

Supplementary information

for the paper

ZnO Nested Shell Magic Clusters as Tetrapod Nuclei

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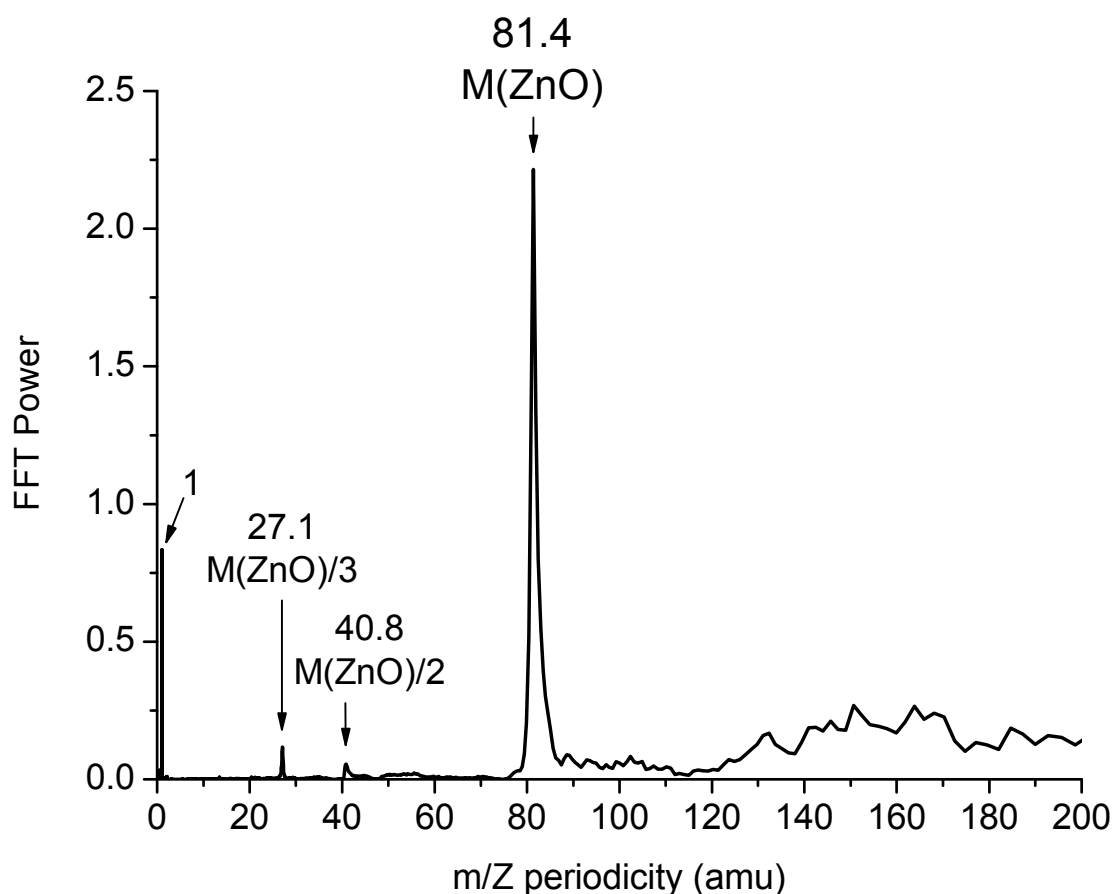


Figure S1. The Fourier transformed TOF mass spectrum of ZnO clusters shown in gray in Figure 1. The FFT power spectrum indicates what frequencies carry most of the energy. The main peak at 81.4 amu corresponds to the mass of $(\text{ZnO})_1$ monomer. The peaks at 40.8 amu and 27.1 amu represent the numbers of double and triple charged ZnO clusters: obviously, they are negligible small. The peak at 1 amu indicates the resolution of the mass spectrometer high enough to resolve the isotopic structure of the clusters, although this structure is observable only for small clusters (see Figure S3).

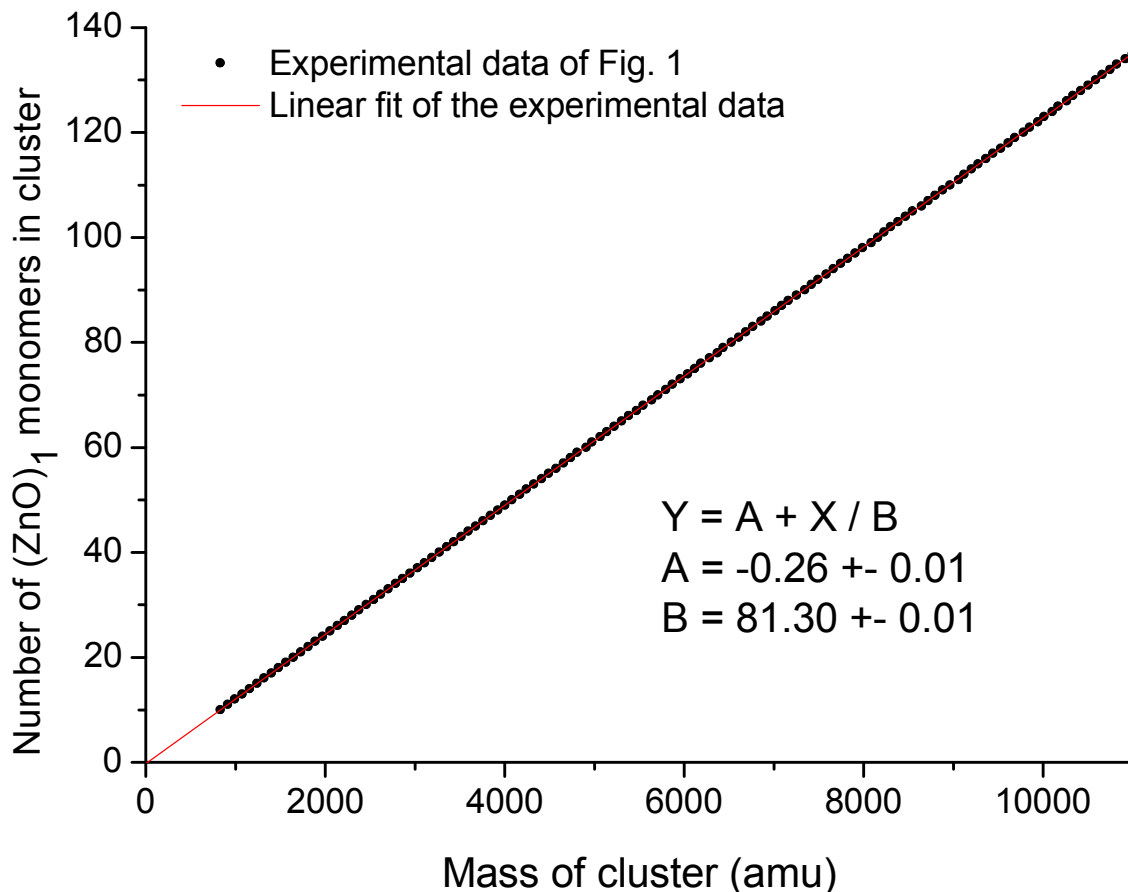


Figure S2. The linear fit (red line) of the series of experimentally detected ZnO clusters (black dots) in the region of masses where the series can be uninterruptedly traced. The dots are the peak positions in the smoothed mass spectrum of Figure 1. Extrapolation of the linear fit to the zero mass gives the y-intercept $A = -0.26$ amu (instrumental error) and, as it is less than 1 amu, proves the stoichiometric composition of the observed $(\text{ZnO})_n$ clusters. The slope $B = 81.3$ amu corresponds to the mass of $(\text{ZnO})_1$ monomer.

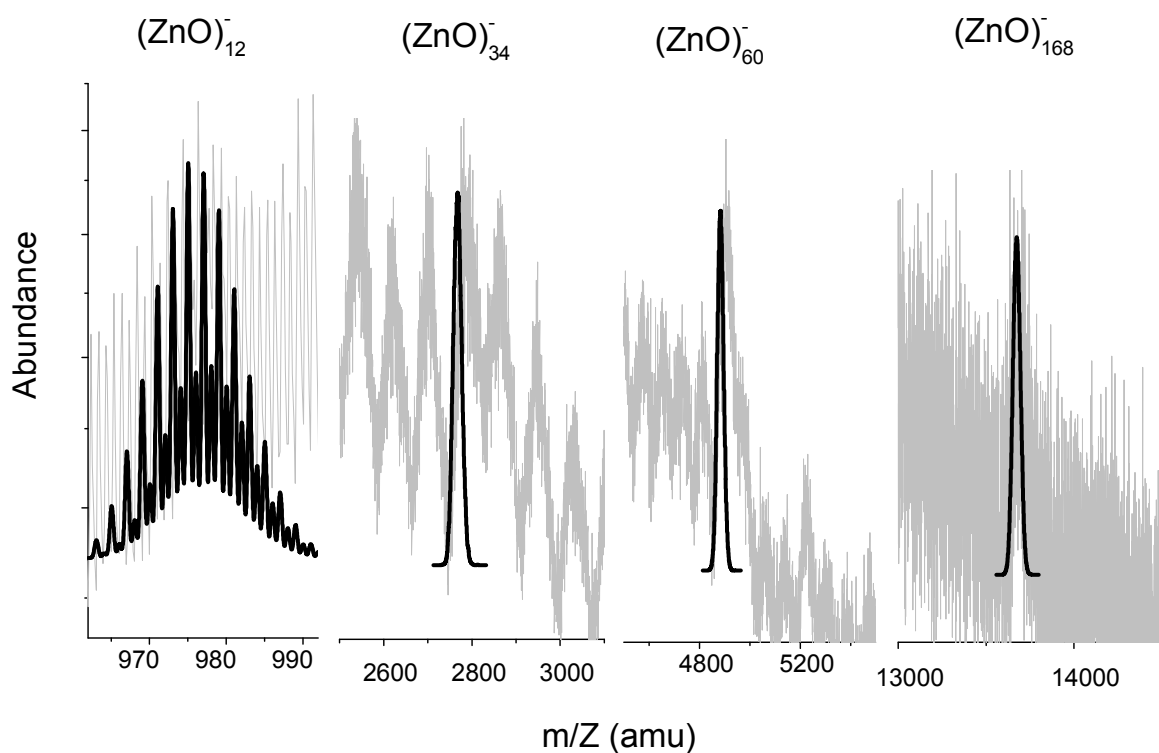


Figure S3. The fragments of the TOF mass spectrum of ZnO clusters (gray line of Figure 1) overlapped by the calculated patterns for the corresponding clusters (black lines) taking into account the natural isotopic distribution of constituting elements of the clusters. The patterns are calculated using ISOPRO software (<http://sites.google.com/site/isoproms/home>) based on Yergey's algorithm (J. A. Yergey. *Int. J. Mass Spectr. and Ion Physics* 1983, **52**, 337) using the following parameters: the empirical type, 30000 molecules, negatively charged by an electron, Gaussian peak shape, resolving power is 1600.

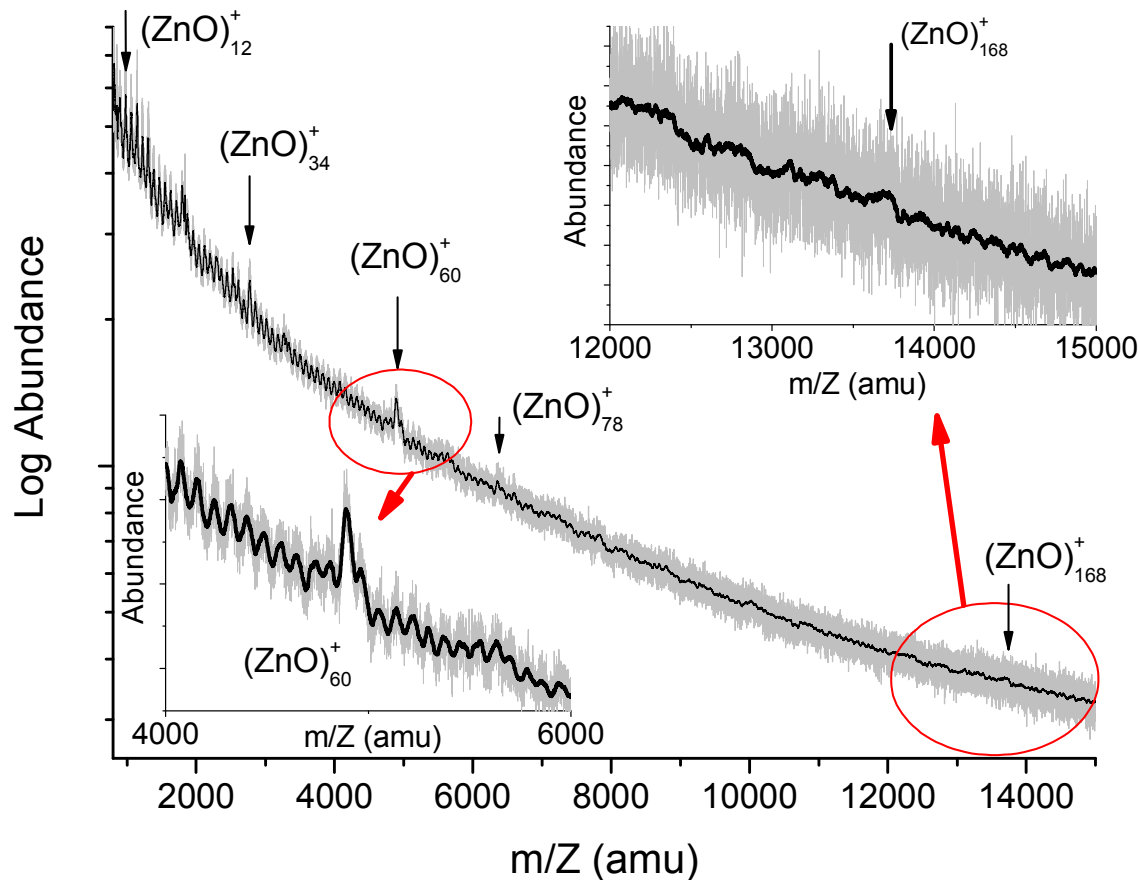


Figure S4. The TOF mass spectrum of positively charged ZnO clusters obtained by laser ablation of ZnO₂ powder mixed with octadecylamine in toluene. Gray line displays measured signal, black line shows the smoothed spectrum (50 point adjacent averaging). The clusters of enhanced stability are pointed and labeled. Insets show the fragments of the spectrum in the vicinity of (ZnO)₆₀ and (ZnO)₁₆₈ cluster mass regions.

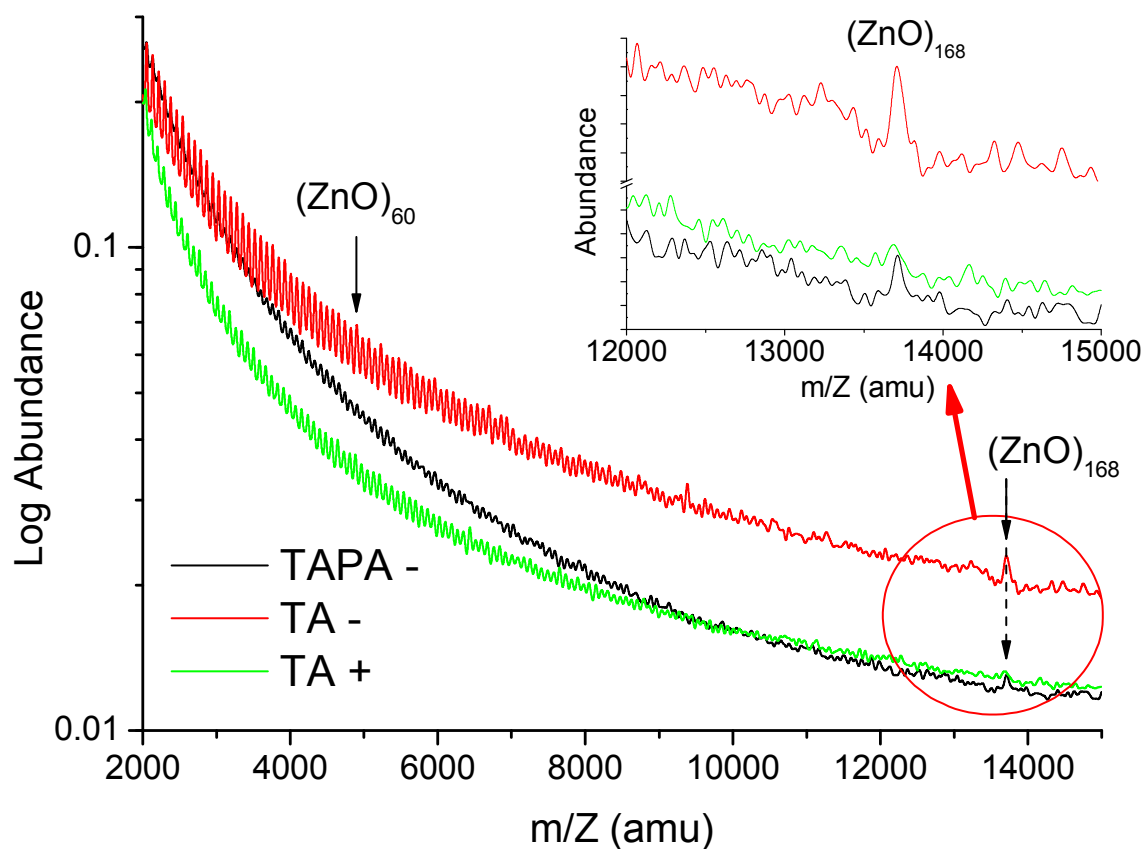
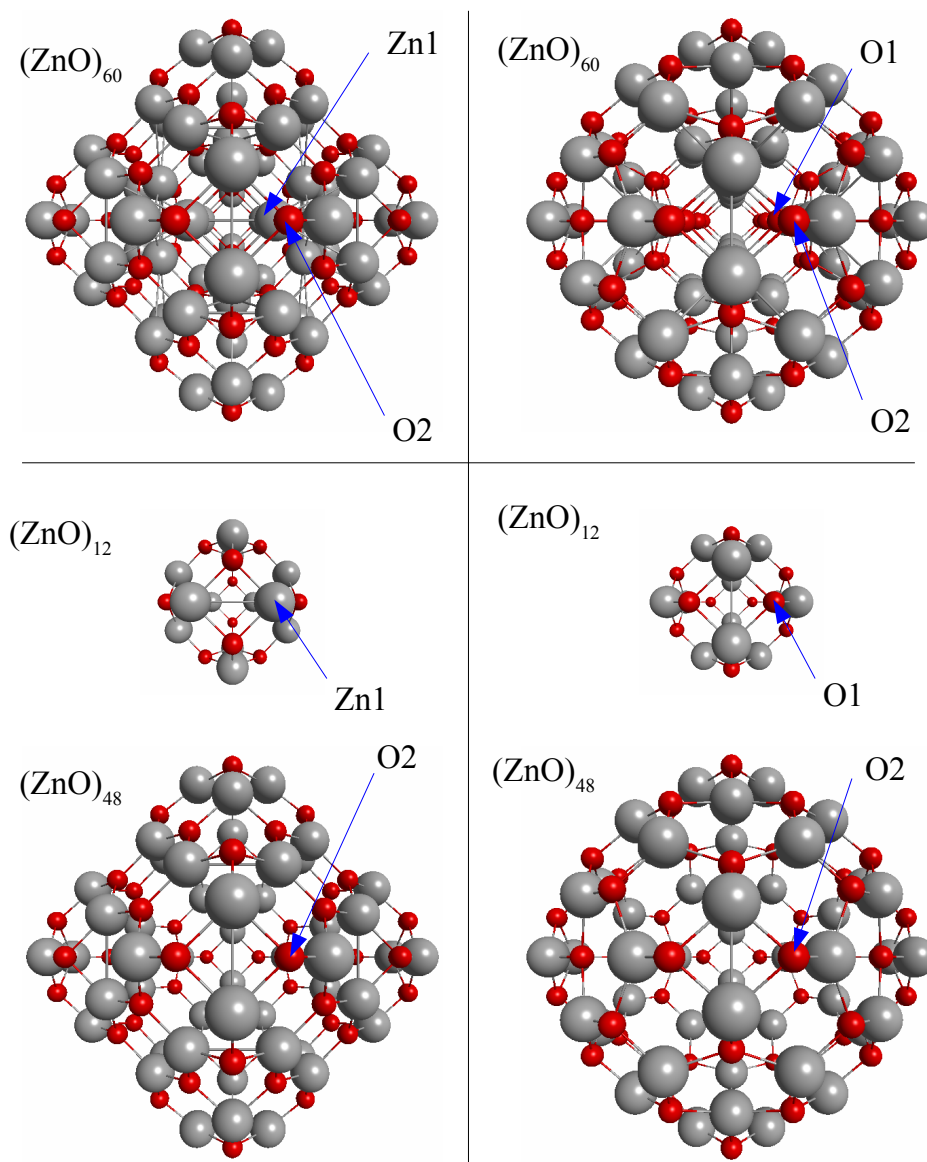


Figure S5. The TOF mass spectra of ZnO clusters obtained by laser ablation of ZnO_2 powder mixed with: trifluoroacetic acid (TA) and picolinic acid (PA) (negatively charged clusters, black line); TA (negatively charged, red line); TA (positively charged, green line). The spectra are 50 point FFT smoothed. Inset shows the fragments of the spectra in the vicinity of $(\text{ZnO})_{168}$ cluster mass region. The positively charged $(\text{ZnO})_{168}^+$ cluster is hardly detectable, same as in Figure S4, where it was produced with octadecylamine.



