

Supporting information

Tunable properties and composition of ZnO films supported on metal surfaces

Yizhen Song, Paulo C. D. Mendes, Sergey M. Kozlov

Department of Chemical and Biomolecular Engineering, Faculty of Engineering, National University of Singapore, 119260, Singapore

Impact of the Hubbard corrections on bulk ZnO properties

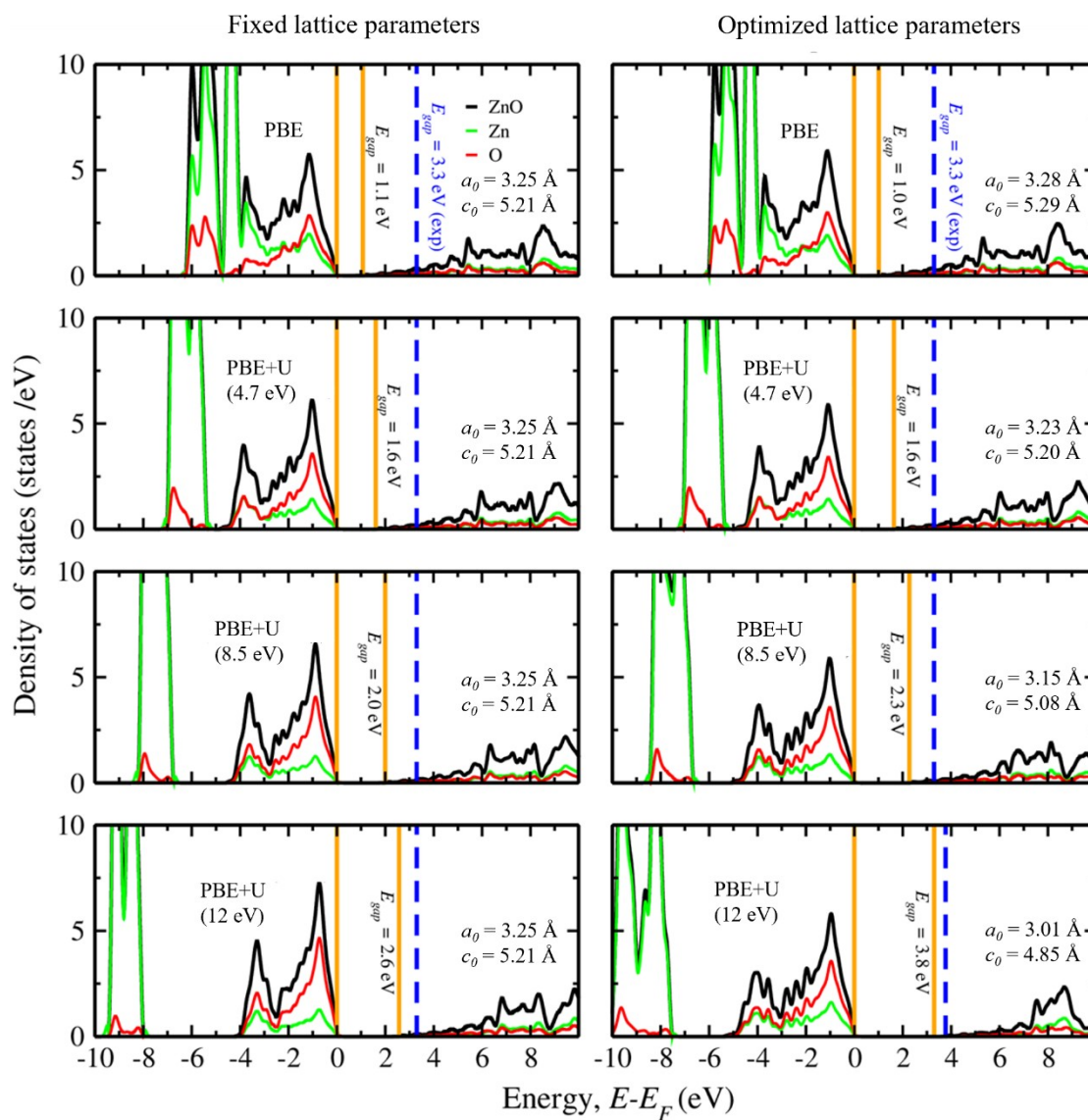


Fig. S1. Density of states calculated with PBE and PBE+U methods for wurtzite ZnO bulk with lattice constants fixed in the reference value of $a_0 = 3.25$ Å, $c_0 = 5.21$ Å (left column) and optimized to the indicated values (right column). The blue vertical dashed lines represent the experimental value of the ZnO bulk band gap¹ and the orange vertical lines show the calculated gap.

Effects of the dispersion and dipole corrections on the reactivity of ZnO

We tested the effects of the zero-damping D3 vdW corrections² and the dipole corrections³ to the PBE functional⁴ on the adsorption energies of H and O vacancy formation energies in the 9/16 ZnO/Cu model (Table S1). The dispersion and dipole corrections have a negligible effect on the adsorption energy of H, and a small impact effect on the formation energy of O vacancies.

Table S1. Effects of dispersion (D3) and dipole corrections (DIPOLE) for 9/16 ZnO/Cu on the O vacancy formation energy, $E_{vac}[O]$, and adsorption energy of the H atom, $E_{ad}[H]$. The ΔE shows the variation of each property with respect to the value calculated with PBE.

	Method	$E_{vac}[O]$ (eV)	ΔE (eV)
O vacancy formation energy	PBE	2.60	0.00
	PBE+D3	2.79	0.19
	PBE+DIPOLE	2.59	-0.01
	Method	$E_{ad}[H]$ (eV)	ΔE (eV)
H atom adsorption energy	PBE	-0.69	0.00
	PBE+D3	-0.70	-0.01
	PBE+DIPOLE	-0.68	0.01

Convergence tests

The convergence test with respect to the sampling of k-points is shown in Table S2. Based on our tests, the k-mesh of 3×3×1 subdivisions was selected and the sampling was transferred to cells of different sizes proportionally to the norms of the reciprocal lattice vectors, as shown in Table S3. Note that the cells in Table S3 were employed in calculations, whereas the illustrations in the article may contain equivalent cells adjusted for clearer visualization.

Table S2. Convergence test for the adsorption of an H atom on 9/16 ZnO/Cu(111) cell composed of 3 Cu layers with respect to the k-mesh sampling. The adsorption energy of the H atom, E_{ad} , the average distance between the two topmost Cu surface layers, $d[Cu-Cu]$, and between ZnO film and topmost Cu layer, $d[ZnO-Cu]$, are given.

k-mesh	$E_{ad}[H]$ (eV)	$d[Cu-Cu]$ (Å)	$d[ZnO-Cu]$ (Å)
1×1×1	-0.50	2.04	2.43
2×2×1	-0.58	2.08	2.54
3×3×1	-0.66	2.09	2.55
4×4×1	-0.69	2.09	2.54
5×5×1	-0.63	2.08	2.55
6×6×1	-0.66	2.09	2.55
7×7×1	-0.68	2.09	2.55

Table S3. **k**-point samplings used in calculations of various cells based on graphitic ZnO. The lengths of the real and reciprocal surface lattice vectors, **a** and **b**, are indicated.

ZnO/M	 a real, Å	 b real, Å	 a reciprocal, Å ⁻¹	 b reciprocal, Å ⁻¹	k -sampling subdivisions		
9/16 Cu	10.21	10.21	0.11	0.11	3	3	1
32/43 Mo	33.48	17.47	0.06	0.11	2	3	1
43/64 Ru	21.68	21.68	0.05	0.05	1	1	1
25/36 Pd	16.50	16.50	0.07	0.07	2	2	1
28/39 Pd	17.18	17.18	0.07	0.07	2	2	1
25/36 Pt	16.63	16.63	0.07	0.07	2	2	1
27/37 Pt	16.86	16.86	0.07	0.07	2	2	1
2×2 9/16 Cu	20.42	20.42	0.06	0.06	2	2	1
31/52 Cu	18.41	18.41	0.06	0.06	2	2	1
49/64 Ag	23.14	23.14	0.05	0.05	1	1	1
31/39 Ag	18.06	18.06	0.06	0.06	2	2	1
49/64 Au	23.08	23.08	0.05	0.05	1	1	1
31/39 Au	18.02	18.02	0.06	0.06	2	2	1
52/27 Sn	23.85	23.85	0.05	0.05	1	1	1
36/31 Pb	19.49	19.49	0.06	0.06	2	2	1

Translations of the ZnO film on Cu(111)

We evaluated the effect of the lateral alignment of the oxide film with metal support using 49/81 ZnO/Cu supercells for *gr*-ZnO(0001) and *wz*-ZnO(0001), whereas 42/63 matching was used for *wz*-Zn(10 $\bar{1}$ 0). To obtain geometrically distinct structures, the films were translated along **a** and **b** lattice vectors by half of the maximum displacement that repeats the structure, $L/(m \times n)$. Here L is the length of the supercell lattice vector, m and n are the number of ZnO and Cu unit cells, composing the supercell. Four unique positions were considered, as shown in Fig. S2, the (i) as-deposited film without translation, film translated (ii) once along **a**, (iii) once along **b**, and (iv) once along each surface lattice vector. All translated structures had relative energies within 1 meV for *gr*-ZnO(0001), 4 meV for *wz*-ZnO(0001) and 37 meV for *wz*-ZnO indicating a negligible effect of translations on the film stability. Translation of the film has a similarly small effect (< 5 meV) on films with one H adsorbed or one O vacancy formed in *gr*-ZnO(0001) if the position of the considered site above the metal surface is constant.

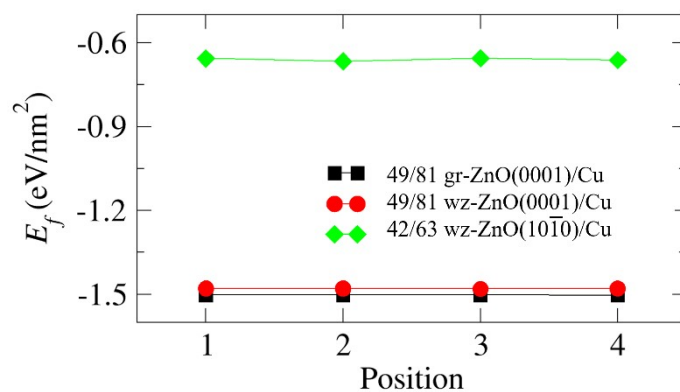
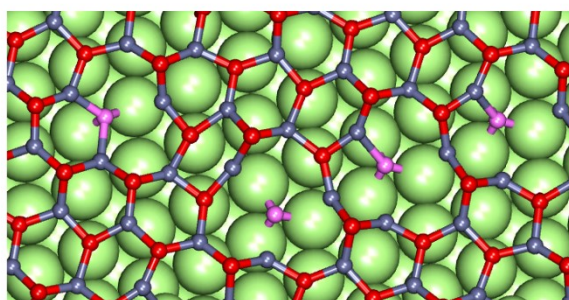


Fig. S2. Translations of different types of ZnO films supported on Cu(111). E_f is the formation energy of metal-supported films. Positions 1 to 4 correspond to 1 - initial arbitrary position, 2 - initial structure shifted along lattice vector \mathbf{b} once, 3 - initial structure shifted along lattice vector \mathbf{a} once, and 4 - initial structure shifted along each lattice vector once. See the discussion above for more details.

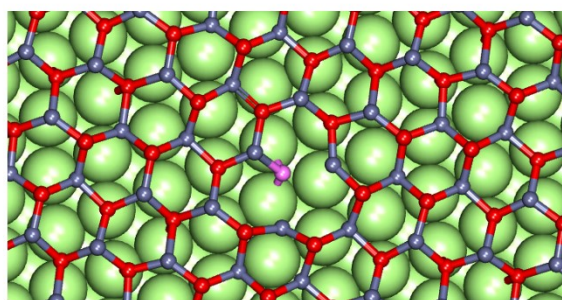
The interaction between ZnO and Mo(110)

A Monolayer of ZnO on Mo surface



● O atom: $d_{\text{Mo-O}} < 2.2 \text{ \AA}$

B 4 layers of ZnO on Mo surface



● O atom ● Zn atom

Fig. S3. Top views of the interface between Mo(110) support and the gr-ZnO(0001) film with the thickness of A) 1 Monolayer and B) 4 layers. O atoms displacing towards the metal support and forming Mo-O bonds with distances $d_{\text{Mo-O}} < 2.2 \text{ \AA}$ are displayed in pink.

Complementary data for the geometric and electronic analyses

Table S4. Charge analysis for ZnO supported on metals derived from the graphitic films, as well as the rumpling defined as the height different of Zn and O planes, $h[\text{Zn-O}]$, and shortest O-M distances, $d[\text{O-M}]$. Average charges on O, Zn, and H atoms, $Q[\text{O}]$, $Q[\text{Zn}]$, $Q[\text{H}]$, as well as the charges on surface metal atoms, $Q[\text{M}]$. The H/ZnO/metal systems were calculated at saturation H coverages under methanol synthesis conditions.

ZnO/M (unit cells)	ZnO/metal				H/ZnO/metal			
	$h[\text{Zn-O}]$ (Å)	$Q[\text{O}]$ (a.u.)	$Q[\text{Zn}]$ (a.u.)	$Q[\text{M}]$ (a.u.)	$Q[\text{H}]$ (a.u.)	$Q[\text{O}]$ (a.u.)	$Q[\text{Zn}]$ (a.u.)	$Q[\text{M}]$ (a.u.)
gr-ZnO	0.00	-1.18	1.18	/	/	/	/	/
43/64 Ru	0.14	-1.12	1.08	-0.01	0.55	-1.21	0.83	-0.13
25/36 Pd	0.19	-1.11	1.14	-0.04	0.54	-1.20	0.93	-0.17
28/39 Pd	0.21	-1.11	1.14	-0.01	0.54	-1.20	0.93	-0.18
25/36 Pt	0.20	-1.10	1.15	-0.07	0.55	-1.20	0.99	-0.22
27/37 Pt	0.23	-1.09	1.15	-0.07	0.55	-1.20	0.99	-0.23
9/16 Cu	0.13	-1.14	1.10	0.01	0.56	-1.20	0.88	-0.07
31/52 Cu	0.15	-1.14	1.12	0.00	0.55	-1.20	0.88	-0.08
49/64 Ag	0.10	-1.15	1.13	0.00	0.56	-1.18	1.02	-0.07
31/39 Ag	0.12	-1.16	1.14	0.00	0.58	-1.16	1.11	-0.03
49/64 Au	0.14	-1.13	1.16	-0.04	0.55	-1.20	0.99	-0.19
31/39 Au	0.16	-1.14	1.17	-0.01	0.56	-1.20	1.02	-0.18
52/27 Sn	0.07	-1.18	1.14	0.13	0.58	-1.19	1.11	0.08
36/31 Pb	0.05	-1.17	1.14	0.01	/	/	/	/

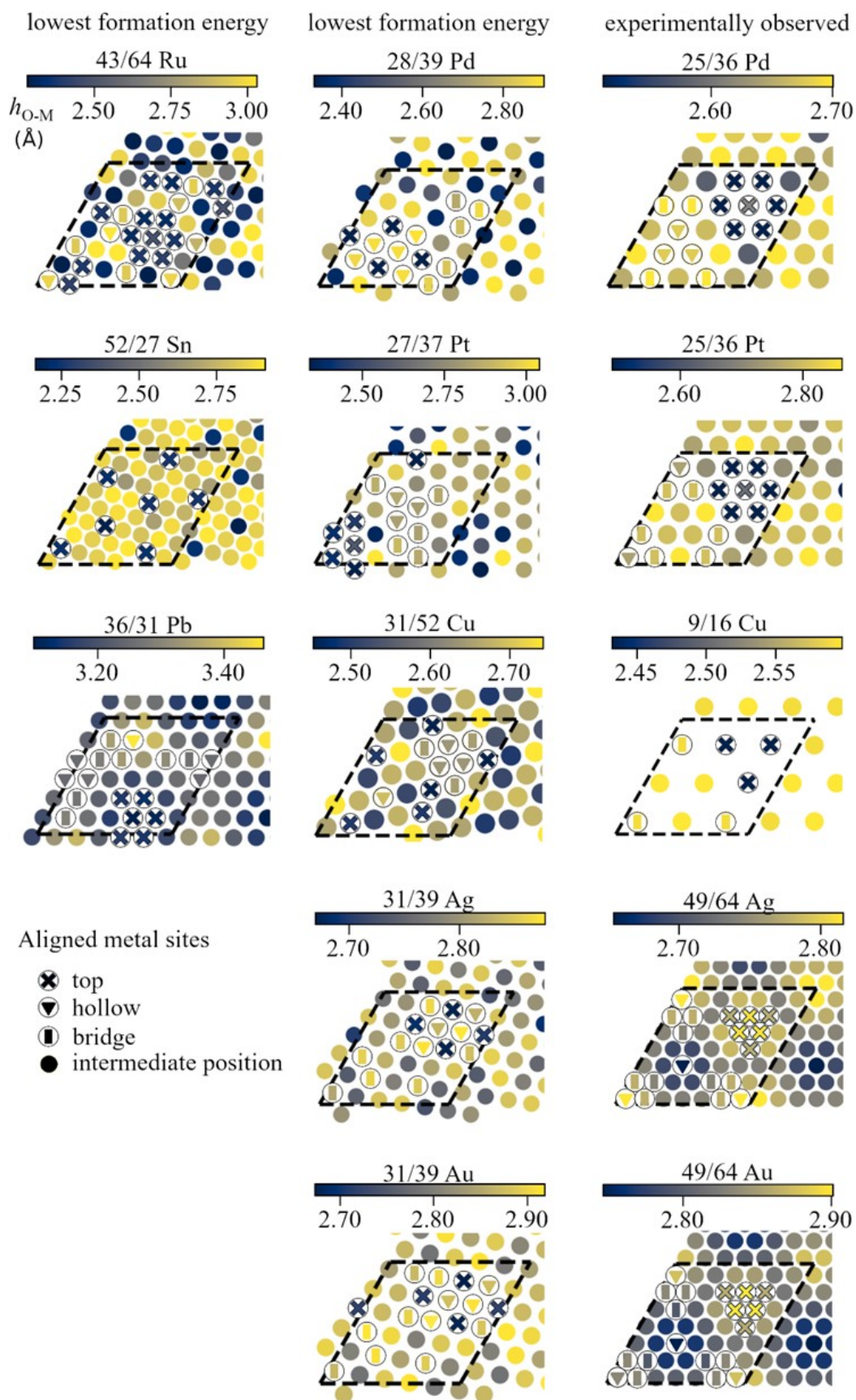


Fig. S4. Color maps of distances between O atoms in supported ZnO films and the planes of metal atoms. The aligned metal site is marked for selected O atoms in each unit cell. The dashed lines show the employed surface cell. The sizes of data points do not represent atomic sizes.

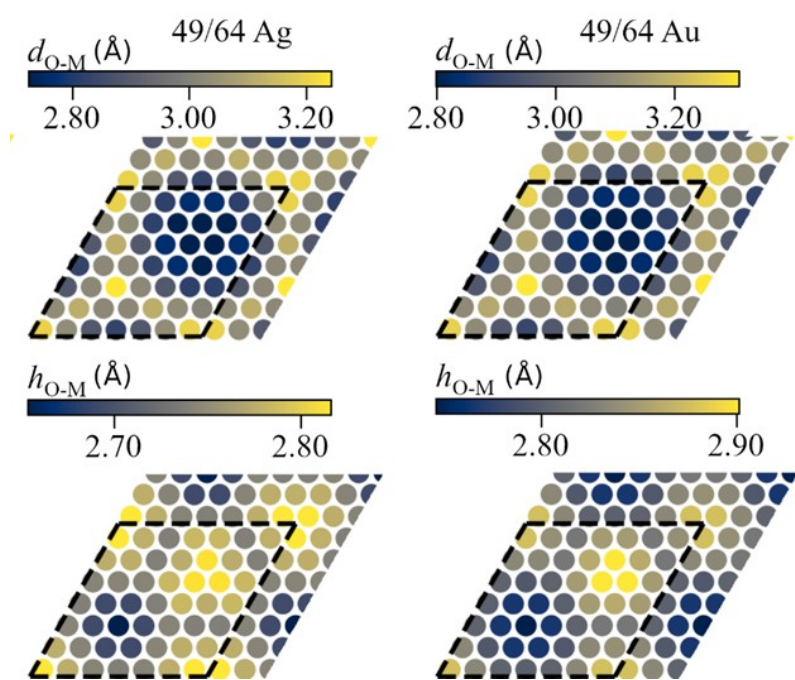


Fig. S5. Patterns observed for the shortest O-M distance and the distance between O atoms and the topmost metal plane for ZnO supported on Ag and Au.

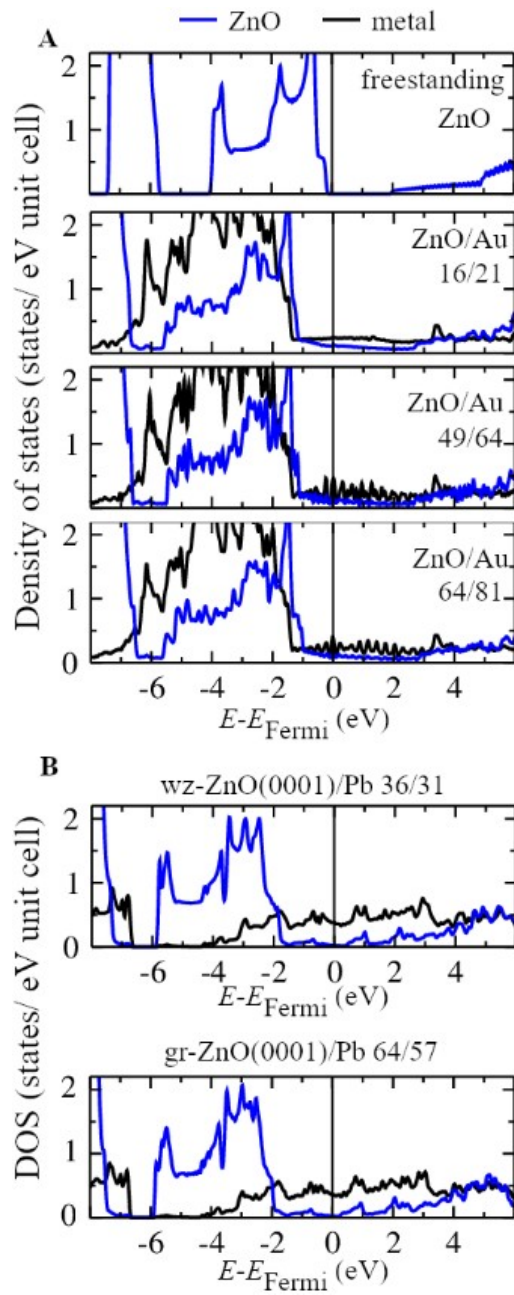


Fig. S6. Similarity in the local density of states projected on ZnO and surface metal atoms per ZnO unit or metal atom for **A)** various matches of gr-ZnO(0001) on Au and **B)** low-strain ZnO/Pb films.

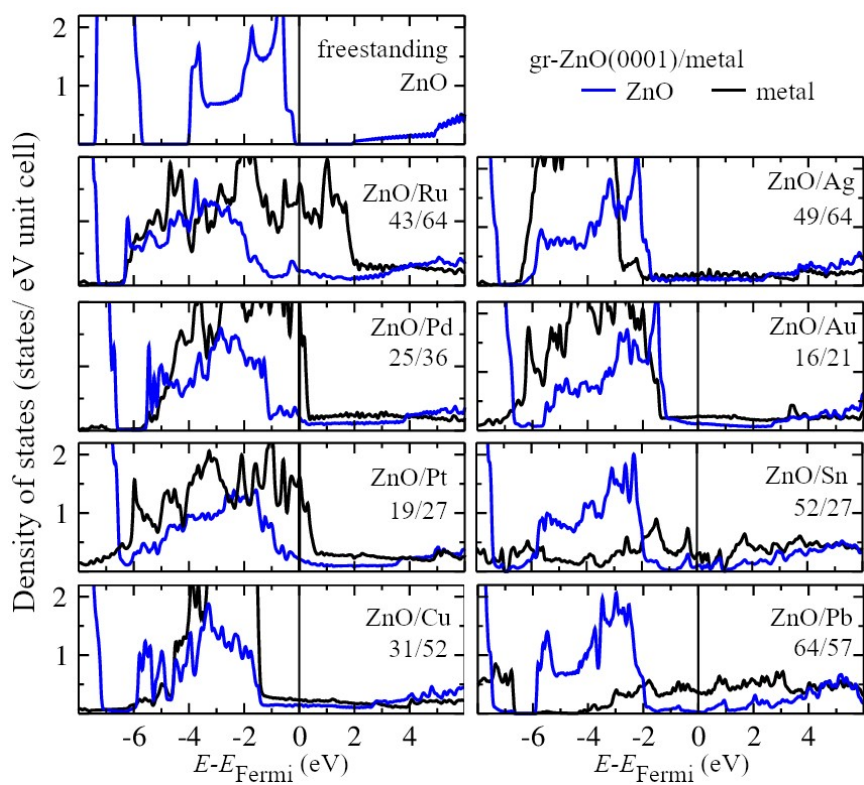


Fig. S7. Local density of states projected on ZnO and surface metal atoms per ZnO unit or metal atom for the freestanding graphitic ZnO(0001) monolayer and the indicated ZnO/M lattice matches corresponding to the lowest possible deformations of gr-ZnO(0001).

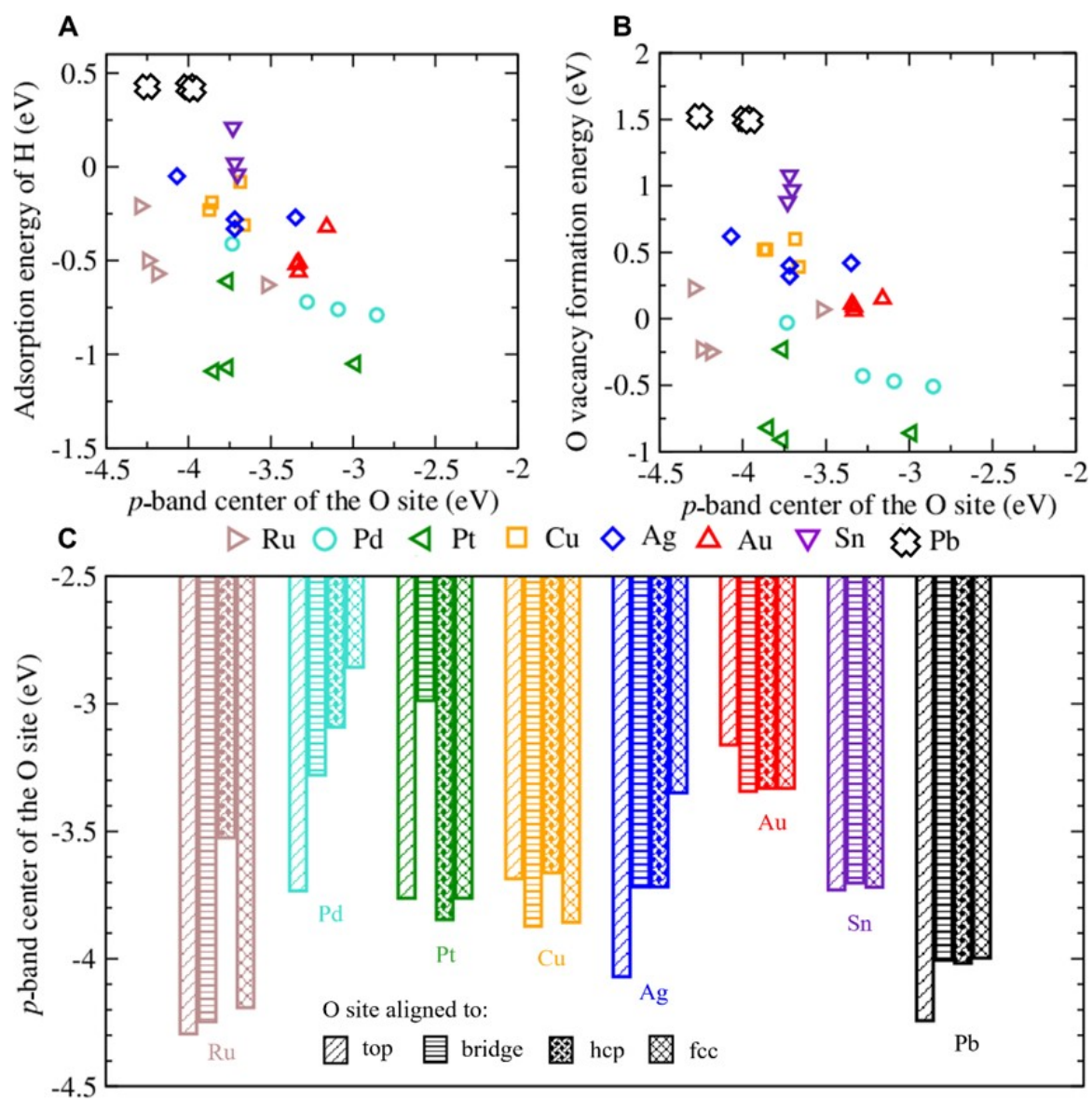


Fig. S8. Analyses of the supported gr-ZnO films with the lowest deformation showing the **A)** adsorption energies of H atoms (at low coverage) and **B)** O vacancy formation energies versus the p -band center of the O atoms for the O sites aligned to top, bridge, and hollow hcp and fcc sites of the metal support, and **C)** variation of the average p -band centers for O atoms aligned to these high-symmetry sites of the metal support.

Table S5. Work function difference of gr-ZnO(0001)/M, $\Delta\phi$, based on the work functions of the films supported on the metal, $\phi^{\text{ZnO/M}}$, and of the bare metal support, ϕ^{M} .

ZnO/M	ϕ^{M} (eV)	$\phi^{\text{ZnO/M}}$ (eV)	$\Delta\phi$ (eV)
gr-ZnO	/	5.7	/
43/64 Ru	4.8	4.5	-0.3
25/36 Pd	5.3	5.1	-0.2
28/39 Pd	5.3	5.2	-0.1
25/36 Pt	5.7	5.3	-0.4
27/37 Pt	5.7	5.5	-0.2
9/16 Cu	4.8	4.5	-0.3
31/52 Cu	4.8	4.6	-0.2
49/64 Ag	4.7	4.6	-0.1
31/39 Ag	4.5	4.4	-0.1
49/64 Au	5.2	5.1	-0.1
31/39 Au	5.2	5.1	-0.1
52/27 Sn	4.3	4.2	-0.1
36/31 Pb	3.8	4.0	0.2

Formation of O vacancies and adsorption of H, O, and OH at various conditions

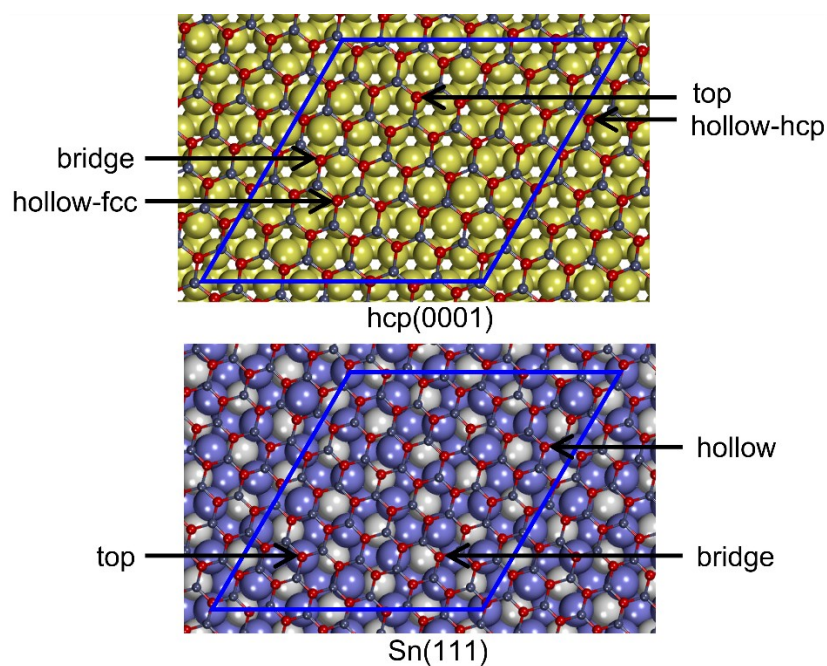


Fig. S9. Classification of O atoms in ZnO films above various sites of non-fcc metal surfaces. The Sn layer positioned below the topmost atoms of the Sn(111) surface is displayed in white for clarity. The same classification was employed to distinguish Zn sites and sites at the centers of the graphitic ZnO rings.

Table S6. Gibbs adsorption energies of single H atoms on O sites of ZnO, $G_{ad}[H]$, and film formation Gibbs free energies under typical hydrogenation conditions of methanol synthesis ($T = 525$ K, $p[H_2] = 1500000$ Pa, $p[H_2O] = 50000$ Pa) for metal-supported ZnO. The top, bridge, hcp and fcc refer to the alignment of the O site above various sites on the metal support. The equilibrium concentrations, θ , of H atoms per total number of O sites under these conditions are also given.

ZnO/M (unit cells)	$G_{ad}[H]$ (eV)				θ	G_f^{**} (eV/nm ²)
	top	bridge	hcp	fcc	[H _{ad}]	
ZnO monolayer	1.15				0	4.89
wz-(1010) 4-layer	0.12				0	2.01
43/64 Ru	-0.21	-0.50	-0.63	-0.57	1	-8.64
25/36 Pd	-0.41	-0.72	-0.76	-0.79	1	-10.52
28/39 Pd	-0.54	-0.69	-0.66	-0.68	1	-10.49
25/36 Pt	-0.60	-1.05	-1.12	-1.14	1	-11.35
27/37 Pt	-0.74	-0.98	-1.04	-1.08	1	-12.32
2x2 9/16 Cu	-0.21	-0.38	-0.30	-0.38	0.83	-1.92
31/52 Cu	-0.08	-0.23	-0.31	-0.19	0.84	-3.17
49/64 Ag	-0.05	-0.28	-0.33	-0.27	0.47	-2.08
31/39 Ag	0.00	-0.03	-0.04	-0.04	0.13	-2.21
49/64 Au	-0.37	-0.67	-0.71	-0.64	0.94	-5.15
31/39 Au	-0.56	-0.62	-0.63	-0.64	0.77	-5.29
52/27 Sn	0.21	-0.04	/ ^a	0.02	0.10	1.62
36/31 Pb	0.58	0.45	0.45	0.49	0	1.41

^a "/" in the table indicates that adsorption on this site is not locally stable

Table S7. Gibbs formation energies of one O vacancy, $G_{vac}[O]$, under ambient conditions ($T = 298.15$ K, $p[O_2] = 20612.2$ Pa, $p[H_2O] = 3171.5$ Pa), and typical hydrogenation conditions of methanol synthesis ($T = 525$ K, $p[H_2] = 1500000$ Pa, $p[H_2O] = 50000$ Pa), and CO oxidation conditions ($T = 450$ K, $p[O_2] = 5000$ Pa) for metal-supported ZnO. The top, bridge, and hollow (hcp, fcc) refer to the alignment of the O site above various sites on the metal support. The equilibrium concentrations, θ , of O vacancies per total number of O sites under hydrogenation conditions are also given.

Equation:	ambient conditions				CO oxidation condition				typical hydrogenation conditions					
	$Zn_xO_x \rightarrow 0.5O_2 + Zn_xO_{x-1}$									$Zn_xO_x + H_2 \rightarrow H_2O + Zn_xO_{x-1}$				
	$G_{vac}[O]$ (eV)				$G_{vac}[O]$ (eV)				$G_{vac}[O]$ (eV)				θ	
ZnO/M (unit cells)	top	bridge	hcp	fcc	top	bridge	hcp	fcc	top	bridge	hcp	fcc	[O _{vac}]	
ZnO monolayer	4.03				3.85				1.62				0	
wz-(1010) 4-layer	3.18				3.00				0.77				0	
43/64 Ru	2.63	2.18	2.48	2.16	2.46	2.00	2.30	1.98	0.23	-0.23	0.07	-0.25	0.19	
25/36 Pd	2.38	1.97	1.93	1.89	2.20	1.80	1.76	1.72	-0.03	-0.43	-0.47	-0.51	breaks	
28/39 Pd	2.22	2.15	2.30	2.27	2.05	1.98	2.13	2.10	-0.19	-0.26	-0.11	-0.14	0.14	
25/36 Pt	2.17	1.43	1.46	1.40	2.00	1.25	1.28	1.22	-0.23	-0.98	-0.95	-1.01	breaks	
27/37 Pt	1.93	1.63	1.70	1.62	1.76	1.45	1.53	1.45	-0.49	-0.79	-0.71	-0.80	breaks	
2x2 9/16 Cu	2.62	2.52	2.50	2.52	2.45	2.35	2.33	2.35	0.22	0.12	0.10	0.12	0	
31/52 Cu	3.01	2.93	2.80	2.92	2.84	2.76	2.63	2.75	0.61	0.53	0.40	0.52	0	
49/64 Ag	3.02	2.80	2.73	2.82	2.85	2.63	2.55	2.65	0.62	0.40	0.32	0.42	0	
31/39 Ag	3.15	3.30	3.33	3.34	2.98	3.13	3.16	3.17	0.78	0.89	0.92	0.93	0	
49/64 Au	2.42	2.24	2.18	2.26	2.25	2.06	2.01	2.08	0.02	-0.17	-0.22	-0.15	0.08	
31/39 Au	2.35	2.41	2.40	2.44	2.18	2.34	2.23	2.27	-0.06	0.00	-0.01	0.03	0.03	
52/27 Sn	3.28	3.28	/ ^a	3.49	3.11	3.20	/	3.31	0.88	0.97	/	1.08	0	
36/31 Pb	3.65	4.57	3.54	3.60	3.48	3.40	3.37	3.43	1.25	1.17	1.14	1.20	0	

^a "/" in the table indicates that adsorption on this site is not locally stable

The formation energy of one OH vacancy in metal-supported hydrogenated ZnO films and the adsorption energies of O and OH for films containing one O vacancy at the most favourable site are shown in Table S8. The energies of OH species abstraction from the surface under hydrogenation conditions were calculated as

$$G_{\text{vac}}[\text{OH}] = E[\text{H}_{k-1}/\text{Zn}_x\text{O}_{x-1}/\text{M}] + G[\text{H}_2\text{O}] - G[\text{H}_k/\text{Zn}_x\text{O}_x/\text{M}] - 0.5 * G[\text{H}_2]$$

where k is the number of H atoms in the hydrogenated film in which the OH vacancies were created. The OH removal energies were calculated for the most stable sites for O vacancy formation.

Table S8. Gibbs OH vacancy formation energies for the saturated hydrogenated ZnO films on metals, $G_{\text{vac}}[\text{OH}]$, and Gibbs adsorption energy of one O, $G_{\text{ad}}[\text{O}]$, and one OH atom, $G_{\text{ad}}[\text{OH}]$ for metal-supported ZnO with an O vacancy under methanol synthesis conditions, $T = 525 \text{ K}$, $p[\text{H}_2] = 1.5 \text{ MPa}$, $p[\text{H}_2\text{O}] = 0.05 \text{ MPa}$.

ZnO/M (unit cells)	From hydrogenated ZnO		For ZnO with one O vacancy	
	$G_{\text{vac}}[\text{OH}]$ (eV)		$G_{\text{ad}}[\text{O}]$ (eV)	$G_{\text{ad}}[\text{OH}]$ (eV)
43/64 Ru	0.24		0.42	-0.10
25/36 Pd	0.72		0.63	-0.17
25/36 Pt	0.78		1.12	0.07
27/37 Pt	0.81		0.78	-0.32
2x2 9/16 Cu	0.95		/	/
31/52 Cu	0.94		/	/
49/64 Ag	0.63		/	/
49/64 Au	0.59		0.46	-0.18
31/39 Au	0.85		0.05	-0.53
52/27 Sn	0.87		/	/
36/31 Pb	/		/	/

Table S9. Gibbs adsorption energies of one O atom above the centers of ZnO rings, $G_{\text{ad}}[\text{O}]$ under ambient conditions ($T = 298.15 \text{ K}$, $p[\text{O}_2] = 20612.2 \text{ Pa}$, $p[\text{H}_2\text{O}] = 3171.5 \text{ Pa}$), and typical hydrogenation conditions of methanol synthesis ($T = 525 \text{ K}$, $p[\text{H}_2] = 1500000 \text{ Pa}$, $p[\text{H}_2\text{O}] = 50000 \text{ Pa}$), and CO oxidation conditions ($T = 450 \text{ K}$, $p[\text{O}_2] = 5000 \text{ Pa}$) for metal-supported ZnO. The top, bridge, and hollow (hcp, fcc) refer to the alignment of the center of ZnO rings above various sites on the metal support.

Equation: ZnO/M (unit cells)	ambient conditions				CO oxidation condition				typical hydrogenation conditions			
	$\text{Zn}_x\text{O}_x + 0.5\text{O}_2 \rightarrow \text{Zn}_x\text{O}_{x+1}$				$\text{Zn}_x\text{O}_x + \text{H}_2\text{O} \rightarrow \text{Zn}_x\text{O}_{x+1} + \text{H}_2$				$\text{Zn}_x\text{O}_x + \text{H}_2\text{O} \rightarrow \text{Zn}_x\text{O}_{x+1} + \text{H}_2$			
	$G_{\text{ad}}[\text{O}]$ (eV)				$G_{\text{ad}}[\text{O}]$ (eV)				$G_{\text{ad}}[\text{O}]$ (eV)			
	top	bridge	hcp	fcc	top	bridge	hcp	fcc	top	bridge	hcp	fcc
ZnO monolayer	3.43				3.62				5.87			
wz-(1010) 4-layer	1.18				1.36				3.59			
43/64 Ru	X ^a	X	X	X	X	X	X	X	X	X	X	X
25/36 Pd	0.32	0.37	0.21	0.55	0.50	0.55	0.39	0.73	2.74	2.78	2.63	2.96
28/39 Pd	X	0.24	0.32	0.46	X	0.42	0.49	0.64	X	2.66	2.73	2.87
25/36 Pt	X	0.19	0.11	0.70	X	0.37	0.29	0.87	X	2.61	2.53	3.11
27/37 Pt	0.27	-0.17	-0.21	0.44	0.45	0.01	-0.03	0.61	2.69	2.45	2.21	2.85
2x2 9/16 Cu	-0.84	X	-0.40	-0.56	-0.66	X	-0.22	-0.38	1.57	X	2.02	1.86
31/52 Cu	-0.76	-0.73	-0.76	-0.65	-0.58	-0.54	-0.57	-0.47	1.66	1.69	1.66	1.77
49/64 Ag	X	-0.26	-0.39	-0.12	X	-0.08	-0.21	0.06	X	2.15	2.03	2.30
31/39 Ag	-0.60	-0.54	-0.54	-0.52	-0.42	-0.36	-0.36	-0.34	1.81	1.88	1.88	1.90
49/64 Au	1.09	0.56	0.46	X	1.27	0.74	0.64	X	3.50	2.97	2.87	X
31/39 Au	0.71	0.69	0.79	0.64	0.89	0.97	0.97	0.82	3.13	3.10	3.20	3.05
52/27 Sn	X	X	/ ^b	-1.34	X	X	/	-1.16	X	X	/	1.07
36/31 Pb	-0.61	-0.96	-1.11	-0.68	-0.43	-0.78	-0.93	-0.50	1.80	1.46	1.31	1.74

^a "X" in the table indicates that O adsorption at this site makes some O in the ZnO film move to the metal surface; ^b "/" in the table indicates that adsorption on this site is not locally stable.

