0.936523000	1.645572000
Zn	1.832401000	-1.201704000	-0.569132000
Cu	-2.872601000	0.490827000	-0.627258000
Cu	-0.793410000	1.177881000	0.372946000
Cu	-1.171571000	-1.083473000	-0.627575000

Cu₃Zn₃O₃ (0.44 eV C₁ ²A)

O	-3.024033000	-0.273578000	-0.741949000
O	-0.263526000	-2.004564000	0.619485000
O	2.859924000	-0.941667000	-0.575647000
Zn	-1.819198000	-1.440651000	-0.190837000
Zn	2.282853000	0.806964000	-0.283636000
Zn	1.397586000	-1.806023000	-0.084097000
Cu	-2.002642000	1.168413000	-0.207585000
Cu	0.325928000	2.181945000	0.053995000
Cu	-0.130739000	0.061704000	0.924004000

Cu₃Zn₃O₃ (0.45 eV C₁ ²A)

O	0.706835000	2.482211000	0.062542000
O	-2.258148000	0.622024000	-0.496475000
O	-0.149118000	-2.161638000	-0.175527000
Zn	-0.841437000	1.684992000	-0.184678000
Zn	1.344364000	-1.201226000	-0.045466000
Zn	-1.710813000	-1.241552000	-0.163394000
Cu	1.898225000	1.138783000	0.086396000
Cu	3.588181000	-0.506246000	0.130840000
Cu	-3.767784000	-0.108647000	0.357999000

Cu₃Zn₃O₃ (0.47 eV C₁ ²A)

O	1.837543000	2.283611000	-0.000001000
O	-1.704096000	2.351171000	0.000001000
O	-1.284640000	-1.130172000	-0.000029000
Zn	0.076089000	2.428231000	0.000002000
Zn	0.526524000	-1.191619000	-0.000017000
Zn	-2.152803000	0.606046000	-0.000009000
Cu	2.185639000	0.533136000	0.000011000
Cu	2.819193000	-1.747243000	0.000003000

Cu	-3.083617000	-1.658881000	0.000018000
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Cu₃Zn₃O₃ (0.80 eV C₁ ²A)

O	0.782735000	-1.837286000	0.100944000
O	2.532962000	0.658363000	0.069984000
O	-0.473142000	2.527135000	-0.138423000
Zn	2.047729000	-0.937017000	-1.164210000
Zn	-1.593033000	1.121911000	-0.068853000
Zn	1.153213000	1.788210000	-0.040374000
Cu	-0.903339000	-1.205476000	0.055687000
Cu	-3.190083000	-0.592569000	-0.062159000
Cu	1.645915000	-0.615017000	1.314853000

Cu₃Zn₃O₃ (1.74 eV C₁ ⁴A)

O	-0.919206000	-1.859616000	0.438114000
O	2.518412000	-1.549810000	-0.481381000
O	2.121622000	1.944825000	-0.104116000
Zn	0.828828000	-1.906583000	-0.051629000
Zn	0.307155000	1.893639000	0.172509000
Zn	2.555313000	0.236558000	-0.314546000
Cu	-2.220388000	-1.032239000	-0.581027000
Cu	-1.893143000	1.322226000	-0.549726000
Cu	-0.731487000	-0.117283000	1.371754000

Cu₃Zn₃O₃ (1.76 eV C₁ ⁴A)

O	-2.502365000	-1.304250000	-0.024553000
O	-1.892157000	2.143987000	-0.523248000
O	1.316163000	1.419739000	0.772355000
Zn	-2.397799000	0.434212000	-0.345340000
Zn	0.705988000	-0.404175000	1.421259000
Zn	-0.212721000	2.065200000	0.057301000
Cu	1.231781000	-1.418328000	-0.878096000
Cu	-0.863700000	-2.003426000	0.150176000
Cu	2.451326000	0.630965000	-0.506322000

Cu₃Zn₃O₃ (1.84 eV C₁ ⁴A)

O	2.489364000	-0.312408000	-0.562022000
O	0.431976000	2.615345000	-0.289491000
O	-2.095958000	0.353940000	0.825750000
Zn	1.619635000	1.277724000	-0.489354000
Zn	-3.065693000	-0.666350000	-0.431763000
Zn	-0.961489000	1.675091000	0.295893000
Cu	0.940351000	-1.316133000	-1.203174000
Cu	-0.522660000	-0.863871000	0.697853000

Cu	1.845184000	-0.918236000	1.159211000
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Cu₃Zn₃O₃ (1.85 eV C₁ ⁴A)