This paper

Wang et al. *J.Phys.Chem.C* 2010, **114**, 5741

Figure S6. Comparison of $(\text{ZnO})_{60}$ nested shell isomers. The top panel shows the onion-like structures of $(\text{ZnO})_{60}$ cluster, left and right, both composed of two concentric shells $(\text{ZnO})_{12}$ and $(\text{ZnO})_{48}$ but with the different orientation of the inner shells. Zinc atoms are shown as gray balls, Oxygen as red. The shown structures are optimized at B3LYP/6-31G theory level within T_h symmetry restrictions. The pictures in the down panel shows the inner and the outer shells vertically spaced one from the other for clarity of the explanation.

The top-left structure, suggested in this paper, is designed to alternate the type of the neighboring atoms of the adjoining tetragonal faces of the inner and the outer shells, as for example Zn1 and O2 in the left pictures. Such structure allows tight hetero-bonding between the shells, thus decreasing the total energy of the cluster.

In contrast, the top-right structure, considered by Wang *et al.* (*J. Phys. Chem. C* 2010, **114**, 5741) and later by Caddeo *et al.* (*Phys. Chem. Chem. Phys.* 2012, **14**, 14293), places the same element atoms of the different shells in proximity, as for example O1 and O2, thus forcing energetically unfavorable homo-bonding. Consequently, the right-panel (ZnO)₆₀ cluster appears swollen compare to the left one, and has higher total energy.

Table S1. The calculated energy differences of the nested cage (this paper), onion-like and sodalite (both from Wang *et al.* *J. Phys. Chem. C* 2010, **114**, 5741) isomers of (ZnO)₆₀ cluster.

	Symmetry restrictions	This paper: nested cage structure (Figure S6, left)	Wang <i>et al.</i>	
			Onion-like structure (Figure S6, right)	Sodalite structure (see Fig. S6_2 below)
Total energy difference with regard to this paper T _h structure	T _h	0	6.076 eV	
	C ₁	-0.234 eV	6.025 eV	5.521 eV

Our calculations at B3LYP/6-31G theory level show that the proposed in this paper T_h symmetric nested shell structure for (ZnO)₆₀ cluster has the total energy 6.076 eV lower than the total energy of the T_h symmetric onion-like structure proposed by Wang *et al.*, and it is 5.521 eV

lower in energy than the sodalite structure, which was found the most stable isomer of $(\text{ZnO})_{60}$ cluster by both Wang *et al.* and Caddeo *et al.* (*Phys. Chem. Chem. Phys.* 2012, **14**, 14293). In other words, our calculations confirm the findings of Wang *et al.* and Caddeo *et al.* in part that the sodalite structure is more stable than the onion-like structure, which they have constructed, but our nested shell structure, which is built of the same shells but alternatively oriented, is much more stable than any of those reported. Our symmetry reduced structure, C_1 , has even lower energy.

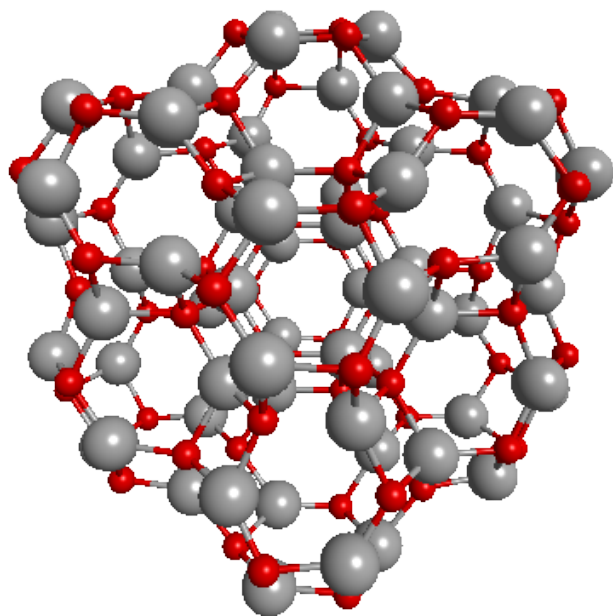


Figure S6_2. The B3LYP/6-31G optimized sodalite structure of $(\text{ZnO})_{60}$.

Table S2. The structures of $(\text{ZnO})_{60}$ cluster and its moieties, the shells $(\text{ZnO})_{12}$ and $(\text{ZnO})_{48}$, optimized at B3LYP/6-31G theory level within the restrictions of T_h symmetry point group (on the left) and C_1 (on the right). Zinc atoms are shown as gray balls, Oxygen as red. The root mean square displacement (RMSD) calculation does not take into account shift and rotation of the clusters as a whole, but just the difference between their structures.

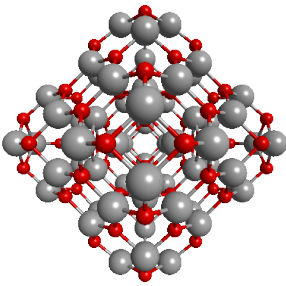
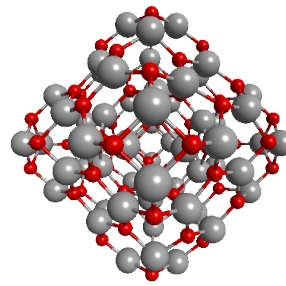
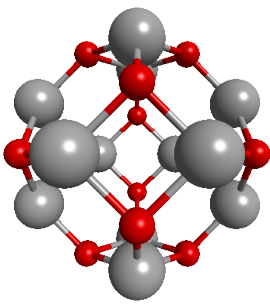
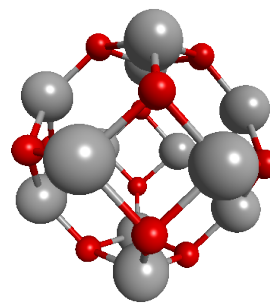
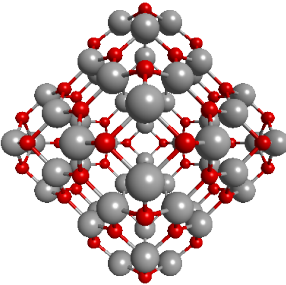
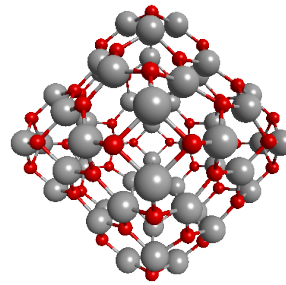
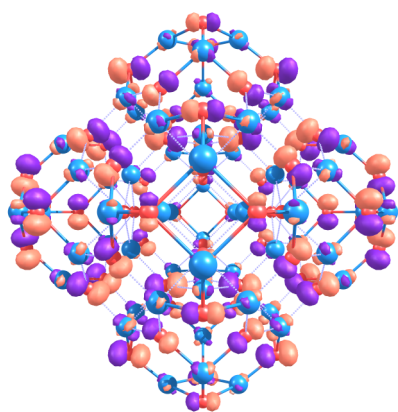
	T_h	RMSD, pm	C_1
$(\text{ZnO})_{60}$		22.1	
$(\text{ZnO})_{12}$		5.0	
$(\text{ZnO})_{48}$		20.6	

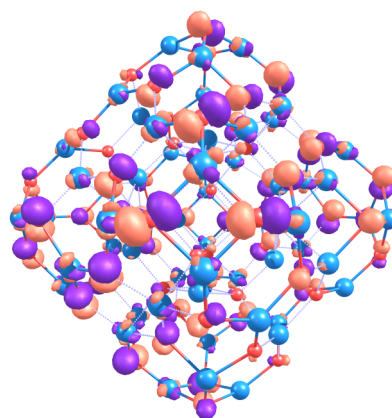
Table S3. The occupancies, energy levels and symmetries of molecular orbitals (MO) of (ZnO)₆₀ clusters of different symmetry point groups near the HOMO energy level, calculated within B3LYP/6-31G theory. Corresponding HOMO-LUMO gaps, the cluster total energies and their differences from the T_h symmetric structure, as well as the first 16 vibrational frequencies of Hessian analysis are listed in the bottom. The degenerate HOMO energies are marked **yellow**. The appearance of the imaginary first vibrational frequency in C_i, C₃ and S₆ structures could be an artifact of the calculations.

MO num ber	Occup ancy	T _h		C ₁		C _i		C ₃		S ₆	
		Energy, eV	Sym.	Energy, eV	Sym.	Energy, eV	Sym.	Energy, eV	Sym.	Energy, eV	Sym.
1133	occ.	-7.004	FG	-7.026	A	-7.026	AU	-7.023	E	-7.023	EU
1134	occ.	-7.004	FG	-7.015	A	-7.015	AG	-7.015	A	-7.015	AG
1135	occ.	-7.004	FG	-6.999	A	-6.999	AU	-6.999	A	-6.996	AU
1136	occ.	-6.966	EU	-6.985	A	-6.985	AU	-6.982	E	-6.982	EU
1137	occ.	-6.966	EU	-6.985	A	-6.982	AU	-6.982	E	-6.982	EU
1138	occ.	-6.814	FG	-6.855	A	-6.852	AG	-6.852	A	-6.849	AG
1139	occ.	-6.814	FG	-6.852	A	-6.849	AG	-6.849	E	-6.849	EG
1140	HOMO	-6.814	FG	-6.852	A	-6.849	AG	-6.849	E	-6.849	EG
1141	LUMO	-3.206	AG	-3.306	A	-3.306	AG	-3.306	A	-3.306	AG
1142	unocc.	-2.484	FU	-2.544	A	-2.544	AU	-2.544	A	-2.542	AU
1143	unocc.	-2.484	FU	-2.542	A	-2.542	AU	-2.542	E	-2.539	EU
1144	unocc.	-2.484	FU	-2.539	A	-2.539	AU	-2.542	E	-2.539	EU
HOMO-LUMO gap, eV		3.608		3.546		3.543		3.543		3.543	
Cluster total energy, Ha		-111265.61841		-111265.62702		-111265.62753		-111265.62748		-111265.62777	
Total energy difference, meV		0		-234		-248		-247		-255	

Hessian	-243.76	2.54	-115.04 ???	176.79 ???	-195.25 ???
analysis:	-40.45	2.38	3.4	23.4	9.22
the list of the	-40.45	2.34	2.39	23.4	9.22
first 16	-23.73	2.06	2.17	2.71	2.36
frequencies.	-23.73	1.96	1.85	2.71	2.36
Translations	-23.73	1.89	1.69	2.18	2.13
and rotations	6.13	39.23	23.71	39.96	25.93
of the cluster	6.13	39.63	38.14	39.96	35.31
are printed	6.13	42.79	39.04	42.85	35.31
blue.	1.81	45.29	42.85	43.41	44.86
Imaginary	1.81	45.81	43.42	43.41	44.86
frequencies	1.81	46.03	44.6	43.66	45.2
are printed	15.75	51.36	44.95	49.09	47.78
red.	15.75	51.51	51.41	50.98	47.78
	15.75	53.04	51.76	50.98	51.68
	22.37	56.16	53.43	55.95	51.68



T_h



C_1

Figure S7. Isosurface of HOMO of $(\text{ZnO})_{60}$ cluster, optimized within T_h and C_1 symmetry, rendered by Chemcraft software (<http://www.chemcraftprog.com>). Blue balls depict Zinc atoms, red – Oxygen, the rendered HOMO is presented by orange and purple isosurfaces. It can be concluded that the HOMO is localized mostly on Oxygen atoms of the outer shell.

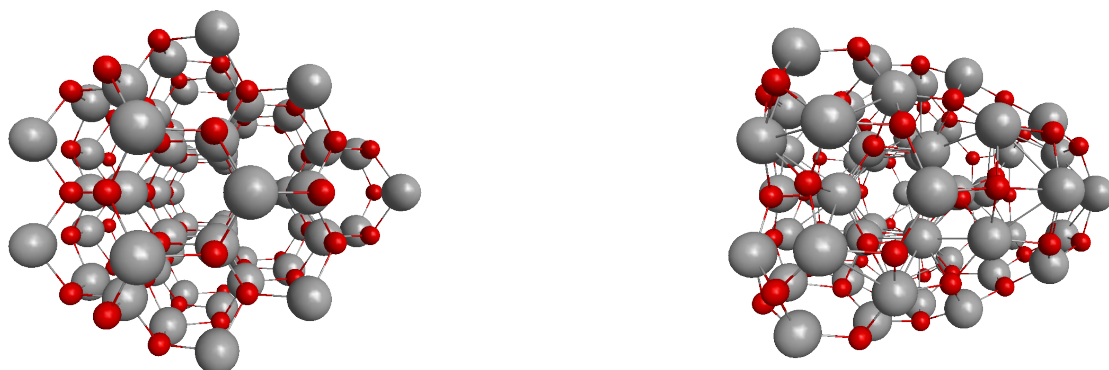


Figure S8. The structure of 60 ZnO pair cut from the bulk wurtzite lattice, which keeps the maximum number of Zn–O bonds (on the left), and its geometry optimized structure at HF/6-31G theory level (on the right). ZnO wurtzite lattice constants $a = 0.325$ nm, $c = 0.52$ nm, $u = 0.382$ were used (Karzel, H. et. al. *Phys. Rev. B* 1996, **53**, 11425).

Table S4. The structures of $(\text{ZnO})_{168}$ cluster and its moieties, the shells $(\text{ZnO})_{12}$, $(\text{ZnO})_{48}$ and $(\text{ZnO})_{108}$, optimized at HF/6-31G theory level within the restrictions of T_h symmetry point group (on the left) and T (on the right). Zinc atoms are shown as gray balls, Oxygen as red.

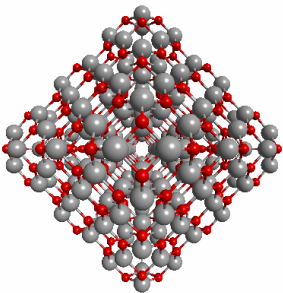
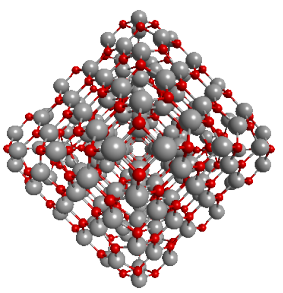
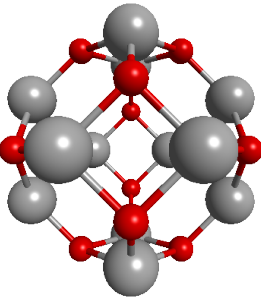
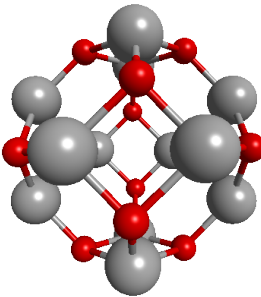
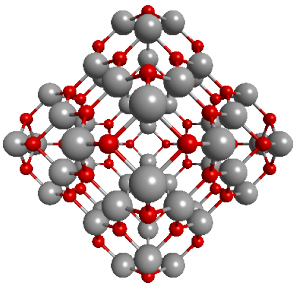
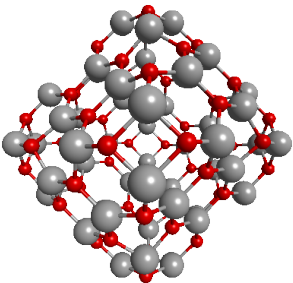
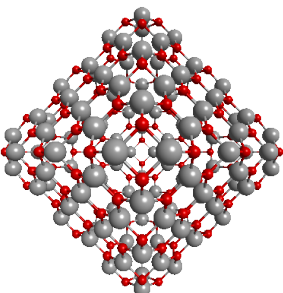
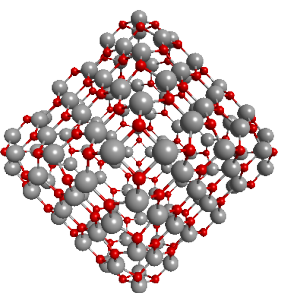
	T_h	RMSD, pm	T
$(\text{ZnO})_{168}$		33.9	
$(\text{ZnO})_{12}$		10.4	
$(\text{ZnO})_{48}$		32.3	
$(\text{ZnO})_{108}$		36.2	

Table S5. The structures of $(\text{ZnO})_{360}$ cluster and its moieties, the shells $(\text{ZnO})_{12}$, $(\text{ZnO})_{48}$, $(\text{ZnO})_{108}$ and $(\text{ZnO})_{192}$, optimized by AM1 method within the T_h symmetry point group are shown in the left column. The corresponding structures without any symmetry restrictions, called C_1 , are shown on the right. Zinc atoms are shown as gray balls, Oxygen as red.

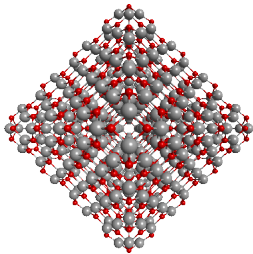
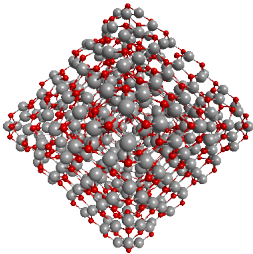
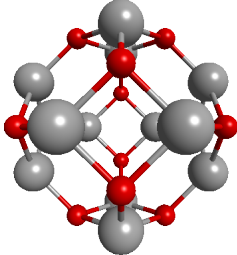
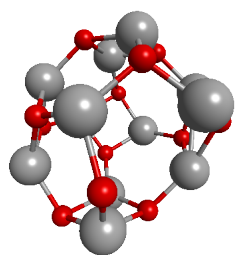
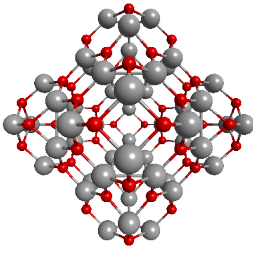
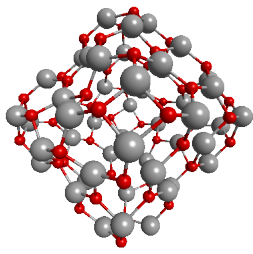
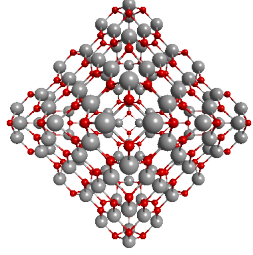
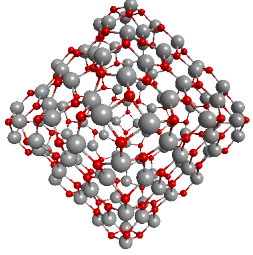
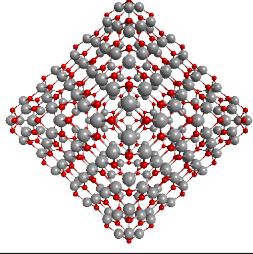
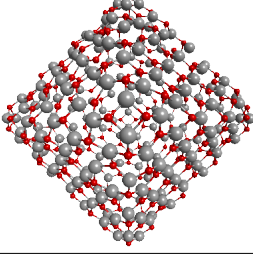
	T_h	RMSD, pm	C_1
$(\text{ZnO})_{360}$		56.3	
$(\text{ZnO})_{12}$		43.5	
$(\text{ZnO})_{48}$		53.2	
$(\text{ZnO})_{108}$		53.3	
$(\text{ZnO})_{192}$		52.9	

Table S6. The bond lengths in T_h symmetric $(\text{ZnO})_{12}$ cluster calculated at different theory levels.