Table S10. Gibbs adsorption energies of one OH moiety above the centers of ZnO rings, $G_{ad}[\text{OH}]$ under ambient conditions ($T = 298.15 \text{ K}$, $p[\text{O}_2] = 20612.2 \text{ Pa}$, $p[\text{H}_2\text{O}] = 3171.5 \text{ Pa}$), and typical hydrogenation conditions of methanol synthesis ($T = 525 \text{ K}$, $p[\text{H}_2] = 1500000 \text{ Pa}$, $p[\text{H}_2\text{O}] = 50000 \text{ Pa}$) for metal-supported ZnO. The top, bridge, and hollow (hcp, fcc) refer to the alignment of the center of ZnO rings above the metal support.

	ambient conditions				typical hydrogenation conditions			
Equation:	$\text{ZnO} + 0.5\text{H}_2\text{O} + 0.25\text{O}_2 \rightarrow \text{OH}/\text{ZnO}$				$\text{ZnO} + \text{H}_2\text{O} \rightarrow \text{OH}/\text{ZnO} + 0.5\text{H}_2$			
ZnO/M (unit cells)	$G_{ad}[\text{OH}]$ (eV)				$G_{ad}[\text{OH}]$ (eV)			
	top	bridge	hcp	fcc	top	bridge	hcp	fcc
ZnO monolayer	1.34				2.56			
wz-(1010) 4-layer	0.44				1.79			
43/64 Ru	-0.71	X ^a	X	-0.77	0.63	X	X	0.57
25/36 Pd	-0.03	-0.22	-0.28	-0.18	1.32	1.13	1.07	1.17
28/39 Pd	-0.26	-0.17	-0.21	X	1.10	1.18	1.14	X
25/36 Pt	X	-0.39	-0.42	0.20	X	0.95	0.92	1.54
27/37 Pt	X	X	-0.60	X	X	X	0.73	X
2x2 9/16 Cu	-0.45	-0.50	-0.52	-0.56	0.90	0.86	0.83	0.80
31/52 Cu	-0.61	-0.73	-0.68	-0.74	0.74	0.62	0.68	0.62
49/64 Ag	-0.42	-0.50	-0.63	-0.34	0.94	0.85	0.72	1.01
31/39 Ag	-0.73	-0.71	-0.68	-0.72	0.63	0.64	0.67	0.63
49/64 Au	0.33	0.00	-0.15	0.35	1.67	1.36	1.20	1.71
31/39 Au	0.12	0.04	0.13	-0.02	1.46	1.39	1.49	1.33
52/27 Sn	-1.39	-0.96	/ ^b	-1.02	-0.04	0.39	/	0.33
36/31 Pb	-0.67	-0.94	-1.08	-0.70	0.67	0.41	0.27	0.64

^a "X" in the table indicates that O adsorption at this site makes some O in the ZnO film move to the metal surface; ^b "/" in the table indicates that adsorption on this site is not locally stable

References

- 1 G. Barcaro, I. O. Thomas and A. Fortunelli, *J. Chem. Phys.*, 2010, **132**, 124703.
- 2 S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
- 3 J. Neugebauer and M. Scheffler, 1992, **46**, 16067–16080.
- 4 J. P. Perdew, K. Burke and M. Ernzerhof, 1996, **77**, 3865–3868.

Structure files of ZnO films on metal surfaces

In this section, the optimized structures of all ZnO/M are provided in XYZ format and accompanied by the matrix of the employed periodic cell dimensions.

Graphitic ZnO on metals

43/64 Ru

```
-21.679999999999997 0.000000000000000 0.000000000000000
10.839999999999999 -18.7754307539999985 0.000000000000000
0.000000000000000 0.000000000000000 19.719999999999989
Ru -8.129999998915903 -17.210811525125902 5.49999999715942
Ru -17.614999998915902 -0.782309615375904 5.49999999715942
Ru -5.419999998915904 -17.210811525125902 5.49999999715942
Ru -16.259999998915902 -3.129238459625904 5.49999999715942
Ru -14.904999998915903 -0.782309615375904 5.49999999715942
Ru -2.709999998915904 -17.210811525125902 5.49999999715942
Ru -14.904999998915901 -5.476167303875904 5.49999999715942
Ru -13.549999998915903 -3.129238459625904 5.49999999715942
Ru -12.194999998915904 -0.782309615375904 5.49999999715942
Ru 0.000000001084098 -17.210811525125902 5.49999999715942
Ru -13.549999998915901 -7.823096148125904 5.49999999715942
Ru -12.194999998915902 -5.476167303875904 5.49999999715942
Ru -10.839999998915903 -3.129238459625904 5.49999999715942
Ru -9.484999998915901 -0.782309615375904 5.49999999715942
Ru 2.710000001084097 -17.210811525125902 5.49999999715942
Ru -12.194999998915902 -10.170024992375902 5.49999999715942
Ru -10.839999998915903 -7.823096148125904 5.49999999715942
Ru -9.484999998915903 -5.476167303875904 5.49999999715942
Ru -8.129999998915901 -3.129238459625904 5.49999999715942
Ru -6.774999998915902 -0.782309615375904 5.49999999715942
Ru 5.420000001084096 -17.210811525125902 5.49999999715942
Ru -10.839999998915903 -12.516953836625902 5.49999999715942
Ru -9.484999998915903 -10.170024992375902 5.49999999715942
Ru -8.129999998915903 -7.823096148125904 5.49999999715942
Ru -6.774999998915900 -5.476167303875904 5.49999999715942
Ru -5.419999998915902 -3.129238459625904 5.49999999715942
Ru -4.064999998915903 -0.782309615375904 5.49999999715942
Ru 8.130000001084097 -17.210811525125902 5.49999999715942
Ru -9.484999998915903 -14.863882680875902 5.49999999715942
Ru -8.129999998915903 -12.516953836625902 5.49999999715942
Ru -6.774999998915904 -10.170024992375902 5.49999999715942
Ru -5.419999998915901 -7.823096148125904 5.49999999715942
Ru -4.064999998915901 -5.476167303875904 5.49999999715942
Ru -2.709999998915903 -3.129238459625904 5.49999999715942
Ru -1.354999998915902 -0.782309615375904 5.49999999715942
Ru -10.839999998915903 -17.210811525125902 5.49999999715942
Ru -6.774999998915904 -14.863882680875902 5.49999999715942
Ru -5.419999998915904 -12.516953836625902 5.49999999715942
Ru -4.064999998915901 -10.170024992375902 5.49999999715942
Ru -2.709999998915902 -7.823096148125904 5.49999999715942
Ru -1.354999998915903 -5.476167303875904 5.49999999715942
Ru 0.000000001084098 -3.129238459625904 5.49999999715942
Ru -20.324999998915903 -0.782309615375904 5.49999999715942
Ru -4.064999998915905 -14.863882680875902 5.49999999715942
Ru -2.709999998915902 -12.516953836625902 5.49999999715942
Ru -1.354999998915902 -10.170024992375902 5.49999999715942
Ru 0.000000001084097 -7.823096148125904 5.49999999715942
Ru 1.355000001084098 -5.476167303875904 5.49999999715942
Ru -18.969999998915902 -3.129238459625904 5.49999999715942
Ru -1.354999998915902 -14.863882680875902 5.49999999715942
Ru 0.000000001084097 -12.516953836625902 5.49999999715942
Ru 1.355000001084097 -10.170024992375902 5.49999999715942
Ru 2.710000001084098 -7.823096148125904 5.49999999715942
```

Ru	-17.614999998915902	-5.476167303875904	5.499999999715942
Ru	1.355000001084097	-14.863882680875902	5.499999999715942
Ru	2.710000001084096	-12.516953836625902	5.499999999715942
Ru	4.065000001084098	-10.170024992375902	5.499999999715942
Ru	-16.259999998915902	-7.823096148125904	5.499999999715942
Ru	4.065000001084096	-14.863882680875902	5.499999999715942
Ru	5.420000001084097	-12.516953836625902	5.499999999715942
Ru	-14.904999998915903	-10.170024992375902	5.499999999715942
Ru	6.775000001084097	-14.863882680875902	5.499999999715942
Ru	-13.549999998915904	-12.516953836625902	5.499999999715942
Ru	-12.194999998915904	-14.863882680875902	5.499999999715942
Ru	-18.972589039879278	0.000846320454145	7.545383758925984
Ru	-17.619383662600548	-2.358734116412478	7.559216325437735
Ru	-16.279433586769187	-0.000087621657263	7.526690390827774
Ru	-16.266991219203256	-4.711801313039359	7.575121055307608
Ru	-14.913484609640056	-2.369970841322084	7.532597554740348
Ru	-13.539157138997709	-0.000786494834802	7.514149953349094
Ru	-14.917669626404392	-7.043780250048000	7.568620674659412
Ru	-13.560315748285500	-4.710350693703994	7.543731584268067
Ru	-12.181587177865291	-2.350948554053566	7.541340726881407
Ru	-10.815905726368118	0.006937520000958	7.555674519372495
Ru	-13.553225240261618	-9.374089677393151	7.541340726881407
Ru	-12.200088611839082	-7.044400242631267	7.544070889888687
Ru	-10.840585258639555	-4.687643966436736	7.544070889888687
Ru	-9.481257822029633	-2.334459767278367	7.568620674659412
Ru	-8.125677274431126	0.003304530725807	7.588709102548655
Ru	-12.170802740361577	-11.730471110203425	7.532597554740348
Ru	-10.820558764365806	-9.388402574472270	7.543731584268067
Ru	-9.479326129521361	-7.043386544931995	7.544070889888687
Ru	-8.139125487348689	-4.676677485823735	7.543731584268067
Ru	-6.787044025085467	-2.331902458546891	7.575121055307608
Ru	-5.427757721321833	-0.010290828740733	7.577638270296341
Ru	-10.827584503108408	-14.079466792592443	7.559216325437735
Ru	-9.465964755711282	-11.731726982413756	7.575121055307608
Ru	-8.121072551565987	-9.397190736673629	7.568620674659412
Ru	-6.785187581873082	-7.050392522553283	7.541340726881407
Ru	-5.435712649998367	-4.674988802474495	7.532597554740348
Ru	-4.073031834291051	-2.337229844995083	7.559216325437735
Ru	-2.721394876888934	-0.008072913079292	7.552364703202727
Ru	-9.486293909364759	-16.414597200351558	7.552364703202727
Ru	-8.135033258454570	-14.069709267389458	7.577638270296341
Ru	-6.774299555228303	-11.740040076769127	7.588709102548655
Ru	-5.426039068255835	-9.412050390051370	7.555674519372495
Ru	-4.0711102555008030	-7.049783478410261	7.514149953349094
Ru	-2.700359089196515	-4.676983897842643	7.526690390827774
Ru	-1.352972545047329	-2.345109830170211	7.545383758925984
Ru	0.000000000000000	0.000000000000000	7.542264916513745
Ru	-6.792372928486552	-16.410005527151498	7.550485234380569
Ru	-5.440520351754563	-14.073750472456046	7.566518277091213
Ru	-4.078534425867395	-11.745986804541428	7.561523188859828
Ru	-2.714326697584841	-9.407944230946539	7.531380776899116
Ru	-1.335367910143011	-7.037130204857180	7.527314300275057
Ru	0.024704801451724	-4.688060482391807	7.550485234380569
Ru	1.367688786253694	-2.352760640569140	7.552364703202727
Ru	-4.077982517768250	-16.413328185150924	7.527314300275057
Ru	-2.721314299739142	-14.076000468114081	7.553780306813396
Ru	-1.357412661541319	-11.740638574298380	7.541413193571868
Ru	0.010483160770853	-9.380703204692846	7.553780306813396
Ru	1.372034740176829	-7.026926683357975	7.566518277091213
Ru	2.722790979776408	-4.695430657869804	7.577638270296341
Ru	-1.335317949800386	-16.422134512799676	7.531380776899116
Ru	0.006397592789819	-14.080665315161321	7.541413193571868
Ru	1.351015068751495	-11.729557618540294	7.541413193571868

Ru	2.706944247658766	-9.370322928727518	7.561523188859828
Ru	4.059976829659422	-7.038695207956681	7.588709102548655
Ru	1.371590178208635	-16.434551774731062	7.561523188859828
Ru	2.710831138968292	-14.094157835193068	7.553780306813396
Ru	4.049644647385226	-11.720782764253777	7.531380776899116
Ru	5.401944794623951	-9.370317883949586	7.555674519372495
Ru	4.068485611577737	-16.450184352185982	7.566518277091213
Ru	5.413350427911260	-14.100403117991897	7.527314300275057
Ru	6.770259694005746	-11.724860780754943	7.514149953349094
Ru	6.767668127034815	-16.452795498456680	7.550485234380569
Ru	8.139792675965706	-14.098359234500096	7.526690390827774
Ru	9.485561584926607	-16.431167244283934	7.545383758925984
Ru	-8.147488347516825	-17.216961709301930	9.687102889261654
Ru	-17.625984863474422	-0.803366042850663	9.663743711976124
Ru	-5.435879469500922	-17.207524421816590	9.635025791024253
Ru	-16.263673818364541	-3.152290239628768	9.700289309866319
Ru	-14.900122978484122	-0.786001783708985	9.588836623265578
Ru	-2.721189259462395	-17.199693298153512	9.604553764274732
Ru	-14.912593414416433	-5.491443155467049	9.735407810120520
Ru	-13.531586151298624	-3.131971348867976	9.648778264985962
Ru	-12.176962948004137	-0.764152486770918	9.639108192828020
Ru	0.013360817188030	-17.198180212643020	9.700651968135368
Ru	-13.567320031304369	-7.807666832205332	9.695799949957218
Ru	-12.189762655517686	-5.478695679078020	9.677353165511260
Ru	-10.817977803171409	-3.121953529543438	9.695799949957218
Ru	-9.482501397122411	-0.773344485269493	9.770669219715812
Ru	2.716783603510736	-17.210603136592809	9.788766730693773
Ru	-12.201840171215171	-10.152711687936929	9.648778264985962
Ru	-10.840429033459671	-7.817296288093657	9.677353165511260
Ru	-9.489808307770346	-5.479438788706037	9.677353165511260
Ru	-8.139432566708040	-3.115024443105391	9.735407810120520
Ru	-6.776041620639771	-0.783576034349668	9.805417653693347
Ru	5.423211666668781	-17.228130629114833	9.757400825775132
Ru	-10.818199662106608	-12.508609567595901	9.700289309866319
Ru	-9.467974015623227	-10.168963157305267	9.735407810120520
Ru	-8.134702162271928	-7.845810394128931	9.695799949957220
Ru	-6.786573674233919	-5.490747719072806	9.648778264985962
Ru	-5.438126516276562	-3.114530948653037	9.700289309866319
Ru	-4.075745820280739	-0.792799927139258	9.742858126320241
Ru	8.144070391118968	-17.222881787196489	9.687102889261654
Ru	-9.488711964714188	-14.849331370707773	9.742858126320241
Ru	-8.130575939057085	-12.515418556265027	9.805417653693347
Ru	-6.768485269392251	-10.176671410056208	9.770669219715812
Ru	-5.413293989740051	-7.847795256727311	9.639108192828020
Ru	-4.070636020703304	-5.478544843298048	9.588836623265578
Ru	-2.722742967742771	-3.109197074123731	9.663743711976124
Ru	-1.359495087925241	-0.776350190397173	9.685755639834211
Ru	-10.832591440987692	-17.209898376340917	9.685755639834211
Ru	-6.791604615733476	-14.858004512866223	9.757400825775132
Ru	-5.423211330365704	-12.522932802923076	9.788766730693773
Ru	-4.060741369474519	-10.187911454778614	9.700651968135368
Ru	-2.694776701639506	-7.818965077729304	9.604553764274732
Ru	-1.344213548652660	-5.464058830605319	9.635025791024253
Ru	0.003417959650147	-3.111018013379285	9.687102889261654
Ru	-20.327913467834783	-0.789182189139618	9.685755639834211
Ru	-4.093861361838497	-14.854996004187607	9.685549302359545
Ru	-2.718335048382835	-12.512254738920848	9.692232863691142
Ru	-1.338865501670692	-10.168659298142041	9.665543265988264
Ru	0.022126770312688	-7.802544812991306	9.685549302359545
Ru	1.368392952316991	-5.464726367896657	9.757400825775132
Ru	-18.955542211752778	-3.133299458030680	9.742858126320241
Ru	-1.364249973438842	-14.850592643501221	9.665543265988264
Ru	0.00000001084097	-12.516953836625902	9.682668626719144

Ru	1.363237063805005	-10.165156176648280	9.692232863691142
Ru	2.706427730107263	-7.817325570361821	9.788766730693773
Ru	-17.613382437050856	-5.476436165263015	9.805417653693347
Ru	1.355097987830123	-14.873450594308579	9.692232863691142
Ru	2.703115478361826	-12.531609568234449	9.665543265988264
Ru	4.047380555538789	-10.164769842456083	9.700651968135368
Ru	-16.269013330233051	-7.825414860552004	9.770669219715812
Ru	4.071734594778100	-14.893320692698795	9.685549302359545
Ru	5.415965964354186	-12.532203133994889	9.604553764274732
Ru	-14.929743059003524	-10.163483012379480	9.639108192828020
Ru	6.780093021405869	-14.879278257455793	9.635025791024253
Ru	-13.549240997560297	-12.510884128870671	9.588836623265578
Ru	-12.171272165530509	-14.862867638903314	9.663743711976124
Ru	-18.994471312577829	-0.006836017275255	11.712940405315349
Ru	-17.517036554157681	-2.270144347278167	11.797856758732149
Ru	-16.227621505632452	0.006602406565952	11.624533654283194
Ru	-16.149688951512967	-4.664464461724636	11.828595581762615
Ru	-14.839926425831099	-2.306885361487852	11.652784133450400
Ru	-13.584919282770890	0.001343631244934	11.623343824523527
Ru	-14.837883700170970	-7.094460986626850	11.828361409091862
Ru	-13.486886850082778	-4.654516135526492	11.703648157738165
Ru	-12.220808336762438	-2.326214929396518	11.682017769656120
Ru	-10.955355581103698	0.082632515502201	11.780021069084315
Ru	-13.555034608093766	-9.420423009692382	11.682017769656120
Ru	-12.166852130871872	-7.036287905210718	11.731566527988578
Ru	-10.850178008832874	-4.720483771996943	11.731566527988578
Ru	-9.565041590506240	-2.378216037971382	11.828361409091862
Ru	-8.158310965587035	0.020648675575488	11.862925493393259
Ru	-12.262215460412566	-11.698310594285893	11.652784133450400
Ru	-10.905627359258087	-9.352728562345714	11.703648157738165
Ru	-9.5029669860295259	-7.018659076792344	11.731566527988578
Ru	-8.127485790659136	-4.768186056127795	11.703648157738165
Ru	-6.804700243156797	-2.457157627945317	11.828595581762615
Ru	-5.352118247387605	-0.026010449601674	11.850593915705215
Ru	-10.955479047915745	-14.035126481244415	11.797856758732149
Ru	-9.565610805330250	-11.653808664330052	11.828595581762615
Ru	-8.117074709322788	-9.302753729401767	11.828361409091862
Ru	-6.744157055143794	-7.028792814911099	11.682017769656120
Ru	-5.417858113756347	-4.770234798226259	11.652784133450400
Ru	-4.047484397926584	-2.470159925477416	11.797856758732149
Ru	-2.657132095565325	0.013904478001979	11.741827912320549
Ru	-9.499392321041242	-16.481239097036141	11.741827912320549
Ru	-8.186466586425151	-14.127355162914762	11.850593915705215
Ru	-6.742962239603562	-11.720450543633767	11.862925493393259
Ru	-5.290760351844455	-9.329130771047229	11.780021069084315
Ru	-4.046376739823121	-7.011217362411011	11.623343824523527
Ru	-2.720471395371522	-4.725199490441495	11.624533654283194
Ru	-1.348684508332179	-2.322318057256072	11.712940405315349
Ru	0.000000000000000	0.000000000000000	11.745087930427504
Ru	-6.792817798446254	-16.523790495025299	11.729723514418943
Ru	-5.403087083224156	-14.184331219170490	11.822306000807924
Ru	-3.959165324933575	-11.739756817748919	11.814129901421424
Ru	-2.655222028009178	-9.337846508493598	11.658876123940317
Ru	-1.406204481448682	-7.025354156675983	11.678040111079151
Ru	-0.073613436316163	-4.630782729768423	11.729723514418943
Ru	1.316524416606559	-2.308096134965828	11.741827912320549
Ru	-4.052762588996547	-16.480562479509061	11.678040111079151
Ru	-2.694757346990007	-14.114054565371463	11.716562715820894
Ru	-1.318202741582564	-11.724635208737851	11.712885395136240
Ru	-0.035751130546764	-9.384675151791958	11.716562715820894
Ru	1.257552370087236	-7.004054471494681	11.822306000807924
Ru	2.698584833812764	-4.622065141483567	11.850593915705215
Ru	-1.425576692980046	-16.405997228691465	11.658876123940317

Ru	-0.027066688311068	-14.054710211177033	11.712885395136240
Ru	1.345269429893634	-11.771516088085120	11.712885395136240
Ru	2.652655024019419	-9.476814595959121	11.814129901421424
Ru	4.061273205190597	-7.075628885941720	11.862925493393259
Ru	1.306510300914159	-16.334290094291976	11.814129901421424
Ru	2.730508477536779	-14.052131790836581	11.716562715820894
Ru	4.080798720989220	-11.807017770814927	11.658876123940317
Ru	5.406115932948155	-9.528932498454973	11.780021069084315
Ru	4.145534713136937	-16.362475817334833	11.822306000807924
Ru	5.458967070445226	-14.044944871814952	11.678040111079151
Ru	6.791296022594015	-11.765557022833915	11.623343824523527
Ru	6.866431234762420	-16.396288283206285	11.729723514418943
Ru	8.108092901003983	-14.056833670124455	11.624533654283194
Ru	9.503155820910015	-16.446276679468678	11.712940405315349
O	7.816975957319168	-16.424095017359470	14.378698415596796
O	4.486009353433939	-15.999469753814356	14.116428359738292
O	1.217537507691016	-15.647853265426754	14.069218056104960
O	-2.009310161713433	-15.095613568296876	14.695404261922663
O	-5.258951841747482	-14.660694032648788	14.116428359738292
O	-8.507342823648116	-14.297681794067287	14.153814204415879
O	-11.753426414309580	-13.836908007872832	14.022231225958302
O	6.549328140059507	-13.368822768895663	14.605384891678218
O	3.237839877723252	-12.967737737891202	14.695404261922663
O	0.00000017344080	-12.516953909850056	14.641550817184513
O	-3.320207106458027	-12.005922628759492	14.069218056104960
O	-6.604387583852551	-11.660506062896095	14.232713876290083
O	-9.846809619045164	-11.253015855009313	14.123715276502105
O	-13.098383533511150	-10.726255058139488	14.681509398405398
O	5.325959954541142	-10.251398371576505	14.071613549006196
O	2.102669650799015	-9.897085835363796	14.069218056104960
O	-1.228529667229802	-9.487510421484505	14.695404261922663
O	-4.625008601088827	-9.037315073847317	14.071613549006196
O	-7.918958589029028	-8.651811123168589	14.068231711357884
O	-11.124886346108189	-8.136144815653820	14.770763450277975
O	-14.373208836940872	-7.591505978571297	14.068231711357884
O	4.043899408254656	-7.225610394266000	14.232713876290083
O	0.772942539261452	-6.890697941209435	14.116428359738292
O	-2.536923972469542	-6.419134946472217	14.605384891678218
O	-5.841598903341293	-5.980405485230008	14.681509398405398
O	-9.071448764559097	-5.566361906011288	14.770763450277975
O	-12.323664838384722	-5.072924252007347	14.770763450277975
O	-15.661992702324730	-4.621335645949245	14.123715276502105
O	-18.968484147123252	-4.259014948756823	14.153814204415879
O	-0.524804497361519	-3.793683611321855	14.378698415596796
O	-3.820172986109224	-3.260311978136806	14.022231225958302
O	-7.011197629850246	-2.901079472714029	14.123715276502105
O	-10.227832521998010	-2.532113873810284	14.068231711357884
O	-13.580017511115495	-2.068770432180668	14.681509398405398
O	-16.946400548633203	-1.678210987662811	14.022231225958302
O	-20.191493485185898	-1.172345994872486	14.716325119934103
O	-1.759534583190060	-0.702911553843010	14.716325119934103
O	-5.044172977196556	-0.218734232726054	14.153814204415879
O	2.560488224377831	-18.664745270510352	14.232713876290083
O	-0.700951301420318	-18.262148284126212	14.071613549006196
O	-4.012404118810030	-17.762904012304571	14.605384891678218
O	-7.292171407925643	-17.333083100868702	14.378698415596796
O	-10.568971882844011	-16.900173424957096	14.716325119934103
Zn	6.066190199053914	-17.095969313776887	14.193488879515822
Zn	2.743957947739054	-16.764936041169520	14.131583835995791
Zn	-0.611993718599038	-16.283603052576925	14.189095428879069
Zn	-3.684355516929902	-15.892224231954030	14.269618991924869
Zn	-6.998638915417676	-15.480920817912711	14.193488879515822
Zn	-10.288936954187635	-15.140859641613813	14.156337257304694

Zn	8.026288139961181	-14.526496451819167	14.197666382558083
Zn	4.765247705033968	-14.020063988331911	14.269618991924869
Zn	1.494345787534265	-13.616545792675153	14.150904396471152
Zn	-1.699447552019208	-13.261299175947478	14.150904396471152
Zn	-5.050839568351694	-12.769299927312902	14.131583835995791
Zn	-8.347170624122786	-12.411818471995010	14.126420854385424
Zn	-11.676940289882312	-11.896510601525698	14.248944365897184
Zn	-14.797021260593176	-11.498476894288043	14.257052405041794
Zn	3.568010805948056	-11.163631209177989	14.189095428879069
Zn	0.205101713536961	-10.673016319704907	14.150904396471152
Zn	-2.956017139381101	-10.103627024694903	14.189095428879069
Zn	-6.388818652531818	-9.764819828033117	14.159545763133938
Zn	-9.752383841364725	-9.273086661912048	14.170329055885876
Zn	-12.787497395591370	-8.870089814633165	14.186605074629279
Zn	-16.102172798181766	-8.360141490978094	14.159545763133938
Zn	2.306881568580558	-8.016625317967403	14.131583835995791
Zn	-1.080892236883940	-7.638573068041461	14.269618991924869
Zn	-4.323516235372844	-7.065357740918492	14.257052405041794
Zn	-7.604528150923341	-6.639252562270022	14.186605074629279
Zn	-10.840000017344078	-6.258476844149944	14.511593859324494
Zn	-13.994536787851999	-5.693075173231565	14.170329055885876
Zn	-17.415364879677874	-5.340659612052241	14.126420854385424
Zn	0.932448665415782	-4.973971156637952	14.193488879515822
Zn	-2.272829076749453	-4.561212975012180	14.197666382558083
Zn	-5.538849418697026	-4.164271504806227	14.248944365897184
Zn	-8.773079419563304	-3.809268699183799	14.170329055885876
Zn	-12.127974505517308	-3.266088155546778	14.186605074629279
Zn	-15.304210342368565	-2.714648427995483	14.248944365897184
Zn	-18.807900697682857	-2.294520057197571	14.156337257304694
Zn	-0.261767017763705	-1.841428442765322	14.279691082581492
Zn	-3.423162400161516	-1.340050833638575	14.156337257304694
Zn	-6.757464544979279	-1.022952450280299	14.126420854385424
Zn	-10.029008601318433	-0.650469213438751	14.159545763133938
Zn	-13.399462552813926	-0.211595899121007	14.257052405041794
Zn	-5.753459115243814	-18.463151859618481	14.197666382558083
Zn	-9.114392641404265	-18.081413295955112	14.279691082581492
Zn	9.376159610387955	-17.628019549606968	14.279691082581492

25/36 Pd

	16.5038722728940215	0.0000000000000000	0.0000000000000000
	8.2519361364470107	14.2927726491398417	0.0000000000000000
	0.0000000000000000	0.0000000000000000	20.0376776414429365
Pd	0.0000000000000000	0.0000000000000000	5.5000000000000034
Pd	1.375322689407816	2.382128774856606	5.5000000000000034
Pd	2.750645378815690	4.764257549713315	5.5000000000000034
Pd	4.125968068223505	7.146386324569921	5.5000000000000034
Pd	5.501290757631321	9.528515099426528	5.5000000000000034
Pd	6.876613447039195	11.910643874283235	5.5000000000000034
Pd	2.750645378815631	0.0000000000000000	5.5000000000000034
Pd	4.125968068223447	2.382128774856606	5.5000000000000034
Pd	5.501290757631321	4.764257549713315	5.5000000000000034
Pd	6.876613447039137	7.146386324569921	5.5000000000000034
Pd	8.251936136446952	9.528515099426528	5.5000000000000034
Pd	9.627258825854826	11.910643874283235	5.5000000000000034
Pd	5.501290757631380	0.0000000000000000	5.5000000000000034
Pd	6.876613447039196	2.382128774856606	5.5000000000000034
Pd	8.251936136447069	4.764257549713315	5.5000000000000034
Pd	9.627258825854884	7.146386324569921	5.5000000000000034
Pd	11.002581515262701	9.528515099426528	5.5000000000000034
Pd	12.377904204670575	11.910643874283235	5.5000000000000034
Pd	8.251936136447011	0.0000000000000000	5.5000000000000034
Pd	9.627258825854826	2.382128774856606	5.5000000000000034
Pd	11.002581515262701	4.764257549713315	5.5000000000000034

Pd	12.377904204670516	7.146386324569921	5.500000000000034
Pd	13.753226894078331	9.528515099426528	5.500000000000034
Pd	15.128549583486205	11.910643874283235	5.500000000000034
Pd	11.002581515262642	0.000000000000000	5.500000000000034
Pd	12.377904204670457	2.382128774856606	5.500000000000034
Pd	13.753226894078333	4.764257549713315	5.500000000000034
Pd	15.128549583486148	7.146386324569921	5.500000000000034
Pd	16.503872272893965	9.528515099426528	5.500000000000034
Pd	17.879194962301838	11.910643874283235	5.500000000000034
Pd	13.753226894078390	0.000000000000000	5.500000000000034
Pd	15.128549583486205	2.382128774856606	5.500000000000034
Pd	16.503872272894078	4.764257549713315	5.500000000000034
Pd	17.879194962301895	7.146386324569921	5.500000000000034
Pd	19.254517651709712	9.528515099426528	5.500000000000034
Pd	20.629840341117585	11.910643874283235	5.500000000000034
Pd	1.373772036770776	0.793147655234788	7.754769638888393
Pd	2.731958824692349	3.182408605581707	7.756561208714535
Pd	4.091069041098146	5.575514484055047	7.758917290096256
Pd	5.468933474636328	7.962045688885289	7.758917290096256
Pd	6.861868851137213	10.335622602072336	7.756561208714535
Pd	8.251936136447011	12.706477338670267	7.754769638888393
Pd	4.122026110002145	0.774741441485798	7.756561208714535
Pd	5.485816046778318	3.167237371332229	7.732328294987211
Pd	6.861804530744198	5.566850406474739	7.721998365893267
Pd	8.251936136447013	7.958297906475386	7.732328294987211
Pd	9.642003421756806	10.335622602072336	7.756561208714535
Pd	11.014940701563416	12.697551219697653	7.774075792414532
Pd	6.874071702908832	0.755212476199513	7.758917290096256
Pd	8.251936136446952	3.159071836190263	7.721998365893267
Pd	9.642067742149706	5.566850406474739	7.721998365893267
Pd	11.034938798257702	7.962045688885289	7.758917290096256
Pd	12.407231927226182	10.327769781959066	7.811215298676704
Pd	13.763377240893229	12.676682367676824	7.811215298676704
Pd	9.629800569985198	0.755212476199513	7.758917290096256
Pd	11.018056226115707	3.167237371332229	7.732328294987211
Pd	12.412803231795884	5.575514484055047	7.758917290096256
Pd	13.787081640860446	7.959975296690124	7.828502216447486
Pd	15.142417965187853	10.314551110470095	7.876553964106520
Pd	16.503872272894021	12.665594704899434	7.828502216447486
Pd	12.381846162891874	0.774741441485798	7.756561208714535
Pd	13.771913448201671	3.182408605581707	7.756561208714535
Pd	15.147726959226917	5.581093148643697	7.811215298676704
Pd	16.503872272894021	7.956443077339496	7.876553964106520
Pd	17.865326580600193	10.314551110470095	7.876553964106520
Pd	19.244367304894702	12.676682367676824	7.811215298676704
Pd	15.130100236123244	0.793147655234788	7.754769638888393
Pd	16.503872272893961	3.190442858884277	7.774075792414532
Pd	17.860017586561014	5.581093148643697	7.811215298676704
Pd	19.220662904927593	7.959975296690124	7.828502216447486
Pd	20.600512618561748	10.327769781959066	7.811215298676704
Pd	21.992803844224508	12.697551219697653	7.774075792414532
Pd	16.503872272894021	1.591802964649126	9.986698871169303
Pd	17.874515437674827	3.979151570649918	10.029015658103855
Pd	19.247021599926740	6.359755146197974	10.062114914126200
Pd	20.619673554401125	8.737258072456333	10.062114914126200
Pd	21.995083646039852	11.116185063591201	10.029015658103855
Pd	23.377266604135507	13.496871166815280	9.986698871169303
Pd	2.749854003023664	1.587628948877882	9.977699753584325
Pd	4.118484767487809	3.971739516146650	9.959109059508968
Pd	5.492053737929345	6.357676395429162	9.950404332038243
Pd	6.871551201993460	8.740190457322932	9.959109059508968
Pd	8.251936136447071	11.117514751384185	9.977699753584325
Pd	9.630477941652538	13.496871166815280	9.986698871169303

Pd	5.498869701941419	1.580842675670363	9.959109059508968
Pd	6.870244218308489	3.966537348838875	9.904601816929867
Pd	8.251936136447009	6.359697951462088	9.904601816929867
Pd	9.632321070900680	8.740190457322932	9.959109059508968
Pd	11.012660899748184	11.116185063591201	10.029015658103855
Pd	12.383304064528993	13.490208664038560	10.029015658103855
Pd	8.251936136447009	1.577419858281514	9.950404332038243
Pd	9.633628054585529	3.966537348838875	9.904601816929867
Pd	11.011818534964672	6.357676395429162	9.950404332038243
Pd	12.388070991386915	8.737258072456333	10.062114914126200
Pd	13.756295106653843	11.114829515974593	10.144693398244392
Pd	15.131220318419633	13.488532079625374	10.062114914126200
Pd	11.005002570952723	1.580842675670363	9.959109059508968
Pd	12.385387505406333	3.971739516146650	9.959109059508968
Pd	13.760722945861302	6.359755146197974	10.062114914126200
Pd	15.127876182572322	8.734083386275456	10.196988667634052
Pd	16.503872272894085	11.117378525728883	10.196988667634052
Pd	17.876524227368407	13.488532079625374	10.062114914126200
Pd	13.7540128269870480	1.587628948877882	9.977699753584325
Pd	15.133229108113211	3.979151570649918	10.029015658103855
Pd	16.503872272894018	6.355886266330492	10.144693398244392
Pd	17.879868363215849	8.734083386275456	10.196988667634052
Pd	19.251449439134195	11.114829515974593	10.144693398244392
Pd	20.624440481259043	13.490208664038560	10.029015658103855
Pd	0.000000000000000	0.000000000000000	12.241789464176279
Pd	1.390737241366181	2.369134558174227	12.262220941965094
Pd	2.805315978655617	4.727721351321614	12.284254463509676
Pd	4.205897736304591	7.100238909187071	12.301895426357866
Pd	5.560267333516204	9.499437070320862	12.284254463509676
Pd	6.895574044767602	11.903791589040530	12.262220941965094
Pd	2.747099333045593	0.019846501925090	12.262220941965094
Pd	4.151427087817273	2.396827546672406	12.235781615235064
Pd	5.544898707906995	4.752218263061947	12.195657629262168
Pd	6.908843750260502	7.114640375149904	12.195657629262168
Pd	8.251936136446952	9.499117555794928	12.235781615235064
Pd	9.608298228126426	11.903791589040530	12.262220941965094
Pd	5.496984781586423	0.065614227497361	12.284254463509676
Pd	6.887991094093505	2.425914010927992	12.195657629262168
Pd	8.251936136447069	4.764257549713315	12.135452857268302
Pd	9.595028522633521	7.114640375149904	12.195657629262168
Pd	10.943604939377813	9.499437070320862	12.284254463509676
Pd	12.332524528670120	11.936843842437835	12.370096852550221
Pd	8.251936136447013	0.092294830765703	12.301895426357866
Pd	9.615881178800517	2.425914010927992	12.195657629262168
Pd	10.958973564987028	4.752218263061947	12.195657629262168
Pd	12.297974536589436	7.100238909187071	12.301895426357866
Pd	13.681702856349062	9.515095802966387	12.435017277588331
Pd	15.104409016256962	11.979295156168083	12.435017277588331
Pd	11.006887491307594	0.065614227497361	12.284254463509676
Pd	12.352445185076631	2.396827546672406	12.235781615235064
Pd	13.698556294238399	4.727721351321614	12.284254463509676
Pd	15.081166112986118	7.091154339145207	12.435017277588331
Pd	16.503872272893965	9.528515099426528	12.481260649820188
Pd	17.903335529531073	11.979295156168085	12.435017277588331
Pd	13.756772939848435	0.019846501925090	12.262220941965094
Pd	15.113135031527847	2.369134558174227	12.262220941965094
Pd	16.503872272894078	4.711857613404114	12.370096852550221
Pd	17.926578432801918	7.091154339145207	12.435017277588331
Pd	19.326041689438973	9.515095802966387	12.435017277588331
Pd	20.675220017118040	11.936843842437835	12.370096852550221
O	1.656214375913477	0.956215785278123	14.947920533600243
O	4.961016352285080	0.958118887946117	14.995990499075777
O	3.310263499355770	3.817306699958953	14.995990499075777

O	8.251936088585749	0.963163991017893	14.961812954777029
O	6.608726377606575	3.815549922620484	14.974666711859777
O	4.960092554930974	6.664804241875029	14.961812954777029
O	11.542855824886532	0.958118887946117	14.995990499075777
O	9.895145799565039	3.815549922620484	14.974666711859777
O	8.251936088585810	6.661672629527086	14.974666711859777
O	6.601183235656496	9.517346886862979	14.995990499075777
O	14.847657801258013	0.956215785278123	14.947920533600243
O	13.193608677815838	3.817306699958953	14.995990499075777
O	11.543779622240523	6.664804241875029	14.961812954777029
O	9.902688941515114	9.517346886862979	14.995990499075777
O	8.251936088585746	12.380340904211700	14.947920533600243
O	16.503872225032765	3.831346920857986	14.872625786165887
O	14.852023045649656	6.681257699503939	14.806474558394475
O	13.212150446231814	9.521600359635682	14.806474558394475
O	11.569979903096883	12.377099101524907	14.872625786165887
O	18.155721404415857	6.681257699503939	14.806474558394475
O	16.503872225032815	9.528515041302631	14.908946105800082
O	14.863999625614914	12.382687064768168	14.806474558394475
O	19.795594003833699	9.521600359635682	14.806474558394475
O	18.143744824450597	12.382687064768168	14.806474558394475
O	21.437764546968644	12.377099101524907	14.872625786165887
Zn	16.503872320755288	1.892154804887803	14.664380985611638
Zn	3.307836094662297	1.909780090179688	14.746898111824656
Zn	18.178943326242621	4.733858735905326	14.708966044921528
Zn	6.597027557095783	1.922251676350682	14.758041838339294
Zn	4.963232536328608	4.752067661472477	14.758041838339294
Zn	19.845753628520079	7.599079084912741	14.737204135030487
Zn	9.906844811520765	1.922251676350682	14.758041838339294
Zn	8.251936184308216	4.764257607837211	14.727059200836266
Zn	6.618141163541098	7.618453485688573	14.758041838339294
Zn	21.493702087061834	10.475189324478251	14.708966044921528
Zn	13.196036273954252	1.909780090179688	14.746898111824656
Zn	11.540639832287939	4.752067661472477	14.758041838339294
Zn	9.885731205075448	7.618453485688573	14.758041838339294
Zn	8.251936184308274	10.473212643152358	14.746898111824656
Zn	23.117154378613506	13.346695333881891	14.664380985611638
Zn	14.828801315267835	4.733858735905326	14.708966044921528
Zn	13.161991012990486	7.599079084912741	14.737204135030487
Zn	11.514042554448624	10.475189324478251	14.708966044921528
Zn	9.890590262897073	13.346695333881891	14.664380985611638
Zn	16.503872320755228	7.624082007904410	14.720762208753857
Zn	14.854584833352510	10.480731732373535	14.720762208753857
Zn	13.189113559936017	13.376497412267900	14.708966044921528
Zn	18.153159808157952	10.480731732373535	14.720762208753857
Zn	16.503872320755281	13.387387302826090	14.737204135030487
Zn	19.818631081574438	13.376497412267900	14.708966044921528

25/36 Pt

	16.6311514935075984	0.0000000000000000	0.0000000000000000
	8.3155757467537992	14.4029996875650852	0.0000000000000000
	0.0000000000000000	0.0000000000000000	20.0896391656700004
Pt	0.0000000000000000	0.0000000000000000	5.500000000000015
Pt	1.385929291125614	2.400499947927480	5.500000000000015
Pt	2.771858582251286	4.800999895855062	5.500000000000015
Pt	4.157787873376900	7.201499843782543	5.500000000000015
Pt	5.543717164502513	9.601999791710023	5.500000000000015
Pt	6.929646455628186	12.002499739637605	5.500000000000015
Pt	2.771858582251227	0.0000000000000000	5.500000000000015
Pt	4.157787873376841	2.400499947927480	5.500000000000015
Pt	5.543717164502514	4.800999895855062	5.500000000000015
Pt	6.929646455628127	7.201499843782543	5.500000000000015
Pt	8.315575746753741	9.601999791710023	5.500000000000015