O	-2.395661000	1.437036000	-0.413427000
O	-1.969555000	-2.096305000	-0.506304000
O	1.327848000	-1.560613000	0.735698000
Zn	-2.351123000	-0.341160000	-0.489238000
Zn	2.542727000	-0.652488000	-0.459490000
Zn	-0.309094000	-2.102964000	0.138198000
Cu	-0.919062000	1.944877000	0.461167000
Cu	1.360972000	1.678492000	-0.655152000
Cu	0.517525000	0.192404000	1.083232000

Cu₃Zn₃O₃ (2.24 eV C₁ ⁴A)

O	1.263436000	-2.315629000	-0.461577000
O	3.448316000	0.328595000	0.392850000
O	0.604750000	2.394665000	0.056923000
Zn	2.543913000	-1.144031000	-0.014815000
Zn	-0.764819000	1.246335000	-0.339866000
Zn	2.138518000	1.548588000	0.268818000
Cu	-0.260398000	-1.378938000	-0.538708000
Cu	-3.082196000	0.722113000	-0.205249000
Cu	-2.176729000	-1.163444000	0.836037000

Cu₃Zn₃O₃ (2.32 eV C₁ ⁴A)

O	2.386395000	1.503048000	-0.423638000
O	-0.901923000	2.395718000	0.555442000
O	-1.532834000	-1.029344000	0.154691000
Zn	0.767931000	2.082136000	0.087916000
Zn	0.188565000	-1.280672000	-0.415185000
Zn	-1.919059000	0.898217000	0.360452000
Cu	2.216778000	-0.177067000	-0.966479000
Cu	2.146496000	-1.457275000	1.129535000
Cu	-3.354178000	-0.915514000	-0.276417000

Cu₃Zn₃O₃ (4.27 eV C_s ⁶A')

O	-0.286883000	-1.933867000	0.000000000
O	-3.061370000	0.360412000	0.000000000
O	-0.538694000	2.831427000	0.000000000
Zn	-1.816841000	-0.912006000	0.000000000
Zn	0.834745000	1.600603000	0.000000000
Zn	-1.994125000	1.811609000	0.000000000
Cu	0.834745000	-1.324815000	1.409795000
Cu	2.481622000	-0.283816000	0.000000000

Cu	0.834745000	-1.324815000	-1.409795000
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Cu₃Zn₃O₃ (4.80 eV C_s ⁶A')

O	2.455107000	-0.123056000	0.000000000
O	0.967758000	-3.318309000	0.000000000
O	-2.113245000	-1.593978000	0.000000000
Zn	1.923904000	-1.822894000	0.000000000
Zn	-1.498775000	0.132578000	0.000000000
Zn	-0.697019000	-2.654823000	0.000000000
Cu	1.314029000	1.240736000	0.000000000
Cu	-0.697019000	2.321648000	1.134027000
Cu	-0.697019000	2.321648000	-1.134027000

Cu₃Zn₃O₃ (4.89 eV C₁ ⁶A)

O	-2.817707000	-0.892442000	-0.141591000
O	0.050768000	-2.975700000	-0.323072000
O	1.959223000	-0.070109000	0.464953000
Zn	-1.508296000	-2.083638000	-0.284334000
Zn	3.592854000	0.665001000	-0.012679000
Zn	1.171121000	-1.649059000	0.050971000
Cu	-2.108196000	0.540133000	0.694424000
Cu	-1.374582000	2.602630000	-0.465729000
Cu	0.337652000	1.117130000	0.025751000

Cu₄Zn₃O₃

Cu₄Zn₃O₃ (0.00 eV C₁ ¹A)

O	0.240771000	2.246950000	0.653081000
O	1.977586000	0.678924000	-2.032793000
O	0.627996000	-2.167374000	-0.398766000
Zn	1.202159000	1.711459000	-0.785647000
Zn	1.117511000	-1.532332000	1.444029000
Zn	1.418249000	-0.917108000	-1.442366000
Cu	0.817032000	0.755601000	1.733184000
Cu	-1.051809000	-1.230210000	-0.321771000
Cu	-1.288899000	1.169691000	0.250394000
Cu	-3.128338000	-0.140894000	-0.360175000

Cu₄Zn₃O₃ (0.10 eV C₁ ¹A)

O	0.197462000	1.929077000	0.934138000
O	-2.842697000	1.507508000	-0.855068000
O	-2.504142000	-1.992173000	-0.443520000
Zn	-1.332457000	1.929182000	-0.013101000
Zn	-0.847343000	-1.946200000	0.340078000