Theory level	Basis set	Zn-O bond length, pm	
		edge between tetragon and hexagon	edge between two hexagons
AM1		204.6	198.2
HF	3-21G	188.7	182.3
B3LYP		187.4	180.0
MP2		189.8	182.8
HF	6-31G	194.8	187.1
B3LYP		195.0	186.5
MP2		197.3	188.8
HF	6-31G(3df)	193.7	185.7
B3LYP		193.9	185.2
MP2		192.3	183.5

Besides the mentioned in the paper, the following basis sets and their extensions were used in these calculations:

3-21G basis set for Oxygen: Binkley, J. S.; Pople, J. A.; Hehre, W. J. Self-consistent molecular orbital methods. 21. Small split-valence basis sets for first-row elements. *J. Am. Chem. Soc.* 1980, **102**, 939–947.

3-21G basis set for Zinc: Dobbs, K. D.; Hehre, W. J. Molecular orbital theory of the properties of inorganic and organometallic compounds 5. Extended basis sets for first-row transition metals. *J. Comput. Chem.* 1987, **8**, 861–879.

Polarization exponents for 6-31G basis set: Hariharan, P. C.; Pople, J. A. The influence of polarization functions on molecular orbital hydrogenation energies. *Theoret. Chim. Acta* 1973, **28**, 213–222.

Multiple polarization, and f functions: Frisch, M. J.; Pople, J. A.; Binkley, J. S. Self-consistent molecular orbital methods 25. Supplementary functions for Gaussian basis sets. *J. Chem. Phys.* 1984, **80**, 3265–3269.

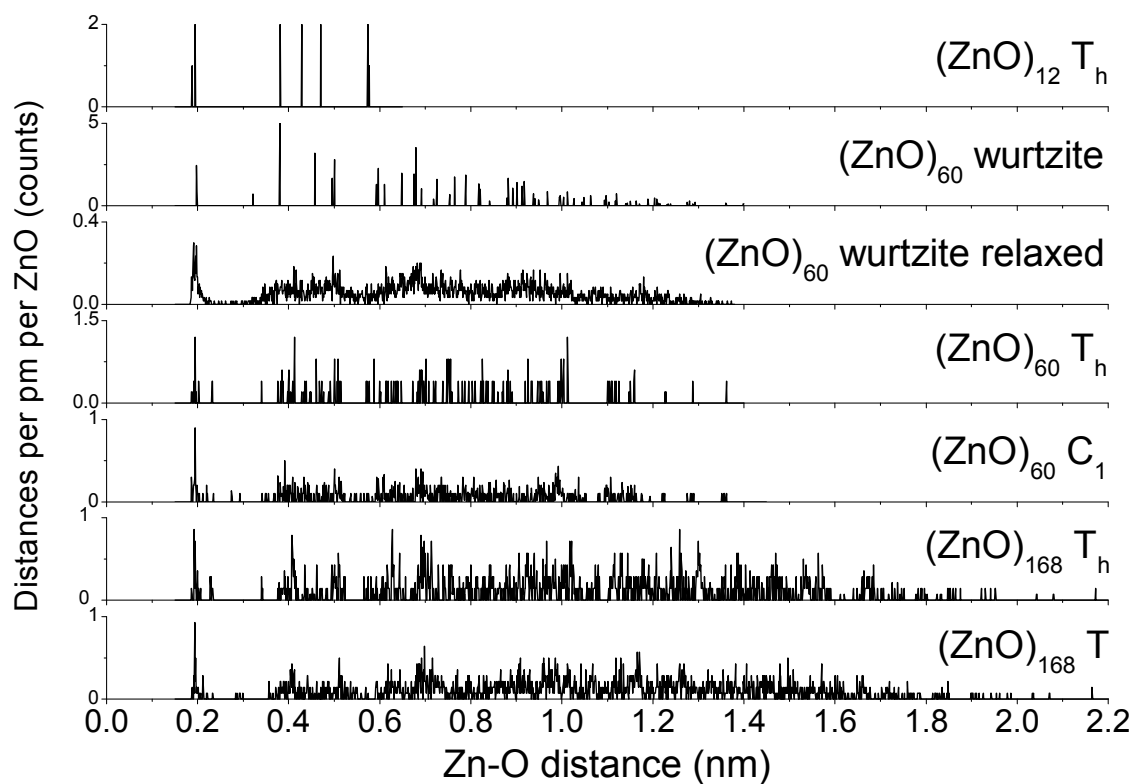


Figure S9. Zn–O distance distributions counted from HF/6-31G optimizations. The panel, labeled “(ZnO)₆₀ wurtzite”, represents the spherical fragment of 60 ZnO pairs, which was cut from the bulk wurtzite ZnO crystal structure, while the result of its geometry optimization is labeled “(ZnO)₆₀ wurtzite relaxed”.

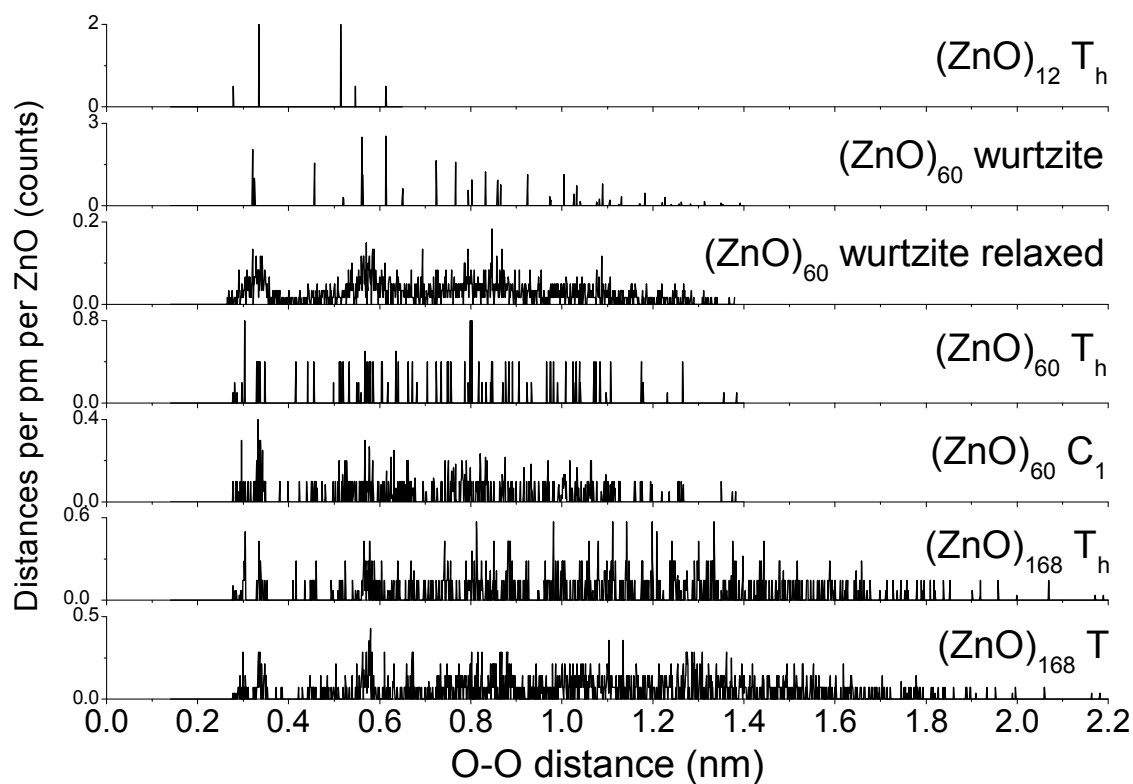


Figure S10. O–O distance distributions counted from HF/6-31G optimizations. The panel, labeled “(ZnO)₆₀ wurtzite”, represents the spherical fragment of 60 ZnO pairs, which was cut from the bulk wurtzite ZnO crystal structure, while the result of its geometry optimization is labeled “(ZnO)₆₀ wurtzite relaxed”.

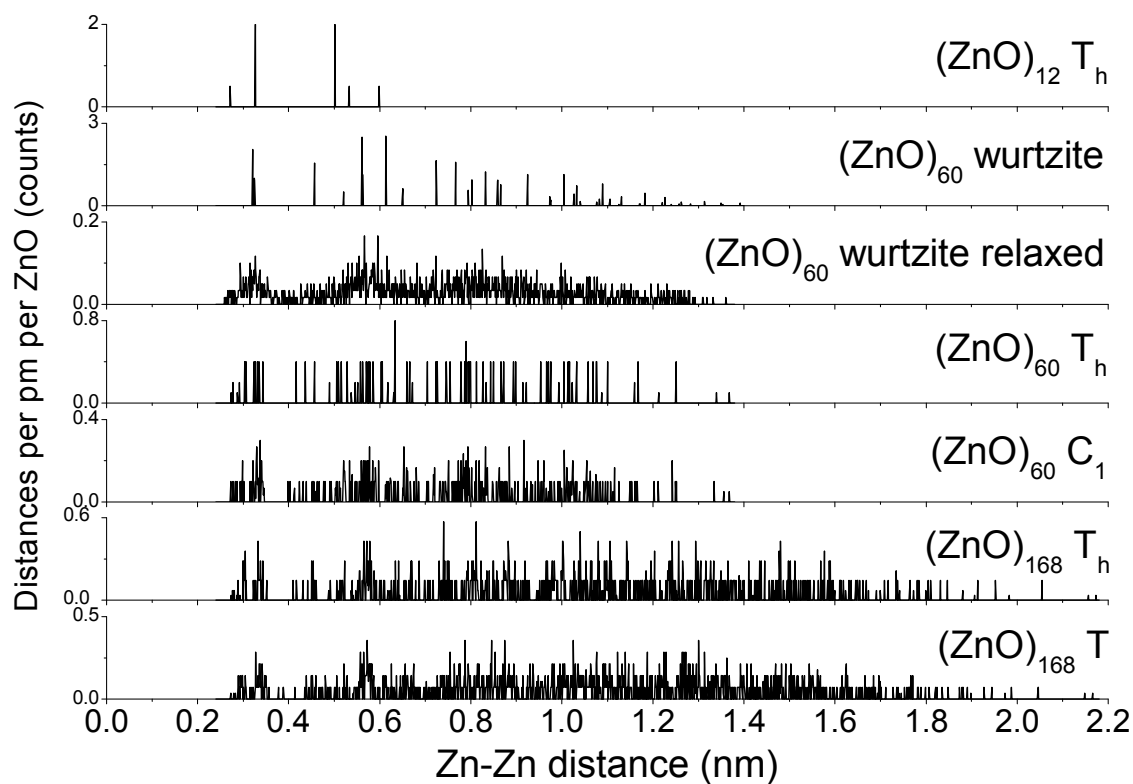


Figure S11. Zn–Zn distance distributions counted from HF/6-31G optimizations. The panel, labeled “(ZnO)₆₀ wurtzite”, represents the spherical fragment of 60 ZnO pairs, which was cut from the bulk wurtzite ZnO crystal structure, while the result of its geometry optimization is labeled “(ZnO)₆₀ wurtzite relaxed”.

Optimized Cartesian coordinates of the clusters, their symmetry point group, calculation theory level, and total energy.

(ZnO)₁₂, T_h, AM1, -154.3021 Hartree

Zn	0.00000000	-2.65369010	1.42534006
Zn	0.00000000	2.65369010	1.42534006
Zn	0.00000000	-2.65369010	-1.42534006
Zn	2.65369010	-1.42534006	0.00000000
Zn	2.65369010	1.42534006	0.00000000
Zn	-2.65369010	-1.42534006	0.00000000
Zn	-2.65369010	1.42534006	0.00000000
Zn	-1.42534006	0.00000000	2.65369010
Zn	-1.42534006	0.00000000	-2.65369010
Zn	1.42534006	0.00000000	-2.65369010
Zn	1.42534006	0.00000000	2.65369010
Zn	0.00000000	2.65369010	-1.42534006
O	0.00000000	-1.42954004	-2.98466992
O	0.00000000	1.42954004	-2.98466992
O	0.00000000	-1.42954004	2.98466992
O	1.42954004	2.98466992	0.00000000
O	1.42954004	-2.98466992	0.00000000
O	-1.42954004	2.98466992	0.00000000
O	-1.42954004	-2.98466992	0.00000000
O	2.98466992	0.00000000	1.42954004
O	2.98466992	0.00000000	-1.42954004
O	-2.98466992	0.00000000	-1.42954004
O	-2.98466992	0.00000000	1.42954004
O	0.00000000	1.42954004	2.98466992

(ZnO)₁₂, T_h, HF/3-21G, -22124.5446 Hartree

Zn	0.00000000	-2.65369010	1.42533994
Zn	0.00000000	2.65369010	1.42533994
Zn	0.00000000	-2.65369010	-1.42533994
Zn	-1.42533994	0.00000000	2.65369010
Zn	1.42533994	0.00000000	-2.65369010
Zn	1.42533994	0.00000000	2.65369010
Zn	-1.42533994	0.00000000	-2.65369010
Zn	2.65369010	-1.42533994	0.00000000
Zn	-2.65369010	1.42533994	0.00000000
Zn	2.65369010	1.42533994	0.00000000
Zn	-2.65369010	-1.42533994	0.00000000
Zn	0.00000000	2.65369010	-1.42533994
O	0.00000000	-1.42954004	-2.98466992
O	0.00000000	1.42954004	-2.98466992
O	0.00000000	-1.42954004	2.98466992
O	2.98466992	0.00000000	1.42954004

O	-2.98466992	0.00000000	-1.42954004
O	-2.98466992	0.00000000	1.42954004
O	2.98466992	0.00000000	-1.42954004
O	1.42954004	2.98466992	0.00000000
O	-1.42954004	-2.98466992	0.00000000
O	1.42954004	-2.98466992	0.00000000
O	-1.42954004	2.98466992	0.00000000
O	0.00000000	1.42954004	2.98466992

(ZnO)₁₂, T_h, B3LYP/3-21G, -22148.4555 Hartree

Zn	0.00000000	-2.52430010	1.29407990
Zn	0.00000000	2.52430010	1.29407990
Zn	0.00000000	-2.52430010	-1.29407990
Zn	-1.29407990	0.00000000	2.52430010
Zn	1.29407990	0.00000000	-2.52430010
Zn	1.29407990	0.00000000	2.52430010
Zn	-1.29407990	0.00000000	-2.52430010
Zn	2.52430010	-1.29407990	0.00000000
Zn	-2.52430010	1.29407990	0.00000000
Zn	2.52430010	1.29407990	0.00000000
Zn	-2.52430010	-1.29407990	0.00000000
Zn	0.00000000	2.52430010	-1.29407990
O	0.00000000	-1.34880996	-2.65660000
O	0.00000000	1.34880996	-2.65660000
O	0.00000000	-1.34880996	2.65660000
O	2.65660000	0.00000000	1.34880996
O	-2.65660000	0.00000000	-1.34880996
O	-2.65660000	0.00000000	1.34880996
O	2.65660000	0.00000000	-1.34880996
O	1.34880996	2.65660000	0.00000000
O	-1.34880996	-2.65660000	0.00000000
O	1.34880996	-2.65660000	0.00000000
O	-1.34880996	2.65660000	0.00000000
O	0.00000000	1.34880996	2.65660000

(ZnO)₁₂, T_h, MP2/3-21G, -22128.9361 Hartree

Zn	2.57469344	-1.30189383	0.00000000
Zn	-2.57469344	-1.30189383	0.00000000
Zn	2.57469344	1.30189383	0.00000000
Zn	-2.57469344	1.30189383	0.00000000
Zn	-1.30189419	0.00000000	2.57469440
Zn	1.30189419	0.00000000	-2.57469440
Zn	-1.30189419	0.00000000	-2.57469440
Zn	1.30189419	0.00000000	2.57469440
Zn	0.00000000	-2.57469559	-1.30189455
Zn	0.00000000	2.57469559	1.30189455

Zn	0.00000000	-2.57469559	1.30189455
Zn	0.00000000	2.57469559	-1.30189455
O	1.37660587	2.68262458	0.00000000
O	-1.37660587	2.68262458	0.00000000
O	1.37660587	-2.68262458	0.00000000
O	-1.37660587	-2.68262458	0.00000000
O	2.68262434	0.00000000	1.37660623
O	-2.68262434	0.00000000	-1.37660623
O	2.68262434	0.00000000	-1.37660623
O	-2.68262434	0.00000000	1.37660623
O	0.00000000	-1.37660599	2.68262434
O	0.00000000	1.37660599	-2.68262434
O	0.00000000	-1.37660599	-2.68262434
O	0.00000000	1.37660599	2.68262434

(ZnO)₁₂, T_h, HF/6-31G, -22229.0194 Hartree

Zn	0.00000000	-2.66440010	1.35992002
Zn	0.00000000	2.66440010	1.35992002
Zn	0.00000000	-2.66440010	-1.35992002
Zn	-1.35992002	0.00000000	2.66440010
Zn	1.35992002	0.00000000	-2.66440010
Zn	1.35992002	0.00000000	2.66440010
Zn	-1.35992002	0.00000000	-2.66440010
Zn	2.66440010	-1.35992002	0.00000000
Zn	-2.66440010	1.35992002	0.00000000
Zn	2.66440010	1.35992002	0.00000000
Zn	-2.66440010	-1.35992002	0.00000000
Zn	0.00000000	2.66440010	-1.35992002
O	0.00000000	-1.39342999	-2.73275995
O	0.00000000	1.39342999	-2.73275995
O	0.00000000	-1.39342999	2.73275995
O	2.73275995	0.00000000	1.39342999
O	-2.73275995	0.00000000	-1.39342999
O	-2.73275995	0.00000000	1.39342999
O	2.73275995	0.00000000	-1.39342999
O	1.39342999	2.73275995	0.00000000
O	-1.39342999	-2.73275995	0.00000000
O	1.39342999	-2.73275995	0.00000000
O	-1.39342999	2.73275995	0.00000000
O	0.00000000	1.39342999	2.73275995

(ZnO)₁₂, T_h, B3LYP/6-31G, -22252.8200 Hartree

Zn	0.00000000	-2.62150002	1.36004996
Zn	0.00000000	2.62150002	1.36004996
Zn	0.00000000	-2.62150002	-1.36004996
Zn	-1.36004996	0.00000000	2.62150002

Zn	1.36004996	0.00000000	-2.62150002
Zn	1.36004996	0.00000000	2.62150002
Zn	-1.36004996	0.00000000	-2.62150002
Zn	2.62150002	-1.36004996	0.00000000
Zn	-2.62150002	1.36004996	0.00000000
Zn	2.62150002	1.36004996	0.00000000
Zn	-2.62150002	-1.36004996	0.00000000
Zn	0.00000000	2.62150002	-1.36004996
O	0.00000000	-1.39082003	-2.76098990
O	0.00000000	1.39082003	-2.76098990
O	0.00000000	-1.39082003	2.76098990
O	2.76098990	0.00000000	1.39082003
O	-2.76098990	0.00000000	-1.39082003
O	-2.76098990	0.00000000	1.39082003
O	2.76098990	0.00000000	-1.39082003
O	1.39082003	2.76098990	0.00000000
O	-1.39082003	-2.76098990	0.00000000
O	1.39082003	-2.76098990	0.00000000
O	-1.39082003	2.76098990	0.00000000
O	0.00000000	1.39082003	2.76098990