Pt	9.701505037879413	12.002499739637605	5.500000000000015
Pt	5.543717164502572	0.000000000000000	5.500000000000015
Pt	6.929646455628186	2.400499947927480	5.500000000000015
Pt	8.315575746753858	4.800999895855062	5.500000000000015
Pt	9.701505037879471	7.201499843782543	5.500000000000015
Pt	11.087434329005085	9.601999791710023	5.500000000000015
Pt	12.473363620130758	12.002499739637605	5.500000000000015
Pt	8.315575746753799	0.000000000000000	5.500000000000015
Pt	9.701505037879413	2.400499947927480	5.500000000000015
Pt	11.087434329005085	4.800999895855062	5.500000000000015
Pt	12.473363620130698	7.201499843782543	5.500000000000015
Pt	13.859292911256311	9.601999791710023	5.500000000000015
Pt	15.245222202381985	12.002499739637605	5.500000000000015
Pt	11.087434329005026	0.000000000000000	5.500000000000015
Pt	12.473363620130639	2.400499947927480	5.500000000000015
Pt	13.859292911256311	4.800999895855062	5.500000000000015
Pt	15.245222202381925	7.201499843782543	5.500000000000015
Pt	16.631151493507538	9.601999791710023	5.500000000000015
Pt	18.017080784633212	12.002499739637605	5.500000000000015
Pt	13.859292911256372	0.000000000000000	5.500000000000015
Pt	15.245222202381985	2.400499947927480	5.500000000000015
Pt	16.631151493507659	4.800999895855062	5.500000000000015
Pt	18.017080784633272	7.201499843782543	5.500000000000015
Pt	19.403010075758885	9.601999791710023	5.500000000000015
Pt	20.788939366884556	12.002499739637605	5.500000000000015
Pt	1.389916532776785	0.802468684349788	7.772797061193651
Pt	2.762117299250888	3.217912223977514	7.775650177754410
Pt	4.123309405153957	5.625457436125668	7.782953115280487
Pt	5.505441401737874	8.019380276975625	7.782953115280487
Pt	6.909840663266233	10.401979826192591	7.775650177754410
Pt	8.315575746753799	12.798062318865510	7.772797061193651
Pt	4.167852382738452	0.783107637394976	7.775650177754410
Pt	5.535210128199455	3.195755057537097	7.762830136269594
Pt	6.914885827101481	5.609688598017418	7.758834110221458
Pt	8.315575746753799	8.011489572490889	7.762830136269594
Pt	9.721310830241361	10.401979826192591	7.775650177754410
Pt	11.111736170264995	12.788635714353450	7.785760436091911
Pt	6.933443750169884	0.758161974463795	7.782953115280487
Pt	8.315575746753737	3.183622491530142	7.758834110221458
Pt	9.716265666405993	5.609688598017418	7.758834110221458
Pt	11.125710091769729	8.019380276975625	7.782953115280487
Pt	12.518511507941527	10.398100554127993	7.825897088739690
Pt	13.885388016498407	12.765600114620863	7.825897088739690
Pt	9.697707743337718	0.758161974463795	7.782953115280487
Pt	11.095941365308143	3.195755057537097	7.762830136269594
Pt	12.507842088353645	5.625457436125668	7.782953115280487
Pt	13.902009318627343	8.026328822386182	7.848658719702491
Pt	15.266724330143106	10.389752181768177	7.912285191354115
Pt	16.631151493507595	12.753341730357802	7.848658719702491
Pt	12.463299110769141	0.783107637394976	7.775650177754410
Pt	13.869034194256706	3.217912223977514	7.775650177754410
Pt	15.264274984950656	5.642298706381205	7.825897088739690
Pt	16.631151493507591	8.026495011593806	7.912285191354115
Pt	17.995578656872080	10.389752181768177	7.912285191354115
Pt	19.376914970516665	12.765600114620863	7.825897088739690
Pt	15.241234960730814	0.802468684349788	7.772797061193651
Pt	16.631151493507542	3.228727946423168	7.785760436091911
Pt	17.998028002064416	5.642298706381205	7.825897088739690
Pt	19.360293668387847	8.026328822386182	7.848658719702491
Pt	20.743791479073543	10.398100554127993	7.825897088739690
Pt	22.150566816750086	12.788635714353450	7.785760436091911
Pt	16.631151493507598	1.613192668715367	10.000097154435467
Pt	18.013964766347225	4.022977842009170	10.043072668516640

Pt	19.383500719433105	6.420765259612915	10.092736853413600
Pt	20.762356026662779	8.809012708020706	10.092736853413600
Pt	22.154132866639372	11.193959343591088	10.043072668516640
Pt	23.549661407955075	13.596403353207402	10.000097154435467
Pt	2.784286752525481	1.607508706071695	9.997237540942507
Pt	4.157872256504653	4.013202008303132	10.000221711423116
Pt	5.531044341145890	6.408649852449718	10.000012952280283
Pt	6.918976985296943	8.795575683590062	10.000221711423116
Pt	8.315575746753860	11.187982275421799	9.997237540942507
Pt	9.712641579060120	13.596403353207402	10.000097154435467
Pt	5.554471017961568	1.594221995671991	10.000221711423116
Pt	6.929026579769459	4.000475361051968	9.975962098631014
Pt	8.315575746753797	6.402048965461146	9.975962098631014
Pt	9.712174508210772	8.795575683590062	10.000221711423116
Pt	11.108170120375831	11.193959343591088	10.043072668516640
Pt	12.490983393215455	13.589062189529917	10.043072668516640
Pt	8.315575746753796	1.585699982665643	10.000012952280283
Pt	9.702124913738137	4.000475361051968	9.975962098631014
Pt	11.100107152361703	6.408649852449718	10.000012952280283
Pt	12.499946960352418	8.809012708020706	10.092736853413600
Pt	13.881064720887945	11.189763130176846	10.186032878181987
Pt	15.252296186277924	13.576221407496551	10.092736853413600
Pt	11.076680475546148	1.594221995671991	10.000221711423116
Pt	12.473279237003062	4.013202008303132	10.000221711423116
Pt	13.878802267582092	6.420765259612915	10.092736853413600
Pt	15.252316400195379	8.805928979418145	10.275568818095978
Pt	16.631151493507659	11.194141416293988	10.275568818095978
Pt	18.010006800737273	13.576221407496551	10.092736853413600
Pt	13.846864740982237	1.607508706071695	9.997237540942507
Pt	15.248338220667980	4.022977842009170	10.043072668516640
Pt	16.631151493507602	6.426473114776482	10.186032878181987
Pt	18.009986586819938	8.805928979418145	10.275568818095978
Pt	19.381238266127259	11.189763130176846	10.186032878181987
Pt	20.771319593799753	13.589062189529917	10.043072668516640
Pt	0.000000000000000	0.000000000000000	12.275028056924304
Pt	1.392525098305484	2.381818529951488	12.301956066017572
Pt	2.809374432120853	4.760606632689210	12.341749328528030
Pt	4.215485979062781	7.168187826933067	12.355645948539822
Pt	5.597456681480677	9.589706744261344	12.341749328528030
Pt	6.949122941764047	12.006128312049372	12.301956066017572
Pt	2.758977903295238	0.015052845564228	12.301956066017572
Pt	4.169139583994627	2.407053861108422	12.301620043373035
Pt	5.566516846262182	4.792290385386899	12.297139308022565
Pt	6.948588953827919	7.186109495414551	12.297139308022565
Pt	8.315575746753739	9.588891965348136	12.301620043373035
Pt	9.682028551743553	12.006128312049372	12.301956066017572
Pt	5.527493497393977	0.052686310614534	12.341749328528030
Pt	6.933503639188063	2.424599806763636	12.297139308022565
Pt	8.315575746753858	4.800999895855062	12.261819465134266
Pt	9.682562539679681	7.186109495414551	12.297139308022565
Pt	11.033694812026926	9.589706744261344	12.341749328528030
Pt	12.421411328196880	12.032494409370653	12.394791720032522
Pt	8.315575746753799	0.066624033698950	12.355645948539822
Pt	9.697647854319536	2.424599806763636	12.297139308022565
Pt	11.064634647245418	4.792290385386899	12.297139308022565
Pt	12.415665514444818	7.168187826933067	12.355645948539822
Pt	13.785201157127439	9.595040818361444	12.520792342490431
Pt	15.214202973021676	12.070144567598447	12.520792342490431
Pt	11.103657996113625	0.052686310614534	12.341749328528030
Pt	12.462011909512849	2.407053861108422	12.301620043373035
Pt	13.821777061386749	4.760606632689210	12.341749328528030
Pt	15.202149677613360	7.140813989170279	12.520792342490431
Pt	16.631151493507538	9.601999791710023	12.585201641949778

Pt	18.048100013993519	12.070144567598447	12.520792342490431
Pt	13.872173590212364	0.015052845564228	12.301956066017572
Pt	15.238626395202116	2.381818529951488	12.301956066017572
Pt	16.631151493507662	4.741010556388975	12.394791720032522
Pt	18.060153309401834	7.140813989170279	12.520792342490431
Pt	19.477101829887754	9.595040818361444	12.520792342490431
Pt	20.840891658818446	12.032494409370653	12.394791720032522
O	1.677412849399895	0.968454729416764	15.112463469936710
O	5.010310032336070	0.970359335382415	15.165209262845096
O	3.345510878018436	3.853876055058258	15.165209262845096
O	8.315575698523427	0.994815731906464	15.226048222892043
O	6.665699512586146	3.848443377202366	15.163732293020626
O	5.019323571786966	6.704091889970981	15.226048222892043
O	11.620841364710900	0.970359335382415	15.165209262845096
O	9.965451884460826	3.848443377202366	15.163732293020626
O	8.315575698523487	6.706112757443795	15.163732293020626
O	6.650776544205851	9.578764121407850	15.165209262845096
O	14.953738547646958	0.968454729416764	15.112463469936710
O	13.285640519028535	3.853876055058258	15.165209262845096
O	11.611827825259889	6.704091889970981	15.226048222892043
O	9.980374852841120	9.578764121407850	15.165209262845096
O	8.315575698523428	12.466090053014895	15.112463469936710
O	16.631151445277222	3.867292647941597	15.076954159950178
O	14.957469956696055	6.745207885288546	14.851273345220237
O	13.320256387424866	9.580944970107433	14.851273345220237
O	11.664749426234668	12.469353275735953	15.076954159950178
O	18.304832933858407	6.745207885288546	14.851273345220237
O	16.631151445277283	9.601999733137870	15.011912096752711
O	14.993937876006042	12.479846344017538	14.851273345220237
O	19.942046503129596	9.580944970107433	14.851273345220237
O	18.268365014548419	12.479846344017538	14.851273345220237
O	21.597553464319773	12.469353275735953	15.076954159950178
Zn	16.631151541737974	1.907814210249399	14.847979352363531
Zn	3.344491502597946	1.930943100053741	14.899041326779150
Zn	18.324653260271493	4.731594424253051	14.822263052518760
Zn	6.658183537033718	1.949792333855677	14.938651901892520
Zn	5.017661435130180	4.791259965292291	14.938651901892520
Zn	20.058115616990072	7.623441218932300	14.852226180870424
Zn	9.972968052934627	1.949792333855677	14.938651901892520
Zn	8.315575794984113	4.800999954427215	14.907231182549870
Zn	6.675053693080634	7.661947564133779	14.938651901892520
Zn	21.695797226675559	10.570587053694162	14.822263052518760
Zn	13.286660087370397	1.930943100053741	14.899041326779150
Zn	11.613490154838164	4.791259965292291	14.938651901892520
Zn	9.956097896887709	7.661947564133779	14.938651901892520
Zn	8.315575794984172	10.541113663174263	14.899041326779150
Zn	23.294511767439882	13.449092670298720	14.847979352363531
Zn	14.937649823204339	4.731594424253051	14.822263052518760
Zn	13.204187466485871	7.623441218932300	14.852226180870424
Zn	11.566505856800271	10.570587053694162	14.822263052518760
Zn	9.967791316036070	13.449092670298720	14.847979352363531
Zn	16.631151541737907	7.677618025906423	14.838190889064137
Zn	14.964587995247406	10.564190762470151	14.838190889064137
Zn	13.260007575333848	13.503818072899525	14.822263052518760
Zn	18.297715088228415	10.564190762470151	14.838190889064137
Zn	16.631151541737971	13.559117112982230	14.852226180870424
Zn	20.002295508141984	13.503818072899525	14.822263052518760

19/27 Pt

	-12.4733636201000007	-7.2014998437999997	0.0000000000000000
	-12.4733636201000007	-21.6044995313000001	0.0000000000000000
	0.0000000000000000	0.0000000000000000	20.0896391656999995
Pt	-19.403010076265502	-24.004999479724535	5.499999999815235

Pt	-18.017080785281856	-21.604499532042333	5.49999999815235
Pt	-16.631151494298297	-19.203999584360286	5.49999999815235
Pt	-15.245222203314650	-16.803499636678083	5.49999999815235
Pt	-13.859292911083646	-14.402999686835393	5.49999999815235
Pt	-12.473363620099999	-12.002499739153190	5.49999999815235
Pt	-11.087434329116443	-9.601999791471144	5.49999999815235
Pt	-9.701505038132796	-7.201499843788941	5.49999999815235
Pt	-8.315575747149149	-4.800999896106738	5.49999999815235
Pt	-15.245222202067204	-21.604499531311060	5.49999999815235
Pt	-13.859292911083557	-19.203999583628857	5.49999999815235
Pt	-12.473363620099999	-16.803499635946810	5.49999999815235
Pt	-11.087434329116352	-14.402999688264607	5.49999999815235
Pt	-9.701505036885347	-12.002499738421918	5.49999999815235
Pt	-8.315575745901700	-9.601999790739713	5.49999999815235
Pt	-6.929646454918144	-7.201499843057666	5.49999999815235
Pt	-5.543717163934497	-4.800999895375464	5.49999999815235
Pt	-4.157787872950850	-2.400499947693262	5.49999999815235
Pt	-11.087434329116354	-19.203999583617797	5.49999999815235
Pt	-9.701505038132707	-16.803499635935594	5.49999999815235
Pt	-8.315575747149149	-14.402999688253548	5.49999999815235
Pt	-6.929646456165503	-12.002499740571345	5.49999999815235
Pt	-5.543717163934498	-9.601999790728655	5.49999999815235
Pt	-4.157787872950850	-7.201499843046451	5.49999999815235
Pt	-2.771858581967293	-4.800999895364405	5.49999999815235
Pt	-1.385929290983647	-2.400499947682202	5.49999999815235
Pt	0.000000000000000	0.000000000000000	5.49999999815235
Pt	-18.010189206606068	-23.244714808033461	7.774267724285473
Pt	-16.617413697598515	-20.798768752145676	7.777795873564348
Pt	-15.247966940005824	-18.359631804138782	7.814852183716391
Pt	-13.901244837114341	-15.970275748614579	7.838671689936939
Pt	-12.525416751567127	-13.594586204891744	7.805412924946813
Pt	-11.099121905972417	-11.193217874320887	7.777795873564348
Pt	-9.673855401913286	-8.793959348061199	7.780827804360028
Pt	-8.275924076489787	-6.421056748351635	7.814852183716391
Pt	-6.910761857061868	-4.050035997428851	7.805412924946813
Pt	-13.860125974338814	-20.794809226139147	7.773701805676022
Pt	-12.494007343992717	-18.383824544115804	7.780827804360028
Pt	-11.125418924157257	-15.989360280151287	7.774267724285473
Pt	-9.716744821234235	-13.591689765395561	7.761125709335436
Pt	-8.284482729536684	-11.176423818215261	7.774267724285473
Pt	-6.880042083918445	-8.782030328324703	7.838671689936939
Pt	-5.520652212405757	-6.422450867986679	7.902639660822745
Pt	-4.165440319167219	-4.053693298160619	7.838671689936939
Pt	-2.778864494294084	-1.628215482923046	7.780827804360028
Pt	-22.176918878076343	-25.620012124453446	7.777795873564348
Pt	-20.790969833750161	-23.223602506637565	7.761125709335436
Pt	-19.385739826662885	-20.796706480327323	7.761125709335436
Pt	-17.983912252918277	-18.362877017299414	7.805412924946813
Pt	-16.624395526523607	-15.972799314256514	7.902639660822745
Pt	-15.275043120123286	-13.612249034496321	7.902639660822745
Pt	-13.896199845051841	-11.226810667129900	7.814852183716391
Pt	-12.481194816454126	-8.807316424163494	7.773701805676022
Pt	-11.078770069507065	-6.405373568597360	7.773701805676022
Pt	-19.400080045990858	-22.409803458081097	9.968653603496977
Pt	-17.999700897305395	-19.992055316245803	9.998798560539674
Pt	-16.600467101935394	-17.570161616125855	10.155561243542831
Pt	-15.242630436886316	-15.186752892989016	10.277453115519068
Pt	-13.903651002442569	-12.792845259990116	10.155561243542831
Pt	-12.497241859851346	-10.401187078734836	10.019141898419344
Pt	-11.086364952158258	-8.015029165675678	9.997885973590218
Pt	-9.690414070600266	-5.622335388543808	10.019141898419344
Pt	-20.787140949152963	-24.826273012130827	9.998798560539674
Pt	-15.232434929848210	-19.983976751621256	10.019141898419344

Pt	-13.855843399196356	-17.576865899866366	10.080273015859534
Pt	-12.499266434324671	-15.175397363987788	10.063874370246651
Pt	-11.106612633941559	-12.793670421823316	9.998798560539674
Pt	-9.697568461569880	-10.406366003787433	9.999394853677508
Pt	-8.294090687334389	-8.018054049869388	10.080273015859534
Pt	-6.915972755921866	-5.644492342783828	10.155561243542831
Pt	-5.554814393317091	-3.236983578826401	10.063874370246651
Pt	-16.636756709658613	-22.405975572860868	9.999394853677508
Pt	-11.085765687823971	-17.598157329031221	9.999394853677508
Pt	-9.707419065491843	-15.203135179732332	9.968653603496977
Pt	-8.312591750064659	-12.797560270747061	9.968653603496977
Pt	-6.892646411310876	-10.393618431565645	10.063874370246651
Pt	-5.530798587856298	-8.012117748303407	10.277453115519068
Pt	-4.173298214209943	-5.607128731646941	10.277453115519068
Pt	-2.796793152421892	-3.211079424644080	10.080273015859534
Pt	-1.398036393444999	-0.794411420515237	9.997885973590218
Pt	-12.462325894596745	-19.996558788909091	9.997885973590218
Pt	-19.446241980921350	-23.961574870472660	12.296385511366593
Pt	-18.039922161860883	-21.612028384982739	12.301005346631205
Pt	-16.632136229071325	-19.272974645797870	12.330708067977227
Pt	-15.180928245133536	-16.848654497286358	12.510514556899723
Pt	-13.772732041562779	-14.360156901558550	12.500097626691389
Pt	-12.413137097280828	-11.968865013763590	12.330708067977227
Pt	-11.084412861733812	-9.604824775882260	12.312313476531530
Pt	-9.743246643302189	-7.201338057724739	12.320857081101410
Pt	-20.848181155295300	-26.370159091358758	12.330708067977227
Pt	-15.249179444023856	-21.605703706615564	12.312313476531530
Pt	-13.838562219340492	-19.240229767132263	12.320857081101410
Pt	-12.414702243338839	-16.800389768809051	12.334434968343855
Pt	-11.028211562026666	-14.387272065204529	12.296385511366593
Pt	-9.683564170688243	-12.018516524326438	12.301005346631205
Pt	-8.342213210338791	-9.654356966804622	12.334434968343855
Pt	-7.000898690400207	-7.234602613848317	12.510514556899723
Pt	-5.624100539113243	-4.747457376035396	12.500097626691389
Pt	-16.663175405374925	-23.955752170066116	12.334434968343855
Pt	-11.086498554542333	-19.199970423902176	12.312313476531530
Pt	-9.696604527750788	-16.779953997090661	12.301005346631205
Pt	-8.315575747149149	-14.402999688253548	12.266756264044020
Pt	-19.419000938699352	-19.263151816683305	12.296385511366593
Pt	-18.023258278376527	-16.899884939145508	12.500097626691389
Pt	-4.157787872950850	-7.201499843046451	12.579241508436011
Pt	-2.764900304666431	-4.722742263965524	12.510514556899723
Pt	-1.364918377557230	-2.364431550242839	12.320857081101410
Pt	0.000000000000000	0.000000000000000	12.281683536306655
O	-20.591635490222487	-23.498984434636601	15.211364699298004
O	-15.995395218563583	-20.164683052927888	15.252968759303455
O	-19.246919259272211	-20.486387041332666	15.211364699298004
O	-11.455807357239472	-16.680236591372299	15.188668995010783
O	-14.768798821196189	-17.099788175736883	14.770224081411602
O	-17.980900807563316	-17.415027027469208	14.817476130915949
O	-10.054899628623943	-13.626627477313233	15.211364699298004
O	-13.347784650652940	-14.065903343418135	14.817476130915949
O	-16.631151459372791	-14.402999755260744	15.020248154880010
O	-8.717604840867779	-10.544860957736745	15.188668995010783
O	-11.959265472930131	-10.971577049812710	15.252968759303455
O	-2.753476876338498	-4.240261005030616	14.770224081411602
O	-7.424451439136321	-7.465950395254347	14.770224081411602
O	-10.700633402607874	-7.896372396660224	15.157288385743893
O	-1.488142282157345	-1.187793197988484	15.157288385743893
O	-6.091405299802195	-4.526569049654615	14.817476130915949
O	-21.938793684130118	-26.475738846220867	15.252968759303455
O	-17.246678558663760	-23.185401558212696	15.188668995010783
O	-12.757951453152970	-19.721833982093102	15.157288385743893

Zn	-22.149394267252440	-24.591789698490572	14.935030555531441
Zn	-17.521642737152742	-21.289042821860772	14.935030555531441
Zn	-8.315575780827212	-14.402999619839255	14.917745891873009
Zn	-12.898595926602468	-17.866869641183673	14.785334730533997
Zn	-16.264613337176097	-18.367159229612732	14.799744886230712
Zn	-7.076201714107772	-11.445248827428587	14.867738357491167
Zn	-11.496750138478916	-14.808545589486402	14.867738357491167
Zn	-14.889370746405525	-15.191862421330120	14.824642200590505
Zn	-5.711853524208382	-8.315494779647054	14.824642200590505
Zn	-10.222417579523626	-11.731166028926694	14.935030555531441
Zn	-13.381357697300707	-12.103488431379510	14.799744886230712
Zn	-4.345503071867551	-5.298641971040387	14.824642200590505
Zn	-9.023865141821373	-8.702052739770505	14.785334730533997
Zn	-12.189706336338503	-9.088324812383155	14.914505111238723
Zn	-3.024266276552426	-2.237076795384412	14.785334730533997
Zn	-7.774119929352104	-5.536851356985956	14.799744886230712
Zn	-23.454517520552084	-27.616932346749252	14.914505111238723
Zn	-18.847139109994860	-24.156704287842942	14.867738357491167
Zn	-14.249230725791222	-20.906741389425772	14.914505111238723

9/16 Cu

	10.2106219202999995	0.0000000000000000	0.0000000000000000
	-5.1053109601999997	8.8426579713999995	0.0000000000000000
	0.0000000000000000	0.0000000000000000	18.5527257741999989
Cu	-3.828983220100012	6.631993478600013	2.0000000000000057
Cu	-2.552655480100000	4.421328985700000	2.0000000000000057
Cu	-1.276327739999982	6.631993478600013	2.0000000000000057
Cu	-1.276327740000012	2.210664492900013	2.0000000000000057
Cu	0.000000000000030	4.421328985700000	2.0000000000000057
Cu	1.276327740000000	6.631993478600013	2.0000000000000057
Cu	0.000000000000000	0.000000000000000	2.0000000000000057
Cu	1.276327739999970	2.210664492900013	2.0000000000000057
Cu	2.552655480099987	4.421328985700000	2.0000000000000057
Cu	3.828983220099957	6.631993478600013	2.0000000000000057
Cu	2.552655480100030	0.000000000000000	2.0000000000000057
Cu	3.828983220100000	2.210664492900013	2.0000000000000057
Cu	5.105310960200017	4.421328985700000	2.0000000000000057
Cu	5.105310960199987	0.000000000000000	2.0000000000000057
Cu	6.381638700199957	2.210664492900013	2.0000000000000057
Cu	7.657966440300017	0.000000000000000	2.0000000000000057
Cu	-2.546220819667711	7.365166589967322	4.062943471260583
Cu	-1.260686302822757	5.167247737964803	4.096947403815631
Cu	0.000000000000080	7.350820466970418	4.096947403815631
Cu	-0.000000000000022	2.954982762965377	4.062943471260583
Cu	1.260686302822654	5.167247737964803	4.096947403815631
Cu	2.546220819667785	7.365166589967322	4.062943471260583
Cu	1.271771468898630	0.734257599953106	4.043011887447451
Cu	2.534847400933457	2.953757233717304	4.046290795321661
Cu	3.814705859546378	5.170537110642095	4.046290795321661
Cu	5.105310960199936	7.374142771593814	4.043011887447451
Cu	3.825452501487182	0.718363627040600	4.046290795321661
Cu	5.105310960200008	2.947552657099991	4.034938353516064
Cu	6.395916060753482	5.170537110642095	4.046290795321661
Cu	6.385169418813036	0.718363627040600	4.046290795321661
Cu	7.675774519466487	2.953757233717304	4.046290795321661
Cu	8.938850451401409	0.734257599953106	4.043011887447451
Cu	-3.827168976461645	8.104722353147046	6.071500847417077
Cu	-2.531168699517027	5.904845930882308	6.125706147510538
Cu	-1.274019971117213	8.082291401078475	6.125706147510538
Cu	-1.257148728299760	3.698178610939245	6.125706147510538
Cu	-0.000000000000033	5.895105314300008	6.260532004952880
Cu	1.274019971117444	8.082291401078475	6.125706147510538
Cu	-0.000000000000002	1.475871236705959	6.071500847417077

Cu	1.257148728299584	3.698178610939245	6.125706147510538
Cu	2.531168699516922	5.904845930882308	6.125706147510538
Cu	3.827168976461621	8.104722353147046	6.071500847417077
Cu	2.544347555828377	1.468979746285394	6.045490712858846
Cu	3.815110842878091	3.692450042123330	6.026089999987105
Cu	5.105310960199977	5.904698478929237	6.045490712858846
Cu	5.105310960200089	1.457757887153343	6.026089999987105
Cu	6.395511077421798	3.692450042123330	6.026089999987105
Cu	7.666274364571674	1.468979746285394	6.045490712858846
Cu	-3.857887096099497	6.633606397964724	8.105806416765256
Cu	-2.589837965033897	4.399861668014248	8.116648179286919
Cu	-1.321345187341054	6.657984313940473	8.316723948728299
Cu	-1.289382848855506	2.184826542334329	8.105806416765256
Cu	0.0000000000000324	4.369347315019081	8.316723948728299
Cu	1.321345187340778	6.657984313940473	8.316723948728299
Cu	0.0000000000000000	0.0000000000000000	8.103774378027691
Cu	1.289382848855755	2.184826542334329	8.105806416765256
Cu	2.589837965034127	4.399861668014248	8.116648179286919
Cu	3.857887096099424	6.633606397964724	8.105806416765256
Cu	2.536806712956056	0.024225031200974	8.105806416765256
Cu	3.837724299826384	2.215711157633055	8.018342809602256
Cu	5.105310960200073	4.411235656233918	8.018342809602256
Cu	5.105310960199743	0.042934635371503	8.116648179286919
Cu	6.372897620473517	2.215711157633055	8.018342809602256
Cu	7.673815207443717	0.024225031200974	8.105806416765256
O	1.711494181945102	0.988131624619847	10.721707397802536
O	-0.000000100400109	3.949591600598747	10.563064991215022
O	-1.684864348016263	6.867862081200592	10.563064991215022
O	5.105310859800011	0.981023661298470	10.728702713857203
O	3.402246844017104	3.930817065150763	10.728702713857203
O	1.684864147216342	6.867862081200592	10.563064991215022
O	8.499127537654772	0.988131624619847	10.721707397802536
O	6.808374875482887	3.930817065150763	10.728702713857203
O	5.105310859800072	6.866394542260339	10.721707397802536
Zn	-0.000000001699813	1.928079433720330	10.485241120248574
Zn	-1.730637774878005	4.895921189994612	10.549323403562633
Zn	-3.435545243643980	7.878618344489819	10.485241120248574
Zn	3.406459357293348	1.966720287838791	10.589318522020323
Zn	1.730637771478118	4.895921189994612	10.549323403562633
Zn	-0.000000001700207	7.893473742610781	10.549323403562633
Zn	6.804162559606587	1.966720287838791	10.589318522020323
Zn	5.105310958500005	4.909217575522486	10.589318522020323
Zn	3.435545240243806	7.878618344489819	10.485241120248574

31/52 Cu

	12.7632774003999998	13.2639869572000002	0.0000000000000000
	-17.8685883606000004	4.4213289856999998	0.0000000000000000
	0.0000000000000000	0.0000000000000000	19.5527034153000017
Cu	-15.315932879749502	4.421328986145987	5.500000000852932
Cu	-14.039605140987446	6.631993478569199	5.500000000852932
Cu	-12.763277399162146	8.842657971876694	5.500000000852932
Cu	-12.763277400175481	4.421328985265583	5.500000000852932
Cu	-11.486949660137075	6.631993479015218	5.500000000852932
Cu	-10.210621921374891	8.842657971438397	5.500000000852932
Cu	-8.934294179549504	11.053322464745987	5.500000000852932
Cu	-7.657966440787446	13.263986957169198	5.500000000852932
Cu	-6.381638698962147	15.474651450476694	5.500000000852932
Cu	-10.210621919325110	4.421328985711602	5.500000000852932
Cu	-8.934294180562926	6.631993478134782	5.500000000852932
Cu	-7.657966440524519	8.842657971884417	5.500000000852932
Cu	-6.381638699975482	11.053322463865582	5.500000000852932
Cu	-5.105310959937075	13.263986957615217	5.500000000852932
Cu	-3.828983221174891	15.474651450038397	5.500000000852932

Cu	-8.934294180300000	2.210664492850000	5.500000000852932
Cu	-7.657966441537854	4.421328985273306	5.500000000852932
Cu	-6.381638699712556	6.631993478580801	5.500000000852932
Cu	-5.105310960950498	8.842657971004012	5.500000000852932
Cu	-3.828983219125110	11.053322464311602	5.500000000852932
Cu	-2.552655480362926	13.263986956734783	5.500000000852932
Cu	-1.276327740324520	15.474651450484416	5.500000000852932
Cu	-6.381638699449501	2.210664493295987	5.500000000852932
Cu	-5.105310960687445	4.421328985719199	5.500000000852932
Cu	-3.828983218862146	6.631993479026693	5.500000000852932
Cu	-2.552655480100000	8.842657971450000	5.500000000852932
Cu	-1.276327741337854	11.053322463873306	5.500000000852932
Cu	0.000000000487445	13.263986957180801	5.500000000852932
Cu	1.276327739249503	15.474651449604014	5.500000000852932
Cu	-3.828983219875481	2.210664492415583	5.500000000852932
Cu	-2.552655479837074	4.421328986165218	5.500000000852932
Cu	-1.276327741074892	6.631993478588399	5.500000000852932
Cu	0.000000000750499	8.842657971895987	5.500000000852932
Cu	1.276327739512554	11.053322464319200	5.500000000852932
Cu	2.552655481337853	13.263986957626694	5.500000000852932
Cu	-1.276327739025108	2.210664492861602	5.500000000852932
Cu	-0.000000000262926	4.421328985284783	5.500000000852932
Cu	1.276327739775481	6.631993479034417	5.500000000852932
Cu	2.552655480324518	8.842657971015583	5.500000000852932
Cu	3.828983220362926	11.053322464765218	5.500000000852932
Cu	5.105310959125108	13.263986957188399	5.500000000852932
Cu	0.000000000000000	0.000000000000000	5.500000000852932
Cu	1.276327738762146	2.210664492423306	5.500000000852932
Cu	2.552655480587445	4.421328985730801	5.500000000852932
Cu	3.828983219349501	6.631993478154014	5.500000000852932
Cu	5.105310961174891	8.842657971461602	5.500000000852932
Cu	6.381638699937074	11.053322463884783	5.500000000852932
Cu	7.657966439975480	13.263986957634417	5.500000000852932
Cu	6.381638700200000	6.631993478600000	5.500000000852932
Cu	7.657966438962147	8.842657971023307	5.500000000852932
Cu	8.934294180787445	11.053322464330801	5.500000000852932
Cu	10.210621919549501	13.263986956754014	5.500000000852932
Cu	-14.041181367315501	5.167487821635743	7.553958470356290
Cu	-12.772704852152696	7.384900010275252	7.589622692331504
Cu	-11.502930870099142	9.575367734008129	7.579120041973680
Cu	-11.497542798490887	5.176719696820228	7.544733017233415
Cu	-10.225742210162196	7.384521377056236	7.557183169189916
Cu	-8.929304076822820	9.581519901657606	7.545897664517518
Cu	-7.636646195640541	11.790133281883580	7.544733017233415
Cu	-6.372821949663082	13.997604838124449	7.553958470356290
Cu	-5.111422405272117	16.203975262641517	7.548246084041399
Cu	-8.938498563486116	5.161551823426436	7.545897664517518
Cu	-7.657966441287821	7.368881642571885	7.544343952349079
Cu	-6.360534148202825	9.584820823724179	7.557183169189916
Cu	-5.086724921221716	11.790365857568982	7.589622692331504
Cu	-3.833193011366481	13.981689232499077	7.580422004236460
Cu	-2.560853836919442	16.192558907641267	7.546111561428426
Cu	-7.646357233374649	2.935801724412967	7.579120041973680
Cu	-6.387622962434986	5.137302727819584	7.557183169189916
Cu	-5.106096680491063	7.363573203515955	7.545897664517518
Cu	-3.824611217326210	9.595475470178904	7.579120041973680
Cu	-2.562799448104933	11.793175218892712	7.603384667560671
Cu	-1.287966995721796	13.984544005883073	7.561484331296468
Cu	-0.003750623044070	16.207841171776249	7.531518961858120
Cu	-5.114469547425605	2.931379060755761	7.589622692331504
Cu	-3.839710326668567	5.139791949896193	7.544733017233415
Cu	-2.563101142889915	7.378566822401274	7.538531082382974
Cu	-1.291721004479238	9.602529452636453	7.562943911840971

Cu	-0.011794133293145	11.797708002973987	7.562082687947906
Cu	1.285814495264789	13.998645682589551	7.538161578146462
Cu	-10.197011477436833	2.951756276710093	7.538531082382974
Cu	-2.559896003821422	2.941552268839807	7.553958470356290
Cu	-1.271249483335587	5.156818236478959	7.531518961858120
Cu	-0.002812626929146	7.378212133361938	7.538161578146462
Cu	1.267531112834615	9.588792295407774	7.546456442516229
Cu	2.565061202816240	11.793205651391935	7.546456442516229
Cu	3.856583988608472	14.002714421061121	7.562943911840971
Cu	0.020536952570854	2.949943025230918	7.546111561428426
Cu	1.296290527041411	5.156302817172150	7.561484331296468
Cu	2.552059630043002	7.354918936667898	7.562082687947906
Cu	3.825374124549144	9.567304953300294	7.546456442516229
Cu	5.117700943450138	11.796675960458110	7.562082687947906
Cu	6.389278094691274	14.008177760315501	7.603384667560671
Cu	-16.582653977301138	5.156706659142660	7.548246084041399
Cu	2.571375842923868	2.953499815500010	7.580422004236460
Cu	3.831487793613663	5.147949920891786	7.603384667560671
Cu	5.093103456070766	7.344059026402419	7.562943911840971
Cu	6.374964571864357	9.572445084148514	7.538161578146462
Cu	7.649642905816926	11.808456076160438	7.561484331296468
Cu	8.919783608642607	14.014113852100911	7.580422004236460
Cu	-10.213786700473253	11.776321829488634	7.538531082382974
Cu	8.932966546579664	9.584643491844794	7.531518961858120
Cu	10.198283324548594	11.806800967227815	7.546111561428426
Cu	-1.279822938226750	0.745963006815821	7.548246084041399
Cu	-15.309872858013533	5.900615282188689	9.610854733070973
Cu	-14.035732106004211	8.108981838319732	9.734086148394697
Cu	5.094236399644166	5.877155811006624	9.688551254747711
Cu	-12.776205804617803	5.909041360765739	9.611369682131439
Cu	-11.498556661254543	8.112268960057889	9.661800884713211
Cu	-10.212663220772782	10.303592769025222	9.583870327145606
Cu	-8.928876193116629	12.525435622591072	9.530421052184758
Cu	-7.658850644372958	14.751088637407126	9.546695966687052
Cu	11.481072741441929	12.538331715183094	9.565510833821353
Cu	-10.219242691203851	5.909188380656543	9.569056930862615
Cu	-8.935841911773686	8.109460357914180	9.571066774586848
Cu	-7.641459761605177	10.316858573394018	9.569056930862615
Cu	-6.363105526582581	12.531327097422785	9.611369682131439
Cu	-5.103569199263672	14.729760168357785	9.610854733070973
Cu	-3.835772756744898	16.937721756399540	9.565510833821353
Cu	-8.922152438034525	3.689093768902748	9.583870327145606
Cu	-7.660388685245904	5.891919664144652	9.571066774586848
Cu	-6.377668723780411	8.105264906541166	9.571066774586848
Cu	-5.093879028234931	10.323236681173427	9.661800884713211
Cu	-3.828138036791183	12.522138631054428	9.734086148394697
Cu	-2.563366635630484	14.712914942066933	9.614805696215033
Cu	-14.050703131478921	3.677012402379745	9.546695966687052
Cu	-6.381463631310536	3.671139287368681	9.661800884713211
Cu	-5.113196867990967	5.880597974549440	9.569056930862615
Cu	-3.839083661992697	8.113958390672034	9.583870327145606
Cu	-2.562662925691416	10.334999902419028	9.688551254747711
Cu	-1.291135181886620	12.517959248010669	9.661637971178452
Cu	0.000356865018304	14.725292240977611	9.546403780000340
Cu	-11.488218306267251	3.689964521119729	9.530421052184758
Cu	-3.834587986536162	3.666276471295815	9.611369682131439
Cu	-2.556804821416117	5.891244784889201	9.530421052184758
Cu	-1.287338744945030	8.121462589490809	9.557480705465297
Cu	-0.013767592772773	10.331696818935045	9.599280140150483
Cu	1.283206012648057	12.524190088179292	9.564614701318972
Cu	2.571751330654262	14.739452704551640	9.557480705465297
Cu	-1.264345544948114	3.678543888813131	9.546695966687052
Cu	0.010621809057944	5.901649890885739	9.546403780000340

Cu	1.275407615890219	8.113180918355349	9.564614701318972
Cu	2.552655481087820	10.316434300328114	9.560896480206909
Cu	3.849084745580486	12.531390618520579	9.599280140150483
Cu	5.126392966247247	14.737147186674340	9.688551254747711
Cu	0.012666455502969	1.473249428517365	9.565510833821353
Cu	1.303202614669727	3.687588860499436	9.614805696215033
Cu	2.567974279031028	5.886851465963226	9.661637971178452
Cu	3.822649287392291	8.086215462644383	9.599280140150483
Cu	5.099352811661715	10.311931893565355	9.564614701318972
Cu	6.381127343055586	12.544492186126105	9.661637971178452
Cu	-5.110029178004607	1.475524459225843	9.734086148394697
Cu	6.373553854490764	8.088387606057552	9.557480705465297
Cu	7.646987766123757	10.322360768236653	9.546403780000340
Cu	8.918130461160752	12.548799097533630	9.614805696215033
Cu	-2.560457263522795	1.476269478053528	9.610854733070973
Cu	-15.321915048620721	4.393357431690246	11.594382802776341
Cu	-14.061181697217791	6.572111344733680	11.741413207288570
Cu	-12.731795512945093	8.833151443640055	11.833658554003238
Cu	-12.765195950704207	4.386621079151494	11.566430794859922
Cu	-11.480385898510386	6.589224249498992	11.664304042167483
Cu	-10.168772635112678	8.842233533149967	11.662081011365558
Cu	-8.923677860953482	11.070099806142768	11.567620969156028
Cu	-7.687065093930041	13.283002423722571	11.566430794859922
Cu	-6.402871691268544	15.493817937916774	11.594382802776341
Cu	-10.230459682480701	4.422134316612042	11.567620969156028
Cu	-8.935718091847221	6.635639783102128	11.603346855187532
Cu	-7.654096692150708	8.842067962745681	11.603346855187532
Cu	-6.421959820050151	11.069022694310604	11.664304042167483
Cu	-5.146382130956267	13.312613870354660	11.741413207288570
Cu	-3.824416938298752	15.498104730258113	11.648764619065503
Cu	-8.978223814780426	2.243571253724611	11.637283325367626
Cu	-7.678523510328850	4.457783749450856	11.662081011365558
Cu	-6.384084536802072	6.628937182752198	11.603346855187532
Cu	-5.126603178421710	8.806627645114890	11.662081011365558
Cu	-3.852957057188354	11.030811615206892	11.833658554003238
Cu	-2.505585591581454	13.295183898185581	11.780411075148315
Cu	-1.246260783173701	15.483906895588465	11.575079400273658
Cu	-6.389146747603318	2.242681870637337	11.833658554003238
Cu	-5.071553602239463	4.448397984790406	11.664304042167483
Cu	-3.819761774302585	6.614410806729472	11.567620969156028
Cu	-2.559188753733447	8.788160411573678	11.637283325367626
Cu	-1.241874737706512	11.024108082487846	11.755919642347250
Cu	0.043822895468541	13.280224978610192	11.608317083103394
Cu	1.273631686971598	15.485607204671329	11.546586615077432
Cu	-3.766335492625935	2.221919713511658	11.741413207288570
Cu	-2.521638276165755	4.437021425725932	11.566430794859922
Cu	-1.284467677141876	6.624180751292151	11.546586615077432
Cu	-0.005503368442106	8.827635180454285	11.591455058189579
Cu	1.298132324687782	11.056451070687030	11.615457103667692
Cu	2.542397046909885	13.276264410874743	11.591455058189579
Cu	-1.249112577847495	2.219469559877258	11.594382802776341
Cu	-0.023048929421777	4.442740011439875	11.575079400273658
Cu	1.240353753219875	6.661826208640743	11.608317083103394
Cu	2.539043735143919	8.859976992512403	11.615457103667692
Cu	3.820790380368299	11.032874836900572	11.615457103667692
Cu	5.062784060873798	13.248756971499718	11.755919642347251
Cu	0.000000000000000	0.000000000000000	11.609694724203401
Cu	1.253733460851736	2.202892369285058	11.648764619065503
Cu	2.502103192379936	4.446494234443479	11.780411075148315
Cu	3.837057113969480	6.676437845228160	11.755919642347251
Cu	5.121072764795451	8.845403309655243	11.591455058189579
Cu	6.373789791511582	11.007251712849063	11.608317083103394
Cu	7.661448839401515	13.207624767470934	11.780411075148315