Zn	-2.875314000	-0.284126000	-0.749098000
Cu	0.029833000	0.053275000	1.387185000
Cu	1.511220000	-1.246677000	0.075653000
Cu	1.728297000	1.240152000	0.001638000
Cu	3.380597000	-0.133682000	-0.927261000

Cu₄Zn₃O₃ (0.41 eV C₁ ¹A)

O	0.254244000	2.345292000	-0.035309000
O	-1.181022000	-2.073804000	0.072571000
O	1.628571000	-0.475073000	-1.679984000
Zn	0.691335000	1.112675000	1.460271000
Zn	0.899701000	1.147935000	-1.272253000
Zn	-2.337475000	-0.559799000	-0.168945000
Cu	2.037228000	-0.603533000	0.282907000
Cu	-0.087517000	-1.186556000	1.383833000
Cu	-1.538143000	1.602971000	-0.154155000
Cu	0.167012000	-1.516181000	-1.079151000

Cu₄Zn₃O₃ (0.43 eV C₁ ¹A)

O	-0.219082000	1.976280000	0.470414000
O	3.212157000	1.553102000	-0.265113000
O	2.706106000	-1.938625000	-0.079425000
Zn	1.510025000	1.961308000	0.056511000
Zn	0.890889000	-1.959309000	0.107809000
Zn	3.177449000	-0.236635000	-0.202780000
Cu	-0.604678000	0.077634000	0.467022000
Cu	-1.497143000	-1.954552000	-0.092663000
Cu	-3.224753000	-0.182054000	-0.165995000
Cu	-2.016334000	1.862869000	-0.203302000

Cu₄Zn₃O₃ (0.61 eV C_s ¹A')

O	0.931242000	2.074114000	0.000000000
O	-2.611534000	1.910019000	0.000000000
O	-1.865102000	-1.533913000	0.000000000
Zn	-0.863460000	2.261723000	0.000000000
Zn	-0.017891000	-1.333231000	0.000000000
Zn	-2.512574000	0.110963000	0.000000000
Cu	1.122249000	0.614083000	1.238975000
Cu	1.122249000	0.614083000	-1.238975000
Cu	1.122249000	-1.489694000	2.210233000
Cu	1.122249000	-1.489694000	-2.210233000

Cu₄Zn₃O₃ (0.71 eV C₁ ¹A)

O	1.330156000	-2.606936000	-0.772788000
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O	3.622343000	-0.077652000	0.166641000
O	1.402063000	2.651828000	0.480384000
Zn	2.523919000	-1.414895000	-0.289853000
Zn	-0.269881000	2.170352000	0.081471000
Zn	2.606677000	1.355778000	0.348886000
Cu	-0.302896000	-2.117695000	-0.222043000
Cu	-1.502535000	-0.047703000	-0.045490000
Cu	-2.467424000	-2.058671000	0.680164000
Cu	-2.508453000	2.049069000	-0.523287000

Cu₄Zn₃O₃ (0.88 eV C_s ¹A')

O	-2.040959000	1.548749000	0.000000000
O	-3.180665000	-1.804991000	0.000000000
O	-0.107139000	-3.549502000	0.000000000
Zn	-2.659118000	-0.104565000	0.000000000
Zn	1.054039000	-2.142178000	0.000000000
Zn	-1.721177000	-2.821946000	0.000000000
Cu	-0.263722000	1.643341000	0.000000000
Cu	1.724893000	0.079959000	0.000000000
Cu	1.724893000	2.285016000	1.165352000
Cu	1.724893000	2.285016000	-1.165352000

Cu₄Zn₃O₃ (1.07 eV C₁ ¹A)

O	0.885096000	2.134394000	0.902690000
O	-0.620968000	-0.887788000	1.817606000
O	-1.461001000	-1.379440000	-1.077371000
Zn	-0.054145000	0.816904000	1.764166000
Zn	-1.559283000	0.446139000	-1.659654000
Zn	0.188558000	-1.296885000	-0.076963000
Cu	1.812310000	0.707568000	0.008270000
Cu	-0.337760000	2.104264000	-0.602804000
Cu	2.533113000	-1.439928000	-0.607303000
Cu	-2.203487000	-1.300252000	0.720118000

Cu₄Zn₃O₃ (1.20 eV C₁ ³A)