(ZnO)₁₂, T_h, MP2/6-31G, -22233.2353 Hartree

Zn	0.00000000	-2.65859628	1.36622596
Zn	0.00000000	2.65859628	1.36622596
Zn	0.00000000	-2.65859628	-1.36622596
Zn	-1.36622596	0.00000000	2.65859628
Zn	1.36622596	0.00000000	-2.65859628
Zn	1.36622596	0.00000000	2.65859628
Zn	-1.36622596	0.00000000	-2.65859628
Zn	2.65859628	-1.36622596	0.00000000
Zn	-2.65859628	1.36622596	0.00000000
Zn	2.65859628	1.36622596	0.00000000
Zn	-2.65859628	-1.36622596	0.00000000
Zn	0.00000000	2.65859628	-1.36622596
O	0.00000000	-1.41723669	-2.78875327
O	0.00000000	1.41723669	-2.78875327
O	0.00000000	-1.41723669	2.78875327
O	2.78875327	0.00000000	1.41723669
O	-2.78875327	0.00000000	-1.41723669
O	-2.78875327	0.00000000	1.41723669
O	2.78875327	0.00000000	-1.41723669
O	1.41723669	2.78875327	0.00000000
O	-1.41723669	-2.78875327	0.00000000
O	1.41723669	-2.78875327	0.00000000
O	-1.41723669	2.78875327	0.00000000
O	0.00000000	1.41723669	2.78875327

(ZnO)₁₂, T_h, HF/6-31G(3df), -22229.4877 Hartree

Zn	0.00000000	-2.60901976	1.33633006
Zn	0.00000000	2.60901976	1.33633006
Zn	0.00000000	-2.60901976	-1.33633006
Zn	-1.33633006	0.00000000	2.60901976
Zn	1.33633006	0.00000000	-2.60901976
Zn	1.33633006	0.00000000	2.60901976
Zn	-1.33633006	0.00000000	-2.60901976
Zn	2.60901976	-1.33633006	0.00000000
Zn	-2.60901976	1.33633006	0.00000000
Zn	2.60901976	1.33633006	0.00000000
Zn	-2.60901976	-1.33633006	0.00000000
Zn	0.00000000	2.60901976	-1.33633006
O	0.00000000	-1.39584994	-2.74233985
O	0.00000000	1.39584994	-2.74233985
O	0.00000000	-1.39584994	2.74233985
O	2.74233985	0.00000000	1.39584994
O	-2.74233985	0.00000000	-1.39584994
O	-2.74233985	0.00000000	1.39584994
O	2.74233985	0.00000000	-1.39584994
O	1.39584994	2.74233985	0.00000000
O	-1.39584994	-2.74233985	0.00000000
O	1.39584994	-2.74233985	0.00000000
O	-1.39584994	2.74233985	0.00000000
O	0.00000000	1.39584994	2.74233985

(ZnO)₁₂, T_h, B3LYP/6-31G(3df), -22253.5520 Hartree

Zn	0.00000000	-2.55823731	1.33357561
Zn	0.00000000	2.55823731	1.33357561
Zn	0.00000000	-2.55823731	-1.33357561
Zn	-1.33357561	0.00000000	2.55823731
Zn	1.33357561	0.00000000	-2.55823731
Zn	1.33357561	0.00000000	2.55823731
Zn	-1.33357561	0.00000000	-2.55823731
Zn	2.55823731	-1.33357561	0.00000000
Zn	-2.55823731	1.33357561	0.00000000
Zn	2.55823731	1.33357561	0.00000000
Zn	-2.55823731	-1.33357561	0.00000000
Zn	0.00000000	2.55823731	-1.33357561
O	0.00000000	-1.39132202	-2.77163076
O	0.00000000	1.39132202	-2.77163076
O	0.00000000	-1.39132202	2.77163076
O	2.77163076	0.00000000	1.39132202
O	-2.77163076	0.00000000	-1.39132202
O	-2.77163076	0.00000000	1.39132202

O	2.77163076	0.00000000	-1.39132202
O	1.39132202	2.77163076	0.00000000
O	-1.39132202	-2.77163076	0.00000000
O	1.39132202	-2.77163076	0.00000000
O	-1.39132202	2.77163076	0.00000000
O	0.00000000	1.39132202	2.77163076

(ZnO)₁₂, T_h, MP2/6-31G(3df), -22237.5867 Hartree

Zn	2.52091336	-1.31868613	0.00000000
Zn	-2.52091336	-1.31868613	0.00000000
Zn	2.52091336	1.31868613	0.00000000
Zn	-2.52091336	1.31868613	0.00000000
Zn	-1.31868613	0.00000000	2.52091599
Zn	1.31868613	0.00000000	-2.52091599
Zn	-1.31868613	0.00000000	-2.52091599
Zn	1.31868613	0.00000000	2.52091599
Zn	0.00000000	-2.52092171	-1.31868637
Zn	0.00000000	2.52092171	1.31868637
Zn	0.00000000	-2.52092171	1.31868637
Zn	0.00000000	2.52092171	-1.31868637
O	1.38047743	2.75630760	0.00000000
O	-1.38047743	2.75630760	0.00000000
O	1.38047743	-2.75630760	0.00000000
O	-1.38047743	-2.75630760	0.00000000
O	2.75630569	0.00000000	1.38047755
O	-2.75630569	0.00000000	-1.38047755
O	2.75630569	0.00000000	-1.38047755
O	-2.75630569	0.00000000	1.38047755
O	0.00000000	-1.38047934	2.75630379
O	0.00000000	1.38047934	-2.75630379
O	0.00000000	-1.38047934	-2.75630379
O	0.00000000	1.38047934	2.75630379

(ZnO)₁₂, C₁, AM1, -154.3021 Hartree

Zn	-2.51081324	-0.05786372	1.66323841
O	-1.09381580	0.19451262	3.11671972
Zn	-0.57106251	1.95600951	2.21784663
O	-2.37228847	1.94040549	1.24848878
Zn	0.35902533	-1.11039746	2.77626252
O	-2.86107683	-1.59759390	0.46482018
Zn	-2.01436019	2.13032627	-0.69194263
O	1.20071447	2.61975813	1.62633491
Zn	-1.16830850	-2.74505043	0.41511515
Zn	-2.44316387	-1.00456393	-1.44779456
O	0.36191016	-2.83239365	1.67217994
O	2.30728483	-0.81235838	2.22863150

Zn	2.44316912	1.00457084	1.44779074
Zn	1.16830444	2.74504924	-0.41511208
O	-2.30728865	0.81235754	-2.22862840
O	-0.36191320	2.83240223	-1.67217863
O	-1.20070922	-2.61975145	-1.62633872
Zn	2.01436400	-2.13032937	0.69194043
O	2.86107302	1.59759259	-0.46481711
Zn	-0.35902935	1.11039650	-2.77625942
Zn	0.57105851	-1.95601070	-2.21784401
O	2.37229252	-1.94040847	-1.24849117
O	1.09381187	-0.19451363	-3.11671686
Zn	2.51081753	0.05786088	-1.66324091

(ZnO)₁₂, C₁, HF/6-31G, -22229.0194 Hartree

Zn	0.02848000	0.95538998	-3.14155006
O	1.90033996	0.88432997	-2.60596991
Zn	1.68366003	-1.02472997	-2.28309011
O	-0.14720000	-0.97518998	-2.94731998
Zn	2.42253995	1.94835997	-1.15857005
O	-1.18794000	2.15482020	-2.37898993
Zn	-1.49246991	-1.60716999	-1.81124008
O	2.13812017	-1.82418990	-0.65393001
Zn	-0.56493002	3.23169994	-0.87968999
Zn	-2.56318998	1.41692996	-1.21282005
O	1.21711004	3.22244000	-0.31041002
O	2.91309977	1.19349003	0.56922001
Zn	2.67791986	-0.64775997	0.80221003
Zn	0.67967004	-2.46253991	0.46908000
O	-2.79836011	-0.42432001	-0.97982997
O	-1.10237002	-2.45327020	-0.10020000
O	-2.02338004	2.59335995	0.24332000
Zn	1.60721004	2.37634015	1.40063000
O	1.30268002	-1.38565004	1.96838999
Zn	-2.30780005	-1.17918992	0.74795997
Zn	-1.56893003	1.79390001	1.87248003
O	0.26194000	1.74435997	2.53671002
O	-1.78560007	-0.11516000	2.19535995
Zn	0.08625000	-0.18622001	2.73094010

(ZnO)₁₂, C₁, B3LYP/6-31G, -22252.8200 Hartree

Zn	0.00000000	-2.62132025	1.36002958
Zn	-0.00000000	2.62132025	1.36002958
Zn	0.00000000	-2.62132025	-1.36002958
Zn	-1.36002946	0.00000004	2.62132025
Zn	1.36002946	-0.00000004	-2.62132025
Zn	1.36002946	-0.00000004	2.62132025

Zn	-1.36002946	0.00000004	-2.62132025
Zn	2.62132025	-1.36002958	-0.00000000
Zn	-2.62132025	1.36002958	0.00000000
Zn	2.62132025	1.36002958	-0.00000000
Zn	-2.62132025	-1.36002958	0.00000000
Zn	-0.00000000	2.62132025	-1.36002958
O	0.00000001	-1.39073062	-2.76118422
O	0.00000000	1.39073062	-2.76118422
O	-0.00000000	-1.39073062	2.76118422
O	2.76118445	0.00000001	1.39073062
O	-2.76118445	-0.00000001	-1.39073062
O	-2.76118445	-0.00000001	1.39073062
O	2.76118445	0.00000001	-1.39073062
O	1.39073062	2.76118422	-0.00000000
O	-1.39073062	-2.76118422	0.00000000
O	1.39073062	-2.76118422	0.00000000
O	-1.39073062	2.76118422	-0.00000000
O	-0.00000001	1.39073062	2.76118422

(ZnO)₁₂, C₁, MP2/6-31G, -22233.2353 Hartree

Zn	-0.00000032	-2.65837717	1.36650479
Zn	-0.00000007	2.65837693	1.36650455
Zn	0.00000029	-2.65837669	-1.36650479
Zn	-1.36650467	-0.00000057	2.65837741
Zn	1.36650467	-0.00000031	-2.65837717
Zn	1.36650491	0.00000020	2.65837741
Zn	-1.36650503	-0.00000011	-2.65837741
Zn	2.65837789	-1.36650503	0.00000003
Zn	-2.65837765	1.36650527	-0.00000006
Zn	2.65837693	1.36650455	-0.00000009
Zn	-2.65837741	-1.36650443	-0.00000001
Zn	-0.00000003	2.65837717	-1.36650455
O	-0.00000003	-1.41705894	-2.78914452
O	-0.00000003	1.41705883	-2.78914404
O	0.00000021	-1.41705894	2.78914428
O	2.78914404	0.00000012	1.41705906
O	-2.78914404	-0.00000009	-1.41705906
O	-2.78914404	-0.00000006	1.41705894
O	2.78914428	-0.00000008	-1.41705906
O	1.41705894	2.78914428	-0.00000014
O	-1.41705894	-2.78914404	-0.00000006
O	1.41705883	-2.78914404	0.00000017
O	-1.41705894	2.78914428	0.00000007
O	-0.00000007	1.41705894	2.78914428

(ZnO)₆₀, T_h, AM1, -771.4869 Hartree

O	0.00000000	-3.06195998	-5.80931997
O	0.00000000	3.06195998	-5.80931997
O	0.00000000	-3.06195998	5.80931997
O	5.80931997	0.00000000	3.06195998
O	-5.80931997	0.00000000	-3.06195998
O	-5.80931997	0.00000000	3.06195998
O	5.80931997	0.00000000	-3.06195998
O	3.06195998	5.80931997	0.00000000
O	-3.06195998	-5.80931997	0.00000000
O	3.06195998	-5.80931997	0.00000000
O	-3.06195998	5.80931997	0.00000000
O	0.00000000	3.06195998	5.80931997
O	2.85994005	-1.42018008	-4.30836010
O	-2.85994005	1.42018008	-4.30836010
O	-2.85994005	-1.42018008	4.30836010
O	4.30836010	2.85994005	1.42018008
O	-4.30836010	2.85994005	-1.42018008
O	-4.30836010	-2.85994005	1.42018008
O	4.30836010	-2.85994005	-1.42018008
O	1.42018008	4.30836010	2.85994005
O	-1.42018008	-4.30836010	2.85994005
O	1.42018008	-4.30836010	-2.85994005
O	-1.42018008	4.30836010	-2.85994005
O	-2.85994005	-1.42018008	-4.30836010
O	-2.85994005	1.42018008	4.30836010
O	2.85994005	-1.42018008	4.30836010
O	2.85994005	1.42018008	-4.30836010
O	-4.30836010	-2.85994005	-1.42018008
O	4.30836010	-2.85994005	1.42018008
O	4.30836010	2.85994005	-1.42018008
O	-4.30836010	2.85994005	1.42018008
O	-1.42018008	-4.30836010	-2.85994005
O	1.42018008	4.30836010	-2.85994005
O	-1.42018008	4.30836010	2.85994005
O	1.42018008	-4.30836010	2.85994005
O	2.85994005	1.42018008	4.30836010
O	1.43560994	0.00000000	-7.29387999
O	-1.43560994	0.00000000	-7.29387999
O	-1.43560994	0.00000000	7.29387999
O	7.29387999	1.43560994	0.00000000
O	-7.29387999	1.43560994	0.00000000
O	-7.29387999	-1.43560994	0.00000000
O	7.29387999	-1.43560994	0.00000000
O	0.00000000	7.29387999	1.43560994
O	0.00000000	-7.29387999	1.43560994
O	0.00000000	-7.29387999	-1.43560994

O	0.00000000	7.29387999	-1.43560994
O	1.43560994	0.00000000	7.29387999
Zn	1.41557002	-2.85146999	-4.33022976
Zn	-1.41557002	2.85146999	-4.33022976
Zn	-1.41557002	-2.85146999	4.33022976
Zn	4.33022976	1.41557002	2.85146999
Zn	-4.33022976	1.41557002	-2.85146999
Zn	-4.33022976	-1.41557002	2.85146999
Zn	4.33022976	-1.41557002	-2.85146999
Zn	2.85146999	4.33022976	1.41557002
Zn	-2.85146999	-4.33022976	1.41557002
Zn	2.85146999	-4.33022976	-1.41557002
Zn	-2.85146999	4.33022976	-1.41557002
Zn	-1.41557002	-2.85146999	-4.33022976
Zn	-1.41557002	2.85146999	4.33022976
Zn	1.41557002	-2.85146999	4.33022976
Zn	1.41557002	2.85146999	-4.33022976
Zn	-4.33022976	-1.41557002	-2.85146999
Zn	4.33022976	-1.41557002	2.85146999
Zn	4.33022976	1.41557002	-2.85146999
Zn	-4.33022976	1.41557002	2.85146999
Zn	-2.85146999	-4.33022976	-1.41557002
Zn	2.85146999	4.33022976	-1.41557002
Zn	-2.85146999	4.33022976	1.41557002
Zn	2.85146999	-4.33022976	1.41557002
Zn	1.41557002	2.85146999	4.33022976
Zn	0.00000000	-1.42223001	-6.92319012
Zn	0.00000000	1.42223001	-6.92319012
Zn	0.00000000	-1.42223001	6.92319012
Zn	6.92319012	0.00000000	1.42223001
Zn	-6.92319012	0.00000000	-1.42223001
Zn	-6.92319012	0.00000000	1.42223001
Zn	6.92319012	0.00000000	-1.42223001
Zn	1.42223001	6.92319012	0.00000000
Zn	-1.42223001	-6.92319012	0.00000000
Zn	1.42223001	-6.92319012	0.00000000
Zn	-1.42223001	6.92319012	0.00000000
Zn	0.00000000	1.42223001	6.92319012
Zn	2.65756011	0.00000000	-5.73937988
Zn	-2.65756011	0.00000000	-5.73937988
Zn	-2.65756011	0.00000000	5.73937988
Zn	5.73937988	2.65756011	0.00000000
Zn	-5.73937988	2.65756011	0.00000000
Zn	-5.73937988	-2.65756011	0.00000000
Zn	5.73937988	-2.65756011	0.00000000
Zn	0.00000000	5.73937988	2.65756011

Zn	0.00000000	-5.73937988	2.65756011
Zn	0.00000000	-5.73937988	-2.65756011
Zn	0.00000000	5.73937988	-2.65756011
Zn	2.65756011	0.00000000	5.73937988
Zn	2.95333004	1.54657996	0.00000000
Zn	-2.95333004	-1.54657996	0.00000000
Zn	-2.95333004	1.54657996	0.00000000
Zn	0.00000000	2.95333004	-1.54657996
Zn	0.00000000	2.95333004	1.54657996
Zn	0.00000000	-2.95333004	-1.54657996
Zn	0.00000000	-2.95333004	1.54657996
Zn	-1.54657996	0.00000000	2.95333004
Zn	1.54657996	0.00000000	2.95333004
Zn	-1.54657996	0.00000000	-2.95333004
Zn	1.54657996	0.00000000	-2.95333004
Zn	2.95333004	-1.54657996	0.00000000
O	3.04848003	0.00000000	-1.48734999
O	-3.04848003	0.00000000	-1.48734999
O	-3.04848003	0.00000000	1.48734999
O	1.48734999	3.04848003	0.00000000
O	-1.48734999	3.04848003	0.00000000
O	-1.48734999	-3.04848003	0.00000000
O	1.48734999	-3.04848003	0.00000000
O	0.00000000	1.48734999	3.04848003
O	0.00000000	-1.48734999	3.04848003
O	0.00000000	-1.48734999	-3.04848003
O	0.00000000	1.48734999	-3.04848003
O	3.04848003	0.00000000	1.48734999

(ZnO)₆₀, T_h, HF/6-31G, -111146.6633 Hartree

O	0.00000000	-2.79109001	-5.48598003
O	0.00000000	2.79109001	-5.48598003
O	0.00000000	-2.79109001	5.48598003
O	5.48598003	0.00000000	2.79109001
O	-5.48598003	0.00000000	-2.79109001
O	-5.48598003	0.00000000	2.79109001
O	5.48598003	0.00000000	-2.79109001
O	2.79109001	5.48598003	0.00000000
O	-2.79109001	-5.48598003	0.00000000
O	2.79109001	-5.48598003	0.00000000
O	-2.79109001	5.48598003	0.00000000
O	0.00000000	2.79109001	5.48598003
O	1.38794994	0.00000000	-6.77734995
O	-1.38794994	0.00000000	-6.77734995
O	-1.38794994	0.00000000	6.77734995
O	6.77734995	1.38794994	0.00000000

O	-6.77734995	1.38794994	0.00000000
O	-6.77734995	-1.38794994	0.00000000
O	6.77734995	-1.38794994	0.00000000
O	0.00000000	6.77734995	1.38794994
O	0.00000000	-6.77734995	1.38794994
O	0.00000000	-6.77734995	-1.38794994
O	0.00000000	6.77734995	-1.38794994
O	1.38794994	0.00000000	6.77734995
O	2.83660984	0.00000000	-1.43250990
O	-2.83660984	0.00000000	-1.43250990
O	-2.83660984	0.00000000	1.43250990
O	1.43250990	2.83660984	0.00000000
O	-1.43250990	2.83660984	0.00000000
O	-1.43250990	-2.83660984	0.00000000
O	1.43250990	-2.83660984	0.00000000
O	0.00000000	1.43250990	2.83660984
O	0.00000000	-1.43250990	2.83660984
O	0.00000000	-1.43250990	-2.83660984
O	0.00000000	1.43250990	-2.83660984
O	2.83660984	0.00000000	1.43250990
O	2.74977016	-1.40522003	-4.12106991
O	-2.74977016	1.40522003	-4.12106991
O	-2.74977016	-1.40522003	4.12106991
O	4.12106991	2.74977016	1.40522003
O	-4.12106991	2.74977016	-1.40522003
O	-4.12106991	-2.74977016	1.40522003
O	4.12106991	-2.74977016	-1.40522003
O	1.40522003	4.12106991	2.74977016
O	-1.40522003	-4.12106991	2.74977016
O	1.40522003	-4.12106991	-2.74977016
O	-1.40522003	4.12106991	-2.74977016
O	-2.74977016	-1.40522003	-4.12106991
O	-2.74977016	1.40522003	4.12106991
O	2.74977016	-1.40522003	4.12106991
O	2.74977016	1.40522003	-4.12106991
O	-4.12106991	-2.74977016	-1.40522003
O	4.12106991	-2.74977016	1.40522003
O	4.12106991	2.74977016	-1.40522003
O	-4.12106991	2.74977016	1.40522003
O	-1.40522003	-4.12106991	-2.74977016
O	1.40522003	4.12106991	-2.74977016
O	-1.40522003	4.12106991	2.74977016
O	1.40522003	-4.12106991	2.74977016
O	2.74977016	1.40522003	4.12106991
Zn	0.00000000	-1.36650002	-6.69758034
Zn	0.00000000	1.36650002	-6.69758034