Cu	6.432101608313867	6.653584277601710	11.637283325367626
Cu	7.668802427307032	8.839514943252235	11.546586615077432
Cu	8.927276152795477	11.022655993071663	11.575079400273658
Cu	10.228649914583773	13.248305799672551	11.648764619065503
O	-0.249856686815082	16.298460356516955	14.387487794847564
O	-11.128727760591795	5.768643468905509	14.294882271474481
O	-9.216816535333631	8.474040099710864	14.283647351997358
O	-7.308432816961645	11.174768169236042	14.294882271474481
O	-5.444817966726918	13.875180109728717	14.182195904989838
O	-9.716151186204792	2.763442880597285	14.315896898050777
O	-7.835636784483569	5.466298723388343	14.283647351997358
O	-5.921446220000695	8.166306162978026	14.283647351997358
O	-4.025169767576507	10.882916815203579	14.098728614619301
O	-2.149295726660464	13.591504761831370	14.139713163199733
O	-6.431121173677212	2.465769816876968	14.098728614619299
O	-4.536738962264364	5.163233347935773	14.294882271474481
O	-2.640447196516152	7.889160840299598	14.315896898050777
O	-0.747283786107568	10.620350561966204	14.161389802664125
O	1.166554390611148	13.318856097315813	14.324315866486060
O	-3.129921046232655	2.199089574515254	14.182195904989838
O	-1.226675059911845	4.898374631052631	14.387487794847564
O	0.645532383066536	7.614824735905741	14.324315866486060
O	2.552655406039679	10.316434318897713	14.335632753594769
O	4.465824190508899	13.022307370033831	14.161389802664125
O	0.178794003502718	1.903505277824853	14.303400106645791
O	2.067336771924741	4.606889966948271	14.139713163199733
O	3.939425815504418	7.306645024250781	14.161389802664125
O	5.845879448015047	10.015622122587212	14.324315866486060
O	7.739925176428573	12.750908227029100	14.139713163199733
O	-3.546224159431951	16.578723119980943	14.303400106645791
O	-14.399160525071444	6.032375301391119	14.182195904989838
O	-12.517608599840415	8.757958352670236	14.098728614619299
O	-10.617301158373348	11.454041263854055	14.315896898050777
O	9.134497968419524	9.752467968239209	14.387487794847564
O	11.025396377621956	12.467074558002970	14.303400106645791
Zn	-12.832127122408838	4.916596171244239	14.157918486881016
Zn	-10.920554242092642	7.651730388204349	14.074275892925732
Zn	-9.044918001001665	10.370994442462038	14.145867943967495
Zn	-7.194627489361933	13.075979008932199	14.157918486881016
Zn	-5.279589578381326	15.804229753718001	14.053978240336466
Zn	-9.564396514670630	4.666689865248538	14.145867943967495
Zn	-7.657966366239680	7.368881624002285	14.032124247067516
Zn	-5.781718214872796	10.052941224911915	14.074275892925732
Zn	-3.883578666335515	12.795955375646162	14.073428528430854
Zn	-1.970064972006860	15.522218707025035	14.129739732896123
Zn	-6.271626645327295	4.401973259774976	14.074275892925732
Zn	-4.364584584833452	7.068960564738610	14.145867943967495
Zn	-2.451988746001539	9.763695451462304	14.087093695296334
Zn	-0.544657934730086	12.525738538350751	14.081543081387654
Zn	1.313811448848458	15.220087775877774	14.195191012759075
Zn	-2.947144490522089	4.114069692714827	14.157918486881016
Zn	-1.074610892843289	6.791737067786528	14.195191012759075
Zn	0.843996166281463	9.506274596483454	14.060321793062897
Zn	2.705366378663583	12.201256558446103	14.060321793062897
Zn	4.576291834680077	14.926952795484706	14.087093695296334
Zn	0.305674255942573	3.796751198862604	14.129739732896123
Zn	2.187998685311340	6.529429988214411	14.081543081387654
Zn	4.108604114272856	9.241771687693204	14.060321793062897
Zn	6.014625908636558	11.894134316057507	14.081543081387654
Zn	-4.845176482120157	1.386629115445621	14.073428528430854
Zn	-16.152380530777059	5.210942278971815	14.053978240336466
Zn	-14.245143953836930	7.924060381799421	14.073428528430854
Zn	5.533663571815749	6.258654597002044	14.087093695296334

Zn 7.418766104488950 8.937478000284916 14.195191012759075
Zn 9.322357373495297 11.630332937177267 14.129739732896123
Zn -1.541928993134351 1.091472840201421 14.053978240336466

49/64 Ag

23.1365338804238370 0.0000000000000000 0.0000000000000000
11.5682669402119185 20.0368260959663935 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.3840878029567101
Ag 0.0000000000000000 0.0000000000000000 5.499999999999975
Ag 1.446033367526490 2.504603261995799 5.499999999999975
Ag 2.892066735052980 5.009206523991598 5.499999999999975
Ag 4.338100102579469 7.513809785987398 5.499999999999975
Ag 5.784133470105959 10.018413047983197 5.499999999999975
Ag 7.230166837632449 12.523016309978996 5.499999999999975
Ag 8.676200205158938 15.027619571974796 5.499999999999975
Ag 10.122233572685429 17.532222833970593 5.499999999999975
Ag 2.892066735052980 0.0000000000000000 5.499999999999975
Ag 4.338100102579469 2.504603261995799 5.499999999999975
Ag 5.784133470105959 5.009206523991598 5.499999999999975
Ag 7.230166837632449 7.513809785987398 5.499999999999975
Ag 8.676200205158938 10.018413047983197 5.499999999999975
Ag 10.122233572685429 12.523016309978996 5.499999999999975
Ag 11.568266940211918 15.027619571974796 5.499999999999975
Ag 13.014300307738409 17.532222833970593 5.499999999999975
Ag 5.784133470105959 0.0000000000000000 5.499999999999975
Ag 7.230166837632449 2.504603261995799 5.499999999999975
Ag 8.676200205158938 5.009206523991598 5.499999999999975
Ag 10.122233572685428 7.513809785987398 5.499999999999975
Ag 11.568266940211918 10.018413047983197 5.499999999999975
Ag 13.014300307738409 12.523016309978996 5.499999999999975
Ag 14.460333675264899 15.027619571974796 5.499999999999975
Ag 15.906367042791388 17.532222833970593 5.499999999999975
Ag 8.676200205158938 0.0000000000000000 5.499999999999975
Ag 10.122233572685428 2.504603261995799 5.499999999999975
Ag 11.568266940211918 5.009206523991598 5.499999999999975
Ag 13.014300307738408 7.513809785987398 5.499999999999975
Ag 14.460333675264899 10.018413047983197 5.499999999999975
Ag 15.906367042791388 12.523016309978996 5.499999999999975
Ag 17.352400410317877 15.027619571974796 5.499999999999975
Ag 18.798433777844366 17.532222833970593 5.499999999999975
Ag 11.568266940211918 0.0000000000000000 5.499999999999975
Ag 13.014300307738408 2.504603261995799 5.499999999999975
Ag 14.460333675264899 5.009206523991598 5.499999999999975
Ag 15.906367042791388 7.513809785987398 5.499999999999975
Ag 17.352400410317877 10.018413047983197 5.499999999999975
Ag 18.798433777844366 12.523016309978996 5.499999999999975
Ag 20.244467145370855 15.027619571974796 5.499999999999975
Ag 21.690500512897348 17.532222833970593 5.499999999999975
Ag 14.460333675264899 0.0000000000000000 5.499999999999975
Ag 15.906367042791388 2.504603261995799 5.499999999999975
Ag 17.352400410317877 5.009206523991598 5.499999999999975
Ag 18.798433777844366 7.513809785987398 5.499999999999975
Ag 20.244467145370859 10.018413047983197 5.499999999999975
Ag 21.690500512897348 12.523016309978996 5.499999999999975
Ag 23.136533880423837 15.027619571974796 5.499999999999975
Ag 24.582567247950330 17.532222833970593 5.499999999999975
Ag 17.352400410317877 0.0000000000000000 5.499999999999975
Ag 18.798433777844366 2.504603261995799 5.499999999999975
Ag 20.244467145370855 5.009206523991598 5.499999999999975
Ag 21.690500512897344 7.513809785987398 5.499999999999975
Ag 23.136533880423837 10.018413047983197 5.499999999999975
Ag 24.582567247950326 12.523016309978996 5.499999999999975
Ag 26.028600615476815 15.027619571974796 5.499999999999975

Ag	27.474633983003308	17.532222833970593	5.499999999999975
Ag	20.244467145370859	0.000000000000000	5.499999999999975
Ag	21.690500512897348	2.504603261995799	5.499999999999975
Ag	23.136533880423837	5.009206523991598	5.499999999999975
Ag	24.582567247950330	7.513809785987398	5.499999999999975
Ag	26.028600615476819	10.018413047983197	5.499999999999975
Ag	27.474633983003308	12.523016309978996	5.499999999999975
Ag	28.920667350529797	15.027619571974796	5.499999999999975
Ag	30.366700718056286	17.532222833970593	5.499999999999975
Ag	1.442038644347851	0.832561399496075	7.902165732973385
Ag	2.878772982603663	3.334395410863573	7.894910092417261
Ag	4.315569211084092	5.845710130756872	7.882223075553684
Ag	5.758068591909906	8.359895770909537	7.879328306894020
Ag	7.207419125569036	10.870244533184215	7.879328306894020
Ag	8.663518069358384	13.376578461999035	7.882223075553684
Ag	10.119982299443485	15.876537855871261	7.894910092417261
Ag	11.568266940211837	18.371703296974104	7.902165732973385
Ag	4.327057623371937	0.825892829231283	7.894910092417261
Ag	5.764918264274711	3.328377111735194	7.869356117629198
Ag	7.205752249479721	5.841168703691872	7.847060144752264
Ag	8.653944132376974	8.361527089597677	7.838624486503826
Ag	10.112542579763915	10.875877242694012	7.847060144752264
Ag	11.568266940211835	13.380071872495863	7.869356117629198
Ag	13.016551580980032	15.876537855871261	7.894910092417261
Ag	14.458435195073676	18.368186676018642	7.901680127808962
Ag	7.220318081937552	0.814537503210356	7.882223075553684
Ag	8.661476609927643	3.319780149580364	7.847060144752264
Ag	10.110590941216852	5.837352401577739	7.818405576176326
Ag	11.568266940211918	8.362121292810915	7.818405576176326
Ag	13.023991300659757	10.875877242694012	7.847060144752264
Ag	14.473015811065302	13.376578461999035	7.882223075553684
Ag	15.913818751962395	15.868092486375120	7.903861853859669
Ag	17.351272053603122	18.357834638324487	7.903861853859669
Ag	10.118916406552705	0.806685791872499	7.879328306894020
Ag	11.568266940211840	3.313771916770903	7.838624486503826
Ag	13.025942939206985	5.837352401577739	7.818405576176326
Ag	14.482589748046706	8.361527089597677	7.838624486503826
Ag	15.929114754854638	10.870244533184215	7.879328306894020
Ag	17.370699031942394	13.366733134793684	7.914440556820850
Ag	18.806711391131387	15.857708243713699	7.925375057250013
Ag	20.245952936056334	18.346818981379798	7.914440556820850
Ag	13.017617473870965	0.806685791872499	7.879328306894020
Ag	14.475057270496031	3.319780149580364	7.847060144752264
Ag	15.930781630943951	5.841168703691872	7.847060144752264
Ag	17.378465288513766	8.359895770909537	7.879328306894020
Ag	18.817190985092736	10.864110280635888	7.920517342334895
Ag	20.254048067959641	13.360098062894737	7.938672156223452
Ag	21.693373594885458	15.853083004161096	7.938672156223452
Ag	23.136533880423841	18.345431630661011	7.920517342334895
Ag	15.916215798486133	0.814537503210356	7.882223075553684
Ag	17.371615616148958	3.328377111735194	7.869356117629198
Ag	18.820964669339592	5.845710130756872	7.882223075553684
Ag	20.261279976309737	8.360100075759023	7.914440556820850
Ag	21.697208353497935	10.860471124876804	7.938672156223452
Ag	23.136533880423755	13.357884063977549	7.945292119584892
Ag	24.579694165962046	15.853083004161096	7.938672156223452
Ag	26.027114824791013	18.346818981379798	7.914440556820850
Ag	18.809476257051578	0.825892829231283	7.894910092417261
Ag	20.257760897819853	3.334395410863573	7.894910092417261
Ag	21.699080578783033	5.847725067233043	7.903861853859669
Ag	23.136533880423674	8.358235704505109	7.925375057250013
Ag	24.575859407349569	10.860471124876804	7.938672156223452
Ag	26.019019692887863	13.360098062894737	7.938672156223452

Ag	27.466356369715960	15.857708243713699	7.925375057250013
Ag	28.921795707244392	18.357834638324487	7.903861853859669
Ag	21.694495236075824	0.832561399496075	7.902165732973385
Ag	23.136533880423833	3.337278839895495	7.901680127808962
Ag	24.573987182064485	5.847725067233043	7.903861853859669
Ag	26.011787784537610	8.360100075759023	7.914440556820850
Ag	27.455876775754941	10.864110280635888	7.920517342334895
Ag	28.902368728904953	13.366733134793684	7.914440556820850
Ag	30.359249008885122	15.868092486375120	7.903861853859669
Ag	31.814632565773991	18.368186676018642	7.901680127808962
Ag	23.136533880424004	1.670479371583920	10.221710042322357
Ag	24.589019734800484	4.174270091283263	10.215122863246435
Ag	26.042089296493156	6.677319282115207	10.219418084425838
Ag	27.489361571810242	9.178992965460090	10.240752157978088
Ag	28.931973577081944	11.677670254199496	10.240752157978088
Ag	30.374850401179053	14.181881652489437	10.219418084425838
Ag	31.816019806515261	16.691801401797171	10.215122863246435
Ag	33.258123248346465	19.201586410174578	10.221710042322357
Ag	2.899074793949026	1.673781612682652	10.215288923124263
Ag	4.350917650349831	4.175503137988840	10.189116648763655
Ag	5.795566677871026	6.675849104782932	10.168706069058544
Ag	7.239250760097971	9.178300688903830	10.165796805257006
Ag	8.684595362573887	11.679793571212175	10.168706069058544
Ag	10.127633974306940	14.181069311995065	10.189116648763655
Ag	11.568266940212002	16.689262870601233	10.215288923124263
Ag	13.014944512501543	19.201586410174578	10.221710042322357
Ag	5.791550616254892	1.680253645982632	10.189116648763653
Ag	7.235944650288471	4.177674591685280	10.138856394969601
Ag	8.679972458249384	6.677165776100633	10.098025517387766
Ag	10.125657981953506	9.181166554922990	10.098025517387766
Ag	11.568266940212004	11.681476912595981	10.138856394969601
Ag	13.008899906117064	14.181069311995065	10.189116648763655
Ag	14.457047954332564	16.691801401797171	10.215122863246435
Ag	15.909533808709137	19.207580698852485	10.215122863246435
Ag	8.679238255509137	1.681183419971426	10.168706069058544
Ag	10.122581416507879	4.178493764942910	10.098025517387766
Ag	11.568266940212002	6.678942031988846	10.064058167202409
Ag	13.010875898470495	9.181166554922990	10.098025517387766
Ag	14.451938517850110	11.679793571212175	10.168706069058544
Ag	15.898217359668784	14.181881652489437	10.219418084425838
Ag	17.351947728285900	16.697616436065200	10.238111426366309
Ag	18.803772775738022	19.214451257328285	10.219418084425838
Ag	11.568266940211918	1.680224718158734	10.165796805257006
Ag	13.013952463916121	4.178493764942910	10.098025517387766
Ag	14.456561422174616	6.677165776100633	10.098025517387766
Ag	15.897283120325865	9.178300688903830	10.165796805257006
Ag	17.341094183765897	11.677670254199496	10.240752157978088
Ag	18.793265287226710	14.186089714758712	10.281623430381352
Ag	20.247652450691085	16.705162175754989	10.281623430381352
Ag	21.693921875152220	19.216988972273345	10.240752157978088
Ag	14.457295624914860	1.681183419971426	10.168706069058544
Ag	15.900589230135537	4.177674591685280	10.138856394969601
Ag	17.340967202552971	6.675849104782932	10.168706069058544
Ag	18.783706189037598	9.178992965460090	10.240752157978088
Ag	20.235553063202570	11.683002008240956	10.298782968544261
Ag	21.689520051462303	14.193317887649647	10.317629639153637
Ag	23.136533880423915	16.707648175451013	10.298782968544261
Ag	24.579145885695624	19.216988972273345	10.240752157978088
Ag	17.344983264169112	1.680253645982632	10.189116648763655
Ag	18.785616230074172	4.175503137988840	10.189116648763655
Ag	20.230978464354681	6.677319282115207	10.219418084425838
Ag	21.682146716959544	9.182400301419225	10.281623430381352
Ag	23.136533880423837	11.687016416633490	10.317629639153637

Ag	24.583547709385371	14.193317887649647	10.317629639153637
Ag	26.025415310156752	16.705162175754989	10.281623430381352
Ag	27.469294985109819	19.214451257328285	10.219418084425838
Ag	20.237459086483074	1.673781612682652	10.215288923124263
Ag	21.684048026047339	4.174270091283263	10.215122863246435
Ag	23.136533880423997	6.678419319802666	10.238111426366309
Ag	24.590921043888290	9.182400301419225	10.281623430381352
Ag	26.037514697645260	11.683002008240956	10.298782968544261
Ag	27.479802473621127	14.186089714758712	10.281623430381352
Ag	28.921120032562094	16.697616436065200	10.238111426366309
Ag	30.363533952138688	19.207580698852485	10.215122863246435
Ag	0.000000000000000	0.000000000000000	12.593243365701683
Ag	1.467193078709170	2.504865011679841	12.585624761595302
Ag	2.951144938613450	4.986834921119407	12.563465679928859
Ag	4.432685649149565	7.464566138968402	12.569156052842430
Ag	5.895524597810937	9.954101350417485	12.588218827007138
Ag	7.320105860210859	12.465724647327811	12.569156052842430
Ag	8.725113683349953	14.987642148317722	12.563465679928859
Ag	10.132586746400957	17.513767111707633	12.585624761595302
Ag	2.902873272520132	0.018193972578922	12.585624761595302
Ag	4.388713294148870	2.533824801772938	12.573051912627818
Ag	5.865224183961382	5.015729634889018	12.528328430670204
Ag	7.322975475727179	7.480972773570366	12.496332436315919
Ag	8.751042211143837	9.954456915911038	12.496332436315919
Ag	10.157129749864275	12.449528136320483	12.528328430670204
Ag	11.568266940211831	14.969176492420367	12.573051912627818
Ag	13.003947134022880	17.513767111707633	12.585624761595302
Ag	5.794298195475500	0.062349026529411	12.563465679928859
Ag	7.276361374309028	2.571568324756900	12.528328430670204
Ag	8.730341784145816	5.040465179194023	12.453271756165217
Ag	10.158538314821250	7.492849233342517	12.412419101179831
Ag	11.568266940211920	9.955895737578350	12.453271756165217
Ag	12.979404130559569	12.449528136320483	12.528328430670204
Ag	14.411420197074055	14.987642148317722	12.563465679928859
Ag	15.876117145581155	17.549687620267882	12.567042940577620
Ag	8.680846729150543	0.106535309670037	12.569156052842430
Ag	10.140200204795260	2.601396406484987	12.496332436315919
Ag	11.568266940212002	5.051127629281504	12.412419101179831
Ag	12.977995565602752	7.492849233342517	12.412419101179831
Ag	14.385491669279997	9.954456915911038	12.496332436315919
Ag	15.816428020212815	12.465724647327811	12.569156052842430
Ag	17.275109102036645	15.025948003665494	12.591905464817547
Ag	18.761235744323852	17.599994854588676	12.591905464817547
Ag	11.568266940212000	0.128623395131563	12.588218827007138
Ag	12.996333675628577	2.601396406484987	12.496332436315919
Ag	14.406192096278025	5.040465179194023	12.453271756165217
Ag	15.813558404696657	7.480972773570366	12.496332436315919
Ag	17.241009282613064	9.954101350417485	12.588218827007138
Ag	18.702185321780370	12.486534188340347	12.629825319657701
Ag	20.185239166727150	15.061814861388301	12.640220129139774
Ag	21.673970728988294	17.633817502816235	12.629825319657701
Ag	14.455687151273130	0.106535309670037	12.569156052842430
Ag	15.860172506114816	2.571568324756900	12.528328430670204
Ag	17.271309696462463	5.015729634889018	12.528328430670204
Ag	18.703848231274108	7.464566138968402	12.569156052842430
Ag	20.164748473215834	9.953300500776070	12.629825319657701
Ag	21.650504769049299	12.499924756501887	12.657706051724171
Ag	23.136533880423755	15.073802678928871	12.657706051724171
Ag	24.599097031859223	17.633817502816235	12.629825319657701
Ag	17.342235684948506	0.062349026529411	12.563465679928859
Ag	18.747820586274795	2.533824801772938	12.573051912627818
Ag	20.185388941810558	4.986834921119407	12.563465679928859
Ag	21.650407238136712	7.447709333678765	12.591905464817547

Ag	23.136533880423841	9.950022469156192	12.640220129139774
Ag	24.622562991798212	12.499924756501887	12.657706051724171
Ag	26.087828594120531	15.061814861388301	12.640220129139774
Ag	27.511832016523989	17.599994854588676	12.591905464817547
Ag	20.233660607903705	0.018193972578922	12.585624761595302
Ag	21.669340801714668	2.504865011679841	12.585624761595302
Ag	23.136533880423841	4.974276951397025	12.567042940577620
Ag	24.622660522711129	7.447709333678765	12.591905464817547
Ag	26.108319287631684	9.953300500776070	12.629825319657701
Ag	27.570882439067148	12.486534188340347	12.629825319657701
Ag	28.997958658811200	15.025948003665494	12.591905464817547
Ag	30.396950615266526	17.549687620267882	12.567042940577620
O	1.650507464077505	0.952920898152393	15.379262519760216
O	4.953073100924468	0.945405393059177	15.339712512731245
O	3.295281664167908	3.816784389873860	15.339712512731245
O	8.259124727455408	0.934387058457217	15.305875544412217
O	6.595390737747458	3.807850587316922	15.306286202603234
O	4.938765319760765	6.685418251973640	15.305875544412217
O	11.568266892286269	0.930425452257668	15.302430312893161
O	9.908099102800065	3.801976232281156	15.257090320286602
O	8.246657579582021	6.679677364299719	15.257090320286602
O	6.589905550567515	9.553200234551030	15.302430312893161
O	14.877409057117129	0.934387058457217	15.305875544412217
O	13.228434681772306	3.801976232281156	15.257090320286602
O	11.568266892286182	6.678941973786620	15.217249446333220
O	9.906825369068059	9.555172324778848	15.257090320286602
O	8.247907484591543	12.417020610929010	15.305875544412217
O	18.183460683648057	0.945405393059177	15.339712512731245
O	16.541143046825241	3.807850587316922	15.306286202603234
O	14.889876204990514	6.679677364299719	15.257090320286602
O	13.229708415504312	9.555172324778848	15.257090320286602
O	11.568266892286349	12.421124746726020	15.306286202603234
O	9.910475455529784	15.274636138426819	15.339712512731245
O	21.486026320495032	0.952920898152393	15.379262519760216
O	19.841252120404452	3.816784389873860	15.339712512731245
O	18.197768464811769	6.685418251973640	15.305875544412217
O	16.546628234004860	9.553200234551030	15.302430312893161
O	14.888626299980828	12.417020610929010	15.305875544412217
O	13.226058329042740	15.274636138426819	15.339712512731245
O	11.568266892286186	18.130984125055083	15.379262519760216
O	23.136533832498184	3.819003534434485	15.341021660338043
O	21.492487350600829	6.690367688415741	15.302404597864978
O	19.847049476179603	9.553193441541195	15.347238946931876
O	18.196832972173148	12.411452269969066	15.347238946931876
O	16.540272080568716	15.267856146129784	15.302404597864978
O	14.875621020653695	18.127324241445812	15.341021660338043
O	24.780580314395543	6.690367688415741	15.302404597864978
O	23.136533832498110	9.557439566454665	15.338730091749333
O	21.492179889141845	12.408515813935567	15.376077175207630
O	19.845252402375188	15.258106225435801	15.338730091749333
O	18.184318562465990	18.115428182780732	15.302404597864978
O	26.426018188816752	9.553193441541195	15.347238946931876
O	24.780887775854382	12.408515813935567	15.376077175207630
O	23.136533832498195	15.256620389455000	15.376077175207630
O	21.486317328491722	18.109006305815843	15.347238946931876
O	28.076234692823210	12.411452269969066	15.347238946931876
O	26.427815262621191	15.258106225435801	15.338730091749333
O	24.786750336504635	18.109006305815843	15.347238946931876
O	29.732795584427656	15.267856146129784	15.302404597864978
O	28.088749102530215	18.115428182780732	15.302404597864978
O	31.397446644342672	18.127324241445812	15.341021660338043
Zn	23.136533928349568	1.906512230050777	15.265162335859028
Zn	3.295945884104924	1.902915273954753	15.241750007314650

Zn	24.783875330275325	4.769601699348894	15.205960185164964
Zn	6.598878553722708	1.895404514322943	15.200268945387755
Zn	4.940907710270951	4.767094252649214	15.200268945387755
Zn	26.429112044799258	7.642250409136031	15.218428443888813
Zn	9.911510607890357	1.889331933467776	15.186955877683980
Zn	8.244560832969519	4.759999446797531	15.162106351760483
Zn	6.591964728067662	7.638954055376606	15.186955877683980
Zn	28.077117277186023	10.505436995775364	15.247667766517861
Zn	13.225023368384790	1.889331933467776	15.186955877683980
Zn	11.568266988137573	4.758154448134758	15.142569466266250
Zn	9.904816094841635	7.639335911219156	15.142569466266250
Zn	8.248721108314879	10.508540281728688	15.186955877683980
Zn	29.732706980797062	13.364244685911480	15.218428443888813
Zn	16.537655422552593	1.895404514322943	15.200268945387755
Zn	14.891973143305787	4.759999446797531	15.162106351760483
Zn	13.231717881433511	7.639335911219156	15.142569466266250
Zn	11.568266988137655	10.516827376978148	15.162106351760483
Zn	9.910296144685811	13.374327503600908	15.200268945387755
Zn	31.397875382359441	16.225385830821782	15.205960185164964
Zn	19.840588092170048	1.902915273954753	15.241750007314650
Zn	18.195626266004350	4.767094252649214	15.200268945387755
Zn	16.544569248207480	7.638954055376606	15.186955877683980
Zn	14.887812867960264	10.508540281728688	15.186955877683980
Zn	13.226237831589327	13.374327503600908	15.200268945387755
Zn	11.568266988137486	16.230995722663415	15.241750007314650
Zn	33.053712895116355	19.083570068244267	15.265162335859028
Zn	21.489192526423821	4.769601699348894	15.205960185164964
Zn	19.843955811899864	7.642250409136031	15.218428443888813
Zn	18.195950579513127	10.505436995775364	15.247667766517861
Zn	16.540360875901897	13.364244685911480	15.218428443888813
Zn	14.875192474339704	16.225385830821782	15.205960185164964
Zn	13.219354961582619	19.083570068244267	15.265162335859028
Zn	23.136533928349479	7.647073801628197	15.215110228463637
Zn	21.487529754042296	10.505599507298461	15.276796021643259
Zn	19.841880905885038	13.355946923723746	15.276796021643259
Zn	18.190827114557425	16.213289282455623	15.215110228463637
Zn	16.522533876265374	19.078664836368784	15.205960185164964
Zn	24.785538102656840	10.505599507298461	15.276796021643259
Zn	23.136533928349408	13.357884122179772	15.306645914400102
Zn	21.490885080192392	16.212105935517247	15.276796021643259
Zn	19.832938992351675	19.067157271491933	15.218428443888813
Zn	26.431186950813931	13.355946923723746	15.276796021643259
Zn	24.782182776506581	16.212105935517247	15.276796021643259
Zn	23.136533928349493	19.062778374988739	15.247667766517861
Zn	28.082240742141536	16.213289282455623	15.215110228463637
Zn	26.440128864347447	19.067157271491933	15.218428443888813
Zn	29.750533980433609	19.078664836368784	15.205960185164964

49/64 Au

	23.0799653379289147	0.0000000000000000	0.0000000000000000
	11.5399826689644573	19.9878363011107325	0.0000000000000000
	0.0000000000000000	0.0000000000000000	20.3667672948810186
Au	0.0000000000000000	0.0000000000000000	5.500000000000021
Au	1.442497833620557	2.498479537638842	5.500000000000021
Au	2.884995667241114	4.996959075277683	5.500000000000021
Au	4.327493500861672	7.495438612916525	5.500000000000021
Au	5.769991334482229	9.993918150555366	5.500000000000021
Au	7.212489168102786	12.492397688194208	5.500000000000021
Au	8.654987001723343	14.990877225833049	5.500000000000021
Au	10.097484835343900	17.489356763471889	5.500000000000021
Au	2.884995667241114	0.0000000000000000	5.500000000000021
Au	4.327493500861672	2.498479537638842	5.500000000000021
Au	5.769991334482229	4.996959075277683	5.500000000000021

Au	7.212489168102787	7.495438612916525	5.500000000000021
Au	8.654987001723343	9.993918150555366	5.500000000000021
Au	10.097484835343900	12.492397688194208	5.500000000000021
Au	11.539982668964457	14.990877225833049	5.500000000000021
Au	12.982480502585014	17.489356763471889	5.500000000000021
Au	5.769991334482229	0.000000000000000	5.500000000000021
Au	7.212489168102786	2.498479537638842	5.500000000000021
Au	8.654987001723343	4.996959075277683	5.500000000000021
Au	10.097484835343900	7.495438612916525	5.500000000000021
Au	11.539982668964457	9.993918150555366	5.500000000000021
Au	12.982480502585014	12.492397688194208	5.500000000000021
Au	14.424978336205573	14.990877225833049	5.500000000000021
Au	15.867476169826130	17.489356763471889	5.500000000000021
Au	8.654987001723343	0.000000000000000	5.500000000000021
Au	10.097484835343900	2.498479537638842	5.500000000000021
Au	11.539982668964457	4.996959075277683	5.500000000000021
Au	12.982480502585016	7.495438612916525	5.500000000000021
Au	14.424978336205573	9.993918150555366	5.500000000000021
Au	15.867476169826130	12.492397688194208	5.500000000000021
Au	17.309974003446687	14.990877225833049	5.500000000000021
Au	18.752471837067244	17.489356763471889	5.500000000000021
Au	11.539982668964457	0.000000000000000	5.500000000000021
Au	12.982480502585014	2.498479537638842	5.500000000000021
Au	14.424978336205571	4.996959075277683	5.500000000000021
Au	15.867476169826130	7.495438612916525	5.500000000000021
Au	17.309974003446687	9.993918150555366	5.500000000000021
Au	18.752471837067244	12.492397688194208	5.500000000000021
Au	20.194969670687801	14.990877225833049	5.500000000000021
Au	21.637467504308358	17.489356763471889	5.500000000000021
Au	14.424978336205571	0.000000000000000	5.500000000000021
Au	15.867476169826128	2.498479537638842	5.500000000000021
Au	17.309974003446687	4.996959075277683	5.500000000000021
Au	18.752471837067244	7.495438612916525	5.500000000000021
Au	20.194969670687801	9.993918150555366	5.500000000000021
Au	21.637467504308358	12.492397688194208	5.500000000000021
Au	23.079965337928915	14.990877225833049	5.500000000000021
Au	24.522463171549472	17.489356763471889	5.500000000000021
Au	17.309974003446687	0.000000000000000	5.500000000000021
Au	18.752471837067244	2.498479537638842	5.500000000000021
Au	20.194969670687801	4.996959075277683	5.500000000000021
Au	21.637467504308358	7.495438612916525	5.500000000000021
Au	23.079965337928915	9.993918150555366	5.500000000000021
Au	24.522463171549472	12.492397688194208	5.500000000000021
Au	25.964961005170032	14.990877225833049	5.500000000000021
Au	27.407458838790589	17.489356763471889	5.500000000000021
Au	20.194969670687801	0.000000000000000	5.500000000000021
Au	21.637467504308358	2.498479537638842	5.500000000000021
Au	23.079965337928915	4.996959075277683	5.500000000000021
Au	24.522463171549472	7.495438612916525	5.500000000000021
Au	25.964961005170029	9.993918150555366	5.500000000000021
Au	27.407458838790586	12.492397688194208	5.500000000000021
Au	28.849956672411146	14.990877225833049	5.500000000000021
Au	30.292454506031703	17.489356763471889	5.500000000000021
Au	1.442439484594453	0.832792824720352	7.999721840629664
Au	2.867738977185308	3.342143873989140	7.986814560410529
Au	4.291325293756849	5.857693386070422	7.988043064626309
Au	5.710064645436221	8.367823526485052	7.998663335522059
Au	7.148267243361337	10.858863497668906	7.998663335522059
Au	8.612734035925726	13.342592887779229	7.988043064626309
Au	10.079470659579890	15.833229558450736	7.986814560410529
Au	11.539982668964374	18.322250651669883	7.999721840629664
Au	4.328250986569786	0.812462868670707	7.986814560410529
Au	5.748376055337349	3.318826462952217	7.961620277867556

Au	7.172066518569327	5.838577201437060	7.944245855850731
Au	8.609839758480049	8.354330898502397	7.937530162606458
Au	10.069659749847887	10.857355897679200	7.944245855850731
Au	11.539982668964377	13.350183375206161	7.961620277867556
Au	13.000494678348852	15.833229558450736	7.986814560410529
Au	14.442021823871096	18.312343213826448	7.997010555278429
Au	7.218573926795498	0.787550027260938	7.988043064626309
Au	8.642389437685813	3.291903201994324	7.944245855850731
Au	10.079733334982990	5.819536754312072	7.912240688715704
Au	11.539982668964374	8.348762792486445	7.912240688715704
Au	13.010305588080856	10.857355897679200	7.944245855850731
Au	14.467231302003025	13.342592887779229	7.988043064626309
Au	15.912774503309969	15.813517832108088	8.013817325921160
Au	17.341444423779990	18.288046721607554	8.013817325921160
Au	10.101780071039254	0.761149276956624	7.998663335522059
Au	11.539982668964376	3.279174504105798	7.937530162606458
Au	13.000232002945761	5.819536754312072	7.912240688715704
Au	14.470125579448704	8.354330898502397	7.937530162606458
Au	15.931698094567405	10.858863497668906	7.998663335522059
Au	17.370274589625620	13.333308239323939	8.057076181664060
Au	18.801778772747451	15.795236365791348	8.073542523797784
Au	20.218118980998742	18.265919417232254	8.057076181664060
Au	12.978185266889486	0.761149276956624	7.998663335522059
Au	14.437575900242930	3.291903201994324	7.944245855850731
Au	15.907898819359415	5.838577201437060	7.944245855850731
Au	17.369900692492521	8.367823526485052	7.998663335522059
Au	18.812659630593732	10.861494101896094	8.077719423548318
Au	20.237781104688139	13.327529700640884	8.131126134085187
Au	21.656876599826276	15.785475199012248	8.131126134085187
Au	23.079965337928826	18.252684398429125	8.077719423548318
Au	15.861391411133251	0.787550027260938	7.988043064626309
Au	17.331589282591406	3.318826462952217	7.961620277867556
Au	18.788640044171899	5.857693386070422	7.988043064626309
Au	20.232120946555710	8.376444945665130	8.057076181664060
Au	21.660869842790692	10.862667702568183	8.131126134085187
Au	23.079965337928833	13.325224200740442	8.165231948321717
Au	24.503054076031383	15.785475199012248	8.131126134085187
Au	25.941811694858920	18.265919417232254	8.057076181664060
Au	18.751714351358956	0.812462868670707	7.986814560410529
Au	20.212226360743436	3.342143873989140	7.986814560410529
Au	21.651295417458815	5.874108048505688	8.013817325921160
Au	23.079965337928829	8.385199870638621	8.073542523797784
Au	24.499060833066963	10.862667702568183	8.131126134085187
Au	25.922149571169516	13.327529700640884	8.131126134085187
Au	27.358151903110208	15.795236365791348	8.073542523797784
Au	28.818486252077683	18.288046721607554	8.013817325921160
Au	21.637525853334292	0.832792824720352	7.999721840629664
Au	23.079965337928826	3.350986174568414	7.997010555278429
Au	24.508635258398858	5.874108048505688	8.013817325921160
Au	25.927809729301956	8.376444945665130	8.057076181664060
Au	27.347271045263923	10.861494101896094	8.077719423548318
Au	28.789656086232046	13.333308239323939	8.057076181664060
Au	30.247156172547705	15.813517832108088	8.013817325921160
Au	31.717908851986557	18.312343213826448	7.997010555278429
Au	23.079965337929004	1.662632366783185	10.370919108500004
Au	24.530209304135830	4.149560716518878	10.368789059860871
Au	25.985311149575697	6.636541654393826	10.399043577658572
Au	27.444268974058001	9.132349087515527	10.438888989358455
Au	28.893253518941915	11.642063938636529	10.438888989358455
Au	30.325207246738188	14.153462194249133	10.399043577658572
Au	31.751444994945611	16.657107826431158	10.368789059860871
Au	33.180066140105019	19.156520117719218	10.370919108500004
Au	2.889888208287273	1.668477734982582	10.363484656930092

Au	4.343830518833877	4.156873618485895	10.342870935790346
Au	5.796480132809829	6.645059857882814	10.340782310158895
Au	7.244823644596758	9.142423319301278	10.343180903010511
Au	8.683432088774726	11.645407324624363	10.340782310158895
Au	10.111939774451349	14.147531912823650	10.342870935790346
Au	11.539982668964537	16.650880831145709	10.363484656930092
Au	12.979864535752986	19.156520117719218	10.370919108500004
Au	5.771873413347067	1.683430769801327	10.342870935790346
Au	7.224768091087084	4.171221802221745	10.295870816518457
Au	8.671908311911828	6.658405106086156	10.268221790390449
Au	10.109588854361821	9.148540850662727	10.268221790390449
Au	11.539982668964537	11.645392696667381	10.295870816518457
Au	12.968025563477729	14.147531912823650	10.342870935790346
Au	14.408485680912396	16.657107826431158	10.368789059860871
Au	15.858729647119223	19.169004059271582	10.368789059860871
Au	8.653030712999644	1.697369118603701	10.340782310158895
Au	10.102302126514546	4.180890344361991	10.268221790390449
Au	11.539982668964541	6.662612100370292	10.236794234326428
Au	12.970376483567257	9.148540850662727	10.268221790390449
Au	14.396533249154356	11.645407324624363	10.340782310158895
Au	15.834723429119810	14.153462194249133	10.399043577658572
Au	17.285502699669998	16.670658764748598	10.414125838790543
Au	18.740069240766509	19.185668753578650	10.399043577658572
Au	11.539982668964539	1.702989662508316	10.343180903010511
Au	12.977663211414532	4.180890344361991	10.268221790390449
Au	14.408057026017250	6.658405106086156	10.268221790390449
Au	15.835141693332318	9.142423319301278	10.343180903010511
Au	17.266677156916085	11.642063938636529	10.438888989358455
Au	18.717438428289789	14.160438252993295	10.493713246717267
Au	20.175385296260750	16.685676303054922	10.493713246717267
Au	21.630980793045087	19.201259576069557	10.438888989358455
Au	14.426934624929439	1.697369118603701	10.340782310158895
Au	15.855197246841991	4.171221802221745	10.295870816518457
Au	17.283485205119256	6.645059857882814	10.340782310158895
Au	18.715661701799995	9.132349087515527	10.438888989358455
Au	20.160313103277481	11.639562197124391	10.531701891930469
Au	21.620610436100741	14.167783146154274	10.567624008486241
Au	23.079965337929004	16.696548207972832	10.531701891930469
Au	24.528949882812910	19.201259576069557	10.438888989358455
Au	17.308091924582012	1.683430769801327	10.342870935790346
Au	18.736134819095202	4.156873618485895	10.342870935790346
Au	20.174619526282299	6.636541654393826	10.399043577658572
Au	21.622018469958022	9.129558046173379	10.493713246717267
Au	23.079965337928993	11.640106309913051	10.567624008486241
Au	24.539320239757245	14.167783146154274	10.567624008486241
Au	25.984545379597229	16.685676303054922	10.493713246717267
Au	27.419861435091487	19.185668753578650	10.399043577658572
Au	20.190077129641804	1.668477734982582	10.363484656930092
Au	21.629721371722177	4.149560716518878	10.368789059860871
Au	23.079965337928996	6.634355072724413	10.414125838790543
Au	24.537912205899957	9.129558046173379	10.493713246717267
Au	25.999617572580519	11.639562197124391	10.531701891930469
Au	27.442492247568197	14.160438252993295	10.493713246717267
Au	28.874427976187995	16.670658764748598	10.414125838790543
Au	30.301201028738785	19.169004059271582	10.368789059860871
Au	0.000000000000000	0.000000000000000	12.863468306002520
Au	1.453970352223038	2.494345726132091	12.852578773678346
Au	2.915702061700048	4.976525117647948	12.839935335266123
Au	4.379508678149008	7.461106495302809	12.857015744798774
Au	5.835593054241024	9.956042979993322	12.871566739541315
Au	7.268229242765652	12.464517282087888	12.857015744798774
Au	8.688036525360015	14.974501686987853	12.839935335266123
Au	10.106801080424447	17.481488176670133	12.852578773678346