O	1.642767000	1.844459000	-0.485411000
O	-1.869912000	2.442067000	-0.340143000
O	-2.933091000	-0.850004000	0.410987000
Zn	-0.109743000	2.258294000	-0.427153000
Zn	-1.351530000	-1.764673000	0.441257000
Zn	-2.554247000	0.838499000	0.045426000
Cu	2.010090000	1.008341000	1.176684000
Cu	1.527311000	0.002648000	-1.097113000
Cu	0.929985000	-1.148377000	1.051908000

Cu	0.558389000	-2.188674000	-1.078698000
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Cu₄Zn₃O₃ (1.27 eV C₁ ¹A)

O	2.418108000	-1.028448000	-0.594172000
O	1.446439000	2.380427000	-0.929692000
O	-1.416721000	1.584470000	1.028751000
Zn	2.117696000	0.713619000	-0.902834000
Zn	-1.936949000	-1.518167000	-0.747728000
Zn	-0.038821000	2.191851000	0.037954000
Cu	1.821494000	-0.931825000	1.308440000
Cu	0.541774000	-1.714731000	-0.521141000
Cu	-0.547663000	-0.228185000	1.068587000
Cu	-2.637688000	0.629543000	-0.051086000

Cu₄Zn₃O₃ (1.29 eV C₁ ³A)

O	-0.429740000	1.837484000	0.719671000
O	2.963970000	1.714592000	-0.331687000
O	2.749365000	-1.813528000	-0.241028000
Zn	1.269719000	1.974583000	0.144088000
Zn	0.971301000	-1.912527000	0.167345000
Zn	3.086457000	-0.074401000	-0.342666000
Cu	-0.590664000	-0.069096000	0.598855000
Cu	-1.469401000	-2.182884000	0.023116000
Cu	-2.847799000	-0.238390000	-0.463751000
Cu	-2.060861000	2.023541000	-0.166450000

Cu₄Zn₃O₃ (1.64 eV C₁ ¹A)

O	1.973210000	-0.115534000	0.019518000
O	-0.428347000	2.595987000	-0.405081000
O	-2.808106000	0.022821000	-0.134594000
Zn	0.798714000	1.349913000	0.071000000
Zn	-1.841906000	-1.360069000	-1.249214000
Zn	-1.887693000	1.557567000	-0.371559000
Cu	0.830681000	-0.558384000	1.919547000
Cu	0.402213000	-1.299792000	-0.514781000
Cu	-1.394079000	-0.454389000	1.200595000
Cu	3.541615000	0.021237000	-0.858655000

Cu₄Zn₃O₃ (1.79 eV C₁ ³A)

O	-1.069296000	2.013343000	0.485207000
O	0.042666000	-2.058879000	-0.437167000
O	1.830147000	1.016569000	-1.339856000
Zn	-0.847942000	0.413293000	1.688249000
Zn	0.402229000	1.790073000	-0.539360000

Zn	-1.765660000	-1.464351000	-0.636678000
Cu	2.574002000	0.265472000	0.333206000
Cu	0.869488000	-1.374661000	1.126038000
Cu	-2.346257000	0.758558000	-0.335471000
Cu	0.968735000	-0.681739000	-1.297283000

Cu₄Zn₃O₃ (1.80 eV C₁ ³A)

O	0.975856000	1.761929000	-0.829562000
O	2.124413000	-1.538600000	-1.514693000
O	-0.135027000	-1.907761000	1.164974000
Zn	1.783589000	0.223216000	-1.390837000
Zn	0.080919000	-0.017138000	1.892660000
Zn	1.047582000	-2.057388000	-0.180030000
Cu	1.648122000	1.765985000	0.945505000
Cu	-1.645174000	-1.009799000	0.345497000
Cu	-0.788815000	1.129084000	-0.525886000
Cu	-3.044638000	0.494548000	-0.772686000

Cu₄Zn₃O₃ (1.90 eV C₁ ¹A)

O	0.362250000	-2.644016000	-0.030156000
O	-2.471504000	-0.468489000	-0.292823000
O	-1.468927000	2.942375000	-0.047712000
Zn	-0.951909000	-1.522443000	-0.149126000
Zn	0.377427000	2.543368000	0.069088000
Zn	-2.118042000	1.329972000	-0.162974000
Cu	1.848946000	-1.568591000	0.004058000
Cu	2.038291000	0.887374000	0.095045000
Cu	3.937662000	-0.532426000	0.010442000
Cu	-4.052444000	-1.171387000	0.244106000

Cu₄Zn₃O₃ (2.17 eV C₁ ¹A)