Zn	0.00000000	-1.36650002	6.69758034
Zn	6.69758034	0.00000000	1.36650002
Zn	-6.69758034	0.00000000	-1.36650002
Zn	-6.69758034	0.00000000	1.36650002
Zn	6.69758034	0.00000000	-1.36650002
Zn	1.36650002	6.69758034	0.00000000
Zn	-1.36650002	-6.69758034	0.00000000
Zn	1.36650002	-6.69758034	0.00000000
Zn	-1.36650002	6.69758034	0.00000000
Zn	0.00000000	1.36650002	6.69758034
Zn	2.68676996	0.00000000	-5.43627024
Zn	-2.68676996	0.00000000	-5.43627024
Zn	-2.68676996	0.00000000	5.43627024
Zn	5.43627024	2.68676996	0.00000000
Zn	-5.43627024	2.68676996	0.00000000
Zn	-5.43627024	-2.68676996	0.00000000
Zn	5.43627024	-2.68676996	0.00000000
Zn	0.00000000	5.43627024	2.68676996
Zn	0.00000000	-5.43627024	2.68676996
Zn	0.00000000	-5.43627024	-2.68676996
Zn	0.00000000	5.43627024	-2.68676996
Zn	2.68676996	0.00000000	5.43627024
Zn	2.80630016	1.43747997	0.00000000
Zn	-2.80630016	-1.43747997	0.00000000
Zn	-2.80630016	1.43747997	0.00000000
Zn	0.00000000	2.80630016	-1.43747997
Zn	0.00000000	2.80630016	1.43747997
Zn	0.00000000	-2.80630016	-1.43747997
Zn	0.00000000	-2.80630016	1.43747997
Zn	-1.43747997	0.00000000	2.80630016
Zn	1.43747997	0.00000000	2.80630016
Zn	-1.43747997	0.00000000	-2.80630016
Zn	1.43747997	0.00000000	-2.80630016
Zn	2.80630016	-1.43747997	0.00000000
Zn	1.38925993	-2.75934005	-4.13196993
Zn	-1.38925993	2.75934005	-4.13196993
Zn	-1.38925993	-2.75934005	4.13196993
Zn	4.13196993	1.38925993	2.75934005
Zn	-4.13196993	1.38925993	-2.75934005
Zn	-4.13196993	-1.38925993	2.75934005
Zn	4.13196993	-1.38925993	-2.75934005
Zn	2.75934005	4.13196993	1.38925993
Zn	-2.75934005	-4.13196993	1.38925993
Zn	2.75934005	-4.13196993	-1.38925993
Zn	-2.75934005	4.13196993	-1.38925993
Zn	-1.38925993	-2.75934005	-4.13196993

Zn	-1.38925993	2.75934005	4.13196993
Zn	1.38925993	-2.75934005	4.13196993
Zn	1.38925993	2.75934005	-4.13196993
Zn	-4.13196993	-1.38925993	-2.75934005
Zn	4.13196993	-1.38925993	2.75934005
Zn	4.13196993	1.38925993	-2.75934005
Zn	-4.13196993	1.38925993	2.75934005
Zn	-2.75934005	-4.13196993	-1.38925993
Zn	2.75934005	4.13196993	-1.38925993
Zn	-2.75934005	4.13196993	1.38925993
Zn	2.75934005	-4.13196993	1.38925993
Zn	1.38925993	2.75934005	4.13196993

(ZnO)₆₀, T_h, B3LYP/6-31G, -111265.6184 Hartree

O	0.00000000	-2.82975006	-5.49104023
O	0.00000000	2.82975006	-5.49104023
O	0.00000000	-2.82975006	5.49104023
O	5.49104023	0.00000000	2.82975006
O	-5.49104023	0.00000000	-2.82975006
O	-5.49104023	0.00000000	2.82975006
O	5.49104023	0.00000000	-2.82975006
O	2.82975006	5.49104023	0.00000000
O	-2.82975006	-5.49104023	0.00000000
O	2.82975006	-5.49104023	0.00000000
O	-2.82975006	5.49104023	0.00000000
O	0.00000000	2.82975006	5.49104023
O	2.74587011	-1.41532993	-4.11396027
O	-2.74587011	1.41532993	-4.11396027
O	-2.74587011	-1.41532993	4.11396027
O	4.11396027	2.74587011	1.41532993
O	-4.11396027	2.74587011	-1.41532993
O	-4.11396027	-2.74587011	1.41532993
O	4.11396027	-2.74587011	-1.41532993
O	1.41532993	4.11396027	2.74587011
O	-1.41532993	-4.11396027	2.74587011
O	1.41532993	-4.11396027	-2.74587011
O	-1.41532993	4.11396027	-2.74587011
O	-2.74587011	-1.41532993	-4.11396027
O	-2.74587011	1.41532993	4.11396027
O	2.74587011	-1.41532993	4.11396027
O	2.74587011	1.41532993	-4.11396027
O	-4.11396027	-2.74587011	-1.41532993
O	4.11396027	-2.74587011	1.41532993
O	4.11396027	2.74587011	-1.41532993
O	-4.11396027	2.74587011	1.41532993
O	-1.41532993	-4.11396027	-2.74587011

O	1.41532993	4.11396027	-2.74587011
O	-1.41532993	4.11396027	2.74587011
O	1.41532993	-4.11396027	2.74587011
O	2.74587011	1.41532993	4.11396027
O	1.38151991	0.00000000	-6.79988003
O	-1.38151991	0.00000000	-6.79988003
O	-1.38151991	0.00000000	6.79988003
O	6.79988003	1.38151991	0.00000000
O	-6.79988003	1.38151991	0.00000000
O	-6.79988003	-1.38151991	0.00000000
O	6.79988003	-1.38151991	0.00000000
O	0.00000000	6.79988003	1.38151991
O	0.00000000	-6.79988003	1.38151991
O	0.00000000	-6.79988003	-1.38151991
O	0.00000000	6.79988003	-1.38151991
O	1.38151991	0.00000000	6.79988003
Zn	1.38346004	-2.76687002	-4.13293982
Zn	-1.38346004	2.76687002	-4.13293982
Zn	-1.38346004	-2.76687002	4.13293982
Zn	4.13293982	1.38346004	2.76687002
Zn	-4.13293982	1.38346004	-2.76687002
Zn	-4.13293982	-1.38346004	2.76687002
Zn	4.13293982	-1.38346004	-2.76687002
Zn	2.76687002	4.13293982	1.38346004
Zn	-2.76687002	-4.13293982	1.38346004
Zn	2.76687002	-4.13293982	-1.38346004
Zn	-2.76687002	4.13293982	-1.38346004
Zn	-1.38346004	-2.76687002	-4.13293982
Zn	-1.38346004	2.76687002	4.13293982
Zn	1.38346004	-2.76687002	4.13293982
Zn	1.38346004	2.76687002	-4.13293982
Zn	-4.13293982	-1.38346004	-2.76687002
Zn	4.13293982	-1.38346004	2.76687002
Zn	4.13293982	1.38346004	-2.76687002
Zn	-4.13293982	1.38346004	2.76687002
Zn	-2.76687002	-4.13293982	-1.38346004
Zn	2.76687002	4.13293982	-1.38346004
Zn	-2.76687002	4.13293982	1.38346004
Zn	2.76687002	-4.13293982	1.38346004
Zn	1.38346004	2.76687002	4.13293982
Zn	0.00000000	-1.36886001	-6.64646006
Zn	0.00000000	1.36886001	-6.64646006
Zn	0.00000000	-1.36886001	6.64646006
Zn	6.64646006	0.00000000	1.36886001
Zn	-6.64646006	0.00000000	-1.36886001
Zn	-6.64646006	0.00000000	1.36886001

Zn	6.64646006	0.00000000	-1.36886001
Zn	1.36886001	6.64646006	0.00000000
Zn	-1.36886001	-6.64646006	0.00000000
Zn	1.36886001	-6.64646006	0.00000000
Zn	-1.36886001	6.64646006	0.00000000
Zn	0.00000000	1.36886001	6.64646006
Zn	2.61667013	0.00000000	-5.40859985
Zn	-2.61667013	0.00000000	-5.40859985
Zn	-2.61667013	0.00000000	5.40859985
Zn	5.40859985	2.61667013	0.00000000
Zn	-5.40859985	2.61667013	0.00000000
Zn	-5.40859985	-2.61667013	0.00000000
Zn	5.40859985	-2.61667013	0.00000000
Zn	0.00000000	5.40859985	2.61667013
Zn	0.00000000	-5.40859985	2.61667013
Zn	0.00000000	-5.40859985	-2.61667013
Zn	0.00000000	5.40859985	-2.61667013
Zn	2.61667013	0.00000000	5.40859985
Zn	2.78132010	1.43526995	0.00000000
Zn	-2.78132010	-1.43526995	0.00000000
Zn	-2.78132010	1.43526995	0.00000000
Zn	0.00000000	2.78132010	-1.43526995
Zn	0.00000000	2.78132010	1.43526995
Zn	0.00000000	-2.78132010	-1.43526995
Zn	0.00000000	-2.78132010	1.43526995
Zn	-1.43526995	0.00000000	2.78132010
Zn	1.43526995	0.00000000	2.78132010
Zn	-1.43526995	0.00000000	-2.78132010
Zn	1.43526995	0.00000000	-2.78132010
Zn	2.78132010	-1.43526995	0.00000000
O	2.83638978	0.00000000	-1.42234993
O	-2.83638978	0.00000000	-1.42234993
O	-2.83638978	0.00000000	1.42234993
O	1.42234993	2.83638978	0.00000000
O	-1.42234993	2.83638978	0.00000000
O	-1.42234993	-2.83638978	0.00000000
O	1.42234993	-2.83638978	0.00000000
O	0.00000000	1.42234993	2.83638978
O	0.00000000	-1.42234993	2.83638978
O	0.00000000	-1.42234993	-2.83638978
O	0.00000000	1.42234993	-2.83638978
O	2.83638978	0.00000000	1.42234993

(ZnO)₆₀, C₁, AM1, -771.5470 Hartree

O	0.03388560	-3.04562998	-5.79572392
O	0.20430031	3.10988951	-5.70359707

O	0.22368176	-3.20278597	5.69100952
O	3.15820551	5.60041809	-0.13167690
O	3.12872481	-5.75523520	0.13272634
O	-3.01552057	5.72841358	0.02228349
O	-3.04915094	-5.82290697	-0.01265861
O	5.70374680	-0.24109329	3.05166578
O	5.68092918	0.10694448	-3.08386636
O	-5.82309246	-0.02136092	-3.08998966
O	-5.78998661	-0.03903531	3.10257411
O	0.11524780	2.95007133	5.76390505
O	4.98149824	-3.54398799	2.02266479
O	-4.76063681	3.27584743	1.90485764
O	-4.79747438	-3.34216571	-1.88650954
O	3.54086661	-2.18632317	4.94332314
O	3.51784110	2.07292032	-4.96686983
O	-2.98186707	-1.49613857	-4.39561844
O	-2.93004560	1.41824067	4.38082170
O	-1.41047060	4.25393629	2.85437989
O	-1.53632975	-4.40793848	-2.92799139
O	2.11112547	4.91579962	-3.44991946
O	2.11146951	-5.03612804	3.45040131
O	4.98353243	3.40819120	-2.04859161
O	2.64219141	-1.13781929	-4.13523531
O	-2.82308269	1.44463563	-4.29250145
O	-2.79853725	-1.52111459	4.28314304
O	1.84403563	4.43421793	3.07908988
O	1.42099929	-4.28679037	-2.80291104
O	-1.16403770	4.14164114	-2.69035053
O	-1.16197443	-4.22327757	2.68101239
O	4.06144476	2.50397515	1.11831868
O	4.04573917	-2.62325859	-1.13648510
O	-4.30974770	2.76934624	-1.34636462
O	-4.29317713	-2.84700680	1.33922172
O	2.67138267	1.03940821	4.11818409
O	1.53980958	0.06317303	-7.13249063
O	-1.33357882	0.08376189	-7.21545458
O	-1.27889156	-0.15802208	7.19640493
O	0.14536810	7.06963634	1.41601038
O	0.07845404	-7.24789476	-1.38999081
O	0.10305684	7.06082678	-1.45392048
O	0.06685163	-7.16660213	1.47430015
O	7.08072662	1.37049878	0.00286801
O	7.07432413	-1.50747561	-0.04356064
O	-7.19835520	1.42305100	0.04280351
O	-7.20660591	-1.46933043	-0.01204575
O	1.59268951	-0.16834114	7.11646032

O	2.68739867	0.02626077	-1.45938528
O	-3.28125191	-0.21486953	-1.51277041
O	-3.26280260	0.09256154	1.48428261
O	-0.20187494	1.52714705	3.12178636
O	-0.23249024	-1.61117029	-3.15332723
O	-0.25186270	1.30395389	-2.84511447
O	-0.23486502	-1.38875258	2.82982397
O	1.17224920	2.93362832	0.13704920
O	1.19047952	-3.00646067	-0.10487915
O	-1.78158951	2.94428802	0.04635346
O	-1.74160802	-3.07468796	-0.11733367
O	2.69889545	-0.10004439	1.44737124
Zn	4.78697777	-2.04030347	3.35868096
Zn	-4.46899843	1.54386866	2.94976211
Zn	-4.50385380	-1.61360812	-2.93888974
Zn	2.00509596	-3.49009371	4.74149227
Zn	1.98886597	3.38359118	-4.75302172
Zn	-1.52646482	-2.95160103	-4.44273710
Zn	-1.44080555	2.84279323	4.42625761
Zn	-3.05206275	4.35130262	1.55903292
Zn	-3.09043169	-4.43341446	-1.55599833
Zn	3.42429399	4.68586206	-1.92218244
Zn	3.42163587	-4.82313633	1.92095101
Zn	4.76980448	1.91175508	-3.38622355
Zn	1.39397573	-2.81695127	-4.27791071
Zn	-1.15339983	2.70022297	-4.22309542
Zn	-1.13294423	-2.78235698	4.21195078
Zn	2.73153973	4.13937998	1.25269234
Zn	2.68066144	-4.23293209	-1.16414559
Zn	-2.82036805	4.26911020	-1.38738585
Zn	-2.81067538	-4.35104132	1.37225938
Zn	4.13999176	0.99562907	2.61682296
Zn	4.10728168	-1.10689569	-2.63022852
Zn	-4.38727856	1.40643537	-2.91463280
Zn	-4.35932255	-1.47286785	2.89393926
Zn	1.51282430	2.79640293	4.26067781
Zn	0.09396056	-1.35161412	-6.82982206
Zn	0.11762345	1.48967397	-6.85646868
Zn	0.15621166	-1.58029878	6.84256554
Zn	1.54498422	6.76455879	-0.04667477
Zn	1.49491429	-6.89505768	0.05376985
Zn	-1.29713714	6.72980356	0.00385544
Zn	-1.35498416	-6.85749578	0.03481586
Zn	6.80487633	-0.09248369	1.39823461
Zn	6.79184723	-0.04190341	-1.43634582
Zn	-6.87348700	0.00610756	-1.39917624

Zn	-6.86207628	-0.05594590	1.42535925
Zn	0.16585313	1.26153123	6.80332232
Zn	2.77724576	0.30705473	-5.59215975
Zn	-2.64721870	0.01698031	-5.73874760
Zn	-2.60030007	-0.09540509	5.72781038
Zn	0.20613681	5.54744291	2.69069958
Zn	0.00157325	-5.74150705	-2.66669512
Zn	0.34035468	5.54876280	-2.72059822
Zn	0.32910705	-5.63829422	2.72179246
Zn	5.55043554	2.61564898	-0.27978575
Zn	5.54007339	-2.74259377	0.25416240
Zn	-5.70798969	2.72724009	0.20415428
Zn	-5.72175312	-2.78109431	-0.18268386
Zn	2.82085013	-0.41039351	5.56922531
Zn	2.56817222	1.44061232	0.03087339
Zn	-3.06069803	-1.51780891	0.10891537
Zn	-3.10439134	1.38850987	-0.14682320
Zn	-1.78121507	0.05911463	2.96866727
Zn	-1.79818177	-0.15604691	-2.99281740
Zn	1.21902931	-0.11726257	-2.86759329
Zn	1.24270284	0.02980305	2.87017488
Zn	-0.21182586	2.73463559	-1.38050926
Zn	-0.22652207	-2.81515932	1.35304451
Zn	-0.34057805	2.85685968	1.57239056
Zn	-0.24108180	-3.06405401	-1.66421425
Zn	2.57808089	-1.51284647	-0.03656371

(ZnO)₆₀, C₁, HF/6-31G, -111146.6629 Hartree

O	0.00293313	-2.74905109	-5.52744579
O	-0.13767537	2.83415604	-5.40508413
O	0.02761231	-2.81396985	5.39839649
O	2.72249985	5.43505621	0.09130754
O	2.75212550	-5.49044991	0.01858719
O	-2.86226463	5.51045322	-0.02580368
O	-2.83273149	-5.41506720	-0.09755532
O	5.45716143	0.06623038	2.78150082
O	5.35919571	-0.02526650	-2.80351210
O	-5.56755972	-0.04604852	-2.78771043
O	-5.46930027	0.04582020	2.79713964
O	-0.11364661	2.76931190	5.52100229
O	4.23709297	-2.93882656	1.54986036
O	-4.08597612	2.72285223	1.33262444
O	-4.36021566	-2.88464117	-1.62510931
O	2.68690896	-1.32160652	4.01082468
O	2.53075886	1.34065878	-4.06399155
O	-3.00651264	-1.54732049	-4.28784847

O	-2.94988489	1.59094048	4.32344294
O	-1.63858914	4.26838589	2.97370553
O	-1.36284220	-4.00226402	-2.75694704
O	1.22891068	4.09357119	-2.57671428
O	1.57517755	-4.31594610	2.86483550
O	4.00129128	2.62545514	-1.29430878
O	2.83853197	-1.56980932	-4.32920790
O	-2.79721117	1.34199083	-4.01739502
O	-2.64049864	-1.31994510	4.05729389
O	1.25226521	4.02227592	2.75060034
O	1.52821112	-4.24856806	-2.98073316
O	-1.68562675	4.33647919	-2.87221622
O	-1.33919001	-4.07370424	2.57046700
O	4.24955320	2.90432262	1.61881483
O	3.97564507	-2.70266390	-1.33953285
O	-4.34746790	2.95904613	-1.55675387
O	-4.11131811	-2.60510969	1.28805065
O	2.89636493	1.56796563	4.28207159
O	1.30394685	0.07749412	-6.77748251
O	-1.46866393	0.05010651	-6.73006725
O	-1.41432214	-0.05730262	6.77085781
O	-0.06733858	6.73002672	1.43976533
O	-0.04310528	-6.71007013	-1.44660902
O	-0.05176029	6.79052305	-1.33258927
O	-0.05816638	-6.77042246	1.32574487
O	6.71397686	1.39762938	-0.02844919
O	6.67760897	-1.37516129	-0.02546178
O	-6.78808451	1.39566278	0.01904658
O	-6.82405376	-1.37718058	0.02243396
O	1.35822940	-0.02982873	6.72361946
O	2.66576529	-0.04973314	-1.55894005
O	-2.93833470	0.20940942	-1.27879000
O	-2.77583456	0.07010040	1.55242169
O	0.14500062	1.27293932	2.88380694
O	-0.25517285	-1.25304139	-2.89017010
O	-0.14132062	1.57818222	-2.71698046
O	0.03129013	-1.55834103	2.71015239
O	1.48964798	2.73655128	0.08836815
O	1.23261654	-2.86480403	-0.22172548
O	-1.34278214	2.88460422	0.21488118
O	-1.59982622	-2.71659756	-0.09453698
O	2.82803535	-0.18958403	1.27214193
Zn	4.11095190	-1.33754528	2.63127685
Zn	-4.15675116	1.47841072	2.82428646
Zn	-4.43937254	-1.58934593	-3.02575707
Zn	1.45474684	-2.82355571	4.07949018