Au	2.887151940763052	0.012002398308513	12.852578773678346
Au	4.353736153741845	2.513630740343459	12.841847645736582
Au	5.813289973610690	4.997776575581736	12.806763416938841
Au	7.263407873465580	7.475807860727262	12.786004270463243
Au	8.697447084496041	9.959636634278002	12.786004270463243
Au	10.118426178877220	12.454491216607641	12.806763416938841
Au	11.539982668964456	14.960574820423812	12.841847645736582
Au	12.973164257504475	17.481488176670133	12.852578773678346
Au	5.767648205304489	0.036809496474930	12.839935335266123
Au	7.234846463697928	2.535568508921358	12.806763416938841
Au	8.683502943368065	5.013422761862459	12.745168276704270
Au	10.117349849030443	7.483969541917147	12.721129523208671
Au	11.539982668964457	9.960990777385815	12.745168276704270
Au	12.961539159051696	12.454491216607641	12.806763416938841
Au	14.391928812568899	14.974501686987853	12.839935335266123
Au	15.840297373426484	17.505048448889475	12.840461849516162
Au	8.651262104347818	0.062212523720043	12.857015744798774
Au	10.105943457933998	2.552391806105467	12.786004270463243
Au	11.539982668964461	5.019897217276444	12.721129523208669
Au	12.962615488898479	7.483969541917147	12.721129523208671
Au	14.382518253432876	9.959636634278002	12.786004270463243
Au	15.811736095163273	12.464517282087888	12.857015744798774
Au	17.253958987769384	14.998003694161909	12.875028964567171
Au	18.718292626616538	17.534303955877398	12.875028964567171
Au	11.539982668964457	0.075750341124087	12.871566739541315
Au	12.974021879994915	2.552391806105467	12.786004270463243
Au	14.396462394560849	5.013422761862459	12.745168276704270
Au	15.816557464463333	7.475807860727262	12.786004270463243
Au	17.244372283687888	9.956042979993322	12.871566739541315
Au	18.689289593042421	12.474037741039117	12.918013944429751
Au	20.151056964521189	15.016230238559187	12.934180864088397
Au	21.621776562944390	17.553254165443033	12.918013944429751
Au	14.428703233581105	0.062212523720043	12.857015744798774
Au	15.845118874230989	2.535568508921358	12.806763416938841
Au	17.266675364318225	4.997776575581736	12.806763416938841
Au	18.700456659779917	7.461106495302809	12.857015744798774
Au	20.147478368026938	9.948380695739306	12.918013944429751
Au	21.607823311966090	12.475282605765489	12.956310580876481
Au	23.079965337928915	15.025107390690485	12.956310580876481
Au	24.538154112913432	17.553254165443033	12.918013944429751
Au	17.312317132624425	0.036809496474930	12.839935335266123
Au	18.726229184187069	2.513630740343459	12.841847645736582
Au	20.164263276228866	4.976525117647948	12.839935335266123
Au	21.615631699081767	7.443364952182167	12.875028964567171
Au	23.079965337928918	9.943212125103091	12.934180864088397
Au	24.552107363891739	12.475282605765489	12.956310580876481
Au	26.008873711336641	15.016230238559187	12.934180864088397
Au	27.441638049241305	17.534303955877398	12.875028964567171
Au	20.192813397165867	0.012002398308513	12.852578773678346
Au	21.625994985705884	2.494345726132091	12.852578773678346
Au	23.079965337928915	4.965575704442514	12.840461849516162
Au	24.544298976776076	7.443364952182167	12.875028964567171
Au	26.012452307830880	9.948380695739306	12.918013944429751
Au	27.470641082815401	12.474037741039117	12.918013944429751
Au	28.905971688088460	14.998003694161909	12.875028964567171
Au	30.319633302431345	17.505048448889475	12.840461849516162
O	1.649941103251527	0.952593909651707	15.722876389863702
O	4.948325301871576	0.949430838804481	15.680300712686428
O	3.296393902853803	3.810659952521319	15.680300712686428
O	8.245311709014203	0.944842358048556	15.651151447961817
O	6.593856863025382	3.806965004407879	15.642088000714134
O	4.940913365525790	6.668228177416920	15.651151447961817
O	11.539982621155987	0.940877697454130	15.647917461984850

O	9.890965969578511	3.802417008760516	15.612701760978803
O	8.238472736535110	6.664619247555726	15.612701760978803
O	6.584815324804445	9.523479214738426	15.647917461984850
O	14.834653533297761	0.944842358048556	15.651151447961817
O	13.188999272733291	3.802417008760516	15.612701760978803
O	11.539982621155900	6.662612042310370	15.593152474186123
O	9.887489388112417	9.520799870614727	15.612701760978803
O	8.235584277667488	12.374765591465636	15.651151447961817
O	18.131639940440380	0.949430838804481	15.680300712686428
O	16.486108379286581	3.806965004407879	15.642088000714134
O	14.841492505776856	6.664619247555726	15.612701760978803
O	13.192475854199383	9.520799870614727	15.612701760978803
O	11.539982621155982	12.373906118115210	15.642088000714134
O	9.888051222138206	15.227745335605166	15.680300712686428
O	21.430024139060446	0.952593909651707	15.722876389863702
O	19.783571339457993	3.810659952521319	15.680300712686428
O	18.139051876786176	6.668228177416920	15.651151447961816
O	16.495149917507366	9.523479214738426	15.647917461984850
O	14.844380964644312	12.374765591465636	15.651151447961816
O	13.191914020173590	15.227745335605166	15.680300712686428
O	11.539982621155906	18.082648307627707	15.722876389863702
O	23.079965290120438	3.812166959320297	15.686895309502434
O	21.433218076047805	6.671839741045846	15.667959882546210
O	19.790499629270670	9.525483191054512	15.696668468381748
O	18.144560267787334	12.376333791321130	15.696668468381748
O	16.494591770125162	15.225791422499775	15.667959882546210
O	14.841416101676405	18.081752734360702	15.686895309502434
O	24.726712504193063	6.671839741045846	15.667959882546210
O	23.079965290120349	9.529007154528337	15.707949998916487
O	21.436300177224343	12.376253647292410	15.747975089563964
O	19.792344940102513	15.223332636756602	15.707949998916487
O	18.141338984197795	18.078041264496072	15.667959882546210
O	26.369430950970219	9.525483191054512	15.696668468381748
O	24.723630403016518	12.376253647292410	15.747975089563964
O	23.079965290120430	15.223165133456867	15.747975089563964
O	21.434025928637105	18.073855445666069	15.696668468381752
O	28.015370312453555	12.376333791321130	15.696668468381752
O	26.367585640138181	15.223332636756602	15.707949998916487
O	24.725904651603784	18.073855445666069	15.696668468381748
O	29.665338810115543	15.225791422499775	15.667959882546210
O	28.018591596042917	18.078041264496072	15.667959882546210
O	31.318514478564474	18.081752734360702	15.686895309502434
Zn	23.079965385737463	1.900764008749958	15.578164823559105
Zn	3.294155225499795	1.901881436652403	15.552422068598633
Zn	24.728530547327598	4.755749779724892	15.528489494304122
Zn	6.588956843534191	1.903128220954211	15.491813103275927
Zn	4.942635781395398	4.754639946149359	15.491813103275927
Zn	26.376716144103575	7.615985479464120	15.537946277201284
Zn	9.889099536855911	1.899366651785463	15.484230046666550
Zn	8.237711915639023	4.756045222458462	15.462624877818286
Zn	6.589449513598029	7.614528139263938	15.484230046666550
Zn	28.019920982412593	10.473139565275261	15.560967088335500
Zn	13.190865896689948	1.899366651785463	15.484230046666550
Zn	11.539982716772935	4.756181289113111	15.454759680150634
Zn	9.888965153385513	7.615827593088694	15.454759680150634
Zn	8.240332693515048	10.473941684241089	15.484230046666550
Zn	29.672686584096969	13.324773741777824	15.537946277201284
Zn	16.491008590011834	1.903128220954211	15.491813103275927
Zn	14.842253517907009	4.756045222458462	15.462624877818286
Zn	13.191000280160356	7.615827593088694	15.454759680150634
Zn	11.539982716773016	10.475746030373717	15.462624877818286
Zn	9.893661654634137	13.330068308186920	15.491813103275927
Zn	31.325630562494396	16.182262188607197	15.528489494304122

Zn	19.785810208046062	1.901881436652403	15.552422068598633
Zn	18.137329652150626	4.754639946149359	15.491813103275927
Zn	16.490515919947828	7.614528139263938	15.484230046666550
Zn	14.839632740030812	10.473941684241089	15.484230046666550
Zn	13.186303778911723	13.330068308186920	15.491813103275927
Zn	11.539982716772929	16.184073601985681	15.552422068598633
Zn	32.973838186806631	19.037454383825558	15.578164823559105
Zn	21.431400224147353	4.755749779724892	15.528489494304122
Zn	19.783214627371368	7.615985479464120	15.537946277201284
Zn	18.14009789062319	10.473139565275261	15.560967088335500
Zn	16.487244187377811	13.324773741777824	15.537946277201284
Zn	14.834300208980551	16.182262188607197	15.528489494304122
Zn	13.186092584668131	19.037454383825558	15.578164823559106
Zn	23.079965385737388	7.618337673476661	15.559924142969692
Zn	21.431821687646075	10.474481804118357	15.612907414081977
Zn	19.787078151290181	13.323261174506985	15.612907414081977
Zn	18.137656626330390	16.178667551462283	15.559924142969692
Zn	16.482865370570593	19.037660808069141	15.528489494304122
Zn	24.728109083828862	10.474481804118355	15.612907414081977
Zn	23.079965385737470	13.325224258800361	15.641443173138564
Zn	21.435221849381659	16.177929797775882	15.612907414081977
Zn	19.783994945743913	19.034913555159140	15.537946277201284
Zn	26.372852620184588	13.323261174506985	15.612907414081977
Zn	24.724708922093278	16.177929797775882	15.612907414081977
Zn	23.079965385737374	19.029393645850682	15.560967088335500
Zn	28.022274145144383	16.178667551462283	15.559924142969692
Zn	26.375935825730863	19.034913555159140	15.537946277201284
Zn	29.677065400904191	19.037660808069141	15.528489494304122

16/21 Au

	-8.6549870017000003	-9.9939181506000008	0.0000000000000000
	-4.3274935009000002	-22.4863158387000013	0.0000000000000000
	0.0000000000000000	0.0000000000000000	20.3667672949000007
Au	-8.654987001281560	-14.990877225107676	5.500000000482850
Au	-7.212489168239470	-12.492397688464138	5.500000000482850
Au	-5.769991334331928	-9.993918150821264	5.500000000482850
Au	-4.327493501289900	-7.495438614177798	5.500000000482850
Au	-2.884995666949631	-4.996959074286412	5.500000000482850
Au	-1.442497833907542	-2.498479537642876	5.500000000482850
Au	0.0000000000000000	0.0000000000000000	5.500000000482850
Au	-10.097484834770631	-22.486315837258068	5.500000000482850
Au	-8.654987001728541	-19.987836300614529	5.500000000482850
Au	-7.212489167820999	-17.489356762971653	5.500000000482850
Au	-5.769991334779002	-14.990877226328347	5.500000000482850
Au	-4.327493500871459	-12.492397688685474	5.500000000482850
Au	-2.884995667829370	-9.993918152041935	5.500000000482850
Au	-1.442497833489071	-7.495438612150389	5.500000000482850
Au	-11.539982668692458	-29.981754451657125	5.500000000482850
Au	-10.097484835650370	-27.483274915013592	5.500000000482850
Au	-8.654987001310101	-24.984795375122204	5.500000000482850
Au	-7.212489168268073	-22.486315838478738	5.500000000482850
Au	-5.769991334360530	-19.987836300835866	5.500000000482850
Au	-4.327493501318441	-17.489356764192326	5.500000000482850
Au	-2.884995667410930	-14.990877226549612	5.500000000482850
Au	-7.201760862368733	-14.154288352054131	7.940846429336481
Au	-5.771777178780248	-11.669426091792083	7.948343060695199
Au	-4.341219776692178	-9.170111274456593	7.927015958666606
Au	-2.892579424867516	-6.657049706393459	7.914876340821587
Au	-1.443445929567684	-4.147735442188392	7.927015958666606
Au	-8.655301134927496	-11.656211182673257	7.939602319154209
Au	-7.215241939914310	-9.163043680900824	7.939602319154209
Au	-8.657092855047534	-21.664661493125251	7.940846429336481
Au	-7.197814796340198	-19.162387272655089	7.927015958666606

Au	-5.757621376807785	-16.654124890833323	7.944207708630727
Au	-4.320797613376475	-14.158864955599686	7.965976151374194
Au	-2.889097543165640	-11.671486553270123	7.944207708630727
Au	-10.098510131882133	-19.164358713333286	7.914876340821587
Au	-8.646377947983172	-16.652743722422009	7.914876340821587
Au	-10.106107288649255	-29.141518134420046	7.940846429336481
Au	-8.663255083526575	-26.640938383896565	7.944207708630727
Au	-7.220130854569366	-24.145494820215863	7.948343060695199
Au	-5.766924429025467	-21.654897274077406	7.939602319154209
Au	-4.318065970150385	-19.151628915992053	7.948343060695199
Au	-11.542625458180103	-26.644242471645931	7.965976151374194
Au	-10.101537933643421	-24.157360551354380	7.965976151374194
Au	-8.655122759480998	-13.318870874964887	10.300974590231053
Au	-7.210607004296532	-10.819782513215912	10.316325793847158
Au	-5.775425597565458	-8.331559356818811	10.300974590231053
Au	-4.342950911042761	-5.836445503262714	10.297767542485106
Au	-2.888161231750333	-3.339802459883589	10.313682096638045
Au	-5.764903017289244	-23.324253429122209	10.316325793847158
Au	-4.334463982346949	-20.822513887910393	10.316325793847158
Au	-10.083988474307290	-20.830719365863018	10.297767542485106
Au	-8.649518915487082	-18.319571194600982	10.255665089411602
Au	-7.210528118950010	-15.806987270774338	10.297767542485106
Au	-5.761750963858124	-13.308427751224990	10.341433556748877
Au	-4.318552611115632	-10.825237916547605	10.313682096638045
Au	-2.885467581492967	-8.334306667762103	10.255665089411602
Au	-1.447494005619983	-5.826356126937085	10.255665089411602
Au	-11.558649007564027	-28.317363280780505	10.341433556748877
Au	-10.105773342957217	-25.831670296403328	10.357136327536297
Au	-8.644561033777853	-23.334676946594513	10.341433556748877
Au	-7.206919147253580	-20.823721908116475	10.300974590231053
Au	-5.775766658868431	-18.315193611869173	10.313682096638045
Au	-4.335515525269379	-15.809501475229604	10.357136327536297
Au	-2.868685134840705	-13.325378054118463	10.357136327536297
Au	-8.726917026637103	-14.971291796567197	12.700343660289835
Au	-7.254025270192670	-12.483240136726300	12.731681715126474
Au	-5.746704575128859	-10.031525292547268	12.740586990172407
Au	-4.308489967272886	-7.567524557701062	12.700343660289835
Au	-2.927800386113989	-5.055263130631584	12.704978517835146
Au	-1.486709953607745	-2.499842891821908	12.740586990172407
Au	0.000000000000000	0.000000000000000	12.744349927308914
Au	-10.025737490947471	-22.474765308577460	12.753911388883903
Au	-8.602060510389949	-19.935335785631676	12.700343660289835
Au	-7.241579602176882	-17.423134760601371	12.704978517835146
Au	-5.815868057954383	-14.934517468263817	12.753911388883903
Au	-4.289764033687263	-12.471577258526311	12.747837524056353
Au	-2.813100514309102	-10.001836098066896	12.704978517835146
Au	-1.442497833489071	-7.495438612150389	12.645311975253497
Au	-11.527145290157659	-30.022304546991890	12.731681715126474
Au	-10.123355456298183	-27.551185201758891	12.753911388883903
Au	-8.655820713467188	-25.027880267254357	12.747837524056353
Au	-7.183790444849677	-22.454923294881830	12.731681715126474
Au	-5.749065973863395	-19.948865804930826	12.740586990172407
Au	-4.364389256345548	-17.467092302219331	12.747837524056353
Au	-2.884995667410930	-14.990877226549612	12.765144794384959
O	-9.394757946478371	-22.479245713822145	15.504616446665729
O	-7.215025925045540	-19.997015358049765	15.559572441164695
O	-5.031430719698299	-17.505773655404308	15.512908380260043
O	-8.285109133964463	-16.879251278773328	15.530444065985156
O	-11.539982656128432	-24.984795449605443	15.500559434145524
O	-6.127477730859321	-14.385833071538158	15.504616446665729
O	-3.989742252560943	-11.874561828232089	15.512908380260043
O	-7.219169636939852	-11.247575676994291	15.565681517380067
O	-1.820318752922125	-9.370054852536654	15.530444065985156

O	-5.055423253048406	-8.737892056021584	15.559572441164695
O	-2.877052577198740	-6.230928077606507	15.530444065985156
O	-10.442725289780331	-28.095389415104542	15.504616446665729
O	-9.367018287691353	-13.739244945444980	15.559572441164695
O	-8.288800993591598	-25.586214568477438	15.512908380260043
O	-6.131101366141816	-23.102941487286007	15.565681517380067
O	-12.614689963603567	-30.609951033935960	15.565681517380067
Zn	-2.541456254354697	-13.107436153097666	15.412253916672878
Zn	-9.024380631461870	-20.597364465268491	15.372812950592639
Zn	-6.846313399942048	-18.134832618971345	15.374206847875094
Zn	-1.442497846038810	-7.495438537445885	15.364788424739615
Zn	-4.687873142470054	-15.635083779463837	15.412253916672878
Zn	-7.942423266068880	-15.006017289443129	15.372812950592639
Zn	-5.795712989724302	-12.500300462531523	15.389831402575286
Zn	-0.364970056262838	-1.869704052768847	15.418319643926811
Zn	-3.627082123684924	-9.988297637846232	15.374206847875094
Zn	-6.853290722178704	-9.375139343613357	15.418319643926811
Zn	-4.670663644851137	-6.870770163323312	15.372812950592639
Zn	-12.241526710258489	-28.750838779375187	15.389831402575286
Zn	-2.509085016189520	-4.357103506120149	15.374206847875094
Zn	-10.080644643891681	-26.224029669076160	15.412253916672878
Zn	-7.927721343299154	-23.709328514828286	15.389831402575286
Zn	-5.764219762240401	-21.235390371052794	15.418319643926811

52/27 Sn

	-20.6510535445999999	-11.9228913230000000	0.0000000000000000
	0.0000000000000000	-23.8457826460000000	0.0000000000000000
	0.0000000000000000	0.0000000000000000	21.7307573058000010
Sn	-18.356492039873871	-15.897188430269289	5.499999999512627
Sn	-16.061930535147745	-11.9228913230000000	5.499999999512627
Sn	-13.767369030421763	-7.948594215730798	5.499999999512627
Sn	-18.356492039873871	-23.845782647192308	5.499999999512627
Sn	-16.061930535147745	-19.871485537538405	5.499999999512627
Sn	-13.767369030421763	-15.897188430269200	5.499999999512627
Sn	-11.472807525695634	-11.9228913230000085	5.499999999512627
Sn	-9.178246018904366	-7.948594214538488	5.499999999512627
Sn	-6.883684514178236	-3.974297107269201	5.499999999512627
Sn	-18.356492039873871	-31.794376861730715	5.499999999512627
Sn	-16.061930535147745	-27.820079754461425	5.499999999512627
Sn	-13.767369030421763	-23.845782647192394	5.499999999512627
Sn	-11.472807525695634	-19.871485539923107	5.499999999512627
Sn	-9.178246018904366	-15.897188429076891	5.499999999512627
Sn	-6.883684514178236	-11.922891321807603	5.499999999512627
Sn	-4.589123009452257	-7.948594214538574	5.499999999512627
Sn	-2.294561504726128	-3.974297107269287	5.499999999512627
Sn	0.0000000000000000	0.0000000000000000	5.499999999512627
Sn	-11.472807525695634	-27.820079754461513	5.499999999512627
Sn	-9.178246018904366	-23.845782645999915	5.499999999512627
Sn	-6.883684514178236	-19.871485538730798	5.499999999512627
Sn	-4.589123009452257	-15.897188431461597	5.499999999512627
Sn	-2.294561504726128	-11.922891321807690	5.499999999512627
Sn	0.0000000000000000	-7.948594214538402	5.499999999512627
Sn	-4.589123009452257	-23.845782646000000	5.499999999512627
Sn	-2.294561504726128	-19.871485538730713	5.499999999512627
Sn	0.0000000000000000	-15.897188431461597	5.499999999512627
Sn	-16.060619223031932	-14.568405306208559	6.514061932323464
Sn	-13.766116137191696	-10.603697050729075	6.507049968847128
Sn	-11.472453848987300	-6.624172344185033	6.555598729071279
Sn	-16.069957913847045	-22.520175955181724	6.578565276532538
Sn	-13.763437823702148	-18.546175079315805	6.499034260396886
Sn	-11.474474148490806	-14.570521182326800	6.531132954924270
Sn	-9.174568489563486	-10.597465309381203	6.569465048019931
Sn	-6.881204416054476	-6.623335947195899	6.531132954924270

Sn	-4.586299476314253	-2.652675745269597	6.514061932323464
Sn	-16.066643170301482	-30.465751374378691	6.530465462711293
Sn	-13.764083659419343	-26.502686460711622	6.578565276532538
Sn	-11.468065517998898	-22.514485525683831	6.578565276532538
Sn	-9.178125090984160	-18.546241627854894	6.555598729071279
Sn	-6.886095124086058	-14.569568047823175	6.569465048019931
Sn	-4.590389928885310	-10.601640608218686	6.569465048019931
Sn	-2.300012951388287	-6.622127834404724	6.507049968847128
Sn	-20.649846585696935	-14.572726133960087	6.533350338119506
Sn	-18.356832761923105	-34.442711306448579	6.533350338119506
Sn	-9.179739849902868	-26.498990953632614	6.499034260396886
Sn	-6.884670868402972	-22.527028097803182	6.530465462711293
Sn	-4.584924456020011	-18.542849083866191	6.507049968847128
Sn	-2.295374980054713	-14.574816839477293	6.531132954924270
Sn	-0.000474604628541	-10.598259996960074	6.555598729071279
Sn	-18.350793050495405	-18.544568465817878	6.530465462711293
Sn	-2.295427741579959	-22.521910497591335	6.533350338119506
Sn	-0.004134845253823	-18.547592917521857	6.514061932323464
Sn	-18.358929415594986	-26.492181905051591	6.499034260396886
Sn	-16.064811530055195	-14.501847529205847	9.389725110226788
Sn	-13.727066084485420	-10.592183948391920	9.394621044736715
Sn	-11.551031291965957	-30.429608581359396	9.449209750229008
Sn	-16.089177722343628	-22.480337925311012	9.484470083171830
Sn	-13.761459742356383	-18.572897174207032	9.372591469634967
Sn	-11.397028647388378	-14.578312572843338	9.410981302945441
Sn	-9.194186029991316	-10.603802781670581	9.456794681315859
Sn	-6.926674708723831	-6.686510023300852	9.410981302945441
Sn	-4.526562597098737	-2.682323989388513	9.389725110226788
Sn	-15.951402755843276	-30.441694517222054	9.426127669351031
Sn	-13.788974501075586	-26.539250318060684	9.484470083171830
Sn	-11.423954867845778	-22.517759698204969	9.484470083171830
Sn	-9.173777384489236	-18.634464894051433	9.449209750229008
Sn	-6.870797941873905	-14.583388600048810	9.456794681315859
Sn	-4.586069570669787	-10.581482583703940	9.456794681315859
Sn	-2.309567338641060	-6.661702723236164	9.394621044736715
Sn	-20.592186859335033	-14.521631505259521	9.411160373501971
Sn	-18.429911871555479	-34.418323832994133	9.411160373501971
Sn	-9.203870903593941	-26.487342974882999	9.372591469634967
Sn	-6.963124925064969	-22.439255399918242	9.426127669351031
Sn	-4.614420121473667	-18.514787297372170	9.394621044736715
Sn	-2.327350188487648	-14.503851372855561	9.410981302945441
Sn	-20.577298412744668	-22.473274462588932	9.449209750229008
Sn	-18.387579408291600	-18.656398020859438	9.426127669351031
Sn	-2.280008358309195	-22.597392599745845	9.411160373501971
Sn	-0.059679417446217	-18.584502450405896	9.389725110226788
Sn	-18.336776443249523	-26.477107788909706	9.372591469634967
Sn	-18.328622211854420	-13.191949670069961	10.500272349153038
Sn	-16.073280487701048	-9.287219027910995	10.301554631149742
Sn	-13.762759144235044	-29.129522575378218	10.698096728105108
Sn	-18.345526978323491	-21.207904959260944	10.698096728105108
Sn	-16.089456779048515	-17.209563378642802	10.207523686398407
Sn	-13.715504519200636	-13.250708886985912	10.356620290627536
Sn	-11.479235367832528	-9.230543116417154	10.457512982040956
Sn	-9.204277149839132	-5.294020490173788	10.363219629853646
Sn	-6.859190684448997	-25.152905298958927	10.207523686398407
Sn	-18.353459625702339	-29.174879260398008	10.207523686398407
Sn	-16.072197150077869	-25.148629838902458	10.455815424049888
Sn	-13.743253735866130	-21.198319348362524	10.455815424049888
Sn	-11.464158737025290	-17.247018913130255	10.363219629853646
Sn	-9.140985409192581	-13.245186739125490	10.504062548318620
Sn	-6.900175489378421	-9.306863694084857	10.504062548318620
Sn	-4.617698254704984	-5.342452863183114	10.356620290627536
Sn	-2.260252433822294	-1.376755359163383	10.500272349153038

Sn	-0.062178898923130	-21.199968939766389	10.500272349153038
Sn	-11.486656205321308	-25.190398754312231	10.455815424049888
Sn	-9.193820966641470	-21.199920403360846	10.698096728105108
Sn	-6.917551031122537	-17.248929209334946	10.457512982040956
Sn	-4.609892643963709	-13.216623532212470	10.504062548318620
Sn	-2.254267145644787	-9.289201643247644	10.457512982040956
Sn	-0.006327368486932	-5.282303907570900	10.301554631149742
Sn	-4.571445692052021	-21.199151033518106	10.301554631149742
Sn	-2.317850770694380	-17.175512218830971	10.356620290627536
Sn	0.017382342264420	-13.227634565695963	10.363219629853646
Sn	-18.390040644053688	-13.225413907557552	13.406849055840462
Sn	-16.306344148669304	-33.049441150692694	13.148192841633222
Sn	-13.843891499119097	-29.052446812103582	13.666512938005214
Sn	-18.238211231869421	-21.176180160499960	13.666512938005214
Sn	-15.969788576798736	-17.183797566733048	13.048292898986848
Sn	-13.608824108287223	-13.224528535696239	13.231116469503458
Sn	-11.523149927600100	-9.313062812251971	13.349283061899749
Sn	-9.029985582765850	-5.322245388908470	13.229486518962903
Sn	-6.896710937910862	-25.269423908087120	13.048292898986848
Sn	-18.435607574490255	-29.084126463179580	13.048292898986848
Sn	-15.972731248756910	-25.202955308352372	13.344408609035195
Sn	-13.840033923142846	-21.257296610991474	13.344408609035195
Sn	-11.526861041238252	-17.081965539012270	13.229486518962903
Sn	-9.220888897471118	-13.327701843427292	13.386007986237988
Sn	-6.931683921760582	-9.196407691234057	13.386007986237988
Sn	-4.648365610864786	-5.447930984765113	13.231116469503458
Sn	-2.258524097505250	-1.306833317874865	13.406849055840462
Sn	-0.002488803041208	-21.236426743567833	13.406849055840462
Sn	-11.489341919365389	-25.077096022233089	13.344408609035195
Sn	-9.220004358211487	-21.308720965396464	13.666512938005214
Sn	-6.824129598333244	-17.245700485772279	13.349283061899749
Sn	-4.498480723303157	-13.244564430761717	13.386007986237988
Sn	-2.303774018666664	-9.209910670975765	13.349283061899749
Sn	-20.468483543102089	-17.045136441083116	13.148192841633222
Sn	-4.527279397428753	-21.442770346224446	13.148192841633222
Sn	-2.393863825448138	-17.096214448538905	13.231116469503458
Sn	-0.094206920595750	-13.364463041079002	13.229486518962903
Sn	-18.155729175900650	-15.891358133680253	14.292610659056461
Sn	-15.948382956828077	-11.858578843699568	14.133021574663100
Sn	-13.985728682839762	-8.006250403927911	14.202911361703830
Sn	-18.424024112527214	-23.997205143612710	14.272141895386593
Sn	-15.927414144946384	-19.679063593947788	14.409177392926457
Sn	-13.841075552071558	-15.834272462445462	14.326196509698086
Sn	-11.438805701844032	-11.908256616781637	14.458024969429104
Sn	-9.271304628789805	-7.904158135641143	14.319673229937839
Sn	-6.792344426914186	-3.941923371007902	14.326196509698086
Sn	-18.461922656818057	-31.623426269688174	14.292610659056461
Sn	-16.295831021643796	-27.799796115117203	14.409177392926457
Sn	-13.767369030421763	-23.845782647192394	14.473358295408934
Sn	-11.570177217973752	-19.737289801225032	14.272141895386593
Sn	-9.170199487131393	-15.999997588727055	14.319673229937839
Sn	-6.883684514178236	-11.922891321807603	14.286742875993562
Sn	-4.593449894015934	-7.985358010878058	14.458024969429104
Sn	-2.295639053031314	-4.104788434282338	14.133021574663100
Sn	0.000000000000000	0.000000000000000	14.522576831868516
Sn	-11.307905760764186	-27.802852996739212	14.272141895386593
Sn	-9.078861922609660	-24.058488228934728	14.409177392926457
Sn	-6.724572964304768	-20.031762450787216	14.202911361703830
Sn	-4.618797948740033	-15.875059341340304	14.458024969429104
Sn	-2.209549426613660	-11.864518241054867	14.319673229937839
Sn	0.059248102544822	-7.730661114284366	14.202911361703830
Sn	-4.684455256481155	-24.022563534631335	14.292610659056461
Sn	-2.407031534740609	-19.805306691018096	14.133021574663100

Sn	-0.017633565614266	-15.992478135546653	14.326196509698086
O	-13.999204418126952	-28.901178036194032	17.135841561329279
O	-17.151193868951907	-29.854628525942935	17.287626204331680
O	-20.352567971298530	-30.697429348016893	17.197977164786771
O	-3.678416443601760	-22.810728271525228	17.226219565371728
O	-6.871643418266742	-23.771838109894357	17.287626204331680
O	-10.078361937598647	-24.742869873671708	17.372077545545253
O	-13.232618825693033	-25.715189735060044	17.397972084042575
O	-16.388772784600459	-26.592012941147999	17.372077545545253
O	-19.494559879032366	-27.481462736882886	17.320320715814756
O	-2.825106852058286	-19.693234098445537	16.382672065431667
O	-6.152918811075519	-20.551500409700999	16.438804697469607
O	-9.273350484924027	-21.518860415515007	17.135841561329279
O	-12.415790086088938	-22.447971971245050	17.397972084042575
O	-15.653698041121290	-23.374186412923216	17.397972084042575
O	-18.728042056131525	-24.296714521026843	16.535630222569836
O	-2.077679591194306	-16.506662428582842	17.238469694377265
O	-5.239810296458926	-17.492924238559610	17.308001523161547
O	-8.487973278690770	-18.340102661053230	17.153774747032134
O	-11.677550855908379	-19.324247900226613	16.535630222569836
O	-14.834972232769006	-20.202465305600583	17.372077545545253
O	-18.029552049852132	-21.117309665134563	17.135841561329279
O	-1.263387564264741	-13.300807853280917	17.272575330524212
O	-4.454116700133592	-14.157604354284878	17.326108628939593
O	-7.590688445008102	-15.141534413546982	17.269562875516353
O	-10.887143589911785	-16.101253046343878	17.272575330524212
O	-14.052364804051907	-17.068049882829904	17.320320715814756
O	-17.279269669814596	-17.910881488159575	17.287626204331680
O	-20.427526228482925	-18.898616568912612	16.438804697469607
O	-0.524072078279865	-10.103640608407717	17.153774747032134
O	-3.742755851140511	-10.925853270570340	17.269562875516353
O	-6.883684470811131	-11.922891384999041	16.564998200305887
O	-10.033786557721770	-12.909602307589829	17.326108628939593
O	-13.256349077437534	-13.793128176081899	17.238469694377265
O	-16.408469540889222	-14.717009775093990	17.197977164786771
O	-19.708228688873302	-15.626020724855689	17.226219565371728
O	-2.881831602749780	-7.714238160223010	17.308001523161547
O	-6.163150152512749	-8.701467489545577	17.326108628939593
O	-9.317609112154353	-9.701286463726024	17.269562875516353
O	-12.529411509094398	-10.561511751445421	17.308001523161547
O	-15.642287466157031	-11.552551344570425	16.382672065431667
O	-18.785264823161079	-12.420980567722951	17.297224586256114
O	-2.183659090087792	-4.522888707212089	16.382672065431667
O	-5.317024739671114	-5.468883545563040	17.238469694377265
O	-8.500522256191577	-6.366613251795313	17.272575330524212
O	-11.639008053397466	-7.324930881959149	17.153774747032134
O	-14.721661915409515	-32.087231141806406	16.438804697469607
O	-17.915461820427890	-33.100599120462412	17.226219565371728
O	-1.364252180226170	-1.366775860956572	17.297224586256114
O	-4.541069442780351	-26.122908997309388	17.197977164786771
O	-7.755182269818690	-26.987835497130554	17.320320715814756
O	-10.896514042928054	-27.916385699166394	16.535630222569836
O	-0.501536406981009	-21.980917722740845	17.297224586256114
Zn	-15.353342133556424	-30.219462062275291	16.924775060538614
Zn	-18.491875872169743	-31.219326667848041	17.016508046674240
Zn	-0.920818014838050	-20.174073476375529	16.998741925646328
Zn	-5.019439184114449	-24.250553451011470	17.016508046674240
Zn	-8.196711136749144	-25.147777061756440	17.221577483270039
Zn	-11.409782691498094	-26.041847466934069	17.130112194170383
Zn	-14.539948057984308	-27.067487435010783	17.252118872000185
Zn	-17.680258337699460	-28.019116637959854	17.221577483270039
Zn	-0.201776036000965	-16.930144065938151	17.055652626435133
Zn	-4.233800333520929	-21.119893250695021	16.627042259642117

Zn	-7.454614204259069	-22.032435806721903	16.924775060538614
Zn	-10.591001339280565	-22.904003186430227	17.252118872000185
Zn	-13.767369073788869	-23.845782584000961	17.200366682950332
Zn	-16.848010241917233	-24.789479845979486	17.130112194170383
Zn	-20.124884682876317	-25.736840101610611	16.971921971915233
Zn	-3.409374787649819	-17.787570206232658	16.893398431230022
Zn	-6.644727286403348	-18.681546816774890	17.031669805785121
Zn	-9.747992422857701	-19.708028619476160	16.938801534494083
Zn	-13.044314292081564	-20.706020446242853	17.130112194170383
Zn	-16.171157826167022	-21.565857134138714	17.252118872000185
Zn	-19.360457449215264	-22.433777280378408	16.938801534494083
Zn	-2.601072940623097	-14.667537919571020	17.248735160790350
Zn	-5.735503325917293	-15.593171415419254	17.125652541887661
Zn	-8.997991863495923	-16.466359078316394	17.041850940766814
Zn	-12.226315119516110	-17.394483805166182	16.971921971915233
Zn	-15.425137751048149	-18.370454057055422	17.221577483270039
Zn	-18.494150887681407	-19.285449887774771	16.924775060538614
Zn	-1.149995792571131	-8.336620417078581	17.031669805785121
Zn	-1.891772357620448	-11.482201190699769	17.041850940766814
Zn	-4.939621367145317	-12.360333856934385	17.055259431749771
Zn	-8.23455255587170	-13.387778076056490	17.055259431749771
Zn	-11.401924098810468	-14.259418392467158	17.248735160790350
Zn	-14.561046952638110	-15.205967387518790	17.055652626435133
Zn	-17.790792169212555	-16.067467637912195	17.016508046674240
Zn	-0.243789311941028	-5.029523211065910	16.627042259642117
Zn	-4.279219324751384	-9.093397069055264	17.125652541887661
Zn	-7.476879758164400	-10.020561854781072	17.055259431749771
Zn	-10.636331028163365	-11.082105302105461	17.125652541887661
Zn	-13.699800396179073	-11.999392310917569	16.893398431230022
Zn	-17.010851240747659	-12.961294064625724	16.998741925646328
Zn	-20.160029040116843	-13.768493401781861	17.214579509128413
Zn	-3.541878492937866	-5.981711265852916	16.893398431230022
Zn	-6.648056641463628	-6.841717478118754	17.248735160790350
Zn	-9.761289457715524	-7.820113517563732	17.041850940766814
Zn	-12.856330601922560	-8.750506556303186	17.031669805785121
Zn	-16.173464033370230	-9.619257324819296	16.627042259642117
Zn	-19.298227525791727	-34.420633104887472	17.214579509128413
Zn	-2.719384425311326	-2.633306249155404	16.998741925646328
Zn	-5.888230690192819	-3.632562333122783	17.055652626435133
Zn	-8.950907421039471	-28.406023848803109	16.971921971915233
Zn	-12.193657351359077	-29.395541855725583	16.938801534494083
Zn	-1.843850657523473	-23.348221248910818	17.214579509128413

64/57 Pb

	-15.7508035509000006	-21.2187048969000003	0.0000000000000000
	26.2513392516000010	-3.0312435566999998	0.0000000000000000
	0.0000000000000000	0.0000000000000000	21.8736514974999992
Pb	-12.250624985946063	-21.218704897809303	5.499999999853009
Pb	-10.500535701114508	-18.187461341109305	5.499999999853009
Pb	-8.750446418907952	-15.156217784106195	5.499999999853009
Pb	-7.000357134076216	-12.124974227406216	5.499999999853009
Pb	-5.250267851869847	-9.093730670403087	5.499999999853009
Pb	-3.500178567038107	-6.062487113703108	5.499999999853009
Pb	-1.750089284831551	-3.031243556700000	5.499999999853009
Pb	0.0000000000000000	0.0000000000000000	5.499999999853009
Pb	-8.750446416792130	-21.218704896899958	5.499999999853009
Pb	-7.000357134585574	-18.187461339896849	5.499999999853009
Pb	-5.250267849753838	-15.156217783196871	5.499999999853009
Pb	-3.500178567547468	-12.124974226193741	5.499999999853009
Pb	-1.750089282715727	-9.093730669493763	5.499999999853009
Pb	-0.000000000509171	-6.062487112490652	5.499999999853009
Pb	1.750089284322380	-3.031243555790653	5.499999999853009
Pb	-5.250267851838304	-21.218704897809413	5.499999999853009

Pb	-3.500178567006566	-18.187461341109433	5.49999999853009
Pb	-1.750089284800197	-15.156217784106303	5.49999999853009
Pb	0.000000000031545	-12.124974227406325	5.49999999853009
Pb	1.750089282238209	-9.093730670403067	5.49999999853009
Pb	3.500178567069760	-6.062487113703066	5.49999999853009
Pb	5.250267849276316	-3.031243556699958	5.49999999853009
Pb	-1.750089282684076	-21.218704896899936	5.49999999853009
Pb	-0.000000000477707	-18.187461339896807	5.49999999853009
Pb	1.750089284354035	-15.156217783196826	5.49999999853009
Pb	3.500178566560589	-12.124974226193720	5.49999999853009
Pb	5.250267851392140	-9.093730669493718	5.49999999853009
Pb	7.000357133598695	-6.062487112490611	5.49999999853009
Pb	8.750446418430249	-3.031243555790611	5.49999999853009
Pb	1.750089282269752	-21.218704897809388	5.49999999853009
Pb	3.500178567101303	-18.187461341109390	5.49999999853009
Pb	5.250267849307861	-15.156217784106280	5.49999999853009
Pb	7.000357134139411	-12.124974227406280	5.49999999853009
Pb	8.750446416345969	-9.093730670403172	5.49999999853009
Pb	10.500535701177705	-6.062487113703193	5.49999999853009
Pb	12.250624983384077	-3.031243556700065	5.49999999853009
Pb	5.250267851423681	-21.218704896900043	5.49999999853009
Pb	7.000357133630240	-18.187461339896934	5.49999999853009
Pb	8.750446418461790	-15.156217783196935	5.49999999853009
Pb	10.500535700668461	-12.124974226193673	5.49999999853009
Pb	12.250624985500199	-9.093730669493695	5.49999999853009
Pb	14.000714267706568	-6.062487112490567	5.49999999853009
Pb	15.750803552538306	-3.031243555790589	5.49999999853009
Pb	8.750446416377622	-21.218704897809346	5.49999999853009
Pb	10.500535701209172	-18.187461341109348	5.49999999853009
Pb	12.250624983415729	-15.156217784106239	5.49999999853009
Pb	14.000714268247467	-12.124974227406261	5.49999999853009
Pb	15.750803550453837	-9.093730670403131	5.49999999853009
Pb	17.500892835285573	-6.062487113703153	5.49999999853009
Pb	19.250982117492129	-3.031243556700044	5.49999999853009
Pb	12.250624985531553	-21.218704896900000	5.49999999853009
Pb	14.000714267738108	-18.187461339896892	5.49999999853009
Pb	15.750803552569845	-15.156217783196912	5.49999999853009
Pb	17.500892834776216	-12.124974226193784	5.49999999853009
Pb	19.250982119607954	-9.093730669493805	5.49999999853009
Pb	21.001071401814514	-6.062487112490697	5.49999999853009
Pb	22.751160686646060	-3.031243555790697	5.49999999853009
Pb	-10.503010564994879	-20.243643469301499	8.346752053071603
Pb	-8.744248780225021	-17.189624014333162	8.331062272508856
Pb	-6.983776123979470	-14.137729349018366	8.320158821440316
Pb	-5.252284667140401	-11.086311800007058	8.319318724282850
Pb	-3.520504647908873	-8.047580718384674	8.331230068630255
Pb	-1.779468526390273	-5.032252753398458	8.346752053071603
Pb	-0.010956135447088	-2.024479734303077	8.350254680501177
Pb	-13.992074603823788	-20.215953321377512	8.350254680501177
Pb	-7.021141885813022	-20.243760996957118	8.331230068630255
Pb	-5.257130238047621	-17.192161081482702	8.309127852291207
Pb	-3.497978137746450	-14.144017150217408	8.307770800409674
Pb	-1.759747424376306	-11.101059577787675	8.309127852291207
Pb	-0.013990987117865	-8.082394865706288	8.331062272508856
Pb	1.730089474699511	-5.075332408712779	8.344671347547660
Pb	3.484792991815349	-2.053847572309184	8.349835662215382
Pb	-3.523633564239704	-20.224160946574109	8.319318724282850
Pb	-1.752736318372033	-17.176034250995052	8.307770800409674
Pb	0.000446605918295	-14.148601949287515	8.307770800409674
Pb	1.748790994599482	-11.132956241347296	8.320158821440316
Pb	3.493977387055188	-8.123246390470531	8.340051300197100
Pb	5.227584855847712	-5.103992125474120	8.356019853269400
Pb	6.970927215460362	-2.072996035007047	8.355969609702623