O	0.167639000	1.906911000	0.707513000
O	1.922941000	-0.775165000	-0.618896000
O	-1.452332000	-1.916901000	-0.807600000
Zn	1.718291000	0.948158000	0.364381000
Zn	-2.067944000	-1.467068000	1.070684000
Zn	0.323389000	-1.563333000	-0.841043000
Cu	-0.880752000	2.228938000	-0.809872000
Cu	-1.151768000	0.684179000	1.321040000
Cu	-1.720639000	0.007402000	-1.135559000
Cu	3.604261000	-0.549880000	0.208225000

Cu₄Zn₃O₃ (2.20 eV C₁ ¹A)

O	-1.630662000	-1.645683000	-1.034035000
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O	1.812768000	-1.062042000	0.073063000
O	0.379962000	1.928456000	0.947659000
Zn	0.075397000	-1.533308000	-0.321762000
Zn	-0.804288000	2.232785000	-0.626919000
Zn	1.783953000	0.817516000	0.556686000
Cu	-2.224447000	-1.385166000	0.779622000
Cu	-1.773693000	0.238050000	-1.335059000
Cu	-0.786299000	0.432118000	1.427165000
Cu	3.537943000	-0.639335000	-0.462544000

Cu₄Zn₃O₃ (3.41 eV C₁ ⁵A)

O	-1.320854000	1.396983000	0.842083000
O	0.304614000	-2.174232000	-0.912752000
O	1.350618000	1.312173000	-1.105279000
Zn	-0.043458000	0.253957000	1.765670000
Zn	-0.381298000	2.212403000	-0.781330000
Zn	-1.412530000	-1.635330000	-0.541236000
Cu	2.291517000	0.689982000	0.367518000
Cu	1.277015000	-1.495050000	0.687493000
Cu	-2.587904000	0.236329000	0.281128000
Cu	0.827772000	-0.438513000	-1.470123000

Cu₄Zn₃O₃ (3.43 eV C₁ ⁵A)

O	0.897065000	1.874955000	0.798986000
O	-2.559244000	1.608196000	-0.259858000
O	-2.270120000	-1.901724000	0.189485000
Zn	-0.805125000	1.862070000	0.048759000
Zn	-0.432292000	-1.806692000	0.259068000
Zn	-2.655041000	-0.178071000	-0.094090000
Cu	0.743346000	0.116467000	1.633870000
Cu	1.937034000	-1.340186000	-0.103499000
Cu	2.089077000	1.105279000	-0.406845000
Cu	0.341996000	-0.190892000	-1.545630000

Cu₄Zn₃O₃ (3.58 eV C_s ⁵A')

O	1.240291000	1.972973000	0.000000000
O	-2.254006000	2.627943000	0.000000000
O	-2.663998000	-0.887196000	0.000000000
Zn	-0.481364000	2.535859000	0.000000000
Zn	-0.900441000	-1.421039000	0.000000000
Zn	-2.687111000	0.880568000	0.000000000
Cu	1.305941000	0.413491000	1.159472000
Cu	1.305941000	0.413491000	-1.159472000
Cu	1.305941000	-1.957826000	1.158826000

Cu	1.305941000	-1.957826000	-1.158826000
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Cu₄Zn₃O₃ (3.59 eV C₁ ⁵A)

O	-1.089817000	1.947741000	0.662855000
O	2.365879000	2.285906000	-0.188424000
O	3.134899000	-1.167417000	-0.412829000
Zn	0.643558000	2.242393000	0.223469000
Zn	1.563791000	-2.050977000	-0.124733000
Zn	2.878631000	0.577381000	-0.314380000
Cu	-0.811920000	-0.024792000	1.037580000
Cu	-0.746820000	-2.277818000	0.270880000
Cu	-2.507593000	-0.866145000	-0.568639000
Cu	-2.411841000	1.527590000	-0.533735000

Cu₄Zn₃O₃ (4.18 eV C₁ ⁵A)

O	1.064930000	1.573186000	-0.995420000
O	2.025553000	-1.828606000	-1.354356000
O	-0.264716000	-1.701751000	1.325082000
Zn	1.816677000	-0.035455000	-1.464231000
Zn	0.236155000	0.247588000	1.888802000
Zn	0.914548000	-2.100627000	0.016705000
Cu	1.844372000	1.759335000	0.712416000
Cu	-1.698904000	-0.779075000	0.502568000
Cu	-0.812789000	1.129315000	-0.615708000
Cu	-3.181904000	0.383949000	-0.773094000