Zn	1.20912778	2.76063681	-4.01640129
Zn	-1.39596653	-2.61645722	-4.17449379
Zn	-1.66476119	3.00081801	4.40206099
Zn	-2.71233130	4.15230894	1.36630452
Zn	-2.85814714	-4.08899689	-1.51784384
Zn	2.65574312	4.05267525	-1.26233828
Zn	2.98089719	-4.37708712	1.57409275
Zn	3.96466899	1.31535733	-2.72500062
Zn	1.55397844	-2.98023582	-4.40835476
Zn	-1.56494606	2.84378338	-4.08634853
Zn	-1.31933415	-2.74048090	4.00986052
Zn	2.74749470	4.10873175	1.51143456
Zn	2.60212374	-4.13225412	-1.37349427
Zn	-3.09125853	4.39729881	-1.58142829
Zn	-2.76590657	-4.03252459	1.25598466
Zn	4.32916498	1.60960519	3.01997089
Zn	4.04634809	-1.45759416	-2.83066201
Zn	-4.22131586	1.35770774	-2.63802576
Zn	-4.07472324	-1.29469705	2.71851444
Zn	1.28547561	2.63659978	4.16825914
Zn	-0.06915778	-1.30055308	-6.71552849
Zn	-0.09196695	1.42644858	-6.63352394
Zn	-0.01839424	-1.40620208	6.62678385
Zn	1.30409229	6.65156031	0.05710233
Zn	1.31343782	-6.69044781	-0.05287857
Zn	-1.42360723	6.71047831	0.04576897
Zn	-1.41427290	-6.63152885	-0.06369878
Zn	6.65155697	0.01229746	1.33738375
Zn	6.58145142	0.01290255	-1.39014208
Zn	-6.76191854	0.00797391	-1.34357715
Zn	-6.69165373	0.00777420	1.38390899
Zn	-0.04129641	1.32080662	6.70911837
Zn	2.60852480	-0.02995532	-5.44283104
Zn	-2.78833342	-0.01182691	-5.40913391
Zn	-2.71890354	0.05070425	5.43621302
Zn	-0.11305393	5.40275240	2.75372887
Zn	0.00256804	-5.38271379	-2.76053309
Zn	-0.15377615	5.46106148	-2.64293599
Zn	0.04359468	-5.44108868	2.63622952
Zn	5.37341118	2.69570923	0.08320975
Zn	5.36188698	-2.70080614	0.02008215
Zn	-5.47225237	2.72118878	-0.02694764
Zn	-5.48366547	-2.67542458	-0.08924738
Zn	2.67797756	0.03208528	5.40273762
Zn	2.77608514	1.29862189	-0.04284313
Zn	-2.88600492	-1.27848291	0.03662593

Zn	-2.76006246	1.54293597	0.18932718
Zn	-1.33023536	-0.05579753	2.83055782
Zn	-1.60215700	0.20183924	-2.70163584
Zn	1.22034752	0.07550948	-2.83742714
Zn	1.49191630	-0.18186682	2.69492435
Zn	-0.01963340	2.85050964	-1.26602376
Zn	-0.09014212	-2.83104563	1.25957859
Zn	0.11901053	2.70183992	1.55466568
Zn	-0.22959681	-2.68184471	-1.56097615
Zn	2.64964628	-1.52287006	-0.19609363

(ZnO)₆₀, C₁, B3LYP/6-31G, -111265.6270 Hartree

O	0.01764000	-2.78187990	-5.50941992
O	-0.14169000	2.87117004	-5.39811993
O	0.02992000	-2.85016012	5.39254999
O	2.75793004	5.42993021	0.09425000
O	2.78503990	-5.47195959	0.03461000
O	-2.89602017	5.49148035	-0.03953000
O	-2.86869001	-5.40809011	-0.10010999
O	5.44025993	0.07933000	2.81506991
O	5.35122967	-0.02838000	-2.84066010
O	-5.54869986	-0.06000000	-2.82217002
O	-5.46175003	0.04838000	2.83240008
O	-0.12729000	2.80215001	5.50129986
O	4.28664970	-2.97654009	1.61784995
O	-4.05914021	2.71819997	1.31929004
O	-4.38443041	-2.91950011	-1.66710007
O	2.68337989	-1.31138003	3.98431993
O	2.51184011	1.34859002	-4.05747986
O	-3.04157019	-1.61373007	-4.33757973
O	-2.98959017	1.63440001	4.35167027
O	-1.70380998	4.31484985	3.00876999
O	-1.34869003	-3.97451997	-2.75188017
O	1.23537004	4.08881998	-2.55823994
O	1.61711001	-4.34434986	2.90376019
O	3.99380994	2.60861015	-1.30376005
O	2.87589002	-1.61198997	-4.35585976
O	-2.79233003	1.33090997	-3.99142003
O	-2.62225008	-1.32729006	4.05070972
O	1.24095011	3.99575019	2.74571991
O	1.59562004	-4.29545021	-3.01513982
O	-1.73032999	4.36588001	-2.91069007
O	-1.34902000	-4.06843996	2.55490994
O	4.27765036	2.94309998	1.66035998
O	3.94951987	-2.69859004	-1.32572007
O	-4.39713001	2.99564004	-1.62473011

O	-4.10569000	-2.58869004	1.29677010
O	2.93074012	1.63108993	4.32590008
O	1.30457997	0.08148000	-6.78804016
O	-1.45710003	0.04396000	-6.72492981
O	-1.41486001	-0.06060000	6.78101015
O	-0.07456000	6.72597027	1.42927003
O	-0.03618000	-6.70553017	-1.43453991
O	-0.04984000	6.80230999	-1.33250010
O	-0.06315999	-6.78081036	1.32687998
O	6.72262001	1.39733005	-0.03382000
O	6.67266989	-1.36524999	-0.01878000
O	-6.78309965	1.38453007	0.01076000
O	-6.83387995	-1.37729001	0.02531000
O	1.34770989	-0.02346000	6.71792030
O	2.63072014	-0.07595000	-1.59631002
O	-2.96702981	0.25806999	-1.21887004
O	-2.74028993	0.09388000	1.59021997
O	0.19396999	1.21133995	2.91135001
O	-0.30446002	-1.19172001	-2.91891003
O	-0.16650000	1.61750996	-2.68229985
O	0.05934000	-1.59798002	2.67535996
O	1.52745998	2.70221996	0.11386999
O	1.17341995	-2.89321995	-0.26945001
O	-1.28287005	2.91292000	0.26385999
O	-1.63743997	-2.68247008	-0.12004000
O	2.86000013	-0.23660000	1.21276999
Zn	4.13194990	-1.34463000	2.63204980
Zn	-4.13528013	1.47338998	2.81933999
Zn	-4.44143009	-1.61607003	-3.05707979
Zn	1.44805002	-2.81938004	4.05840015
Zn	1.20415008	2.78416014	-4.01688004
Zn	-1.40125000	-2.61559010	-4.19363976
Zn	-1.69218993	3.02994990	4.40481997
Zn	-2.71161008	4.17046976	1.37206006
Zn	-2.85135007	-4.06618023	-1.51076996
Zn	2.67850995	4.05584002	-1.25895000
Zn	3.01021004	-4.38044977	1.60338008
Zn	3.96604013	1.31268001	-2.74937987
Zn	1.58051002	-3.00926018	-4.40998983
Zn	-1.56162000	2.84255981	-4.06691980
Zn	-1.31736004	-2.76514983	4.01349020
Zn	2.74451995	4.08923006	1.50617003
Zn	2.60195994	-4.15093994	-1.37746000
Zn	-3.12182999	4.40023041	-1.60832000
Zn	-2.79101014	-4.03610992	1.25500000
Zn	4.33161020	1.63505995	3.04592013

Zn	4.02435017	-1.45295000	-2.82534003
Zn	-4.24005985	1.36346996	-2.63772988
Zn	-4.07670021	-1.29244006	2.74217010
Zn	1.29138005	2.63475013	4.18548012
Zn	-0.05719000	-1.30578005	-6.65151024
Zn	-0.08846000	1.42132998	-6.56303024
Zn	-0.02142000	-1.40068996	6.55810022
Zn	1.29821992	6.58312988	0.05379000
Zn	1.31795001	-6.62557983	-0.03862000
Zn	-1.42965996	6.64603996	0.03441000
Zn	-1.41022992	-6.56271029	-0.06068000
Zn	6.58718014	0.02409000	1.34183002
Zn	6.50999022	0.01363000	-1.38560998
Zn	-6.69769001	-0.00417000	-1.35053003
Zn	-6.62083006	0.00578000	1.37764990
Zn	-0.05269000	1.32588995	6.64293003
Zn	2.55043983	-0.06089000	-5.40893984
Zn	-2.73218989	-0.03828000	-5.36894989
Zn	-2.66167998	0.08228000	5.40255022
Zn	-0.13933000	5.36255980	2.69783998
Zn	0.03097000	-5.34226990	-2.70315003
Zn	-0.18570000	5.42846012	-2.58492994
Zn	0.07269000	-5.40748024	2.57974005
Zn	5.33926010	2.63786006	0.11087999
Zn	5.32228994	-2.64773011	0.04890000
Zn	-5.43179035	2.66611004	-0.05547000
Zn	-5.44976997	-2.61689997	-0.11971001
Zn	2.62257981	0.05796000	5.36139965
Zn	2.78173995	1.25642991	-0.07980000
Zn	-2.89326000	-1.23721004	0.07139000
Zn	-2.68378997	1.56736994	0.23491001
Zn	-1.28625000	-0.09455000	2.83620024
Zn	-1.62782991	0.24836999	-2.62720013
Zn	1.17764997	0.11166000	-2.84328008
Zn	1.52005005	-0.22632000	2.62046981
Zn	0.01585000	2.85871005	-1.22358000
Zn	-0.12673001	-2.83921003	1.21736991
Zn	0.16415000	2.62687016	1.58044994
Zn	-0.27334002	-2.60509014	-1.58618999
Zn	2.57603002	-1.54871011	-0.23868999

(ZnO)₁₆₈, T_h, AM1, -2160.0311 Hartree

O	0.00000000	-3.04189992	-5.98662996
O	0.00000000	3.04189992	-5.98662996
O	0.00000000	-3.04189992	5.98662996
O	5.98662996	0.00000000	3.04189992

O	-5.98662996	0.00000000	-3.04189992
O	-5.98662996	0.00000000	3.04189992
O	5.98662996	0.00000000	-3.04189992
O	3.04189992	5.98662996	0.00000000
O	-3.04189992	-5.98662996	0.00000000
O	3.04189992	-5.98662996	0.00000000
O	-3.04189992	5.98662996	0.00000000
O	0.00000000	3.04189992	5.98662996
O	2.86122012	-1.37433994	-4.36909008
O	-2.86122012	1.37433994	-4.36909008
O	-2.86122012	-1.37433994	4.36909008
O	4.36909008	2.86122012	1.37433994
O	-4.36909008	2.86122012	-1.37433994
O	-4.36909008	-2.86122012	1.37433994
O	4.36909008	-2.86122012	-1.37433994
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O	-1.37433994	-4.36909008	2.86122012
O	1.37433994	-4.36909008	-2.86122012
O	-1.37433994	4.36909008	-2.86122012
O	-2.86122012	-1.37433994	-4.36909008
O	-2.86122012	1.37433994	4.36909008
O	2.86122012	-1.37433994	4.36909008
O	2.86122012	1.37433994	-4.36909008
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O	1.37433994	-4.36909008	2.86122012
O	2.86122012	1.37433994	4.36909008
O	1.48277998	0.00000000	-7.54879999
O	-1.48277998	0.00000000	-7.54879999
O	-1.48277998	0.00000000	7.54879999
O	7.54879999	1.48277998	0.00000000
O	-7.54879999	1.48277998	0.00000000
O	-7.54879999	-1.48277998	0.00000000
O	7.54879999	-1.48277998	0.00000000
O	0.00000000	7.54879999	1.48277998
O	0.00000000	-7.54879999	1.48277998
O	0.00000000	-7.54879999	-1.48277998
O	0.00000000	7.54879999	-1.48277998
O	1.48277998	0.00000000	7.54879999
Zn	1.42468989	-2.87764001	-4.38697004
Zn	-1.42468989	2.87764001	-4.38697004

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Zn	4.38697004	1.42468989	2.87764001
Zn	-4.38697004	1.42468989	-2.87764001
Zn	-4.38697004	-1.42468989	2.87764001
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Zn	-4.38697004	1.42468989	2.87764001
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Zn	1.42468989	2.87764001	4.38697004
Zn	0.00000000	-1.54425001	-7.44328022
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Zn	10.11816978	0.00000000	-2.69455004
Zn	2.69455004	10.11816978	0.00000000
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O	0.00000000	-1.43795002	-11.64830971
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O	4.29910994	-1.42508006	-7.19827986
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Zn	2.87603998	-1.43856001	-8.72161007
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Zn	8.72161007	2.87603998	1.43856001

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Zn	-8.72161007	-2.87603998	1.43856001
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Zn	1.43856001	8.72161007	2.87603998
Zn	-1.43856001	-8.72161007	2.87603998
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Zn	1.43856001	-8.72161007	2.87603998
Zn	2.87603998	1.43856001	8.72161007
O	3.08143997	0.00000000	-10.18313980
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O	0.00000000	10.18313980	3.08143997
O	0.00000000	-10.18313980	3.08143997
O	0.00000000	-10.18313980	-3.08143997
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O	3.08143997	0.00000000	10.18313980
Zn	1.42028999	0.00000000	-11.26912022
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(ZnO)₁₆₈, T_h, HF/6-31G, -311212.4008 Hartree

O	0.00000000	-2.84345007	-5.59236002
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(ZnO)₁₆₈, C₁, AM1, -2160.3074 Hartree

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(ZnO)₁₆₈, C₁, HF/6-31G, -311212.4034 Hartree

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(ZnO)₃₆₀, T_h, AM1, -4628.4434 Hartree

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(ZnO)₃₆₀, C₁, AM1, -4629.0735 Hartree

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Zn	4.25204897	2.84659600	-5.94911385
Zn	-5.73798704	-4.27726030	-2.62376785
Zn	5.63830328	-4.33463526	2.78960609
Zn	6.15043116	4.49267101	-3.34116602
Zn	-5.99186802	4.62801170	3.21767902
Zn	-3.20420194	-6.12552786	-4.34280396
Zn	2.88963199	5.64152288	-4.47161770
Zn	-2.83148718	5.84820890	4.35706377
Zn	2.72511196	-5.77568722	4.44099188
Zn	4.59533167	3.05444717	5.86861897
Zn	2.51390600	-1.37449408	-8.39362144
Zn	-2.86379504	1.29791701	-8.27617455
Zn	-3.57226205	-1.64345300	9.40274525
Zn	9.24268246	3.34447813	1.60451102
Zn	-9.20448780	3.41071105	-1.90124905
Zn	-8.60242939	-2.72429395	1.53532195
Zn	8.96365547	-3.26414299	-2.05203891
Zn	1.45001698	8.39654064	2.47592902
Zn	-1.68893504	-8.90593433	3.18386006
Zn	1.78057289	-9.28126431	-3.44487476
Zn	-1.38252604	8.29121399	-2.59987020
Zn	-3.15128708	-1.75378895	-8.50431728
Zn	-2.57562208	1.44211900	8.58355045
Zn	2.92179084	-1.48530698	8.88710308
Zn	3.23782110	1.80594099	-9.07476997
Zn	-8.89865208	-3.12815619	-1.59478700
Zn	8.56711769	-2.82499886	1.17270505
Zn	8.46470356	2.50559807	-1.50330102
Zn	-8.40115166	2.80478120	1.36959708
Zn	-1.28028500	-8.45502853	-2.54152393
Zn	1.75081503	8.84340858	-3.32638001
Zn	-1.72588098	8.96584892	3.23023510
Zn	1.32288003	-8.75746346	2.92017508
Zn	3.01715207	1.52990198	8.86773014
Zn	1.35617399	-0.19939700	-11.31211853
Zn	-1.61904407	0.10122800	-11.16081333

Zn	-1.58730888	0.34006801	11.59866333
Zn	11.47100258	1.45484900	-0.42407399
Zn	-11.30246353	1.36594403	0.07007900
Zn	-11.54299355	-1.64254498	0.12538300
Zn	11.38320827	-1.50051606	-0.17589700
Zn	0.31586900	11.30816841	1.38943207
Zn	-0.17068401	-11.69833088	1.56398499
Zn	-0.19007000	-11.48654556	-1.48639107
Zn	-0.27437299	11.25219917	-1.52597702
Zn	1.36556900	-0.19873200	11.59792900
Zn	5.63718987	-0.04655700	-7.26139688
Zn	-5.72576189	-0.06606100	-7.04262400
Zn	-5.76806593	0.21595299	7.40763903
Zn	7.28907490	5.67944193	-0.27399999
Zn	-7.15438080	5.71257687	0.05216100
Zn	-7.40367699	-5.90197372	0.02161800
Zn	7.16213799	-5.87399101	-0.27813601
Zn	0.00695700	7.24629498	5.65317631
Zn	-0.13477001	-7.37512684	6.23795700
Zn	-0.16323701	-7.27555799	-5.67132378
Zn	0.00587700	7.07677603	-5.72248888
Zn	6.11929989	0.11356900	7.36149502
Zn	1.73205698	-7.61662912	-9.05938530
Zn	-1.23589194	6.97187424	-8.60388184
Zn	-1.62046397	-7.22286606	8.95772171
Zn	8.83940220	1.58386898	7.27580309
Zn	-8.92080402	1.84441197	-7.69934988
Zn	-9.11014271	-1.76427603	7.76029301
Zn	8.59049034	-1.21564698	-7.14361095
Zn	7.67148495	9.03939533	1.79418898
Zn	-7.25832129	-8.68432236	1.39155006
Zn	7.63974333	-8.98822689	-1.98455095
Zn	-7.57642126	9.00873280	-1.86245501
Zn	-1.36387801	-7.00315619	-8.56686497
Zn	-1.99004495	7.65960598	8.94416142
Zn	1.37413096	-7.16154194	8.77901649
Zn	1.71314394	7.75230598	-9.07567024
Zn	-8.55678749	-1.14788389	-6.93339491
Zn	8.76245117	-1.34298790	7.06907511
Zn	8.99089622	1.86941600	-7.70016193
Zn	-8.70348930	1.33679700	7.10119200
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Zn	7.08102179	8.63811588	-1.31698108
Zn	-7.01077271	8.61359978	1.25840497
Zn	7.02888393	-8.62847328	1.01252902
Zn	1.02661800	7.14445925	8.58319473