Pb	-0.015282720819712	-20.197967760134208	8.320158821440316
Pb	1.766609808023635	-17.175432693048407	8.309127852291207
Pb	3.525650381180403	-14.158180603918701	8.319318724282850
Pb	5.274757489794986	-11.157667034778873	8.335130823606132
Pb	6.996208359220303	-8.137181199482377	8.356442185284632
Pb	8.715851691362950	-5.101624210637723	8.361138030723581
Pb	10.449699726866466	-2.056450986692520	8.343142317643521
Pb	3.507971917142589	-20.196634470460680	8.331062272508856
Pb	5.291378683521895	-17.177311635158212	8.331230068630255
Pb	7.056624633355892	-14.172017534869656	8.343142317643521
Pb	8.784313736239657	-11.147555329410292	8.353692321908955
Pb	10.484912590879279	-8.112016131484868	8.364929188076580
Pb	12.205116279716318	-5.064904740246655	8.353692321908955
Pb	13.951137407630856	-2.020484024251785	8.335130823606132
Pb	7.032211241185452	-20.192757127799915	8.346752053071603
Pb	8.810339321214199	-17.176450379578146	8.355969609702623
Pb	10.560746021971381	-14.150987367952222	8.361138030723581
Pb	12.283291451009223	-11.113739727712009	8.364929188076580
Pb	13.983670910411204	-8.055436151103253	8.364929188076580
Pb	15.706229438059140	-5.021547126196328	8.356442185284632
Pb	1.718609271834934	-23.214198435785597	8.340051300197100
Pb	10.536823377904803	-20.205105409606976	8.349835662215382
Pb	12.306930116764365	-17.170731105573125	8.356019853269400
Pb	14.049437155020561	-14.122463684621295	8.356442185284632
Pb	15.762444940544018	-11.068731938824405	8.353692321908955
Pb	17.475277238965674	-8.028580431710054	8.361138030723581
Pb	19.217359983888215	-5.006468777433978	8.356019853269400
Pb	5.240124163184790	-23.210583687264428	8.344671347547660
Pb	-12.220481492284589	-17.182737256341575	8.344671347547660
Pb	-10.462854509090121	-14.131208524243869	8.340051300197100
Pb	17.525980054873859	-14.103040951269472	8.335130823606132
Pb	19.245550592077642	-11.052723488737822	8.343142317643521
Pb	20.970608415625740	-8.031745595714677	8.355969609702623
Pb	22.730258582580149	-5.022239028383711	8.349835662215382
Pb	8.752762889070874	-23.228220294819412	8.350254680501177
Pb	-12.236195802235391	-19.214811821492219	11.201368101939845
Pb	-10.462984415787526	-16.164844909009670	11.184319427349676
Pb	-8.696423613495657	-13.100515205871414	11.156372838878523
Pb	-6.964637588286234	-10.038444872600099	11.164091140807320
Pb	21.013159234019117	-10.034824766221492	11.197984253856248
Pb	22.739287764440139	-7.024572028878083	11.206516423652557
Pb	24.494974645350531	-4.021036307165733	11.208728717961701
Pb	10.521532337436067	-22.233995711044493	11.208728717961701
Pb	-8.765665992407316	-19.210565248855630	11.187083061174976
Pb	-6.994596131987076	-16.165397109347293	11.138759880841501
Pb	-5.226930094200050	-13.109848101655807	11.131377762484957
Pb	-3.489239677340333	-10.070720417650890	11.143498510494791
Pb	-1.753468831253116	-7.053376400734138	11.187083061174976
Pb	-0.021881564554097	-4.045686132390621	11.201368101939845
Pb	1.735367969513402	-1.026159992089772	11.208728717961701
Pb	-5.284683996128603	-19.205114888567632	11.143498510494791
Pb	-3.509111791847918	-16.162734353746366	11.119145867184868
Pb	-1.742246948342938	-13.129601320229359	11.119145867184868
Pb	-0.001810792275805	-10.109751959374670	11.138759880841501
Pb	1.732861569136846	-7.106315695583122	11.184319427349676
Pb	3.461256778632470	-4.085931336170018	11.201725117082260
Pb	5.214349648773789	-1.044861571503478	11.206516423652557
Pb	-1.783877010627883	-19.190435091182717	11.131377762484957
Pb	0.001090889991158	-16.176317676524150	11.119145867184868
Pb	1.760539250427941	-13.168370159480126	11.131377762484957
Pb	3.503368536483070	-10.168367079274100	11.156372838878523
Pb	5.219572583176483	-7.147679830400560	11.206473432471608
Pb	6.936581874852561	-4.097591011126623	11.223525051715326

Pb	8.684369253713353	-1.034606360077663	11.197984253856248
Pb	1.746139074062881	-19.193504281778040	11.138759880841501
Pb	3.523655823268934	-16.192818044281477	11.143498510494791
Pb	5.289306220669122	-13.199172937667262	11.164091140807320
Pb	7.012297077410213	-10.187636847529845	11.198609528962283
Pb	8.707919850900943	-7.131782001075233	11.231866774668507
Pb	10.416152108774957	-4.060115335111768	11.218171493865205
Pb	-3.574936482582588	-22.231035540232511	11.164091140807320
Pb	5.268866969260142	-19.204711702729011	11.187083061174976
Pb	7.054346464567828	-16.211760884000714	11.197984253856248
Pb	8.808622668789216	-13.199238450168245	11.218171493865205
Pb	10.518344202702620	-10.149143329204229	11.229562171156529
Pb	12.202751200535259	-7.065825177367161	11.229562171156529
Pb	13.922438398422537	-4.010252540834614	11.198609528962283
Pb	-0.057212773187411	-22.199771065354483	11.156372838878523
Pb	8.798237543286364	-19.211758408099662	11.206516423652557
Pb	10.580862673211300	-16.193896828990898	11.223525051715326
Pb	12.322880165036759	-13.142777648380040	11.231866774668507
Pb	14.030779549062423	-10.066223503728484	11.229562171156529
Pb	15.721074940562588	-7.006632359025949	11.231866774668507
Pb	17.451480648781086	-3.977686095412720	11.206473432471608
Pb	3.479854996450383	-22.197492745907340	11.184319427349676
Pb	12.308427646616897	-19.209446486206389	11.201725117082260
Pb	14.080821720342433	-16.155826084486719	11.206473432471608
Pb	15.817139476467549	-13.083302621935411	11.198609528962283
Pb	17.527100174735530	-10.021838225020115	11.218171493865205
Pb	19.234430404236143	-6.989704170182478	11.223525051715326
Pb	20.982190527050637	-3.985814187923595	11.201725117082260
Pb	7.007809516589489	-22.208155396617158	11.201368101939845
Pb	-12.289799550523853	-21.185654273955286	14.039235495680463
Pb	-10.518393228129565	-18.047165541998499	14.046680985402947
Pb	-8.665300074163927	-14.971577746770567	14.034423310822902
Pb	-6.813273088104909	-11.962667686279898	14.014672725576133
Pb	-5.026427749332367	-8.982135436414540	14.043049866704504
Pb	-3.335871885266129	-6.012296535806409	14.059188548325077
Pb	-1.701879322674247	-3.013842700520508	14.039235495680463
Pb	0.000000000000000	0.000000000000000	14.042289929234823
Pb	-8.876066073167639	-21.101506425422084	14.059188548325077
Pb	-7.070894421029264	-18.014115518414126	14.029803619942447
Pb	-5.206271328892491	-15.023367907154034	13.998731428059363
Pb	-3.360746618106414	-12.070495078252367	14.001307287909729
Pb	-1.564698754450174	-9.119316498261238	14.029803619942447
Pb	0.130428489072469	-6.117169940002564	14.046680985402947
Pb	1.757557057134945	-3.055925954662165	14.034088944549746
Pb	-5.458832210682864	-21.080651299620200	14.043049866704504
Pb	-3.617074867821151	-18.093949304764816	14.001307287909729
Pb	-1.750089284800197	-15.156217784106303	13.986069037643192
Pb	0.093053107143637	-12.229501270172111	13.998731428059363
Pb	1.867419072754696	-9.259789586659034	14.034423310822902
Pb	3.544233996256007	-6.186696373909810	14.045142161810610
Pb	5.168438954740085	-3.053188903931744	14.046732929079038
Pb	-1.984192893485876	-21.137838631008748	14.014672725576133
Pb	-0.137049628451150	-18.215784173173851	13.998731428059363
Pb	1.727553635727567	-15.304208967482818	14.001307287909729
Pb	3.547198131391085	-12.368147033211226	14.014672725576133
Pb	5.295859938934587	-9.343587255843914	14.042673060284306
Pb	6.935099294601036	-6.191879168735573	14.057989518869249
Pb	8.564066367878477	-2.978180111144105	14.055376437838255
Pb	1.547613147009239	-21.237286018889048	14.034423310822902
Pb	3.385325325279439	-18.335221333824634	14.029803619942447
Pb	5.234992105614943	-15.405866616284040	14.043049866704504
Pb	7.030691869986553	-12.404601856247307	14.053646945949019
Pb	8.738630002810446	-9.292493244189284	14.046505076836963

Pb	10.345550455537426	-6.069887597788980	14.053595297953434
Pb	11.993292985284324	-2.917700394139645	14.053646945949019
Pb	5.137696888857093	-21.304317868498938	14.046680985402947
Pb	6.961670108233768	-18.354850389271505	14.059188548325077
Pb	8.797682152662114	-15.344159364056607	14.055376437838255
Pb	10.584437330707539	-12.255495144087099	14.053595297953434
Pb	12.250624985500199	-9.093730669493695	14.025648682946521
Pb	13.834489036254006	-5.952872511293672	14.046505076836963
Pb	15.511625357685126	-2.945799168638263	14.042673060284306
Pb	8.741411018798113	-21.269156377842855	14.039235495680463
Pb	10.560455376675254	-18.247354568925523	14.046732929079038
Pb	12.395310710670714	-15.148036702352115	14.057989518869249
Pb	14.178755913235548	-12.035826254817042	14.046505076836963
Pb	15.821887166055038	-8.955809268423922	14.053595297953434
Pb	17.421464947028255	-5.941276139212310	14.057989518869249
Pb	19.121386028174832	-3.007292047446318	14.045142161810610
Pb	12.268266683574499	-21.199896416498945	14.034088944549746
Pb	14.086254927869163	-18.087203588943872	14.045142161810610
Pb	15.944389659880578	-14.991805583999044	14.042673060284306
Pb	17.727890097028833	-11.958889759913175	14.053646945949019
Pb	19.390126435959697	-8.958852533280513	14.055376437838255
Pb	21.022980620884962	-5.980648537442605	14.046732929079038
Pb	22.726051215790847	-3.025369637320110	14.034088944549746
O	9.386277148904457	-19.294932491063346	17.269663940801632
O	6.145585890371187	-18.884662072030743	17.228584599794942
O	2.895387277358624	-18.514727508201450	17.165775293183966
O	-0.377270084552967	-18.178056498086303	17.140314846622847
O	-3.670763005168727	-17.845006569762894	17.139483234601737
O	-6.981382213911667	-17.500063728807348	17.165775293183966
O	-10.296687950143347	-17.115643082716510	17.208706452392519
O	12.654357785077440	-19.716883275217370	17.257856327780019
O	11.317611354627216	-16.655985333246353	17.286112561711136
O	8.066877459627499	-16.212726782438629	17.267836335502185
O	4.810905320516390	-15.819072751270673	17.177861774057138
O	1.538806937150552	-15.475175753120384	17.139483234601737
O	-1.750089265374081	-15.156217857765499	17.129186948971387
O	-5.053487885485976	-14.834194820567273	17.140314846622847
O	-8.359081059907892	-14.485162396350004	17.160732503829248
O	14.596591056639536	-17.109498816434581	17.231555385408807
O	13.271149827267637	-14.049416547395420	17.302650479026394
O	10.011496238058454	-13.577888254893379	17.318223295130426
O	6.747948071481423	-13.150412234195672	17.222865388899166
O	3.470433886904143	-12.779078811496374	17.156665567047920
O	0.180490177066913	-12.456402250399107	17.140314846622847
O	-3.118311724953856	-12.148471246169404	17.139483234601737
O	-6.419013639720962	-11.823681708156640	17.156665567047920
O	16.542944159903740	-14.483445478657755	17.207589745978254
O	15.251935814223376	-11.433898183360863	17.318401537427896
O	11.996654746210474	-10.979617101129667	17.376957766612840
O	8.723325144805486	-10.522858432792717	17.318401537427896
O	5.436835543149802	-10.116130806569648	17.207589745978254
O	2.13557708811831	-9.768190801003648	17.160732503829248
O	-1.164272857993797	-9.453862334165665	17.165775293183966
O	-4.456537381535815	-9.142802425539204	17.177861774057138
O	18.515152696914715	-11.830848008399105	17.222865388899166
O	17.253583705476501	-8.790794381442334	17.318223295130426
O	14.010835625267024	-8.370732257294250	17.376957766612840
O	10.744384636475367	-7.930842872550676	17.376957766612840
O	7.448612790961011	-7.499688266605061	17.302650479026394
O	4.135783193620703	-7.117512907938305	17.231555385408807
O	0.826298054318159	-6.774933665897185	17.208706452392519
O	-2.468999434493623	-6.454140486037057	17.228584599794942
O	20.507730191794586	-9.157464380170563	17.267836335502185

O	19.266236409731430	-6.120616970753855	17.286112561711136
O	16.032112389724215	-5.732087416974109	17.302650479026394
O	12.776614047348895	-5.324435616942919	17.318401537427896
O	9.486795065993014	-4.912509592516971	17.318223295130426
O	6.168027242019108	-4.504589929096291	17.286112561711136
O	2.848838649609314	-4.131797322867439	17.257856327780019
O	-0.454773255649515	-3.782311623031319	17.254009763556692
O	22.517298790510651	-6.473727877205631	17.269663940801632
O	21.248678573265813	-3.432511632889910	17.257856327780019
O	18.019500756117516	-3.054180508723614	17.231555385408807
O	14.772095304899322	-2.681615945747188	17.207589745978254
O	11.488774241131832	-2.299931986257905	17.222865388899166
O	8.177267354955671	-1.911001070487311	17.267836335502185
O	4.848299066962646	-1.512531864827526	17.269663940801632
O	1.537144872518077	-1.130499952876273	17.251572720264164
O	24.503725228531486	-3.797200184944757	17.251572720264164
O	7.452344469305249	-21.964947545508789	17.254009763556692
O	4.220122101278053	-21.578076822560892	17.208706452392519
O	0.9732555565408926	-21.215300373820941	17.160732503829248
O	-2.301688040155209	-20.865893049399670	17.156665567047920
O	-5.604635735102521	-20.506778396486496	17.177861774057138
O	-8.926854248849592	-20.129851010984883	17.228584599794942
O	-12.247839009777980	-19.721394404756396	17.254009763556692
O	10.711004906903305	-22.353492093153562	17.251572720264164
Zn	7.647112622852841	-20.070376890903013	17.214585320617722
Zn	4.416130142423720	-19.679938429928239	17.160165772037082
Zn	1.165445351651098	-19.316195248187608	17.122768512248776
Zn	-2.117433803207776	-18.968804321918000	17.115298028045739
Zn	-5.425013196394806	-18.612096813422685	17.125276668277223
Zn	-8.750856087607373	-18.234460037109510	17.160165772037082
Zn	-12.075441963670443	-17.824020598580717	17.202211832640657
Zn	10.894233537595863	-20.458309273242993	17.214366006595647
Zn	9.561446606515403	-17.397129362096216	17.228885368827623
Zn	6.330803119517368	-16.982305143140039	17.192945183555846
Zn	3.080251738500293	-16.610855608985567	17.125276668277223
Zn	-0.198162624136030	-16.275011057923830	17.105207165337443
Zn	-3.494956102142091	-15.940828966778529	17.105207165337443
Zn	-6.810502857437805	-15.601156017049869	17.122768512248776
Zn	-10.132315071904250	-15.219505536789180	17.160004676736996
Zn	12.817673663939503	-17.818087803081006	17.215738811079305
Zn	11.498739967032899	-14.758728799236518	17.251004963380325
Zn	8.262803777958178	-14.313425365690279	17.224825843257186
Zn	5.008029454308865	-13.913935500796915	17.147325243489821
Zn	1.735379805976812	-13.568054075203861	17.115298028045739
Zn	-1.557149182724958	-13.252813109366867	17.105207165337443
Zn	-4.868213911772115	-12.931794736947364	17.115298028045739
Zn	-8.180444944379886	-12.585921409298637	17.134974431847194
Zn	14.767528186212919	-15.213274404990617	17.204343483868229
Zn	13.483813037311197	-12.155987293994507	17.293116780086976
Zn	10.233195730456689	-11.682322670269858	17.300575393442394
Zn	6.971962202636848	-11.246018770668917	17.208177869383970
Zn	3.691030410508381	-10.872514521586545	17.134974431847194
Zn	0.394789598358923	-10.551301866709863	17.122768512248776
Zn	-2.905506451108566	-10.245700711660975	17.125276668277223
Zn	-6.204996634684861	-9.924656291008892	17.147325243489821
Zn	16.753892579275135	-12.589042561390078	17.208177869383970
Zn	15.501126076182363	-9.546579528824109	17.300575393442394
Zn	12.250624964498975	-9.093730597956407	17.336924269826049
Zn	8.982038837993651	-8.630574446508261	17.293116780086976
Zn	5.692492957186105	-8.213660823297410	17.204343483868229
Zn	2.386214716856643	-7.865353342510692	17.160004676736996
Zn	-0.915541963819427	-7.554254667031474	17.160165772037082
Zn	-4.209097408822874	-7.244915872316248	17.192945183555846

Zn	18.764923826635087	-9.937437667396541	17.224825843257186
Zn	17.532599817933779	-6.912383005859370	17.251004963380325
Zn	14.286023019767185	-6.494630051244547	17.293116780086976
Zn	11.017553086857870	-6.052289594775257	17.300575393442394
Zn	7.720535108530132	-5.610079988773488	17.251004963380325
Zn	4.411585643454830	-5.222630574273023	17.215738811079305
Zn	1.102201954685447	-4.880298560562266	17.202211832640657
Zn	-2.192903578222737	-4.560922529309945	17.214585320617722
Zn	20.786168410991788	-7.270927989227113	17.228885368827623
Zn	19.522615586102589	-4.240473416515196	17.215738811079305
Zn	16.291853750097896	-3.854256565581200	17.204343483868229
Zn	13.026020111584938	-3.446130461810228	17.208177869383970
Zn	9.724147288903652	-3.030328760782405	17.224825843257186
Zn	6.404259875989731	-2.613134442545894	17.228885368827623
Zn	3.086806841845815	-2.236771827113421	17.214366006595647
Zn	-0.208327968987796	-1.890665113834870	17.210801936200212
Zn	22.770834514055540	-4.586110693512683	17.214366006595647
Zn	5.722972099981915	-22.764333974926245	17.202211832640657
Zn	2.495832446044526	-22.383794254769356	17.160004676736996
Zn	-0.760853375131573	-22.010217203184045	17.134974431847194
Zn	-4.053300728627082	-21.630061342263417	17.147325243489821
Zn	-7.371973619697572	-21.241432118612938	17.192945183555846
Zn	-10.704476953633186	-20.837353713856267	17.214585320617722
Zn	-14.009275514699361	-20.453789528258785	17.210801936200212
Zn	8.967335574684261	-23.124198491975591	17.210801936200212

Wurtzite ZnO(0001) on metals

25/36 Ru

194

Lattice="16.26 0.0 0.0 8.13 14.0815730655 0.0 0.0 0.0 20.3467162508"

Ru	16.26000000	1.56461923	5.50000000
Ru	17.61500000	3.91154807	5.50000000
Ru	18.97000000	6.25847692	5.50000000
Ru	20.32500000	8.60540576	5.50000000
Ru	21.68000000	10.95233461	5.50000000
Ru	23.03500000	13.29926345	5.50000000
Ru	2.71000000	1.56461923	5.50000000
Ru	4.06500000	3.91154807	5.50000000
Ru	5.42000000	6.25847692	5.50000000
Ru	6.77500000	8.60540576	5.50000000
Ru	8.13000000	10.95233461	5.50000000
Ru	9.48500000	13.29926345	5.50000000
Ru	5.42000000	1.56461923	5.50000000
Ru	6.77500000	3.91154807	5.50000000
Ru	8.13000000	6.25847692	5.50000000
Ru	9.48500000	8.60540576	5.50000000
Ru	10.84000000	10.95233461	5.50000000
Ru	12.19500000	13.29926345	5.50000000
Ru	8.13000000	1.56461923	5.50000000
Ru	9.48500000	3.91154807	5.50000000
Ru	10.84000000	6.25847692	5.50000000
Ru	12.19500000	8.60540576	5.50000000
Ru	13.55000000	10.95233461	5.50000000
Ru	14.90500000	13.29926345	5.50000000
Ru	10.84000000	1.56461923	5.50000000
Ru	12.19500000	3.91154807	5.50000000
Ru	13.55000000	6.25847692	5.50000000
Ru	14.90500000	8.60540576	5.50000000
Ru	16.26000000	10.95233461	5.50000000
Ru	17.61500000	13.29926345	5.50000000
Ru	13.55000000	1.56461923	5.50000000
Ru	14.90500000	3.91154807	5.50000000

Ru	16.26000000	6.25847692	5.50000000
Ru	17.61500000	8.60540576	5.50000000
Ru	18.97000000	10.95233461	5.50000000
Ru	20.32500000	13.29926345	5.50000000
Ru	24.36739875	14.06852423	7.57236832
Ru	17.59450673	2.34390500	7.53609415
Ru	18.96237209	4.71311730	7.53609415
Ru	20.32500000	7.06688421	7.57236832
Ru	21.67240557	9.39823303	7.59760328
Ru	23.02209423	11.73596236	7.59760328
Ru	10.82713464	14.06533730	7.53609415
Ru	4.06500000	2.34692884	7.51061654
Ru	5.42762791	4.71311730	7.53609415
Ru	6.77575365	7.05735377	7.56833568
Ru	8.12530684	9.39042498	7.57967770
Ru	9.47102918	11.72570793	7.56833568
Ru	13.56286536	14.06533730	7.53609415
Ru	6.79549327	2.34390500	7.53609415
Ru	8.14278964	4.70124179	7.54659987
Ru	9.48677945	7.04375614	7.55836183
Ru	10.83831797	9.38468952	7.55836183
Ru	12.19500000	11.71987601	7.54659987
Ru	16.28260125	14.06852423	7.57236832
Ru	9.49972447	2.33929790	7.56833568
Ru	10.84346149	4.69391393	7.55836183
Ru	12.19500000	7.04078653	7.55972772
Ru	13.55168203	9.38468952	7.55836183
Ru	14.91897082	11.72570793	7.56833568
Ru	18.97531134	14.06973727	7.59760328
Ru	12.19500000	2.34150965	7.57967770
Ru	13.54653851	4.69391393	7.55836183
Ru	14.90322055	7.04375614	7.55836183
Ru	16.26469316	9.39042498	7.57967770
Ru	17.62790577	11.73596236	7.59760328
Ru	21.67468866	14.06973727	7.59760328
Ru	14.89027553	2.33929790	7.56833568
Ru	16.24721036	4.70124179	7.54659987
Ru	17.61424635	7.05735377	7.56833568
Ru	18.97759443	9.39823303	7.59760328
Ru	20.32500000	11.73464422	7.62936105
Ru	16.25748350	1.56236868	9.66588873
Ru	17.61470088	3.91172077	9.62469415
Ru	18.97069079	6.26178154	9.66588873
Ru	20.32500000	8.60007200	9.77136105
Ru	21.68541272	10.94920957	9.78082346
Ru	23.03961917	13.30193033	9.77136105
Ru	2.72089273	1.57090815	9.58157045
Ru	4.06500000	3.89897023	9.58157045
Ru	5.41930921	6.26178154	9.66588873
Ru	6.77296957	8.60618232	9.72871000
Ru	8.12831227	10.95370473	9.72871000
Ru	9.48179272	13.29820938	9.66588873
Ru	5.40910727	1.57090815	9.58157045
Ru	6.77529912	3.91172077	9.62469415
Ru	8.13476342	6.25840870	9.68051193
Ru	9.48824679	8.60353123	9.71192003
Ru	10.84244079	10.94824348	9.68051193
Ru	12.19500000	13.29891805	9.62469415
Ru	8.13251649	1.56236868	9.66588873
Ru	9.48732263	3.91570742	9.68051193
Ru	10.84194363	6.25959907	9.68068223
Ru	12.19500000	8.60316145	9.68068223
Ru	13.54755921	10.94824348	9.68051193

Ru	14.90820728	13.29820938	9.66588873
Ru	10.83965730	1.56247255	9.72871000
Ru	12.19500000	3.91529715	9.71192003
Ru	13.54805637	6.25959907	9.68068223
Ru	14.90175321	8.60353123	9.71192003
Ru	16.26168773	10.95370473	9.72871000
Ru	17.61038083	13.30193033	9.77136105
Ru	13.55034270	1.56247255	9.72871000
Ru	14.90267737	3.91570742	9.68051193
Ru	16.25523658	6.25840870	9.68051193
Ru	17.61703043	8.60618232	9.72871000
Ru	18.96458728	10.94920957	9.78082346
Ru	20.32500000	13.30551352	9.78082346
Ru	0.12892934	0.07443739	11.77684625
Ru	1.40999639	2.37564965	11.65229293
Ru	2.71262525	4.63186902	11.65229293
Ru	4.06500000	6.89191175	11.77684625
Ru	5.45529050	9.33575905	11.85387543
Ru	6.83764075	11.73005991	11.85387543
Ru	2.76237114	0.03326787	11.65229293
Ru	4.06500000	2.34692884	11.66269630
Ru	5.41737475	4.63186902	11.65229293
Ru	6.80935197	6.96465148	11.75045029
Ru	8.18606484	9.35534633	11.77870750
Ru	9.56811087	11.74296207	11.75045029
Ru	5.36762886	0.03326787	11.65229293
Ru	6.72000361	2.37564965	11.65229293
Ru	8.09383625	4.67297854	11.70048329
Ru	9.50149804	7.02327330	11.74860416
Ru	10.86341593	9.38218428	11.74860416
Ru	12.19500000	11.77640252	11.70048329
Ru	8.00107066	0.07443739	11.77684625
Ru	9.43624109	2.41474605	11.75045029
Ru	10.83308211	4.71690203	11.74860416
Ru	12.19500000	7.04078653	11.74044332
Ru	13.52658407	9.38218428	11.74860416
Ru	14.82188913	11.74296207	11.75045029
Ru	10.81264975	0.05654064	11.85387543
Ru	12.19500000	2.41166694	11.77870750
Ru	13.55691789	4.71690203	11.74860416
Ru	14.88850196	7.02327330	11.74860416
Ru	16.20393516	9.35534633	11.77870750
Ru	17.55235925	11.73005991	11.85387543
Ru	13.57735025	0.05654064	11.85387543
Ru	14.95375891	2.41474605	11.75045029
Ru	16.29616375	4.67297854	11.70048329
Ru	17.58064803	6.96465148	11.75045029
Ru	18.93470950	9.33575905	11.85387543
Ru	20.32500000	11.73464422	11.83450026
O	0.76245617	0.44020427	14.02010728
O	4.06500000	0.46659113	14.70449963
O	2.43657977	3.28709770	14.70449963
O	7.36754383	0.44020427	14.02010728
O	5.69342022	3.28709770	14.70449963
O	4.06500000	6.16037798	14.02010728
O	10.64018800	0.43081176	14.10098912
O	8.96380493	3.23984007	14.54928888
O	7.28768627	6.14296275	14.54928888
O	5.69318793	8.99926722	14.10098912
O	13.74981200	0.43081176	14.10098912
O	12.19500000	3.26263716	14.74716907
O	10.55615865	6.09460104	14.52250785
O	8.92302666	8.92986122	14.74716907

O	7.24799993	11.69228061	14.10098912
O	15.42619507	3.23984007	14.54928888
O	13.83384135	6.09460104	14.52250785
O	12.19500000	8.93315752	14.52250785
O	10.51888134	11.73955678	14.54928888
O	17.10231373	6.14296275	14.54928888
O	15.46697333	8.92986122	14.74716907
O	13.87111866	11.73955678	14.54928888
O	18.69681207	8.99926722	14.10098912
O	17.14200007	11.69228061	14.10098912
O	20.32500000	11.73464422	15.11816769
Zn	17.08884311	2.40243493	14.25612293
Zn	4.06500000	2.34692884	14.44686762
Zn	18.65885188	5.12176989	14.25612293
Zn	7.30115690	2.40243493	14.25612293
Zn	5.73114812	5.12176989	14.25612293
Zn	20.32500000	8.04293396	14.16656903
Zn	10.62162701	2.39432324	14.23280739
Zn	8.92443795	5.15252665	14.32724924
Zn	7.38435826	8.00143720	14.23280739
Zn	21.77020062	10.90025726	14.23527080
Zn	13.76837300	2.39432324	14.23280739
Zn	12.19500000	5.13746073	14.33690488
Zn	10.54667150	7.99244943	14.33690488
Zn	8.95773125	10.72659916	14.23280739
Zn	23.52211487	13.58049935	14.16656903
Zn	15.46556205	5.15252665	14.32724924
Zn	13.84332850	7.99244943	14.33690488
Zn	12.19500000	10.81730629	14.32724924
Zn	10.62499123	13.59815479	14.25612293
Zn	17.00564175	8.00143720	14.23280739
Zn	15.43226875	10.72659916	14.23280739
Zn	13.76500877	13.59815479	14.25612293
Zn	18.87979938	10.90025726	14.23527080
Zn	17.12788513	13.58049935	14.16656903
Zn	20.32500000	13.40341815	14.23527080

28/39 Pd

212

Lattice="-12.3779042047 -11.9106438743 0.0 4.1259680682 -16.674901424 0.0 0.0 0.0 20.6643938922"

Pd	-11.00258152	-14.29277265	5.50000000
Pd	-9.62725883	-11.91064387	5.50000000
Pd	-8.25193614	-9.52851510	5.50000000
Pd	-6.87661345	-7.14638632	5.50000000
Pd	-9.62725883	-16.67490142	5.50000000
Pd	-8.25193614	-14.29277265	5.50000000
Pd	-6.87661345	-11.91064387	5.50000000
Pd	-5.50129076	-9.52851510	5.50000000
Pd	-4.12596807	-7.14638632	5.50000000
Pd	-2.75064538	-4.76425755	5.50000000
Pd	-1.37532269	-2.38212878	5.50000000
Pd	0.00000000	0.00000000	5.50000000
Pd	-9.62725883	-21.43915897	5.50000000
Pd	-8.25193614	-19.05703020	5.50000000
Pd	-6.87661345	-16.67490142	5.50000000
Pd	-5.50129076	-14.29277265	5.50000000
Pd	-4.12596807	-11.91064387	5.50000000
Pd	-2.75064538	-9.52851510	5.50000000
Pd	-1.37532269	-7.14638633	5.50000000
Pd	0.00000000	-4.76425755	5.50000000
Pd	-8.25193614	-23.82128775	5.50000000
Pd	-6.87661345	-21.43915897	5.50000000
Pd	-5.50129076	-19.05703020	5.50000000

Pd	-4.12596807	-16.67490142	5.50000000
Pd	-2.75064538	-14.29277265	5.50000000
Pd	-1.37532269	-11.91064387	5.50000000
Pd	0.00000000	-9.52851510	5.50000000
Pd	1.37532269	-7.14638632	5.50000000
Pd	-6.87661345	-26.20341652	5.50000000
Pd	-5.50129076	-23.82128775	5.50000000
Pd	-4.12596807	-21.43915897	5.50000000
Pd	-2.75064538	-19.05703020	5.50000000
Pd	-1.37532269	-16.67490142	5.50000000
Pd	-0.00000000	-14.29277265	5.50000000
Pd	1.37532269	-11.91064387	5.50000000
Pd	-1.37532269	-21.43915897	5.50000000
Pd	-0.00000000	-19.05703020	5.50000000
Pd	1.37532269	-16.67490142	5.50000000
Pd	2.75064538	-14.29277265	5.50000000
Pd	-9.63103493	-13.49908600	7.78479613
Pd	-8.24676482	-11.11782883	7.78658915
Pd	-6.87555764	-8.73194359	7.79181862
Pd	-5.49170790	-6.35114583	7.78147817
Pd	-8.25873239	-15.88424628	7.77842926
Pd	-6.87970958	-13.49746698	7.78614317
Pd	-5.50314607	-11.11877613	7.78953874
Pd	-4.12678025	-8.73399372	7.78698256
Pd	-2.75240226	-6.35727970	7.78631829
Pd	-1.38232942	-3.96820307	7.79168283
Pd	-0.00880568	-1.59026010	7.79061613
Pd	-11.00037194	-11.11863269	7.78164678
Pd	-8.24832348	-20.65626358	7.78791359
Pd	-6.87759713	-18.27068251	7.77633658
Pd	-5.50117828	-15.88155917	7.78446009
Pd	-4.13279746	-13.49862719	7.79231844
Pd	-2.74808381	-11.11545283	7.78762602
Pd	-1.37415902	-8.73656996	7.79240069
Pd	-0.00201426	-6.35605409	7.78655788
Pd	-11.00806004	-15.88360422	7.78333957
Pd	-6.87048332	-23.03176085	7.79361547
Pd	-5.49370090	-20.64671954	7.78001961
Pd	-4.12448901	-18.25830777	7.78438079
Pd	-2.75823170	-15.87491401	7.78643802
Pd	-1.38066955	-13.49052380	7.78049438
Pd	0.00005745	-11.11917868	7.78597952
Pd	1.37278997	-8.73576191	7.78728811
Pd	-9.63320418	-18.27444075	7.77886030
Pd	-5.49971005	-25.40698361	7.79371239
Pd	-4.12013513	-23.03253415	7.78526856
Pd	-2.74196159	-20.63990843	7.77983090
Pd	-1.38112529	-18.25292495	7.78740646
Pd	0.00289712	-15.87269062	7.78426602
Pd	1.37991028	-13.50109350	7.78965721
Pd	-9.62260966	-23.03143763	7.79156720
Pd	-4.12289947	-3.96181787	7.79209953
Pd	1.37373137	-18.25733334	7.79519066
Pd	2.75371981	-15.88300126	7.79224820
Pd	-8.24486019	-25.40454516	7.79148832
Pd	-11.01824876	-12.70484654	10.02368869
Pd	-9.61452671	-10.32996719	10.01791047
Pd	-4.13201853	-24.60122211	10.05249506
Pd	-2.72795454	-22.22870939	10.00431649
Pd	-9.62513526	-15.08862018	10.02397575
Pd	-8.24872539	-12.70594720	10.04710954
Pd	-6.87318009	-10.31740821	10.03981684
Pd	-5.48322358	-7.92240399	10.04249593

Pd	-4.11724317	-5.55475792	10.04116184
Pd	-2.73078728	-3.15827045	10.05307418
Pd	2.74019501	-17.47232500	10.07130528
Pd	-8.24159544	-26.99023909	10.02163426
Pd	-9.62268098	-19.86598479	10.03329984
Pd	-8.27270452	-17.48516233	10.00313823
Pd	-6.88767679	-15.08243289	10.00778039
Pd	-5.52802980	-12.69320142	10.04892191
Pd	-4.12562609	-10.31937551	10.01965138
Pd	-2.75480607	-7.93989126	10.04278586
Pd	-1.37818280	-5.56627489	10.01644179
Pd	0.00005233	-3.18447606	10.03344916
Pd	-8.23789893	-22.26734309	10.04890498
Pd	-6.87000168	-19.85646478	10.02224921
Pd	-5.50367729	-17.47602035	10.02403932
Pd	-4.13965704	-15.09291392	10.04649545
Pd	-2.76001142	-12.69709944	10.03997446
Pd	-1.37290703	-10.33984063	10.04632564
Pd	0.01375371	-7.94178929	10.04789022
Pd	1.37967667	-5.58479084	10.03975527
Pd	-6.85967915	-24.60393234	10.07256456
Pd	-5.49223156	-22.23108510	10.02175945
Pd	-4.10830564	-19.82586108	10.02483146
Pd	-2.78210887	-17.45448911	10.05100489
Pd	-1.38509832	-15.06530907	10.00648091
Pd	-0.01291556	-12.70345585	10.03843361
Pd	1.37317372	-10.33308224	10.01662015
Pd	-1.37662737	-19.83650893	10.03226603
Pd	-0.00854080	-17.45872280	10.02334088
Pd	1.37581058	-15.10718102	10.04248170
Pd	2.75356905	-12.70905084	10.03876272
Pd	-10.98007141	-14.30166280	12.29626282
Pd	-9.65145907	-11.92606071	12.28376601
Pd	-8.24388423	-9.50179908	12.31011101
Pd	-6.86067086	-7.12311403	12.29913721
Pd	-9.63484320	-16.67929114	12.31017192
Pd	-8.24665673	-14.30462657	12.33643858
Pd	-6.91313369	-11.87032648	12.39407631
Pd	-5.48052999	-9.49370359	12.28700238
Pd	-4.09726551	-7.11994676	12.39491424
Pd	-2.72480346	-4.74077053	12.28435475
Pd	-1.30559685	-2.38874478	12.39153303
Pd	4.11698044	-16.63764280	12.30787374
Pd	-9.60695169	-21.48948408	12.25288929
Pd	-8.24390207	-19.07314102	12.32003270
Pd	-6.91749422	-16.69242776	12.20243026
Pd	-5.52640115	-14.27810605	12.29640111
Pd	-4.16551785	-11.89885894	12.28566174
Pd	-2.74437832	-9.54512113	12.29597443
Pd	-1.37200527	-7.15826178	12.30311880
Pd	0.01047865	-4.81355599	12.27074166
Pd	-8.26233310	-23.88593290	12.39147260
Pd	-6.87302357	-21.43418023	12.30481798
Pd	-5.50412631	-19.07005114	12.32635559
Pd	-4.19248924	-16.66021102	12.40057985
Pd	-2.77531310	-14.28250854	12.31267188
Pd	-1.40151413	-11.92854074	12.39431977
Pd	0.00548660	-9.54115925	12.30081055
Pd	1.40482593	-7.19651336	12.39568022
Pd	-6.83093221	-26.21375962	12.27663834
Pd	-5.47620087	-23.76564248	12.40009929
Pd	-4.08789162	-21.40142230	12.20889941
Pd	-2.72103223	-19.02718120	12.36557962

Pd	-1.41232774	-16.63413792	12.22992770
Pd	-0.00581175	-14.30175984	12.29243392
Pd	1.35191985	-11.91857076	12.30205275
Pd	-1.36043775	-21.42571333	12.31956831
Pd	0.01013007	-19.05875920	12.29562641
Pd	1.33524484	-16.70228278	12.38116422
Pd	2.73090253	-14.31252824	12.29946413
O	-5.40832058	-23.20353656	14.66924239
O	-8.35838197	-24.45740971	14.70707582
O	0.80573644	-17.14729925	14.78161156
O	-2.16069412	-18.58593354	14.84442879
O	-5.13541315	-19.93677234	15.06345903
O	-8.08546326	-21.23617996	15.18877376
O	1.09092339	-13.92724479	15.17590170
O	-1.83612264	-15.32260748	15.18756355
O	-4.75445195	-16.66124373	14.68016657
O	-7.74255514	-18.01471089	15.12526454
O	1.37024506	-10.68677706	15.16620194
O	-1.54384702	-12.06826328	14.65004448
O	-4.48334018	-13.43783747	15.20807834
O	-7.45979309	-14.79937053	15.00085562
O	-10.42064609	-16.14817366	15.06680590
O	1.64073325	-7.43985837	14.64701271
O	-1.28669465	-8.83312255	15.19826995
O	-4.21252247	-10.22060442	15.19567963
O	-7.14401610	-11.59877064	14.64892701
O	-10.12214149	-12.92873685	15.13809852
O	-1.00173489	-5.60366995	15.18189082
O	-3.95381836	-6.99763937	14.64957515
O	-6.87359547	-8.37561718	15.19652667
O	-9.83225658	-9.71796050	15.16836024
O	-0.73863188	-2.38987008	14.67853627
O	-3.65208787	-3.76712774	15.21645539
O	-2.48074538	-21.81173656	15.14080987
O	3.75382231	-15.82329933	15.03866918
Zn	-7.29440542	-22.85917777	14.71170386
Zn	2.10304838	-12.38532638	14.81447124
Zn	-1.10353773	-17.00158442	14.74458360
Zn	-4.05140605	-18.44603702	14.71558232
Zn	-7.00589206	-19.72683148	14.83693929
Zn	-9.92595692	-21.10500095	14.77668948
Zn	-0.75221430	-13.83399405	14.79150682
Zn	-3.65738086	-15.07678413	14.79488396
Zn	-6.68400363	-16.50188953	14.72933103
Zn	-9.57622744	-17.80721050	14.76057315
Zn	-0.45874294	-10.47087203	14.78339548
Zn	-3.46605231	-11.90229941	14.80121466
Zn	-6.30082597	-13.33762244	14.74259315
Zn	-9.34081906	-14.61242114	14.83384856
Zn	0.09912006	-4.12715495	14.77951306
Zn	-0.28343503	-7.29505208	14.78345495
Zn	-3.12391074	-8.74084103	14.79494988
Zn	-6.04007043	-10.01686755	14.80033498
Zn	-9.06944542	-11.39978765	14.78173899
Zn	-11.95909893	-12.75961296	14.76057220
Zn	-2.83574145	-5.42108217	14.79795195
Zn	-5.87767617	-6.83321516	14.78541255
Zn	-4.57835927	-24.94426667	14.78368938
Zn	-7.54352288	-26.20499046	14.77129394
Zn	1.46518926	-18.92796246	14.73649882
Zn	-1.36668669	-20.32257982	14.83612721
Zn	-4.31213841	-21.60987767	14.73823356
Zn	1.90658008	-15.57488080	14.78416500

27/37 Pt

202

Lattice="-13.8592929113 -9.6019997917 0.0 1.3859292911 -16.8034996355 0.0 0.0 0.0 20.7163554165"

Pt	-12.47336362	-12.00249974	5.50000000
Pt	-11.08743433	-9.60199979	5.50000000
Pt	-9.70150504	-7.20149984	5.50000000
Pt	-12.47336362	-16.80349964	5.50000000
Pt	-11.08743433	-14.40299969	5.50000000
Pt	-9.70150504	-12.00249974	5.50000000
Pt	-8.31557575	-9.60199979	5.50000000
Pt	-6.92964646	-7.20149984	5.50000000
Pt	-5.54371716	-4.80099990	5.50000000
Pt	-12.47336362	-21.60449953	5.50000000
Pt	-11.08743433	-19.20399958	5.50000000
Pt	-9.70150504	-16.80349964	5.50000000
Pt	-8.31557575	-14.40299969	5.50000000
Pt	-6.92964646	-12.00249974	5.50000000
Pt	-5.54371716	-9.60199979	5.50000000
Pt	-4.15778787	-7.20149984	5.50000000
Pt	-2.77185858	-4.80099990	5.50000000
Pt	-1.38592929	-2.40049995	5.50000000
Pt	0.00000000	0.00000000	5.50000000
Pt	-11.08743433	-24.00499948	5.50000000
Pt	-9.70150504	-21.60449953	5.50000000
Pt	-8.31557575	-19.20399958	5.50000000
Pt	-6.92964646	-16.80349964	5.50000000
Pt	-5.54371717	-14.40299969	5.50000000
Pt	-4.15778787	-12.00249974	5.50000000
Pt	-2.77185858	-9.60199979	5.50000000
Pt	-1.38592929	-7.20149984	5.50000000
Pt	0.00000000	-4.80099990	5.50000000
Pt	-6.92964646	-21.60449953	5.50000000
Pt	-5.54371716	-19.20399958	5.50000000
Pt	-4.15778787	-16.80349964	5.50000000
Pt	-2.77185858	-14.40299969	5.50000000
Pt	-1.38592929	-12.00249974	5.50000000
Pt	-0.00000000	-9.60199979	5.50000000
Pt	-2.77185858	-19.20399958	5.50000000
Pt	-1.38592929	-16.80349964	5.50000000
Pt	-0.00000000	-14.40299969	5.50000000
Pt	-11.11257310	-11.20722051	7.80399907
Pt	-9.69967265	-8.80388328	7.78613521
Pt	-8.28968261	-6.40001161	7.78606313
Pt	-11.11683778	-15.98268855	7.79897756
Pt	-9.73124376	-13.59558646	7.79920778
Pt	-8.32154975	-11.19761178	7.78994577
Pt	-6.90390780	-8.78761763	7.79229987
Pt	-5.49992587	-6.39585508	7.82973168
Pt	-4.12771007	-4.01984159	7.87308310
Pt	-11.09007487	-20.79754206	7.77416855
Pt	-9.70881668	-18.39558186	7.78100735
Pt	-8.32518756	-16.00472764	7.78830546
Pt	-6.93445335	-13.60462310	7.78085271
Pt	-5.52880581	-11.18824757	7.78458096
Pt	-4.12725443	-8.77270013	7.82086800
Pt	-2.75286795	-6.38442805	7.88601387
Pt	-1.39826500	-4.00771112	7.90466649
Pt	-0.02964396	-1.62686831	7.82916470
Pt	-12.48727439	-8.81930885	7.78780862
Pt	-9.69651652	-23.20992956	7.77674415
Pt	-8.30237508	-20.80683234	7.77883067
Pt	-6.91589977	-18.41589567	7.79351404

Pt	-5.53754166	-16.02234920	7.79095818
Pt	-4.14882051	-13.61013561	7.78572668
Pt	-2.76156151	-11.18588225	7.79597767
Pt	-1.38540071	-8.76785505	7.81980211
Pt	-0.02250101	-6.37113193	7.84985063
Pt	-12.51128205	-13.59465290	7.84368145
Pt	-5.51031626	-20.81582369	7.80565239
Pt	-4.13763863	-18.43530188	7.82179438
Pt	-2.76928411	-16.03561380	7.80157299
Pt	-1.38495771	-13.61220385	7.78876351
Pt	-0.00252208	-11.18791298	7.78425046
Pt	-12.49144216	-18.37875688	7.79200806
Pt	-1.39415936	-18.44513226	7.85662265
Pt	-0.01151881	-16.03553671	7.79589750
Pt	-12.47805059	-23.21482154	7.77769380
Pt	-12.48925458	-10.40975400	10.06300695
Pt	-11.09561498	-8.00818334	10.01455688
Pt	-8.30529291	-22.41090481	10.01148348
Pt	-12.48474081	-15.18894603	10.11574243
Pt	-11.10966674	-12.79815777	10.08713750
Pt	-9.71561623	-10.40458309	10.03825665
Pt	-8.31136232	-8.00274358	10.02459843
Pt	-6.91672704	-5.60734462	10.06260101
Pt	-4.14282140	-20.02058035	10.11667476
Pt	-12.46421387	-19.99493258	10.01546767
Pt	-11.08593496	-17.59717300	10.02883948
Pt	-9.71121371	-15.20658267	10.03284892
Pt	-8.32908732	-12.80457570	10.02053306
Pt	-6.93154366	-10.39609500	10.01359112
Pt	-5.52681278	-7.99345417	10.08158718
Pt	-4.14167928	-5.61952279	10.20276628
Pt	-2.78189114	-3.20868355	10.24759973
Pt	-0.01095827	-17.61710794	10.09974363
Pt	-12.48442066	-24.80752843	10.02312163
Pt	-11.08699968	-22.40657046	9.99627659
Pt	-9.69486122	-20.00399051	10.00765294
Pt	-8.31368589	-17.61405705	10.02618022
Pt	-6.92968601	-15.21467118	10.01482021
Pt	-5.53841057	-12.79956527	10.00337883
Pt	-4.14268357	-10.39044523	10.04525992
Pt	-2.75549799	-7.98348546	10.16718169
Pt	-1.37897257	-5.59488334	10.25586860
Pt	-0.02388492	-3.19914059	10.20149885
Pt	-6.92001158	-20.02125924	10.03308808
Pt	-5.53794685	-17.62100594	10.05451022
Pt	-4.14665377	-15.21428163	10.02737440
Pt	-2.76063136	-12.79881148	10.02957431
Pt	-1.37557282	-10.39093228	10.05017917
Pt	-0.00247895	-7.98719368	10.08866605
Pt	-2.77542903	-17.62543275	10.11975796
Pt	-1.38602701	-15.20817228	10.03672367
Pt	0.00204130	-12.79764098	10.01880086
Pt	-12.41713513	-11.94271189	12.42263464
Pt	-11.06775149	-9.56269391	12.35795632
Pt	-9.71415514	-7.19613363	12.32491659
Pt	-12.41159817	-16.84622089	12.36802310
Pt	-11.02687425	-14.40503533	12.38095522
Pt	-9.66857887	-11.98322252	12.36239219
Pt	-8.31750371	-9.59624393	12.34011031
Pt	-6.97703105	-7.21113357	12.37272924
Pt	-5.61723274	-4.81728059	12.41988713
Pt	-12.45587324	-21.62055522	12.31593256
Pt	-11.06651822	-19.22725618	12.33970897

Pt	-9.69097115	-16.81915849	12.35803635
Pt	-8.30580157	-14.40194156	12.32322300
Pt	-6.92603511	-12.01033185	12.30290229
Pt	-5.57311148	-9.64774951	12.33193475
Pt	-4.20517636	-7.28006499	12.48946966
Pt	-2.80380970	-4.81819499	12.53453632
Pt	-1.37408577	-2.32396684	12.49586424
Pt	-12.45443059	-26.33954939	12.36179804
Pt	-11.07861493	-23.98506182	12.32410805
Pt	-9.70845132	-21.61200667	12.29405554
Pt	-8.33665306	-19.21662566	12.33837830
Pt	-6.95908594	-16.79987011	12.33988857
Pt	-5.55341642	-14.39868390	12.30147358
Pt	-4.15682128	-12.03542008	12.32813662
Pt	-2.75594902	-9.67940750	12.37834149
Pt	-1.33378710	-7.28518783	12.49264971
Pt	0.06226426	-4.80423264	12.50724013
Pt	-6.97011876	-21.61846793	12.37141836
Pt	-5.61934752	-19.20963369	12.36852422
Pt	-4.19845708	-16.76605519	12.37209746
Pt	-2.77126155	-14.39513636	12.35517847
Pt	-1.36815712	-12.03200173	12.35619300
Pt	0.04566914	-9.66158354	12.35460083
Pt	-2.84946807	-19.18047411	12.49123607
Pt	-1.39824224	-16.73842158	12.37370653
Pt	0.01015051	-14.38320678	12.35667264
O	-11.17147282	-22.52329719	15.22071367
O	-6.44736002	-19.34642856	15.22881327
O	-9.72327068	-19.62226363	15.22957341
O	-1.88519445	-16.06035542	15.35060786
O	-5.04091488	-16.38401532	15.12938699
O	-8.29331147	-16.71622795	15.22787479
O	-11.57544200	-16.98383021	15.36387076
O	-0.55949708	-13.10550870	15.24124049
O	-3.77356789	-13.37830288	15.22650443
O	-6.98298035	-13.76815090	15.18795092
O	-10.23945927	-14.10954985	15.19258908
O	-13.01368051	-19.82700922	15.23975220
O	-2.46181496	-10.41197187	15.22385836
O	-5.68747162	-10.76132076	15.19863432
O	-8.91421331	-11.16234235	15.19640676
O	-12.13664223	-11.42343457	15.09182752
O	-1.02480245	-7.56600920	14.81640169
O	-4.33707478	-7.77178690	14.73979847
O	-7.55488081	-8.17312739	15.27929833
O	-10.76437900	-8.46211177	15.22817320
O	0.36609493	-4.74344546	14.77358148
O	-2.89045240	-4.89161131	14.93673776
O	-6.10857125	-5.20304901	15.41642574
O	-7.94045217	-22.30111114	15.21362037
O	-1.43573881	-1.98603423	14.77872732
O	-3.20249461	-19.05768434	14.71443078
O	1.28551800	-15.83987177	15.28732723
Zn	-12.84648856	-21.69971847	14.95415322
Zn	-8.17132795	-18.58268558	14.96047420
Zn	-11.41883352	-18.84096831	14.98739928
Zn	-3.54534712	-15.22516907	14.96861443
Zn	-6.77715353	-15.62743448	14.92049473
Zn	-10.00855017	-15.98199319	14.99099800
Zn	-13.18694756	-16.25701975	14.84027604
Zn	-2.24701059	-12.29622878	14.97747803
Zn	-5.49155050	-12.63309322	14.96714279
Zn	-8.69653942	-13.02690579	14.92687517

Zn	-11.85400467	-13.26415271	14.80919381
Zn	-0.84810132	-9.52365699	14.88330072
Zn	-4.17113593	-9.74380128	14.77247173
Zn	-7.41721733	-10.03198248	14.94921702
Zn	-10.57130990	-10.31151339	14.93150205
Zn	-13.71972886	-10.43329821	14.88074147
Zn	-2.73499278	-6.78075417	14.82429339
Zn	-6.12910163	-7.02762078	14.94696308
Zn	-9.24555737	-7.37068084	14.96175194
Zn	-11.02892700	-24.38355734	14.96683797
Zn	-1.31238206	-3.86718874	14.79622924
Zn	-4.67899981	-4.16933231	14.86190306
Zn	-6.41671599	-21.22078731	15.01960446
Zn	-9.62363761	-21.48405385	14.93086241
Zn	-1.72594478	-17.81781779	14.80907702
Zn	-5.00308283	-18.22874907	14.80757185
Zn	-0.37016232	-14.96502849	15.00055684

13/21 Cu

110

Lattice="-7.6579664403 -8.8426579714 0.0 3.8289832201 -11.0533224643 0.0 0.0 0.0 20.1794196661"

Cu	-6.38163870	-11.05332246	5.50000000
Cu	-5.10531096	-8.84265797	5.50000000
Cu	-3.82898322	-6.63199348	5.50000000
Cu	-2.55265548	-4.42132899	5.50000000
Cu	-1.27632774	-2.21066449	5.50000000
Cu	0.00000000	0.00000000	5.50000000
Cu	-5.10531096	-13.26398696	5.50000000
Cu	-3.82898322	-11.05332246	5.50000000
Cu	-2.55265548	-8.84265797	5.50000000
Cu	-1.27632774	-6.63199348	5.50000000
Cu	-0.00000000	-4.42132899	5.50000000
Cu	-3.82898322	-15.47465145	5.50000000
Cu	-2.55265548	-13.26398696	5.50000000
Cu	-1.27632774	-11.05332246	5.50000000
Cu	-0.00000000	-8.84265797	5.50000000
Cu	1.27632774	-6.63199348	5.50000000
Cu	-2.55265548	-17.68531594	5.50000000
Cu	-1.27632774	-15.47465145	5.50000000
Cu	-0.00000000	-13.26398696	5.50000000
Cu	1.27632774	-11.05332246	5.50000000
Cu	2.55265548	-8.84265797	5.50000000
Cu	-5.10515074	-10.31717338	7.56212272
Cu	-3.82970689	-8.10601101	7.55809348
Cu	-2.55474460	-5.89516778	7.55764842
Cu	-1.28235303	-3.68578137	7.56188849
Cu	0.00450675	-1.47458208	7.55565798
Cu	-6.37850340	-8.10647079	7.56209335
Cu	-3.83405004	-12.53016151	7.56355888
Cu	-2.54644972	-10.31441864	7.57059495
Cu	-1.27308243	-8.10749535	7.56278168
Cu	-0.00217003	-5.89273249	7.58064105
Cu	1.27728563	-3.68523166	7.55616603
Cu	-2.55785501	-14.73097853	7.56823836
Cu	-1.27568690	-12.52926509	7.54780321
Cu	0.00141579	-10.31249512	7.56200819
Cu	1.27410107	-8.10556264	7.55885837
Cu	-5.10466390	-14.73541072	7.56668906
Cu	-5.10472799	-5.89880840	7.57185103
Cu	0.00173330	-14.74324316	7.56211845
Cu	1.27371076	-12.53455967	7.56390423
Cu	2.55153700	-10.31216965	7.56099628
Cu	-3.83060380	-16.94534184	7.55203522

Cu	-6.37560766	-9.57464710	9.60985227
Cu	-5.10480681	-7.39214882	9.62030023
Cu	-3.81811510	-5.15787270	9.61031345
Cu	-2.55699275	-2.96358328	9.62685216
Cu	2.55625780	-11.79298082	9.57298705
Cu	-3.82130542	-18.41574684	9.58933893
Cu	-5.11145270	-11.79910808	9.60099084
Cu	-3.83432420	-9.56967673	9.59382825
Cu	-2.55050755	-7.36850237	9.58380941
Cu	-1.30070757	-5.14970570	9.61438353
Cu	-0.00443336	-2.95400779	9.57952154
Cu	-3.84013750	-13.99309699	9.63878315
Cu	-2.54145330	-11.80568404	9.57987240
Cu	-1.25645833	-9.56962640	9.62572420
Cu	0.00306011	-7.38559278	9.61167857
Cu	1.29039217	-5.14183188	9.60753021
Cu	-2.56438872	-16.21288320	9.58578199
Cu	-1.27187680	-13.99511408	9.58721976
Cu	-0.00929401	-11.78916329	9.58166445
Cu	1.26903192	-9.57031535	9.61288604
Cu	2.55320708	-7.36887344	9.58709313
Cu	-6.41241739	-11.05795580	11.61412434
Cu	-5.11261069	-8.88639236	11.75030510
Cu	-3.82473727	-6.65061687	11.62741691
Cu	-2.58198999	-4.41574837	11.79540238
Cu	-1.25958952	-2.20667530	11.62408831
Cu	3.80613939	-11.03076538	11.62623831
Cu	-5.09994133	-13.22702649	11.76878342
Cu	-3.79525719	-11.05654253	11.55525577
Cu	-2.54732842	-8.82788112	11.62624244
Cu	-1.27617238	-6.63399303	11.61717329
Cu	-0.01299122	-4.43310441	11.61948377
Cu	-3.84593501	-15.48725622	11.66274269
Cu	-2.52986290	-13.28206626	11.67608928
Cu	-1.29037523	-11.05094474	11.65072099
Cu	0.03138457	-8.84613215	11.79204667
Cu	1.28095861	-6.61147762	11.59816494
Cu	-2.52857273	-17.68114760	11.65096269
Cu	-1.29857543	-15.47389359	11.57795693
Cu	-0.00040709	-13.23861790	11.64732872
Cu	1.27403950	-11.07943398	11.58875611
Cu	2.57512667	-8.84055351	11.62562316
O	0.63494121	-12.15325499	14.42881711
O	-2.00137334	-14.01728550	14.37811354
O	-4.66347432	-15.90175258	14.39000564
O	0.31940063	-8.92010286	14.03238886
O	-2.31745993	-10.81225572	14.45954353
O	-4.97468191	-12.69044825	14.06098228
O	0.05065926	-5.69973712	14.51346614
O	-2.59975829	-7.57197686	14.51228199
O	-5.24085831	-9.41761138	14.05203617
O	-0.24260351	-2.46453528	14.45084626
O	-2.87283098	-4.34661855	14.03838558
O	-1.72319395	-17.25129547	14.39896857
O	3.29035061	-10.29318482	14.36459136
Zn	-1.22126527	-12.31585221	14.12742016
Zn	-3.84531231	-14.23168869	14.09333903
Zn	1.13405491	-7.19476083	14.18764065
Zn	-1.58147902	-9.11164478	14.16173655
Zn	-4.15166027	-10.97712422	14.12718417
Zn	0.78621531	-4.00770717	14.16007385
Zn	-1.78486114	-5.91316270	14.19411151
Zn	-4.43651061	-7.68629928	14.14769061

Zn	-7.13813868	-9.62183826	14.11458413
Zn	-2.09848355	-2.59811935	14.14624702
Zn	-0.94686847	-15.55612962	14.18070958
Zn	-3.58768313	-17.43246850	14.15599083
Zn	1.43134625	-10.47462401	14.15452179

31/39 Ag

218

Lattice="-13.0143003077 -12.52301631 0.0 4.3381001026 -17.532222834 0.0 0.0 0.0 21.0108040538"

Ag	-11.56826694	-15.02761957	5.50000000
Ag	-10.12223357	-12.52301631	5.50000000
Ag	-8.67620021	-10.01841305	5.50000000
Ag	-7.23016684	-7.51380979	5.50000000
Ag	-10.12223357	-17.53222283	5.50000000
Ag	-8.67620020	-15.02761957	5.50000000
Ag	-7.23016684	-12.52301631	5.50000000
Ag	-5.78413347	-10.01841305	5.50000000
Ag	-4.33810010	-7.51380978	5.50000000
Ag	-2.89206673	-5.00920652	5.50000000
Ag	-1.44603337	-2.50460326	5.50000000
Ag	0.00000000	0.00000000	5.50000000
Ag	-10.12223357	-22.54142936	5.50000000
Ag	-8.67620021	-20.03682610	5.50000000
Ag	-7.23016684	-17.53222283	5.50000000
Ag	-5.78413347	-15.02761957	5.50000000
Ag	-4.33810010	-12.52301631	5.50000000
Ag	-2.89206673	-10.01841305	5.50000000
Ag	-1.44603337	-7.51380979	5.50000000
Ag	0.00000000	-5.00920652	5.50000000
Ag	-8.67620021	-25.04603262	5.50000000
Ag	-7.23016684	-22.54142936	5.50000000
Ag	-5.78413347	-20.03682610	5.50000000
Ag	-4.33810010	-17.53222283	5.50000000
Ag	-2.89206674	-15.02761957	5.50000000
Ag	-1.44603337	-12.52301631	5.50000000
Ag	0.00000000	-10.01841305	5.50000000
Ag	1.44603337	-7.51380979	5.50000000
Ag	-7.23016684	-27.55063588	5.50000000
Ag	-5.78413347	-25.04603262	5.50000000
Ag	-4.33810010	-22.54142936	5.50000000
Ag	-2.89206674	-20.03682610	5.50000000
Ag	-1.44603337	-17.53222283	5.50000000
Ag	-0.00000000	-15.02761957	5.50000000
Ag	1.44603337	-12.52301631	5.50000000
Ag	-1.44603337	-22.54142936	5.50000000
Ag	0.00000000	-20.03682610	5.50000000
Ag	1.44603337	-17.53222283	5.50000000
Ag	2.89206673	-15.02761957	5.50000000
Ag	-10.12846120	-14.19082139	7.86994531
Ag	-8.67575851	-11.68470546	7.87288839
Ag	-7.23051493	-9.17899865	7.86436064
Ag	-5.78438314	-6.67184422	7.87351821
Ag	-8.67858038	-16.69913642	7.87264840
Ag	-7.23538486	-14.19647223	7.87395863
Ag	-5.78351269	-11.68641216	7.87136824
Ag	-4.33901341	-9.18464845	7.87045670
Ag	-2.88995921	-6.67741040	7.87193366
Ag	-1.44653746	-4.17595198	7.87399362
Ag	-0.00118399	-1.67407493	7.87261482
Ag	-11.56856229	-11.68762813	7.87557062
Ag	-8.67271859	-21.71105098	7.86756064
Ag	-7.23383041	-19.20227221	7.86894042
Ag	-5.78858445	-16.69705277	7.87030504

Ag	-4.34497569	-14.19315658	7.86518373
Ag	-2.89588410	-11.68573504	7.86985406
Ag	-1.44427899	-9.18438377	7.86137980
Ag	-0.00347493	-6.67719656	7.87254913
Ag	-11.56616530	-16.69855754	7.86832640
Ag	-7.22567497	-24.21103685	7.87414613
Ag	-5.78303557	-21.70432153	7.86801393
Ag	-4.34067074	-19.19985595	7.87436049
Ag	-2.89372143	-16.69316046	7.87064888
Ag	-1.45113095	-14.19286357	7.87322597
Ag	0.00490946	-11.68760349	7.87246753
Ag	1.44768190	-9.18679444	7.87121568
Ag	-10.12118630	-19.20668829	7.87500262
Ag	-5.78302860	-26.71920577	7.87176642
Ag	-4.33525020	-24.20778505	7.87135254
Ag	-2.89185041	-21.70448883	7.87089549
Ag	-1.44794413	-19.19952488	7.86921675
Ag	-0.00387430	-16.69528429	7.87354168
Ag	1.44393615	-14.19535677	7.86762910
Ag	-10.12189262	-24.21101911	7.87309382
Ag	0.00199172	-21.70118858	7.86728561
Ag	1.44188737	-19.19853249	7.87365618
Ag	2.89469680	-16.69370643	7.87216272
Ag	-8.67875564	-26.71478364	7.87086700
Ag	-11.58217632	-13.35597557	10.21672503
Ag	-10.11908159	-10.86006527	10.22375079
Ag	-4.33954977	-25.87762392	10.20511058
Ag	-2.89525864	-23.37596662	10.22134589
Ag	-10.11650915	-15.85553091	10.20781498
Ag	-8.68883371	-13.35702601	10.19796580
Ag	-7.22306749	-10.83231779	10.20280838
Ag	-5.78449237	-8.34375853	10.19866359
Ag	-4.32959065	-5.82767306	10.19973344
Ag	-2.88599800	-3.33223908	10.21012301
Ag	2.89262369	-18.36301666	10.19599895
Ag	-8.66784007	-28.36946758	10.21882633
Ag	-10.10913855	-20.89056343	10.20464613
Ag	-8.68051235	-18.36466620	10.21708338
Ag	-7.22543929	-15.87272821	10.21939362
Ag	-5.79253633	-13.35523202	10.20350428
Ag	-4.33990117	-10.85274958	10.22648090
Ag	-2.88384322	-8.35854725	10.19666287
Ag	-1.45103755	-5.84290167	10.22771926
Ag	0.01174338	-3.35811386	10.21063282
Ag	-8.67513114	-23.38382732	10.21108121
Ag	-7.23188580	-20.87220569	10.20682320
Ag	-5.80083974	-18.37076633	10.20547039
Ag	-4.34110612	-15.85640468	10.20531208
Ag	-2.91592169	-13.35678433	10.19992880
Ag	-1.44364530	-10.85135239	10.19639826
Ag	-0.00482502	-8.35117238	10.20002014
Ag	1.44460272	-5.84689815	10.20081358
Ag	-7.22527119	-25.88532434	10.19916639
Ag	-5.77672006	-23.35803625	10.21010949
Ag	-4.33042907	-20.87297476	10.20808951
Ag	-2.89404881	-18.35466805	10.20284711
Ag	-1.44669706	-15.85757168	10.22312338
Ag	0.00052240	-13.36412660	10.19817082
Ag	1.44934188	-10.84907127	10.22659171
Ag	-1.44161920	-20.87603408	10.20499884
Ag	-0.02153398	-18.36641395	10.21539442
Ag	1.44621263	-15.87094064	10.20894242
Ag	2.87429458	-13.35849971	10.20646556

Ag	-11.55974801	-15.02600978	12.56103184
Ag	-10.14699968	-12.56392678	12.57557669
Ag	-8.67450258	-10.00528762	12.56636963
Ag	-7.22867241	-7.53975177	12.56624850
Ag	-10.15867517	-17.51025519	12.55119013
Ag	-8.63334093	-15.03023346	12.55465904
Ag	-7.26499394	-12.48579773	12.50751619
Ag	-5.75821522	-9.99193829	12.58306562
Ag	-4.31476045	-7.49388764	12.49914073
Ag	-2.89687197	-4.97613008	12.58473361
Ag	-1.38915688	-2.49724221	12.52754731
Ag	4.30074698	-17.48303454	12.55939273
Ag	-10.10070404	-22.56473316	12.59364853
Ag	-8.66854982	-20.01564813	12.56248979
Ag	-7.24656149	-17.54748987	12.59176645
Ag	-5.77020430	-15.00550524	12.56769129
Ag	-4.37229161	-12.52497646	12.58621117
Ag	-2.87867050	-10.03119330	12.57245454
Ag	-1.44748197	-7.52395749	12.56871533
Ag	-0.00428079	-5.05674955	12.58768473
Ag	-8.68298907	-25.09682237	12.52852723
Ag	-7.25684296	-22.53885621	12.56437135
Ag	-5.76404463	-20.06897592	12.54939531
Ag	-4.38545849	-17.53518857	12.52706479
Ag	-2.89053511	-15.02833898	12.56812941
Ag	-1.46986313	-12.54280763	12.49896749
Ag	-0.01527445	-10.01094365	12.56978535
Ag	1.47469590	-7.54548777	12.50822089
Ag	-7.17941562	-27.54002936	12.58399800
Ag	-5.78796188	-24.99762229	12.52825718
Ag	-4.31920061	-22.52562918	12.59097343
Ag	-2.85916603	-20.00357833	12.53376002
Ag	-1.47688644	-17.50459173	12.59124944
Ag	0.03506335	-15.02255694	12.56704191
Ag	1.41363041	-12.49854776	12.57590543
Ag	-1.45881822	-22.56048194	12.56589529
Ag	0.00659358	-20.05537576	12.56409152
Ag	1.41388795	-17.57902986	12.53901919
Ag	2.87891597	-15.02484045	12.56114968
O	1.14625101	-18.60999963	15.35652560
O	-1.52573031	-20.48426832	15.42304147
O	-4.17705037	-22.35077889	15.22811462
O	-6.82621122	-24.20638883	15.38670619
O	-9.48461208	-26.04481129	15.40541974
O	0.85892466	-15.38919460	15.36295019
O	-1.78401936	-17.25718495	15.24556406
O	-4.45263155	-19.10788875	15.39156771
O	-7.10832457	-20.96736407	15.43567828
O	-9.77731230	-22.81587418	15.25874500
O	0.59372766	-12.16343563	15.36540969
O	-2.07259262	-14.01235118	15.41212614
O	-4.72808609	-15.88485277	15.43285725
O	-7.38608367	-17.73242937	15.23158723
O	-10.05607446	-19.59656255	15.40122380
O	0.30513581	-8.92087392	15.41668136
O	-2.35039452	-10.78321681	15.38623126
O	-5.00056930	-12.64923267	15.30983482
O	-7.67836509	-14.51081937	15.37549334
O	-10.32469205	-16.37081741	15.40603385
O	0.02042915	-5.68231564	15.29609682
O	-2.64046137	-7.55897596	15.41926872
O	-5.30116574	-9.42171137	15.33744660
O	-7.93972647	-11.28502830	15.40886614

O	-10.60641487	-13.12441319	15.30937884
O	-0.27147110	-2.47078241	15.37657494
O	-2.91814770	-4.33126000	15.30479325
O	-5.56907347	-6.18081967	15.40464991
O	-8.23290729	-8.04035360	15.41190108
O	-6.56036511	-27.43949423	15.28538169
O	3.81469811	-16.77485909	15.32277536
Zn	-0.71390064	-18.80765705	15.23564257
Zn	-3.38604918	-20.64123059	15.21877839
Zn	-6.05326052	-22.50603326	15.23755690
Zn	-8.68853586	-24.35119248	15.21904852
Zn	1.66839109	-13.70014168	15.25322413
Zn	-1.00843044	-15.54119392	15.23327541
Zn	-3.65916046	-17.41459772	15.22336704
Zn	-6.31245473	-19.27987710	15.22868293
Zn	-8.96831386	-21.11598388	15.24724530
Zn	1.36217689	-10.45903372	15.26127046
Zn	-1.27443128	-12.31793023	15.24180206
Zn	-3.93238203	-14.19547209	15.27506580
Zn	-6.58639155	-16.02730817	15.24121377
Zn	-9.26196173	-17.90881055	15.22672295
Zn	1.09271934	-7.22526804	15.22916105
Zn	-1.55921345	-9.08503302	15.30050091
Zn	-4.21271786	-10.94539637	15.26677436
Zn	-6.87080671	-12.82282906	15.22287370
Zn	-9.54529557	-14.67436017	15.22929658
Zn	0.82785443	-3.98363595	15.24748019
Zn	-1.84581683	-5.87360428	15.25042052
Zn	-4.50540698	-7.72072214	15.24272130
Zn	-7.17187948	-9.57943468	15.27757375
Zn	-9.79695196	-11.42898589	15.23047828
Zn	-12.47272786	-13.31343860	15.21494590
Zn	-2.13936937	-2.62313398	15.21046731
Zn	-0.45294433	-22.01231299	15.25007331
Zn	-3.08693101	-23.88771940	15.24700803
Zn	-5.75321960	-25.74169380	15.21877578
Zn	-8.43597945	-27.58624507	15.22873083
Zn	1.94499517	-16.91230889	15.21098844

31/39 Au

218

Lattice="-12.9824805026 -12.4923976882 0.0 4.3274935009 -17.4893567635 0.0 0.0 0.0 20.9934835457"

Au	-11.53998267	-14.99087723	5.50000000
Au	-10.09748484	-12.49239769	5.50000000
Au	-8.65498700	-9.99391815	5.50000000
Au	-7.21248917	-7.49543861	5.50000000
Au	-10.09748483	-17.48935676	5.50000000
Au	-8.65498700	-14.99087723	5.50000000
Au	-7.21248917	-12.49239769	5.50000000
Au	-5.76999133	-9.99391815	5.50000000
Au	-4.32749350	-7.49543861	5.50000000
Au	-2.88499567	-4.99695908	5.50000000
Au	-1.44249783	-2.49847954	5.50000000
Au	0.00000000	0.00000000	5.50000000
Au	-10.09748484	-22.48631584	5.50000000
Au	-8.65498700	-19.98783630	5.50000000
Au	-7.21248917	-17.48935676	5.50000000
Au	-5.76999133	-14.99087723	5.50000000
Au	-4.32749350	-12.49239769	5.50000000
Au	-2.88499567	-9.99391815	5.50000000
Au	-1.44249783	-7.49543861	5.50000000
Au	0.00000000	-4.99695908	5.50000000
Au	-8.65498700	-24.98479538	5.50000000

Au	-7.21248917	-22.48631584	5.50000000
Au	-5.76999133	-19.98783630	5.50000000
Au	-4.32749350	-17.48935676	5.50000000
Au	-2.88499567	-14.99087723	5.50000000
Au	-1.44249783	-12.49239769	5.50000000
Au	0.00000000	-9.99391815	5.50000000
Au	1.44249783	-7.49543861	5.50000000
Au	-7.21248917	-27.48327491	5.50000000
Au	-5.76999133	-24.98479538	5.50000000
Au	-4.32749350	-22.48631584	5.50000000
Au	-2.88499567	-19.98783630	5.50000000
Au	-1.44249783	-17.48935676	5.50000000
Au	-0.00000000	-14.99087723	5.50000000
Au	1.44249783	-12.49239769	5.50000000
Au	-1.44249783	-22.48631584	5.50000000
Au	0.00000000	-19.98783630	5.50000000
Au	1.44249783	-17.48935676	5.50000000
Au	2.88499567	-14.99087723	5.50000000
Au	-10.10486297	-14.15440031	7.95416792
Au	-8.65247859	-11.66115526	7.95802421
Au	-7.21120103	-9.15949410	7.94851121
Au	-5.76983334	-6.65906447	7.96087326
Au	-8.65824403	-16.65461425	7.95271839
Au	-7.21636712	-14.16273899	7.96060186
Au	-5.76982950	-11.65895540	7.95433894
Au	-4.32664851	-9.16384531	7.95586596
Au	-2.88769456	-6.66173332	7.95633537
Au	-1.44279074	-4.16484068	7.95336255
Au	-0.00478012	-1.66825954	7.95765518
Au	-11.53908396	-11.65917091	7.95773743
Au	-8.65530802	-21.66143977	7.94676880
Au	-7.21952792	-19.15395318	7.94789926
Au	-5.77145479	-16.65861339	7.95173313
Au	-4.33321524	-14.15737630	7.94767935
Au	-2.88732602	-11.66091541	7.95687901
Au	-1.44117731	-9.16371003	7.94782094
Au	-0.00812310	-6.66205433	7.95693134
Au	-11.54004164	-16.65842215	7.94979990
Au	-7.20892580	-24.15377016	7.96099705
Au	-5.76830483	-21.65123745	7.94731188
Au	-4.32772985	-19.15364053	7.95922426
Au	-2.88317802	-16.64888556	7.95126761
Au	-1.44328132	-14.15485393	7.96140950
Au	0.00353014	-11.65825769	7.96184421
Au	1.44205964	-9.16190984	7.95574384
Au	-10.10047202	-19.15977959	7.96043046
Au	-5.76884220	-26.65827041	7.95478983
Au	-4.32759063	-24.15218731	7.95247053
Au	-2.88270644	-21.65510078	7.95023263
Au	-1.44528633	-19.15253346	7.94937166
Au	-0.00061488	-16.65510964	7.95468228
Au	1.44012636	-14.16024474	7.95097520
Au	2.88186776	-11.66118812	7.95223014
Au	0.00416095	-21.64820698	7.94574260
Au	1.43873334	-19.14891196	7.95920230
Au	2.89013597	-16.65081337	7.95504002
Au	-8.65571123	-26.64774098	7.95448464
Au	-11.55851808	-13.32383253	10.33586393
Au	-10.09060816	-10.84052898	10.34490573
Au	-4.32778724	-25.81658730	10.32513341
Au	-2.88508309	-23.32201907	10.34002276
Au	-10.09664251	-15.81969237	10.32467362
Au	-8.66776272	-13.33026972	10.32512815

Au	-7.20439809	-10.81306625	10.32546167
Au	-5.76863657	-8.32552347	10.32367489
Au	-4.32418549	-5.81297552	10.32594795
Au	-2.88018706	-3.32109048	10.32757735
Au	2.88069055	-18.31254444	10.32303056
Au	-8.64472995	-28.30121957	10.33930728
Au	-10.08573045	-20.83607461	10.32618377
Au	-8.66430875	-18.31884558	10.33258134
Au	-7.21029123	-15.83320259	10.34016685
Au	-5.77872397	-13.32306013	10.32585671
Au	-4.32788079	-10.82638870	10.34668699
Au	-2.87974913	-8.33373522	10.32345271
Au	-1.45229577	-5.82810362	10.34513837
Au	0.00372762	-3.34653161	10.32937659
Au	-8.65185158	-23.33011545	10.32657074
Au	-7.21446522	-20.82144285	10.31806249
Au	-5.78401280	-18.32625808	10.32433708
Au	-4.33051423	-15.81712842	10.32206360
Au	-2.90398131	-13.32280357	10.32735208
Au	-1.44047617	-10.82437598	10.32649790
Au	-0.00324581	-8.32962245	10.32470106
Au	1.43481916	-5.83421195	10.32428240
Au	-7.20262947	-25.82544241	10.32211110
Au	-5.76047977	-23.30573549	10.32987933
Au	-4.31803163	-20.82245851	10.32536086
Au	-2.88857039	-18.30676754	10.32076330
Au	-1.44061310	-15.81283081	10.34329569
Au	0.00064080	-13.32532833	10.32842177
Au	1.44659446	-10.82131714	10.34718772
Au	-1.43953859	-20.82066695	10.32028188
Au	-0.02096850	-18.31554292	10.33407548
Au	1.44273924	-15.82747323	10.32856615
Au	2.87189618	-13.32351984	10.32448569
Au	-11.53803417	-14.99393472	12.75387112
Au	-10.11866087	-12.51774834	12.77305361
Au	-8.65183637	-9.97377211	12.76204238
Au	-7.19941506	-7.50345173	12.76996067
Au	-10.12864916	-17.48602241	12.75412518
Au	-8.64140052	-14.99590258	12.76278256
Au	-7.24620825	-12.46409007	12.72249735
Au	-5.75296334	-9.97370791	12.77752895
Au	-4.30935022	-7.47357520	12.72133353
Au	-2.88211094	-4.97022398	12.77046987
Au	-1.40934670	-2.48232844	12.73805346
Au	4.30186849	-17.45403910	12.76433408
Au	-10.08009627	-22.51044888	12.76924841
Au	-8.64481383	-19.97805923	12.75808699
Au	-7.23098635	-17.49536088	12.76484702
Au	-5.77395260	-14.96522678	12.76532939
Au	-4.35454929	-12.48210399	12.77617709
Au	-2.88029684	-9.99401798	12.77625850
Au	-1.43677580	-7.50466715	12.76800054
Au	-0.00835212	-5.02883616	12.77358046
Au	-8.64758379	-25.02343772	12.73269898
Au	-7.22596465	-22.48191984	12.75555174
Au	-5.75309312	-20.00818941	12.74715206
Au	-4.36951249	-17.47984539	12.73461731
Au	-2.89845548	-14.98218285	12.76458318
Au	-1.46147276	-12.49900742	12.72797953
Au	-0.01284549	-9.99676482	12.77465016
Au	1.46173971	-7.52716177	12.72618815
Au	-7.17445237	-27.47912105	12.77705642
Au	-5.76321082	-24.94864932	12.74117099

Au	-4.30657031	-22.47187777	12.76431767
Au	-2.86018580	-19.95065110	12.73724496
Au	-1.46927012	-17.45450380	12.76932194
Au	0.01542031	-14.97762981	12.77104908
Au	1.42966415	-12.47921015	12.77407660
Au	-1.44557888	-22.47931492	12.76489536
Au	0.00715965	-19.98629048	12.75669290
Au	1.41648632	-17.50508494	12.75051939
Au	2.87616540	-14.98872894	12.75634565
O	1.15059989	-18.58213008	15.62728165
O	-1.51815191	-20.44727635	15.66335996
O	-4.17453445	-22.29993059	15.43084215
O	-6.82437905	-24.14362329	15.63330823
O	-9.47133495	-25.98485517	15.64493936
O	0.86226405	-15.36242942	15.62628698
O	-1.77338104	-17.22969403	15.47268068
O	-4.43596953	-19.07072611	15.63399373
O	-7.09463145	-20.91193130	15.67157025
O	-9.75759626	-22.75624989	15.47660113
O	0.58359104	-12.13748607	15.62971668
O	-2.06412006	-13.99129762	15.65556155
O	-4.70789493	-15.85577394	15.67614825
O	-7.36036526	-17.68762447	15.43557369
O	-10.02719329	-19.54006365	15.64129734
O	0.30533482	-8.89861364	15.67498238
O	-2.34505815	-10.76220854	15.66222627
O	-4.98735894	-12.62435789	15.55857498
O	-7.64670554	-14.46989986	15.64406781
O	-10.28985295	-16.32130663	15.65788429
O	0.03072975	-5.67040558	15.56156213
O	-2.62930535	-7.54313609	15.66986732
O	-5.28781390	-9.39783870	15.60410389
O	-7.92426801	-11.25192516	15.64834155
O	-10.57455310	-13.09287102	15.56756969
O	-0.25648404	-2.46397618	15.62552478
O	-2.90857452	-4.32599580	15.54251121
O	-5.55751279	-6.17531990	15.64714359
O	-8.22094346	-8.02124906	15.67284204
O	-6.54869290	-27.36385734	15.55196422
O	3.80086812	-16.73566990	15.59774563
Zn	-0.70004561	-18.77999788	15.44814614
Zn	-3.36896628	-20.59294794	15.40003483
Zn	-6.05696272	-22.45106513	15.42800545
Zn	-8.67860844	-24.30029101	15.40330037
Zn	1.65272650	-13.67076904	15.47927652
Zn	-0.99709932	-15.51377242	15.44580305
Zn	-3.65046841	-17.38173756	15.40837369
Zn	-6.28777246	-19.24041891	15.41128131
Zn	-8.94733268	-21.05588140	15.43815474
Zn	1.34923794	-10.43778570	15.48262354
Zn	-1.28087766	-12.29552407	15.44749582
Zn	-3.92099476	-14.16816013	15.49170047
Zn	-6.55953272	-15.97873355	15.45006161
Zn	-9.23994543	-17.85601867	15.41849320
Zn	1.09589474	-7.21387919	15.42419457
Zn	-1.55342236	-9.06936973	15.53986728
Zn	-4.20258997	-10.92058961	15.50829472
Zn	-6.85769083	-12.78179698	15.41657382
Zn	-9.50580707	-14.63170389	15.44437616
Zn	0.83731463	-3.97494864	15.47001403
Zn	-1.83173986	-5.86318577	15.48106854
Zn	-4.48555506	-7.70510412	15.43552866
Zn	-7.15616066	-9.54986467	15.50858486

Zn	-9.77968941	-11.39424332	15.45095456
Zn	-12.43883677	-13.27403164	15.42335272
Zn	-2.11680462	-2.62528690	15.41105305
Zn	-0.45104892	-21.97177258	15.45389278
Zn	-3.08099164	-23.83832653	15.44911398
Zn	-5.74655390	-25.66773394	15.42187614
Zn	-8.42130961	-27.52151157	15.44995166
Zn	1.93821126	-16.88736497	15.42406981

31/16 Sn

158

Lattice="-9.1782460198 15.8971884307 0.0 -9.1782460198 -15.8971884307 0.0 0.0 0.0 22.3574735566"

Sn	-13.76736903	0.00000000	5.50000000
Sn	-11.47280752	3.97429711	5.50000000
Sn	-9.17824602	7.94859422	5.50000000
Sn	-6.88368451	11.92289132	5.50000000
Sn	-11.47280752	-3.97429711	5.50000000
Sn	-9.17824602	0.00000000	5.50000000
Sn	-6.88368451	3.97429711	5.50000000
Sn	-4.58912301	7.94859422	5.50000000
Sn	-9.17824602	-7.94859422	5.50000000
Sn	-6.88368451	-3.97429711	5.50000000
Sn	-4.58912301	0.00000000	5.50000000
Sn	-2.29456150	3.97429711	5.50000000
Sn	-6.88368451	-11.92289132	5.50000000
Sn	-4.58912301	-7.94859422	5.50000000
Sn	-2.29456150	-3.97429711	5.50000000
Sn	0.00000000	0.00000000	5.50000000
Sn	-11.47224301	1.32702034	6.58373666
Sn	-9.17925691	5.30533196	6.58970351
Sn	-6.88170651	9.26995725	6.55182371
Sn	-13.77229283	-2.65354143	6.58970351
Sn	-9.18048085	-2.65016983	6.58373666
Sn	-6.88201420	1.32314950	6.58373666
Sn	-4.58813123	5.30182995	6.55724577
Sn	-11.47245762	-6.62594092	6.60188162
Sn	-6.88178399	-6.62607099	6.55724577
Sn	-4.58318833	-2.65179052	6.58970351
Sn	-2.29290705	1.32612493	6.60188162
Sn	-9.17824602	-10.59812562	6.63214198
Sn	-13.76937338	5.29981599	6.60188162
Sn	-11.47674332	9.27334825	6.55182371
Sn	-9.17628823	13.25107136	6.55182371
Sn	-16.06482284	1.32424104	6.55724577
Sn	-11.43270262	1.31004385	9.46857165
Sn	-9.24364925	5.27638358	9.47073501
Sn	-6.84954155	9.24197814	9.41274406
Sn	-13.71502662	-2.69483265	9.47073501
Sn	-9.18554898	-2.60743861	9.46857165
Sn	-6.91648646	1.29739476	9.46857165
Sn	-4.52119877	5.28286365	9.43339489
Sn	-11.52526957	-6.62592917	9.48903550
Sn	-6.93167552	-6.67455304	9.43339489
Sn	-4.57606219	-2.58155093	9.47073501
Sn	-2.26651126	1.28038256	9.48903550
Sn	-9.17824602	-10.59812562	9.51851483
Sn	-13.74295723	5.34554661	9.48903550
Sn	-11.51705642	9.25948214	9.41274406
Sn	-9.16814008	13.29291659	9.41274406
Sn	-16.08186377	1.39168940	9.43339489
Sn	-13.74425735	2.65855715	10.40218677
Sn	-11.47319512	6.67086217	10.57058950
Sn	-9.17824602	10.59812562	10.24836430