Zn	4.51836729	-5.93024492	-7.54846573
Zn	-4.40286589	6.05601501	-7.57685518
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Zn	7.31086731	4.48847103	5.79616022
Zn	-7.41057873	4.63655424	-6.05473042
Zn	-7.42193174	-4.47003698	6.06103277
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Zn	5.85885286	7.37921524	4.38986778
Zn	-5.83693075	-7.27559423	4.45452309
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Zn	-4.85066700	6.19315529	7.51157713
Zn	4.16671610	-5.58255196	7.08382082
Zn	4.95209217	5.93978834	-6.98284006
Zn	-7.23565912	-4.43268204	-5.75649834
Zn	7.07410002	-4.15057087	5.49464989
Zn	7.70679712	4.76001978	-6.15911436
Zn	-7.44931698	4.34572840	5.90179014
Zn	-6.18849516	-7.54947901	-4.64560986
Zn	5.96630001	7.46409369	-4.40136003
Zn	-5.94820213	7.46476889	4.43515301
Zn	5.51732588	-7.06613493	4.03646517
Zn	4.20529985	5.79519892	7.18066835
Zn	3.08949113	-4.25995922	-10.31538773
Zn	-2.82865119	4.36290979	-9.97842598
Zn	-3.13256097	-4.54507399	10.36432552
Zn	10.57363605	3.32686090	4.61580706
Zn	-10.46128368	3.20987797	-4.66910982
Zn	-10.42041874	-3.14907002	4.48435402
Zn	10.27039623	-2.98470497	-4.90142918
Zn	4.28328657	10.28155804	3.09461808
Zn	-4.38516092	-10.20338917	2.86437702
Zn	4.75563002	-10.63103962	-3.53090000
Zn	-4.24048901	10.24369431	-3.18249106
Zn	-3.03997111	-4.56443501	-10.01066780
Zn	-3.30927110	4.39393902	10.34552479
Zn	2.94420910	-4.34640980	10.29024696
Zn	3.36525488	4.69001007	-10.75629520
Zn	-10.12294006	-2.78756404	-4.40364981
Zn	9.94267654	-2.67793012	3.96148491
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Zn	-9.79919147	2.77001119	4.24981403
Zn	-4.38483715	-10.05075741	-3.11055303
Zn	4.68753624	10.17755604	-3.03468394
Zn	-4.68341112	10.19310188	2.95324707

Zn	4.12197828	-9.93509674	2.53834796
Zn	2.64706302	4.34224701	9.96064568
Zn	1.60473800	-2.96611786	-12.92028522
Zn	-1.03454006	2.77072597	-12.62976074
Zn	-1.59562099	-2.77621007	13.09424782
Zn	13.34942150	1.95762408	3.20000291
Zn	-13.34352875	2.06482410	-3.47572112
Zn	-12.98207951	-1.51911902	3.03726006
Zn	12.85519123	-1.34483600	-3.05825806
Zn	3.07624102	12.99346638	1.69748497
Zn	-3.03559589	-12.99096394	1.42415094
Zn	3.33840084	-13.38428020	-2.11948299
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Zn	-1.43927896	-2.77498913	-12.67903233
Zn	-1.84016001	3.18127489	13.09866810
Zn	1.50602591	-2.98848319	13.09633636
Zn	1.98010600	3.41516495	-13.42367554
Zn	-12.76296520	-1.03337204	-2.74333692
Zn	12.85193539	-1.12761605	2.49778104
Zn	12.98986053	1.71958399	-3.15673113
Zn	-12.73011780	1.38852203	2.71373510
Zn	-2.84932303	-12.88453102	-1.51825404
Zn	2.81218004	12.72662067	-1.40500498
Zn	-2.78511000	12.73573303	1.29930604
Zn	2.71692300	-12.91830826	1.03640902
Zn	1.26912200	2.88898301	12.87935352
Zn	5.95890570	-2.89738584	-9.01985931
Zn	-5.84519958	3.04101896	-8.91653728
Zn	-6.26606178	-3.07025409	9.10179043
Zn	8.93757057	6.16600084	2.98817897
Zn	-8.86693192	6.18513918	-3.13187194
Zn	-8.99234772	-5.97169685	3.10955286
Zn	8.87769127	-6.08174181	-3.34938788
Zn	2.85000587	8.88471222	5.90613604
Zn	-2.95417786	-8.70576954	5.93610430
Zn	3.03282309	-8.92986965	-6.28265810
Zn	-2.84188223	8.83526325	-5.99432611
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Zn	-6.11208296	3.05162096	9.00855637
Zn	5.73197842	-2.73571491	8.54416943
Zn	6.10789776	3.18956900	-8.78615856
Zn	-8.63584709	-5.87030888	-3.07399201
Zn	8.42538071	-5.60933208	2.47727323
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Zn	-3.04249382	-8.86861897	-5.92801714

Zn	3.23405910	8.67067146	-6.06124306
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Zn	2.73394799	-8.56047249	5.66524506
Zn	5.74761295	2.94623399	8.65500259
Zn	4.30117321	-1.20237708	-11.26529312
Zn	-4.34792185	1.64171505	-11.39147186
Zn	-4.80939102	-1.74543500	12.12283039
Zn	12.02012157	4.78804302	1.72154307
Zn	-11.98622799	4.86136055	-1.91643298
Zn	-11.47440434	-4.42078018	1.52339303
Zn	11.77330589	-4.45161581	-1.94726408
Zn	1.23087001	11.23659134	4.32259893
Zn	-1.48651898	-11.63052273	4.40993786
Zn	1.75895798	-12.01631451	-4.89268112
Zn	-1.22584808	11.18214703	-4.41706800
Zn	-4.33775902	-1.41229510	-11.32952976
Zn	-4.52028704	1.37548602	11.41255283
Zn	4.33093214	-1.32534802	11.55264950
Zn	4.69830894	1.84822202	-11.94638252
Zn	-11.59918785	-4.32036066	-1.49843800
Zn	11.32343578	-4.28077888	1.02903795
Zn	11.32162952	4.42020798	-1.36338997
Zn	-11.17781353	4.27352905	1.05697894
Zn	-1.32325101	-11.26708794	-4.41179609
Zn	1.86597502	11.72690201	-4.56516123
Zn	-1.86803305	11.79851151	4.48554897
Zn	1.42765903	-11.54039669	4.25048828
Zn	4.27587891	1.60245597	11.65104580
Zn	0.03440100	-1.35979497	-15.25738430
Zn	0.01811600	1.45735192	-15.33219147
Zn	-0.03535300	-1.28117001	15.47449493
Zn	15.42765236	0.12988999	1.25911295
Zn	-15.40745449	0.20532300	-1.51771200
Zn	-15.34566307	0.17881301	1.32362103
Zn	15.36386299	0.18339100	-1.55965590
Zn	1.41725600	15.28454018	0.00861900
Zn	-1.38285792	-15.41595364	-0.21605700
Zn	1.45093107	-15.48104572	-0.27847001
Zn	-1.39441299	15.28347111	-0.14496800
Zn	-0.17065001	1.53483605	15.42942905
Zn	2.73282099	0.28768799	-14.12056160
Zn	-2.64446306	-0.10516400	-14.00549793
Zn	-2.84629703	-0.09508900	14.31290054
Zn	14.19633198	2.84760594	0.12822300
Zn	-14.09164810	2.83697510	-0.35578600
Zn	-14.28323078	-2.52828288	-0.03343700

Zn	14.18822193	-2.58092809	-0.40010798
Zn	-0.23357099	14.08348083	2.63383222
Zn	0.02097500	-14.36934948	2.50390100
Zn	0.23529701	-14.20116234	-2.93144417
Zn	0.25484198	14.04783249	-2.75627995
Zn	2.60559106	0.30373001	14.25796700
Zn	0.24505100	-5.57998991	-11.21172714
Zn	0.54972303	5.64774370	-11.07300854
Zn	0.11625800	-5.60067511	11.39460468
Zn	11.34259701	0.28558302	5.52184725
Zn	-11.27057743	0.40002099	-5.70117998
Zn	-11.29253674	-0.23825300	5.66899872
Zn	11.26450348	0.39058301	-5.77898312
Zn	5.62017202	11.22889423	0.31095102
Zn	-5.71679592	-11.28734779	0.05834200
Zn	5.63539076	-11.31197643	-0.49791199
Zn	-5.57893324	11.21204853	-0.39103600
Zn	-0.47619802	5.72772980	11.26631260
Zn	7.00236607	0.36926800	-10.00950909
Zn	-6.91703081	0.22849600	-9.87593746
Zn	-7.13503313	-0.24174200	10.08705330
Zn	10.00510311	7.08598185	0.23405799
Zn	-9.93082047	7.06054497	-0.35192201
Zn	-10.07273197	-6.92578030	-0.07758200
Zn	9.97394657	-6.97731781	-0.51223099
Zn	-0.45576400	9.97553062	6.94352007
Zn	-0.01235900	-10.10719299	6.99410200
Zn	0.20606700	-9.96041393	-7.11414814
Zn	0.40872902	9.89026070	-6.99093533
Zn	6.95708990	0.10056700	10.08436871

Unrelaxed (ZnO)₆₀ bulk wurtzite fragment, C₁

Zn	13.13471985	6.50000000	11.01360035
Zn	11.25833035	6.50000000	13.61359978
Zn	14.07291031	4.87500000	13.61359978
Zn	13.13471985	9.75000000	11.01360035
Zn	11.25833035	9.75000000	13.61359978
Zn	15.94929981	8.12500000	11.01360035
Zn	14.07291031	8.12500000	13.61359978
Zn	16.88750076	6.50000000	13.61359978
Zn	13.13471985	13.00000000	11.01360035
Zn	11.25833035	13.00000000	13.61359978
Zn	15.94929981	11.37500000	11.01360035
Zn	14.07291031	11.37500000	13.61359978
Zn	18.76387978	9.75000000	11.01360035
Zn	16.88750076	9.75000000	13.61359978

Zn	19.70207977	8.12500000	13.61359978
Zn	14.07291031	14.62500000	13.61359978
Zn	16.88750076	13.00000000	13.61359978
Zn	19.70207977	11.37500000	13.61359978
Zn	10.32013988	8.12500000	16.21360016
Zn	13.13471985	6.50000000	16.21360016
Zn	11.25833035	6.50000000	18.81360054
Zn	15.94929981	4.87500000	16.21360016
Zn	14.07291031	4.87500000	18.81360054
Zn	10.32013988	11.37500000	16.21360016
Zn	13.13471985	9.75000000	16.21360016
Zn	11.25833035	9.75000000	18.81360054
Zn	15.94929981	8.12500000	16.21360016
Zn	14.07291031	8.12500000	18.81360054
Zn	18.76387978	6.50000000	16.21360016
Zn	16.88750076	6.50000000	18.81360054
Zn	13.13471985	13.00000000	16.21360016
Zn	11.25833035	13.00000000	18.81360054
Zn	15.94929981	11.37500000	16.21360016
Zn	14.07291031	11.37500000	18.81360054
Zn	18.76387978	9.75000000	16.21360016
Zn	16.88750076	9.75000000	18.81360054
Zn	21.57847023	8.12500000	16.21360016
Zn	19.70207977	8.12500000	18.81360054
Zn	15.94929981	14.62500000	16.21360016
Zn	14.07291031	14.62500000	18.81360054
Zn	18.76387978	13.00000000	16.21360016
Zn	16.88750076	13.00000000	18.81360054
Zn	21.57847023	11.37500000	16.21360016
Zn	19.70207977	11.37500000	18.81360054
Zn	22.51666069	9.75000000	18.81360054
Zn	10.32013988	8.12500000	21.41360092
Zn	13.13471985	6.50000000	21.41360092
Zn	15.94929981	4.87500000	21.41360092
Zn	10.32013988	11.37500000	21.41360092
Zn	13.13471985	9.75000000	21.41360092
Zn	15.94929981	8.12500000	21.41360092
Zn	14.07291031	8.12500000	24.01359940
Zn	18.76387978	6.50000000	21.41360092
Zn	13.13471985	13.00000000	21.41360092
Zn	15.94929981	11.37500000	21.41360092
Zn	14.07291031	11.37500000	24.01359940
Zn	18.76387978	9.75000000	21.41360092
Zn	16.88750076	9.75000000	24.01359940
Zn	15.94929981	14.62500000	21.41360092
Zn	18.76387978	13.00000000	21.41360092

O	10.32013988	8.12500000	13.00000000
O	13.13471985	6.50000000	13.00000000
O	15.94929981	4.87500000	13.00000000
O	10.32013988	11.37500000	13.00000000
O	13.13471985	9.75000000	13.00000000
O	14.07291031	8.12500000	10.39999962
O	15.94929981	8.12500000	13.00000000
O	18.76387978	6.50000000	13.00000000
O	13.13471985	13.00000000	13.00000000
O	14.07291031	11.37500000	10.39999962
O	15.94929981	11.37500000	13.00000000
O	16.88750076	9.75000000	10.39999962
O	18.76387978	9.75000000	13.00000000
O	15.94929981	14.62500000	13.00000000
O	18.76387978	13.00000000	13.00000000
O	10.32013988	8.12500000	18.20000076
O	11.25833035	6.50000000	15.60000038
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O	14.07291031	4.87500000	15.60000038
O	15.94929981	4.87500000	18.20000076
O	10.32013988	11.37500000	18.20000076
O	11.25833035	9.75000000	15.60000038
O	13.13471985	9.75000000	18.20000076
O	14.07291031	8.12500000	15.60000038
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O	16.88750076	6.50000000	15.60000038
O	18.76387978	6.50000000	18.20000076
O	11.25833035	13.00000000	15.60000038
O	13.13471985	13.00000000	18.20000076
O	14.07291031	11.37500000	15.60000038
O	15.94929981	11.37500000	18.20000076
O	16.88750076	9.75000000	15.60000038
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O	19.70207977	8.12500000	15.60000038
O	21.57847023	8.12500000	18.20000076
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O	15.94929981	14.62500000	18.20000076
O	16.88750076	13.00000000	15.60000038
O	18.76387978	13.00000000	18.20000076
O	19.70207977	11.37500000	15.60000038
O	21.57847023	11.37500000	18.20000076
O	22.51666069	9.75000000	15.60000038
O	11.25833035	6.50000000	20.79999924
O	13.13471985	6.50000000	23.39999962
O	14.07291031	4.87500000	20.79999924
O	11.25833035	9.75000000	20.79999924

O	13.13471985	9.75000000	23.39999962
O	14.07291031	8.12500000	20.79999924
O	15.94929981	8.12500000	23.39999962
O	16.88750076	6.50000000	20.79999924
O	11.25833035	13.00000000	20.79999924
O	13.13471985	13.00000000	23.39999962
O	14.07291031	11.37500000	20.79999924
O	15.94929981	11.37500000	23.39999962
O	16.88750076	9.75000000	20.79999924
O	18.76387978	9.75000000	23.39999962
O	19.70207977	8.12500000	20.79999924
O	14.07291031	14.62500000	20.79999924
O	16.88750076	13.00000000	20.79999924
O	19.70207977	11.37500000	20.79999924

Relaxed (ZnO)₆₀ bulk wurtzite fragment, C₁, HF/6-31G, -111146.2717 Hartree

Zn	12.39437962	7.70363998	11.45318031
Zn	11.01984024	6.54108000	13.61096001
Zn	14.43048954	5.38006020	13.46889019
Zn	14.88492966	9.77309990	10.43957043
Zn	10.81381035	9.74726009	13.34609985
Zn	15.62413979	7.33975983	11.52307034
Zn	13.56013966	8.15221977	13.91390991
Zn	17.17950058	6.53966999	13.56853962
Zn	12.40804958	11.40114975	11.57308960
Zn	11.18566036	12.98686981	13.57110977
Zn	15.02272987	12.64435959	11.68653011
Zn	13.65715027	11.43453979	13.99911976
Zn	18.36704063	9.55580997	12.10964966
Zn	16.08381081	9.72502995	13.32754993
Zn	20.12807083	7.76440001	13.72665977
Zn	14.42605972	14.38469028	13.69404984
Zn	17.10663986	12.77017021	13.53884029
Zn	20.05215073	11.63175964	13.59770012
Zn	10.35597038	8.05426979	16.30964088
Zn	12.84595013	6.12179995	16.16988945
Zn	11.22095013	6.55818987	18.97302055
Zn	15.85993958	5.18876982	16.49324989
Zn	14.30226040	5.26351023	19.33190918
Zn	10.34088993	11.50275040	16.31090927
Zn	12.70672035	9.81072998	16.25449944
Zn	10.91656017	9.74042034	19.01114082
Zn	15.83205986	8.01146030	15.73003960
Zn	13.83662987	8.08193016	18.17336082
Zn	18.93172073	6.42708015	16.50687027
Zn	17.50702095	5.68894005	19.27020073

Zn	12.89457989	13.35231018	16.33110046
Zn	11.27439022	12.71467018	19.18884087
Zn	15.87302971	11.37238026	15.89960957
Zn	13.97811985	11.39972019	18.38287926
Zn	18.77149010	9.83493042	15.20798969
Zn	17.34775925	9.78020954	17.77589035
Zn	21.77503967	7.99626017	16.40546989
Zn	20.49711037	7.26177979	19.34753036
Zn	15.94174957	14.22459984	16.54217911
Zn	14.30078983	14.26840973	19.36010933
Zn	18.85658073	12.51877975	16.61022949
Zn	17.51732063	13.84381008	19.26173973
Zn	21.58494949	11.39048958	16.39451027
Zn	20.45627022	12.25339985	19.35556984
Zn	22.51461029	9.74265003	18.26926041
Zn	11.07901001	7.92662001	21.78348923
Zn	12.45256996	5.61651993	21.92433929
Zn	15.29634953	6.78715992	21.78603935
Zn	11.50209999	11.28032970	22.21032906
Zn	13.46761990	9.73176003	20.97602081
Zn	16.05279922	8.17737961	19.57552910
Zn	13.54656982	8.29881001	23.61795998
Zn	18.19095993	8.35951996	21.19432068
Zn	12.45565033	13.87139988	22.07398033
Zn	16.33662987	11.20785046	19.78842926
Zn	13.81908989	11.55195045	23.88845062
Zn	20.27161980	9.85017967	21.70712090
Zn	16.42440033	9.79049015	23.23896027
Zn	15.27970982	12.73054981	21.75905037
Zn	18.36462021	11.76111984	21.83181000
O	10.73005962	8.01455021	12.41625023
O	12.87572956	6.46563005	12.99705982
O	15.95250034	5.62273979	12.35138035
O	10.72049046	11.50658035	12.46168995
O	12.88823032	9.84204960	13.15511036
O	14.01972008	8.07756996	10.61518002
O	15.47344971	7.89432001	13.69865036
O	18.52433968	7.65934992	12.75454044
O	13.06801987	13.07878017	12.94641018
O	14.03349972	11.44493961	10.59195995
O	15.47933960	11.52577019	13.40919018
O	16.50709915	9.24075031	11.39363003
O	20.00712013	9.68043041	13.71498013
O	15.92463970	14.07052994	12.56365013
O	18.36849022	11.50121021	12.70259953
O	10.39214993	8.05722046	18.17093086

O	11.00817013	6.46907997	15.47364044
O	12.99285984	6.19165993	18.17462921
O	14.33076954	5.14041996	15.37154961
O	15.96401024	4.99467993	18.38229942
O	10.34654999	11.41687965	18.16927910
O	10.77814960	9.77217007	15.42022038
O	12.84576035	9.79135990	18.22599030
O	13.58738041	8.08498955	15.89857006
O	15.89890957	8.20209026	17.66781044
O	17.23381996	6.28321981	15.56879044
O	19.09394073	6.28353024	18.40526009
O	11.15723991	12.99164009	15.44371033
O	12.99466991	13.21667004	18.30986977
O	13.77668953	11.44184971	15.92850971
O	15.93282032	11.29508018	17.87495041
O	16.82699013	9.72089005	15.21835995
O	18.94696999	10.46164989	16.96604919
O	20.39855003	7.09733009	15.46940041
O	21.93674088	7.93356991	18.34952927
O	14.31023026	14.44431019	15.55862999
O	15.95456028	14.51710033	18.42107010
O	17.12801933	12.96839046	15.58314037
O	19.07336044	13.22224045	18.42954063
O	20.37457085	12.34986019	15.29502010
O	21.85874939	11.49973011	18.35710907
O	22.51955986	9.72307968	16.26432991
O	11.02818012	6.24834013	20.79785919
O	12.20934010	7.09287977	23.14390945
O	14.17483997	5.26852989	21.24124908
O	11.31853008	9.64918041	20.96594048
O	13.04166985	10.02355957	22.98170090
O	14.27554989	8.07977962	20.29356003
O	15.41827011	8.14922047	23.21331024
O	16.99677086	6.85417986	20.73901939
O	11.22167969	12.84471989	21.03037071
O	12.36114025	12.64367962	23.52598000
O	14.47951984	11.31460953	20.41243935
O	15.63729000	11.55912971	23.33849907
O	17.36796951	9.58471012	19.80924988
O	18.24720955	9.91664982	22.53311920
O	20.10741997	8.15009022	20.98316002
O	14.13444996	14.23314953	21.25859070
O	17.07331085	12.73289013	20.83383942
O	20.16057014	11.63735008	21.17168045

Onion-like structure of (ZnO)₆₀ in Figure S6 right, T_h, B3LYP/6-31G, -111265.3951 Hartree

O	0.00000000	-2.45234466	-4.67312479
O	0.00000000	2.45234466	-4.67312479
O	0.00000000	-2.45234466	4.67312479
O	4.67312479	0.00000000	2.45234466
O	-4.67312479	0.00000000	-2.45234466
O	-4.67312479	0.00000000	2.45234466
O	4.67312479	0.00000000	-2.45234466
O	2.45234466	4.67312479	0.00000000
O	-2.45234466	-4.67312479	0.00000000
O	2.45234466	-4.67312479	0.00000000
O	-2.45234466	4.67312479	0.00000000
O	0.00000000	2.45234466	4.67312479
O	1.41986704	0.00000000	-6.36720991
O	-1.41986704	0.00000000	-6.36720991
O	-1.41986704	0.00000000	6.36720991
O	6.36720991	1.41986704	0.00000000
O	-6.36720991	1.41986704	0.00000000
O	-6.36720991	-1.41986704	0.00000000
O	6.36720991	-1.41986704	0.00000000
O	0.00000000	6.36720991	1.41986704
O	0.00000000	-6.36720991	1.41986704
O	0.00000000	-6.36720991	-1.41986704
O	0.00000000	6.36720991	-1.41986704
O	1.41986704	0.00000000	6.36720991
O	0.00000000	-2.83152723	-1.44309235
O	0.00000000	2.83152723	-1.44309235
O	0.00000000	-2.83152723	1.44309235
O	1.44309235	0.00000000	2.83152723
O	-1.44309235	0.00000000	-2.83152723
O	-1.44309235	0.00000000	2.83152723
O	1.44309235	0.00000000	-2.83152723
O	2.83152723	1.44309235	0.00000000
O	-2.83152723	-1.44309235	0.00000000
O	2.83152723	-1.44309235	0.00000000
O	-2.83152723	1.44309235	0.00000000
O	0.00000000	2.83152723	1.44309235
O	3.20357823	-1.81096268	-4.53660059
O	-3.20357823	1.81096268	-4.53660059
O	-3.20357823	-1.81096268	4.53660059
O	4.53660059	3.20357823	1.81096268
O	-4.53660059	3.20357823	-1.81096268
O	-4.53660059	-3.20357823	1.81096268
O	4.53660059	-3.20357823	-1.81096268
O	1.81096268	4.53660059	3.20357823
O	-1.81096268	-4.53660059	3.20357823
O	1.81096268	-4.53660059	-3.20357823

O	-1.81096268	4.53660059	-3.20357823
O	-3.20357823	-1.81096268	-4.53660059
O	-3.20357823	1.81096268	4.53660059
O	3.20357823	-1.81096268	4.53660059
O	3.20357823	1.81096268	-4.53660059
O	-4.53660059	-3.20357823	-1.81096268
O	4.53660059	-3.20357823	1.81096268
O	4.53660059	3.20357823	-1.81096268
O	-4.53660059	3.20357823	1.81096268
O	-1.81096268	-4.53660059	-3.20357823
O	1.81096268	4.53660059	-3.20357823
O	-1.81096268	4.53660059	3.20357823
O	1.81096268	-4.53660059	3.20357823
O	3.20357823	1.81096268	4.53660059
Zn	0.00000000	-1.27032042	-6.17370653
Zn	0.00000000	1.27032042	-6.17370653
Zn	0.00000000	-1.27032042	6.17370653
Zn	6.17370653	0.00000000	1.27032042
Zn	-6.17370653	0.00000000	-1.27032042
Zn	-6.17370653	0.00000000	1.27032042
Zn	6.17370653	0.00000000	-1.27032042
Zn	1.27032042	6.17370653	0.00000000
Zn	-1.27032042	-6.17370653	0.00000000
Zn	1.27032042	-6.17370653	0.00000000
Zn	-1.27032042	6.17370653	0.00000000
Zn	0.00000000	1.27032042	6.17370653
Zn	2.55423045	0.00000000	-4.81170225
Zn	-2.55423045	0.00000000	-4.81170225
Zn	-2.55423045	0.00000000	4.81170225
Zn	4.81170225	2.55423045	0.00000000
Zn	-4.81170225	2.55423045	0.00000000
Zn	-4.81170225	-2.55423045	0.00000000
Zn	4.81170225	-2.55423045	0.00000000
Zn	0.00000000	4.81170225	2.55423045
Zn	0.00000000	-4.81170225	2.55423045
Zn	0.00000000	-4.81170225	-2.55423045
Zn	0.00000000	4.81170225	-2.55423045
Zn	2.55423045	0.00000000	4.81170225
Zn	-1.40073049	-2.76646280	0.00000000
Zn	1.40073049	2.76646280	0.00000000
Zn	1.40073049	-2.76646280	0.00000000
Zn	0.00000000	-1.40073049	2.76646280
Zn	0.00000000	-1.40073049	-2.76646280
Zn	0.00000000	1.40073049	2.76646280
Zn	0.00000000	1.40073049	-2.76646280
Zn	2.76646280	0.00000000	-1.40073049

Zn	-2.76646280	0.00000000	-1.40073049
Zn	2.76646280	0.00000000	1.40073049
Zn	-2.76646280	0.00000000	1.40073049
Zn	-1.40073049	2.76646280	0.00000000
Zn	1.84478080	-3.09538531	-4.39408541
Zn	-1.84478080	3.09538531	-4.39408541
Zn	-1.84478080	-3.09538531	4.39408541
Zn	4.39408541	1.84478080	3.09538531
Zn	-4.39408541	1.84478080	-3.09538531
Zn	-4.39408541	-1.84478080	3.09538531
Zn	4.39408541	-1.84478080	-3.09538531
Zn	3.09538531	4.39408541	1.84478080
Zn	-3.09538531	-4.39408541	1.84478080
Zn	3.09538531	-4.39408541	-1.84478080
Zn	-3.09538531	4.39408541	-1.84478080
Zn	-1.84478080	-3.09538531	-4.39408541
Zn	-1.84478080	3.09538531	4.39408541
Zn	1.84478080	-3.09538531	4.39408541
Zn	1.84478080	3.09538531	-4.39408541
Zn	-4.39408541	-1.84478080	-3.09538531
Zn	4.39408541	-1.84478080	3.09538531
Zn	4.39408541	1.84478080	-3.09538531
Zn	-4.39408541	1.84478080	3.09538531
Zn	-3.09538531	-4.39408541	-1.84478080
Zn	3.09538531	4.39408541	-1.84478080
Zn	-3.09538531	4.39408541	1.84478080
Zn	3.09538531	-4.39408541	1.84478080
Zn	1.84478080	3.09538531	4.39408541

Onion-like structure of (ZnO)₆₀ in Figure S6 right, C₁, B3LYP/6-31G, -111265,3970 Hartree

O	5.56898928	0.89722455	3.27553582
Zn	4.99806499	2.65250158	2.76791906
Zn	6.08566380	0.78262520	1.43559349
O	5.86697674	2.64799261	1.06239951
Zn	4.05773115	-0.23830606	3.63653374
O	3.14519000	3.10255837	2.87881517
O	2.96572089	0.61818993	4.99661875
Zn	2.42730451	2.36085153	4.55970573
O	4.51351547	-2.04791594	3.09422874
Zn	5.07377243	-2.19330478	1.31018007
O	5.24184179	-0.50366718	0.30473283
Zn	4.59310150	2.92169547	-0.35444263
O	3.63822818	4.57670975	-0.00040095
Zn	2.81539607	4.63791990	1.68386424
Zn	5.46037388	0.08446559	-1.56626880
O	5.18386650	1.90864503	-1.90402806

O	4.62760258	-3.56545973	0.12081020
Zn	3.10794520	-3.20861983	3.51167893
O	2.52142167	-4.65560389	2.47305536
Zn	3.20993829	-4.62784910	0.73469561
O	5.00924158	-1.32863712	-2.70432544
Zn	4.02415848	2.21317506	-3.33881760
Zn	3.85889697	-0.80944979	-4.09152269
O	3.47063398	0.94636542	-4.60547733
Zn	1.53219330	-0.49406186	5.44891644
O	-0.21669525	0.05892865	5.84120083
O	0.74729812	3.11206245	4.88957214
Zn	-0.54449201	1.83334219	5.35081720
Zn	2.45127845	4.93167639	-1.40126801
O	1.12815237	5.34763908	2.06513309
O	0.73239082	5.66325188	-1.23641717
Zn	0.10335340	5.65244198	0.52450615
Zn	4.35564232	-2.83067298	-1.65810609
O	1.71260774	-2.20187974	4.47773409
Zn	0.23798554	4.25455189	3.40239716
O	2.69022393	3.56591368	-2.80461168
O	3.99367619	-4.28946257	-2.85934377
Zn	2.50356364	-5.32543325	-2.25039005
Zn	2.77011466	-3.75773382	-4.23228884
O	1.44717729	-5.08105326	-3.82808995
O	1.73933947	-4.94804525	-0.54133588
O	2.25303102	-1.92373383	-4.36730957
Zn	1.78787315	4.16317368	-4.37789249
O	-1.44708824	5.08101749	3.82822657
Zn	0.49449989	-3.45822883	5.24302578
O	-0.06128624	-4.97627401	4.21677923
O	-1.27282548	-2.88876581	5.70969582
Zn	-1.78796768	-4.16325235	4.37781000
Zn	-2.77002192	3.75769663	4.23241854
Zn	-2.50346398	5.32540178	2.25052118
O	-3.99358106	4.28943014	2.85947204
O	0.06118735	4.97618294	-4.21682215
O	1.27272987	2.88868093	-5.70977306
Zn	-0.49458894	3.45813322	-5.24306679
O	-2.25300336	1.92366970	4.36733866
Zn	-1.59693551	-1.09183276	5.10134792
Zn	0.58908546	-4.85495901	2.40941501
Zn	1.59692001	1.09176719	-5.10139799
Zn	-0.58912742	4.85495853	-2.40943480
O	-1.73934305	4.94804430	0.54141134
O	-0.73244631	-5.66320419	1.23637164
Zn	-0.10336925	-5.65242910	-0.52453417

O	-3.47064233	-0.94638377	4.60540390
Zn	-3.85890770	0.80944824	4.09152222
Zn	-3.20996237	4.62789869	-0.73459768
O	-2.52145338	4.65559816	-2.47296643
Zn	0.54452884	-1.83346677	-5.35080767
O	0.21670406	-0.05905140	-5.84117937
O	-0.74727309	-3.11218715	-4.88958740
Zn	-1.53216672	0.49395922	-5.44885683
Zn	-2.42727447	-2.36095810	-4.55971861
O	-2.96569586	-0.61828029	-4.99656248
O	-4.62763596	3.56552052	-0.12070624
Zn	-3.10791278	3.20858645	-3.51158214
Zn	-5.07374668	2.19334960	-1.31008077
O	-4.51346970	2.04788351	-3.09411550
Zn	-4.02419424	-2.21317124	3.33873653
O	-5.00927734	1.32864785	2.70434880
O	-5.18392372	-1.90863574	1.90396798
Zn	-5.46041298	-0.08444020	1.56627214
Zn	-2.45135188	-4.93166637	1.40116870
O	-1.12819564	-5.34768105	-2.06515336
O	-3.63833570	-4.57674265	0.00032007
Zn	-2.81546664	-4.63799095	-1.68392944
O	-5.86701679	-2.64794636	-1.06246543
O	-5.56899738	-0.89718431	-3.27557802
Zn	-6.08566236	-0.78256863	-1.43563640
Zn	-4.99809361	-2.65247083	-2.76798010
O	-3.14523005	-3.10260487	-2.87884307
Zn	-4.05767059	0.23828945	-3.63648105
O	-5.24183464	0.50367391	-0.30472022
Zn	-4.59316397	-2.92169571	0.35438082
Zn	-0.23794442	-4.25463533	-3.40238714
O	-2.69027758	-3.56592226	2.80453229
Zn	-4.35563898	2.83070707	1.65819359
O	-1.71263516	2.20178866	-4.47768307
O	-2.69375467	-1.68251264	0.15959577
Zn	-3.08386922	0.25694811	-0.20747392
Zn	-1.88341343	-1.80010200	-1.67733800
O	-2.39183402	0.10199706	-2.08994460
O	-0.91270965	-0.68884355	2.96833634
Zn	-1.33090174	1.16955233	2.54729795
O	0.32264772	-2.80915904	1.44871533
Zn	1.03816271	-2.89468408	-0.36191875
Zn	1.33089793	-1.16958725	-2.54729581
O	0.91272855	0.68881232	-2.96834350
O	-0.32263798	2.80914307	-1.44870317
Zn	-1.03817153	2.89466906	0.36192816

Zn	-1.54498351	-2.09717131	1.67947471
Zn	0.96877146	-1.31747890	2.63393760
O	-0.08280604	-2.48358607	-1.98123336
Zn	1.54498708	2.09714389	-1.67948222
O	-2.50876379	1.67812979	0.99705589
O	0.08280592	2.48354292	1.98122871
O	2.39186168	-0.10204798	2.08997250
Zn	1.88340020	1.80003417	1.67733228
Zn	3.08386707	-0.25698563	0.20749082
O	2.69374847	1.68246710	-0.15960228
O	2.50875497	-1.67815042	-0.99704725
Zn	-0.96875077	1.31743240	-2.63390231

Sodalite structure of (ZnO)₆₀ in Figure S6_2, C₁, B3LYP/6-31G, -111265,4155 Hartree

Zn	1.82264996	-0.07737630	4.59546614
O	-1.93171597	0.03289900	4.71050406
O	0.93532085	-1.68895030	4.71052551
Zn	-0.97706753	-1.53956771	4.59652662
O	0.99417335	1.65302837	4.70836544
Zn	-0.84516579	1.61382186	4.59500074
O	3.07917523	0.52047527	3.22989225
Zn	2.07420874	2.36310124	3.26284003
Zn	1.00939226	-2.97862649	3.26395178
O	-1.08856034	-2.92690277	3.23073673
Zn	-3.08648944	0.61341333	3.26443219
O	-1.99046671	2.40305758	3.22869015
O	2.00210619	-2.36712718	1.60284781
Zn	3.01247430	-0.66821659	1.59748220
O	1.04944503	2.91712236	1.60064161
Zn	-0.92765212	2.93720865	1.59664869
Zn	-2.08448267	-2.27315927	1.59945357
O	-3.05524135	-0.55088907	1.60229754
Zn	2.95317602	-4.17090559	1.66442192
O	5.04193926	-0.67166096	1.62846851
O	4.89098406	-4.08964872	1.50814879
Zn	5.76013756	-2.47548962	1.40291345
O	-3.10335445	-4.02893496	1.63119674
Zn	-5.09278440	-0.47115898	1.66405284
Zn	-5.02415752	-3.74689770	1.40426874
O	-5.99149895	-2.18971944	1.50842118
O	-1.93896329	4.69694138	1.62647951
Zn	2.13722968	4.64128304	1.66185820
O	1.09802306	6.27901077	1.50854349
Zn	-0.73436975	6.21957874	1.40211797
Zn	4.99991226	0.68375343	3.02461815
O	3.19746828	3.91739297	3.10661435

O	6.06493473	2.18525124	3.17896008
Zn	5.02923107	3.84460545	3.06343222
O	1.79646301	-4.72819757	3.10868907
Zn	-1.90878868	-4.67184973	3.02615023
Zn	0.81729037	-6.27718592	3.06238270
O	-1.13780832	-6.34329844	3.17843318
O	-4.99475622	0.80935133	3.10856295
Zn	-3.09170294	3.98438096	3.02348089
Zn	-5.84763861	2.43221617	3.06315207
O	-4.92430067	4.15710068	3.17777157
Zn	4.89378738	-5.13688993	-0.10957294
O	6.92842484	-1.92937815	-0.02696617
O	5.94532633	-4.75094795	-1.60021639
Zn	6.83249569	-3.01887822	-1.52483225
Zn	2.00470281	6.80907488	-0.10694554
O	-1.79182673	6.95973396	-0.02671792
O	1.14257443	7.52393103	-1.59845781
Zn	-0.80111474	7.42384338	-1.52365696
Zn	-6.90034962	-1.66954470	-0.10914052
O	-5.13420534	-5.03191185	-0.02571136
Zn	-6.03005266	-4.40574932	-1.52419531
O	-7.09008551	-2.77380466	-1.60048413
Zn	-3.22753143	-5.32076359	0.00166710
O	-6.17931509	0.13221745	0.00023953
Zn	-2.99555063	5.45309353	-0.00133113
Zn	6.22569036	-0.13350925	-0.00009326
O	2.97327542	-5.41353703	0.00064631
O	0.81894535	-7.56562567	1.59923720
Zn	-1.11893535	-7.38420248	1.52564275
Zn	1.70982015	-6.88662863	0.10790725
Zn	6.95531082	2.72303057	1.52495050
O	6.14290714	4.49139166	1.60010874
O	7.00413799	1.63068283	0.02716927
Zn	5.10992384	4.92353630	0.10923491
Zn	-5.83458900	4.65958261	1.52385294
O	-6.96399975	3.07465601	1.59994411
O	-4.91334105	5.24686909	0.02534207
Zn	-6.82235575	1.96338403	0.10878646
O	-2.08760500	-6.87656736	0.02835695
Zn	-1.00017619	-6.18232059	-1.40053928
O	-2.13907599	-4.60985041	-1.62558544
O	0.82769400	-6.31916618	-1.50858235
Zn	-1.05253315	-2.89633822	-1.59624696
Zn	1.93669498	-4.72782135	-1.66232550
O	0.92370683	-2.95793128	-1.60160732
O	3.02744126	-4.05000973	-3.10657978

Zn	1.97193706	-2.44904900	-3.26350594
O	3.05520630	-0.65073496	-3.23169827
Zn	4.86081696	-4.05671549	-3.06372142
O	5.96641493	-2.44301343	-3.17889571
Zn	4.96644449	-0.89737260	-3.02507329
O	5.06620121	0.45494720	-1.62857652
Zn	5.86028385	2.22687459	-1.40238345
O	5.06260157	3.87746263	-1.50875366
Zn	3.12987399	4.04199839	-1.66502702
O	2.10315394	2.28039193	-1.60281587
Zn	3.03810620	0.53812909	-1.59841645
O	-5.09813404	-3.94306684	-3.17778873
Zn	-3.25971413	-3.84883523	-3.02333593
O	-2.09139895	-2.31651640	-3.22844052
Zn	-5.94618988	-2.17981839	-3.06311607
O	-5.02393389	-0.59568161	-3.10690928
Zn	-3.10896897	-0.48193273	-3.26280141
Zn	-5.06728697	0.68848622	-1.66346550
O	-3.02861118	0.68114614	-1.60136223
O	-5.89177084	2.44406343	-1.50858259
Zn	-4.85832930	3.95814681	-1.40410709
O	-2.92658377	4.15654182	-1.63002920
Zn	-1.70570874	4.74836874	-3.02465415
O	-0.86466920	6.38575172	-3.17699933
Zn	1.08620250	6.23730373	-3.06188393
O	1.99855721	4.64760303	-3.11027694
O	3.20311880	5.28220701	-0.00135600
Zn	1.13705087	2.93350077	-3.26466966
O	-0.96082914	2.97027016	-3.22940946
Zn	-1.98374379	2.35894179	-1.59882092
O	0.92301446	-1.69349861	-4.70912361
Zn	-0.91271794	-1.57627678	-4.59382486
Zn	-0.90978134	1.57965791	-4.59568548
O	-1.93067813	0.04950334	-4.70872402
O	1.00695848	1.64764571	-4.71091795
Zn	1.82474840	-0.00026239	-4.59669924
O	-1.03971267	-1.71246958	0.00223943
Zn	-2.03059196	0.04317291	0.00058966
O	-0.96406257	1.75340557	-0.00137920
Zn	0.97570497	-1.77598965	0.00119334
Zn	1.05248332	1.73380005	-0.00159818
O	2.00548315	-0.04308677	-0.00063366