Sn	-16.01324654	-1.28781087	10.35283958
Sn	-11.47679428	-1.31330547	10.54263327
Sn	-9.16632779	2.64725392	10.54263327
Sn	-6.87602269	6.56318952	10.35283958
Sn	-13.80790758	-5.32291530	10.57058950
Sn	-9.19761839	-5.28356039	10.40218677
Sn	-6.89161599	-1.33394845	10.54263327
Sn	-4.59286232	2.62500323	10.40218677
Sn	-11.46767509	-9.26354392	10.54746609
Sn	-6.87774983	-9.28271274	10.54746609
Sn	-4.64546883	-5.27537865	10.35283958
Sn	-2.25363537	-1.34794687	10.57058950
Sn	-9.18931315	-13.24812021	10.54746609
Sn	-13.73669694	2.80059619	13.28024903
Sn	-11.42318777	6.65364851	13.48425131
Sn	-9.17824602	10.59812562	13.08650701
Sn	-15.92794833	-1.50655596	13.21061665
Sn	-11.41590497	-1.36256736	13.44077640
Sn	-9.23943449	2.61915317	13.44077640
Sn	-7.10811059	6.59869164	13.21061665
Sn	-13.81800378	-5.27100085	13.48425131
Sn	-9.32440801	-5.34803240	13.28024903
Sn	-6.87939860	-1.25658582	13.44077640
Sn	-4.47363311	2.54743620	13.28024903
Sn	-11.50416597	-9.39608462	13.44244929
Sn	-6.97428800	-9.18484035	13.44244929
Sn	-4.49867914	-5.09213569	13.21061665
Sn	-2.29354650	-1.38264767	13.48425131
Sn	-9.05628409	-13.21345189	13.44244929
Sn	-13.78364426	0.08264870	14.19473768
Sn	-11.47406975	4.00328677	14.46968119
Sn	-9.17884563	8.10650774	14.42014154
Sn	-7.02014183	11.84341528	14.42014154
Sn	-11.49728219	-3.98988506	14.46968119
Sn	-9.17824602	0.00000000	14.51317183
Sn	-6.80397102	3.94706752	14.19473768
Sn	-4.76369579	7.82853093	14.18199708
Sn	-9.29660016	-7.91790564	14.44634383
Sn	-6.94712278	-4.02971622	14.19473768
Sn	-4.56338611	-0.01340171	14.46968119
Sn	-2.26196152	3.85645513	14.44634383
Sn	-15.97617638	4.06145051	14.44634383
Sn	-4.60581447	-7.73737811	14.18199708
Sn	-11.33575060	11.84445384	14.42014154
Sn	-18.16522779	-0.09115282	14.18199708
O	-15.40934411	-2.78370790	17.30868239
O	-14.17766965	0.17456815	16.47342045
O	-13.08633500	3.23560033	17.41706127
O	-11.78459694	6.32455743	17.32287114
O	-10.64998489	9.37715644	17.20527454
O	-9.49976691	12.48317346	17.20527454
O	-13.35229796	-5.41944483	17.32287114
O	-12.14034893	-2.33653169	17.39215425
O	-10.98473198	0.69188180	17.27226028
O	-9.72069036	3.73352222	17.39215425
O	-8.47345873	6.78814319	17.30868239
O	-7.38498626	9.93404696	17.20527454
O	-11.25803930	-8.02292869	17.29034945
O	-10.02631362	-5.00230450	17.41706127
O	-8.87419026	-1.91040364	17.27226028
O	-7.67581582	1.21852183	17.27226028
O	-6.52735375	4.24234379	16.47342045
O	-5.25730707	7.45589073	16.41591820

O	-9.17824602	-10.59812562	17.27875612
O	-7.88079104	-7.49678708	17.27628021
O	-6.82971466	-4.41691194	16.47342045
O	-5.67369876	-1.39699053	17.39215425
O	-4.42208944	1.76670417	17.41706127
O	-3.33456545	4.87202251	17.27628021
O	-16.31938156	2.62476457	17.27628021
O	-5.90816342	-10.08457027	17.29034945
O	-4.68172471	-7.12357811	16.41591820
O	-3.65193521	-4.00443529	17.30868239
O	-2.39784315	-0.90511261	17.32287114
O	-10.36853534	-13.68687790	17.29034945
O	-17.59570628	-0.33231263	16.41591820
Zn	-13.87787564	-1.73788331	17.09121925
Zn	-12.69191565	1.44578205	17.08367498
Zn	-11.54250446	4.40735701	17.19872724
Zn	-10.28894981	7.49544790	17.17333982
Zn	-9.17824602	10.59812562	17.15830310
Zn	-8.01531548	13.58254451	16.81596950
Zn	-11.81299993	-4.25118637	17.19872724
Zn	-10.64528041	-1.18784564	17.22853599
Zn	-9.47343332	1.86441187	17.22853599
Zn	-8.33348230	4.93894030	17.09121925
Zn	-7.17512871	8.09878878	16.81596950
Zn	-15.11414242	-4.70962165	17.17333982
Zn	-9.72042571	-6.86103814	17.15155819
Zn	-8.67349518	-3.76581818	17.08367498
Zn	-7.41602432	-0.67656623	17.22853599
Zn	-6.16932723	2.32003614	17.08367498
Zn	-5.00008562	5.51164957	16.71264765
Zn	-12.93891836	-7.22327884	17.09948929
Zn	-7.68610611	-9.41025589	17.22498554
Zn	-6.49409767	-6.37421783	16.71264765
Zn	-5.32338011	-3.20105699	17.09121925
Zn	-4.17923367	-0.15617063	17.19872724
Zn	-2.96532285	2.96097768	17.15155819
Zn	-10.95304134	-9.89982941	17.22498554
Zn	-14.84898950	3.90006046	17.15155819
Zn	-13.55345283	6.86847721	17.09948929
Zn	-12.34429387	10.11304356	16.81596950
Zn	-2.13164583	-2.78582625	17.17333982
Zn	-1.04236687	0.35480164	17.09948929
Zn	-8.89559061	-12.48429156	17.22498554
Zn	-16.04055476	0.86256826	16.71264765

36/31 Pb

196

Lattice="-12.2506249841 -15.1562177835 0.0 7.0003571337 -18.1874613402 0.0 0.0 0.0 22.5003677483"

Pb	-10.50053570	-18.18746134	5.50000000
Pb	-8.75044642	-15.15621778	5.50000000
Pb	-7.00035713	-12.12497423	5.50000000
Pb	-5.25026785	-9.09373067	5.50000000
Pb	-3.50017857	-6.06248711	5.50000000
Pb	-1.75008928	-3.03124356	5.50000000
Pb	0.00000000	0.00000000	5.50000000
Pb	-8.75044642	-21.21870490	5.50000000
Pb	-7.00035713	-18.18746134	5.50000000
Pb	-5.25026785	-15.15621778	5.50000000
Pb	-3.50017857	-12.12497423	5.50000000
Pb	-1.75008928	-9.09373067	5.50000000
Pb	-0.00000000	-6.06248711	5.50000000
Pb	-7.00035713	-24.24994845	5.50000000
Pb	-5.25026785	-21.21870490	5.50000000

Pb	-3.50017857	-18.18746134	5.50000000
Pb	-1.75008928	-15.15621778	5.50000000
Pb	0.00000000	-12.12497423	5.50000000
Pb	1.75008928	-9.09373067	5.50000000
Pb	-5.25026785	-27.28119201	5.50000000
Pb	-3.50017857	-24.24994845	5.50000000
Pb	-1.75008928	-21.21870490	5.50000000
Pb	-0.00000000	-18.18746134	5.50000000
Pb	1.75008928	-15.15621778	5.50000000
Pb	3.50017857	-12.12497423	5.50000000
Pb	-3.50017857	-30.31243557	5.50000000
Pb	-1.75008928	-27.28119201	5.50000000
Pb	-0.00000000	-24.24994846	5.50000000
Pb	1.75008928	-21.21870490	5.50000000
Pb	3.50017857	-18.18746134	5.50000000
Pb	5.25026785	-15.15621778	5.50000000
Pb	-8.77667466	-17.16859827	8.28855483
Pb	-7.00650406	-14.14133488	8.28047276
Pb	-5.23397875	-11.12446243	8.28518778
Pb	-3.48155828	-8.09156950	8.29727454
Pb	-1.76116345	-5.06172103	8.30464680
Pb	-0.02016290	-2.00960912	8.30684905
Pb	-10.51167027	-14.12398990	8.28441455
Pb	-7.02346160	-20.20833459	8.28967948
Pb	-5.26926900	-17.18391045	8.28942948
Pb	-3.49587571	-14.16951612	8.29022632
Pb	-1.73311571	-11.13399031	8.28472342
Pb	0.00811647	-8.09492934	8.28774163
Pb	1.72566038	-5.04866980	8.29466628
Pb	-5.24895156	-23.22446970	8.29474794
Pb	-3.50784241	-20.21016852	8.30873502
Pb	-1.75084726	-17.20024768	8.31348639
Pb	0.01424175	-14.17571132	8.30024512
Pb	1.75861455	-11.12764947	8.28322322
Pb	-8.75646276	-23.23800162	8.28288072
Pb	-3.48696226	-26.24373127	8.29173397
Pb	-1.74233509	-23.21958998	8.31144374
Pb	0.00258783	-20.20869060	8.32144793
Pb	1.75742024	-17.18703765	8.31060252
Pb	3.51428417	-14.14677173	8.30050044
Pb	-6.99673140	-26.25988621	8.28742549
Pb	-8.73635365	-11.09098205	8.28248619
Pb	0.02377601	-26.25640074	8.29195253
Pb	1.75932787	-23.23421439	8.29963852
Pb	3.49707059	-20.20873038	8.31910007
Pb	5.24599332	-17.16339715	8.30847863
Pb	-5.24066711	-29.27562607	8.28772400
Pb	-10.53520399	-16.11769237	11.14989632
Pb	-8.74736289	-13.09894173	11.12862697
Pb	-6.95599035	-10.08474480	11.14425869
Pb	-5.20187238	-7.06823755	11.18211217
Pb	3.50751607	-22.21958778	11.22731400
Pb	5.22146869	-19.16408910	11.21652488
Pb	-5.26050177	-31.26990429	11.16023332
Pb	-8.78724019	-19.18167565	11.15606137
Pb	-7.02916252	-16.16803829	11.13947192
Pb	-5.24584279	-13.15742787	11.13570046
Pb	-3.46902741	-10.13579663	11.15221074
Pb	-1.73065632	-7.08068847	11.18814053
Pb	-0.02694215	-4.01738271	11.18657737
Pb	-7.02256231	-22.22738221	11.16580511
Pb	-5.28356607	-19.21857410	11.16650146
Pb	-3.52038787	-16.21235637	11.16052991

Pb	-1.74229056	-13.18652942	11.15269382
Pb	0.01276917	-10.12962345	11.16180874
Pb	1.73737557	-7.06844535	11.17212513
Pb	-5.23867884	-25.23158072	11.16720883
Pb	-3.49355800	-22.23020159	11.20929374
Pb	-1.76057240	-19.23406417	11.21986749
Pb	-0.00360251	-16.20962523	11.20632754
Pb	1.75148974	-13.15396817	11.17773641
Pb	3.49657438	-10.10344209	11.16168596
Pb	-3.47900199	-28.24809365	11.14728047
Pb	-1.70457404	-25.23596459	11.17339449
Pb	0.03080624	-22.23133629	11.22590898
Pb	1.74144777	-19.20555395	11.23597706
Pb	3.48822704	-16.15906551	11.20770216
Pb	-6.99739088	-28.25792313	11.18060848
Pb	-10.56648770	-18.04552456	13.98059634
Pb	-8.80262712	-15.05079164	13.96163086
Pb	-6.95025004	-12.13139787	13.96274525
Pb	-5.11184747	-9.16783150	13.98832868
Pb	-3.36727288	-6.08151097	14.01419201
Pb	-1.74246680	-2.90349808	14.03023301
Pb	-5.27594698	-33.16008538	14.00037385
Pb	-8.78596958	-21.16850315	13.97348120
Pb	-7.11831384	-18.15225880	13.97823988
Pb	-5.34008387	-15.21133571	13.96863614
Pb	-3.50312110	-12.23763008	13.97049637
Pb	-1.68749250	-9.17456806	13.98488576
Pb	0.03794874	-6.01292426	13.99010103
Pb	-7.00937206	-24.24486039	13.96356533
Pb	-5.30746035	-21.26528850	13.98873905
Pb	-3.64043130	-18.27657885	14.00263153
Pb	-1.86908029	-15.27617566	13.99695465
Pb	-0.04314965	-12.20917037	13.97618803
Pb	1.75577686	-9.09053144	13.96697750
Pb	-5.19307501	-27.22618256	13.97193656
Pb	-3.42119513	-24.29383315	13.99072237
Pb	-1.74523456	-21.31542954	14.03825649
Pb	-0.09759560	-18.26197099	14.04669398
Pb	1.66217092	-15.16908045	14.01557393
Pb	3.47292080	-12.09925308	13.97335647
Pb	-3.45061936	-30.20031005	13.97045229
Pb	-1.61589903	-27.28296366	13.97426018
Pb	0.14726524	-24.32369717	14.01947891
Pb	1.78030378	-21.24231326	14.04958885
Pb	3.44176883	-18.10428338	14.04123726
Pb	5.23929162	-15.03982781	14.00630500
O	-4.25856595	-26.87971503	17.21384066
O	-2.22608763	-24.32544546	17.25389744
O	-5.40334472	-23.82195696	17.25625663
O	-0.16115977	-21.79156171	17.38855642
O	-3.33928977	-21.27678697	17.30360900
O	-6.53251764	-20.78787616	17.25076947
O	1.90649555	-19.28433542	17.45553971
O	-1.27865701	-18.74356268	17.33026431
O	-4.47190817	-18.24440441	17.20494205
O	-7.68682415	-17.77429720	17.17634627
O	3.95343247	-16.79283662	17.33860946
O	0.76050281	-16.23075466	17.33068044
O	-2.43995397	-15.70444373	17.17807151
O	-5.65563612	-15.22280672	17.12861552
O	-8.88031318	-14.76311000	17.10695911
O	-6.27457189	-29.42845879	17.23229412
O	2.78811266	-13.73040903	17.27831566

O	-0.41969624	-13.18365954	17.22162241
O	-3.63976967	-12.67574050	17.14292971
O	-6.86406515	-12.20518934	17.09214488
O	-3.07885469	-29.92486964	17.13782986
O	-7.43792492	-26.36455771	17.24345433
O	1.60894010	-10.68306624	17.25120029
O	-1.62184285	-10.15489503	17.22381243
O	-4.85256530	-9.65461502	17.15357782
O	-1.06742072	-27.36688523	17.15046348
O	-8.59881459	-23.32312588	17.24033642
O	0.42803473	-7.66026530	17.26232583
O	-2.81243679	-7.13864074	17.25334981
O	0.96387624	-24.82222252	17.22088561
O	-9.74967362	-20.30732664	17.23994802
O	-0.73383315	-4.65303350	17.28685597
O	3.03700120	-22.31727510	17.38039187
O	-10.91464451	-17.30359514	17.18291053
O	5.11328213	-19.83141395	17.32187456
O	-5.09825371	-32.47420435	17.17339064
Zn	-5.69801216	-25.66872647	17.19035813
Zn	-3.66709656	-23.11661324	17.21755583
Zn	-6.85704101	-22.63485110	17.19786622
Zn	-1.59432538	-20.58733966	17.29673984
Zn	-4.78996965	-20.09513067	17.20529049
Zn	-8.00495777	-19.62993534	17.18139502
Zn	0.48004118	-18.08354105	17.33193115
Zn	-2.71924566	-17.56068289	17.18254539
Zn	-5.94017052	-17.08371490	17.13178742
Zn	-9.16949599	-16.62706508	17.11288507
Zn	2.52453556	-15.58707953	17.27089619
Zn	-0.67576272	-15.04132020	17.19018441
Zn	-3.90247123	-14.53428465	17.10802249
Zn	-7.13574129	-14.06589140	17.07646814
Zn	-10.35790306	-13.59875570	17.09684293
Zn	4.54000090	-13.06172065	17.20065173
Zn	1.34791889	-12.53898893	17.20165888
Zn	-1.87750874	-12.01056527	17.15864920
Zn	-5.11355737	-11.51175954	17.08996485
Zn	-8.33959171	-11.03440302	17.08651289
Zn	-4.53638099	-28.73246015	17.15674864
Zn	3.36410116	-10.01927894	17.19547960
Zn	0.14637955	-9.51481157	17.20180659
Zn	-3.09260732	-8.98964626	17.17006841
Zn	-6.32635747	-8.48132611	17.12470950
Zn	-2.52429484	-26.16963163	17.16194030
Zn	2.18190921	-7.00361614	17.19818779
Zn	-1.04839357	-6.50311482	17.21525279
Zn	-4.28433144	-5.96762195	17.22900968
Zn	-0.48895806	-23.62429905	17.23811677
Zn	1.01638522	-4.00502499	17.18537013
Zn	-2.20879627	-3.49573829	17.28536067
Zn	1.58943647	-21.12729091	17.37201138
Zn	-0.14212651	-0.99270110	17.17377886
Zn	3.66147151	-18.64902228	17.32987724
Zn	5.69762740	-16.13116011	17.19637696

Wurtzite ZnO(10-10) on metals

20/27 Ru

148

Lattice="-12.195 -11.7346442213 0.0 0.0 -14.0815730655 0.0 0.0 0.0 20.6581941874"

Ru	-10.84000000	-12.51695384	5.50000000
Ru	-9.48500000	-10.17002499	5.50000000
Ru	-8.13000000	-7.82309615	5.50000000
Ru	-6.77500000	-19.55774037	5.50000000
Ru	-10.84000000	-17.21081152	5.50000000
Ru	-9.48500000	-14.86388268	5.50000000
Ru	-8.13000000	-12.51695384	5.50000000
Ru	-6.77500000	-10.17002499	5.50000000
Ru	-5.42000000	-7.82309615	5.50000000
Ru	-4.06500000	-5.47616730	5.50000000
Ru	-2.71000000	-3.12923846	5.50000000
Ru	-1.35500000	-14.86388268	5.50000000
Ru	0.00000000	-12.51695384	5.50000000
Ru	-10.84000000	-21.90466921	5.50000000
Ru	-9.48500000	-19.55774037	5.50000000
Ru	-8.13000000	-17.21081153	5.50000000
Ru	-6.77500000	-14.86388268	5.50000000
Ru	-5.42000000	-12.51695384	5.50000000
Ru	-4.06500000	-10.17002499	5.50000000
Ru	-2.71000000	-7.82309615	5.50000000
Ru	-1.35500000	-5.47616730	5.50000000
Ru	0.00000000	-3.12923846	5.50000000
Ru	-5.42000000	-17.21081152	5.50000000
Ru	-4.06500000	-14.86388268	5.50000000
Ru	-2.71000000	-12.51695384	5.50000000
Ru	-1.35500000	-10.17002499	5.50000000
Ru	0.00000000	-7.82309615	5.50000000
Ru	-10.84464936	-14.07534824	7.54202031
Ru	-9.49214302	-11.73053562	7.56963035
Ru	-8.11548247	-9.38452387	7.57211731
Ru	-6.77088534	-7.04850688	7.57812221
Ru	-10.81885047	-18.78877420	7.54627331
Ru	-9.46726588	-16.41748524	7.53539780
Ru	-8.14020797	-14.06932194	7.56016869
Ru	-6.77530582	-11.72791938	7.56737695
Ru	-5.42626954	-9.38952902	7.57299413
Ru	-4.06138995	-7.04971522	7.57564356
Ru	-2.72975605	-4.71169777	7.55449875
Ru	-1.36384445	-2.34623561	7.54999159
Ru	-12.19485638	-11.74322081	7.54898848
Ru	-10.83274249	-23.47084793	7.56008875
Ru	-9.45797156	-21.12765605	7.56734651
Ru	-8.12027142	-18.77910449	7.55380517
Ru	-6.77714671	-16.43410141	7.56376375
Ru	-5.42974970	-14.07587200	7.55567371
Ru	-4.07788938	-11.73611219	7.55575724
Ru	-2.70754334	-9.38885176	7.56157384
Ru	-1.35550565	-7.05743910	7.53975733
Ru	-0.00331412	-4.69414791	7.53224832
Ru	-5.41891290	-18.78756904	7.57330386
Ru	-4.08418560	-16.44431672	7.55568565
Ru	-2.71374281	-14.08736257	7.55645457
Ru	-1.34586995	-11.74178604	7.55581459
Ru	-12.17947445	-21.12694343	7.54753450
Ru	-10.85923755	-12.51837743	9.70094860
Ru	-9.47674134	-10.15919063	9.69911148
Ru	-8.11116844	-7.82685973	9.74417505
Ru	-6.76310321	-19.56190885	9.73031047

Ru	-10.82416968	-17.19787694	9.58612000
Ru	-9.50011183	-14.85376215	9.67588695
Ru	-8.14680524	-12.49574508	9.68882395
Ru	-6.77735736	-10.17978114	9.73701781
Ru	-5.41025153	-7.83137719	9.73031105
Ru	-4.07368405	-5.50429949	9.71376206
Ru	-2.71813545	-3.14463074	9.68191385
Ru	-1.35780310	-14.87248576	9.65926943
Ru	-12.18034717	-24.25835702	9.68474861
Ru	-10.80739435	-21.90175348	9.68403660
Ru	-9.45129328	-19.55542004	9.68855922
Ru	-8.11881507	-17.20512770	9.69607434
Ru	-6.80111806	-14.85546813	9.65865386
Ru	-5.42255387	-12.51174924	9.71415159
Ru	-4.06823945	-10.17420750	9.68402569
Ru	-2.69992115	-7.83369248	9.69540206
Ru	-1.34767867	-5.49998689	9.63309965
Ru	-0.01135259	-3.12966381	9.62829357
Ru	-5.43568212	-17.22669789	9.69907733
Ru	-4.06989624	-14.86392031	9.67668244
Ru	-2.71429835	-12.52303296	9.65821572
Ru	-1.33084868	-10.16149915	9.65137924
Ru	-12.16735151	-19.56551879	9.64928566
Ru	-10.91513392	-14.10380089	11.76215036
Ru	-9.56663419	-11.74773053	11.75307817
Ru	-8.13066878	-9.38480481	11.82161276
Ru	-6.74673063	-7.04725865	11.80088564
Ru	-10.79405816	-18.67717131	11.68535137
Ru	-9.51270815	-16.40930152	11.69036686
Ru	-8.23098669	-14.05515813	11.69871162
Ru	-6.78842634	-11.79739176	11.81209666
Ru	-5.42104536	-9.42063860	11.77033101
Ru	-3.98143490	-7.11324071	11.80977799
Ru	-2.64466582	-4.73685637	11.70878882
Ru	-1.37929193	-2.44040779	11.69980732
Ru	-0.06040834	-14.03118175	11.77608458
Ru	-10.86063369	-23.48493116	11.73894622
Ru	-9.47509538	-21.03881805	11.79789481
Ru	-8.10474897	-18.73250044	11.74982345
Ru	-6.77367165	-16.36117151	11.76620416
Ru	-5.44467012	-14.08852486	11.72275749
Ru	-4.08837167	-11.74852024	11.72270913
Ru	-2.64007612	-9.44688380	11.74234368
Ru	-1.29567163	-7.06206925	11.69245987
Ru	-12.19092011	-16.47776929	11.62017378
Ru	-5.35361309	-18.78062506	11.81882180
Ru	-4.03967001	-16.43620797	11.70714177
Ru	-2.74397989	-14.13839524	11.70869373
Ru	-1.29668451	-11.67177365	11.69079801
Ru	-12.15755283	-21.11056513	11.70322839
O	-9.69920424	-20.54461847	13.98165871
O	-0.61160256	-8.13052531	15.04474989
O	-5.94339894	-15.54698433	13.84713316
O	-8.91234001	-14.95490976	14.95892269
O	-10.87375607	-17.44398523	13.83040071
O	-1.74982220	-5.01214681	14.94501098
O	-2.27488021	-10.52590052	13.79928173
O	-5.27210146	-9.96456002	15.13442360
O	-6.95319733	-12.37794270	14.03082842
O	-10.06370035	-11.87122524	15.01854907
O	-11.88524271	-14.31754449	13.90839026
O	-2.89351839	-16.09588457	14.92195353
O	-3.62774074	-7.41752308	14.00244686

O	-6.67509432	-6.95854647	15.04196288
O	-8.32073669	-9.38289321	14.01900199
O	-11.49335678	-22.93675623	15.07797800
O	-4.85099301	-18.52655579	13.99340344
O	-7.92586112	-18.04268515	14.99174411
O	-0.85143259	-13.70090922	13.88537834
O	-3.96405592	-13.08693397	14.94905776
Zn	-11.25636538	-19.38443886	14.12004506
Zn	-0.61010680	-9.96071053	14.57308071
Zn	-7.34320831	-14.26682169	14.20154983
Zn	-9.14073865	-16.73730324	14.39219915
Zn	-0.14662350	-4.44174240	14.19644047
Zn	-1.86457777	-6.83242099	14.47078055
Zn	-3.86502169	-9.35200237	14.06051199
Zn	-5.22928158	-11.76595331	14.59684676
Zn	-8.49894454	-11.27431600	14.19646772
Zn	-10.12556558	-13.63362586	14.36079577
Zn	-1.26807541	-1.46046167	14.20210175
Zn	-3.03910144	-3.78063675	14.26719218
Zn	-5.15676047	-6.30963552	14.19487044
Zn	-6.60746536	-8.77366161	14.57842265
Zn	-9.96176775	-22.44043637	14.10446533
Zn	-11.39344397	-24.72907664	14.52085547
Zn	-6.35745296	-17.40157457	14.22608330
Zn	-8.00351757	-19.84935681	14.48169948
Zn	-2.49721240	-12.53917023	13.89530403
Zn	-4.10173598	-14.83233741	14.16696637

28/36 Pd

200

Lattice="-16.5038722729 -14.2927726491 0.0 5.5012907576 -9.5285150994 0.0 0.0 0.0 20.9758718289"

Pd	-13.75322689	-14.29277265	5.50000000
Pd	-12.37790421	-11.91064387	5.50000000
Pd	-11.00258152	-9.52851510	5.50000000
Pd	-12.37790420	-16.67490142	5.50000000
Pd	-11.00258152	-14.29277265	5.50000000
Pd	-9.62725883	-11.91064387	5.50000000
Pd	-8.25193614	-9.52851510	5.50000000
Pd	-6.87661345	-7.14638632	5.50000000
Pd	-5.50129076	-4.76425755	5.50000000
Pd	-11.00258152	-19.05703020	5.50000000
Pd	-9.62725883	-16.67490142	5.50000000
Pd	-8.25193614	-14.29277265	5.50000000
Pd	-6.87661345	-11.91064388	5.50000000
Pd	-5.50129076	-9.52851510	5.50000000
Pd	-4.12596807	-7.14638632	5.50000000
Pd	-2.75064538	-4.76425755	5.50000000
Pd	-1.37532269	-2.38212877	5.50000000
Pd	0.00000000	0.00000000	5.50000000
Pd	-9.62725883	-21.43915897	5.50000000
Pd	-8.25193614	-19.05703020	5.50000000
Pd	-6.87661345	-16.67490142	5.50000000
Pd	-5.50129076	-14.29277265	5.50000000
Pd	-4.12596807	-11.91064387	5.50000000
Pd	-2.75064538	-9.52851510	5.50000000
Pd	-1.37532269	-7.14638632	5.50000000
Pd	-0.00000000	-4.76425755	5.50000000
Pd	1.37532269	-2.38212877	5.50000000
Pd	-4.12596807	-16.67490142	5.50000000
Pd	-2.75064538	-14.29277265	5.50000000
Pd	-1.37532269	-11.91064387	5.50000000
Pd	0.00000000	-9.52851510	5.50000000
Pd	1.37532269	-7.14638632	5.50000000

Pd	2.75064538	-4.76425755	5.50000000
Pd	1.37532269	-11.91064387	5.50000000
Pd	2.75064538	-9.52851510	5.50000000
Pd	4.12596807	-7.14638632	5.50000000
Pd	-12.37279411	-13.49503222	7.78607742
Pd	-11.00637936	-11.11465659	7.79350849
Pd	-9.63871030	-8.71906260	7.77872111
Pd	-11.00965772	-15.88359920	7.77519856
Pd	-9.63454941	-13.49502980	7.78345619
Pd	-8.26227605	-11.09902457	7.78520531
Pd	-6.88950307	-8.72818219	7.80338101
Pd	-5.51755642	-6.34468430	7.78072166
Pd	-4.14249169	-3.96227238	7.77898957
Pd	-9.62509629	-18.25929002	7.78396658
Pd	-8.26411985	-15.88239085	7.77625814
Pd	-6.89092160	-13.47997331	7.76604965
Pd	-5.51923772	-11.09835048	7.78974280
Pd	-4.14359920	-8.72028733	7.77819502
Pd	-2.76240641	-6.34538967	7.77526807
Pd	-1.39049751	-3.96093265	7.77508408
Pd	-0.00596404	-1.58362622	7.77288615
Pd	-15.13059017	-13.49138612	7.77478235
Pd	-8.24398666	-20.64207585	7.77483719
Pd	-6.88587906	-18.26087761	7.79387611
Pd	-5.51291697	-15.87150111	7.76455038
Pd	-4.14334994	-13.48285623	7.77253818
Pd	-2.77169386	-11.10074286	7.77660325
Pd	-1.38688727	-8.72411121	7.77865747
Pd	-0.01193661	-6.34289843	7.77608222
Pd	1.36844360	-3.96313500	7.77636753
Pd	-13.76029927	-15.87540193	7.77661389
Pd	-2.75820275	-15.87399201	7.77928254
Pd	-1.39497058	-13.48699174	7.77760598
Pd	-0.01305947	-11.10909862	7.77731716
Pd	1.36329796	-8.72760640	7.77429823
Pd	2.74404944	-6.34877661	7.77288142
Pd	-12.38196797	-18.26109854	7.77725928
Pd	2.73711079	-11.10822344	7.77774533
Pd	4.11973071	-8.72738962	7.77550582
Pd	-11.00641014	-20.63945416	7.77528556
Pd	-13.75460269	-12.70489877	10.01595288
Pd	-6.90069615	-19.86598746	10.05049476
Pd	-5.52104416	-17.42970832	10.02208774
Pd	-12.39532035	-15.08608297	10.02189627
Pd	-10.99988968	-12.69111103	10.06024846
Pd	-9.64731974	-10.28623928	10.02234583
Pd	-8.26025507	-7.91278694	10.04185025
Pd	-1.39656056	-15.07046248	10.02345677
Pd	-0.01473256	-12.68848881	10.02429774
Pd	-11.01411215	-17.47345994	10.02350319
Pd	-9.67653899	-15.11503205	10.01336029
Pd	-8.27846029	-12.65590634	10.01043016
Pd	-6.90324741	-10.31475468	10.07983262
Pd	-5.53203486	-7.91570763	10.04437948
Pd	-4.15131274	-5.54312271	10.01128684
Pd	-2.77623978	-3.15868565	10.02120592
Pd	4.10595117	-10.31879405	10.00908200
Pd	-11.01730102	-22.22728332	10.01510799
Pd	-9.63082649	-19.84956152	10.01087465
Pd	-8.25585223	-17.45332793	10.06092378
Pd	-6.89611185	-15.06802552	9.97354601
Pd	-5.51746097	-12.66778766	10.02218953
Pd	-4.15761626	-10.29640755	10.02639528

Pd	-2.76515057	-7.92110491	10.02305272
Pd	-1.40276915	-5.55513522	10.01633707
Pd	-0.00967501	-3.17123755	10.01751598
Pd	-15.15388656	-15.10037992	10.01498916
Pd	-4.13658257	-15.06574276	9.99819432
Pd	-2.78287838	-12.67153287	10.02249479
Pd	-1.40532812	-10.30812673	10.01193160
Pd	-0.02540374	-7.92438698	10.01874455
Pd	1.35605868	-5.55515054	10.01125721
Pd	-13.76795473	-17.46453736	10.02100332
Pd	1.34594044	-10.32170223	10.01944786
Pd	2.73955690	-7.93781960	10.01632169
Pd	-12.40289211	-19.86784244	10.01515362
Pd	-13.80106036	-14.31725353	12.25522621
Pd	-12.42137038	-11.92026675	12.35729375
Pd	-5.56130006	-18.99213772	12.26015939
Pd	-12.40033763	-16.67845278	12.31081918
Pd	-11.03997324	-14.29881575	12.33441006
Pd	-9.66491882	-11.82563933	12.33755354
Pd	-8.28832661	-9.46227891	12.32421074
Pd	-6.91001957	-7.09206312	12.35623115
Pd	-5.53084707	-4.74325691	12.29120546
Pd	-11.04847385	-19.08641749	12.24557137
Pd	-9.68508000	-16.68283798	12.36658766
Pd	-8.33490101	-14.26224227	12.14814329
Pd	-6.90814069	-11.89736711	12.35025969
Pd	-5.54236678	-9.47315913	12.32828186
Pd	-4.14467738	-7.12015119	12.29257819
Pd	-2.78877848	-4.73729526	12.28135313
Pd	-1.38999113	-2.38300524	12.28076729
Pd	-0.03328911	0.00152863	12.28448419
Pd	-9.64373227	-21.44308226	12.28188137
Pd	-8.28865458	-19.05794611	12.33088957
Pd	-6.90763049	-16.60444565	12.32472527
Pd	-5.51435237	-14.27147559	12.21343480
Pd	-4.14885019	-11.84562604	12.33471175
Pd	-2.78440257	-9.50419893	12.28673269
Pd	-1.40567407	-7.12516127	12.33367083
Pd	-0.03489031	-4.77457194	12.27007530
Pd	1.35163569	-2.39463392	12.33153663
Pd	-4.15267473	-16.63702079	12.31384816
Pd	-2.78552843	-14.24353811	12.28596337
Pd	-1.39585347	-11.89004416	12.28993674
Pd	-0.03850327	-9.50193301	12.28079569
Pd	1.35813934	-7.14855050	12.28064342
Pd	2.72017732	-4.76289680	12.29200977
Pd	1.34272019	-11.88764926	12.33745840
Pd	2.71506697	-9.54066334	12.27407526
Pd	4.09381083	-7.15953703	12.32758349
O	-12.45788439	-15.43498703	15.42051094
O	-9.55314830	-14.20399593	15.50925066
O	-9.65380412	-11.26463909	14.54544710
O	-6.84831001	-9.90214942	15.57294794
O	-6.88891519	-6.85361722	14.53680262
O	-4.15192192	-5.41860548	15.34905251
O	-9.66986064	-17.14645007	14.56460959
O	-6.86231211	-16.00616546	14.52532637
O	-6.86670726	-12.88126230	14.56359967
O	-4.12459843	-11.60128425	14.52812111
O	-4.13684498	-8.51756156	15.34128783
O	-1.42049629	-7.09138719	14.50669302
O	-1.42004306	-3.98166510	15.32992360
O	1.31617918	-2.52790658	14.51688054

O	-15.20183985	-13.76688858	15.32698489
O	-12.40619829	-12.41559389	14.54340338
O	-6.88553200	-18.99278263	15.46625147
O	-4.10684114	-17.75567143	15.28994046
O	-4.15660413	-14.66847073	15.44831984
O	-1.40382002	-13.30111107	15.33601414
O	-1.40148469	-10.18206311	15.34648099
O	1.32354450	-8.74683968	15.34849465
O	1.29597038	-5.63843719	15.32811898
O	-12.44231227	-18.51435807	15.35434464
O	1.32157862	-11.86263442	14.51361183
O	4.03827430	-10.40411445	15.33474965
O	4.04815222	-7.29284736	14.50828133
O	-9.71746764	-20.21788446	15.31377095
Zn	-10.67773028	-15.62065568	15.00622607
Zn	-10.58780814	-12.90864012	14.67876958
Zn	-7.80555146	-11.28191621	14.82863257
Zn	-7.82152802	-8.46378912	14.90088861
Zn	-5.00589989	-6.97483432	14.80804768
Zn	0.35996746	-13.48220344	14.82006036
Zn	-7.84390349	-17.62505916	14.69325059
Zn	-7.92819514	-14.45084672	14.64839426
Zn	-5.03263849	-13.26253217	14.66454116
Zn	-5.12065024	-10.02425794	14.87902998
Zn	-2.38087430	-8.71217534	14.80955555
Zn	-2.38459276	-5.47605398	14.79882384
Zn	0.34312342	-4.14383108	14.80582814
Zn	0.29927372	-0.94235138	14.78447220
Zn	-13.44860740	-13.99274858	14.80717582
Zn	-7.94662570	-20.38872743	14.81904297
Zn	-10.66457412	-9.68338415	14.80888536
Zn	-5.00331415	-16.20844629	14.82875992
Zn	-2.39575264	-14.79073792	14.83259304
Zn	-2.24794258	-11.74226678	14.81277174
Zn	0.36702349	-10.23893749	14.79962109
Zn	0.45819918	-7.20804375	14.79436941
Zn	3.06429983	-5.68855470	14.79780735
Zn	-13.31574829	-16.97586625	14.80406517
Zn	-2.29929931	-2.44427541	14.79113948
Zn	3.08378172	-8.91114862	14.81242330
Zn	-10.58011016	-21.77018070	14.75464681
Zn	-10.70246908	-18.74418940	14.78581070

22/28 Pt

156

Lattice="1.3859292911 16.8034996355 0.0 -9.7015050379 16.8034996355 0.0 0.0 0.0 21.0278333531"

Pt	-8.31557575	28.80599938	5.50000000
Pt	-8.31557575	24.00499948	5.50000000
Pt	-6.92964646	26.40549943	5.50000000
Pt	-8.31557575	19.20399958	5.50000000
Pt	-6.92964646	21.60449953	5.50000000
Pt	-5.54371716	24.00499948	5.50000000
Pt	-8.31557575	14.40299969	5.50000000
Pt	-6.92964646	16.80349964	5.50000000
Pt	-5.54371716	19.20399958	5.50000000
Pt	-4.15778787	21.60449953	5.50000000
Pt	-6.92964646	12.00249974	5.50000000
Pt	-5.54371716	14.40299969	5.50000000
Pt	-4.15778787	16.80349964	5.50000000
Pt	-2.77185858	19.20399958	5.50000000
Pt	-5.54371716	9.60199979	5.50000000
Pt	-4.15778787	12.00249974	5.50000000
Pt	-2.77185858	14.40299969	5.50000000

Pt	-1.38592929	16.80349964	5.50000000
Pt	-4.15778787	7.20149984	5.50000000
Pt	-2.77185858	9.60199979	5.50000000
Pt	-1.38592929	12.00249974	5.50000000
Pt	0.00000000	14.40299969	5.50000000
Pt	-2.77185858	4.80099990	5.50000000
Pt	-1.38592929	7.20149984	5.50000000
Pt	0.00000000	9.60199979	5.50000000
Pt	-1.38592929	2.40049995	5.50000000
Pt	0.00000000	4.80099990	5.50000000
Pt	0.00000000	0.00000000	5.50000000
Pt	-6.92235713	29.63867611	7.78800162
Pt	-6.91413048	24.81979949	7.79325289
Pt	-5.53252117	27.22650995	7.78808136
Pt	-6.92578346	20.03936427	7.81928852
Pt	-5.53207614	22.42347595	7.80212370
Pt	-4.13858579	24.82699002	7.78829513
Pt	-6.93168417	15.24305282	7.78752323
Pt	-5.54479006	17.64395835	7.79700127
Pt	-4.15263006	20.03324179	7.79679387
Pt	-2.75406476	22.42842233	7.78019957
Pt	-5.53999680	12.83698142	7.79481713
Pt	-4.15945084	15.23516431	7.78952992
Pt	-2.77129195	17.64597908	7.79865948
Pt	-1.36176213	20.03290422	7.79193802
Pt	-4.14786719	10.42633395	7.79146364
Pt	-2.76558843	12.83294847	7.78630491
Pt	-1.38723995	15.24267800	7.78658439
Pt	0.01283939	17.64454356	7.79089584
Pt	-2.74988322	8.02367806	7.79898289
Pt	-1.37152746	10.41730239	7.79066308
Pt	0.00101156	12.83311819	7.79528214
Pt	-8.31476788	32.03494919	7.78620184
Pt	-1.36553026	5.62408989	7.80928538
Pt	0.01812425	8.01528350	7.79666850
Pt	-8.30509314	27.22861997	7.79018089
Pt	0.01723648	3.23717648	7.83023599
Pt	-8.30236500	22.41781126	7.81404608
Pt	-8.31306605	17.64724672	7.80442249
Pt	-8.30504026	30.46482380	10.03274491
Pt	-8.28921099	25.65251907	10.04036149
Pt	-6.91042536	28.06189561	10.02814638
Pt	-8.27769425	20.87851872	10.14228456
Pt	-6.89552780	23.25074591	10.04360302
Pt	-5.50160820	25.66739595	10.03311459
Pt	-8.32469556	16.04988189	10.03756129
Pt	-6.93738365	18.46451313	10.05938975
Pt	-5.52851321	20.83789231	10.08284258
Pt	-4.11815676	23.25569117	10.02241594
Pt	-6.92914905	13.67217794	10.03397886
Pt	-5.54120510	16.06730959	10.03440509
Pt	-4.16435145	18.47225055	10.05834047
Pt	-2.72438362	20.85387360	10.02552679
Pt	-5.52529814	11.24878950	10.02842084
Pt	-4.14323836	13.66562103	10.03056351
Pt	-2.77919470	16.05448553	10.03492635
Pt	-1.37209883	18.46308062	10.03891182
Pt	-4.13029973	8.85237522	10.04737658
Pt	-2.74701053	11.25210306	10.02440695
Pt	-1.38719485	13.67014324	10.03248737
Pt	0.00669291	16.06629885	10.02660948
Pt	-2.73975759	6.45072905	10.03640450
Pt	-1.33557781	8.84416282	10.05824490

Pt	0.01928044	11.24161746	10.03099950
Pt	-1.35214345	4.04226891	10.09875126
Pt	0.02496289	6.43928926	10.06769636
Pt	0.00442856	1.67406024	10.07496488
Pt	-8.28195762	28.89406345	12.30927771
Pt	-8.27330803	24.09774801	12.33598556
Pt	-6.87454866	26.49448050	12.31488321
Pt	-8.32785217	19.28536421	12.39487261
Pt	-6.86283766	21.74066220	12.40218394
Pt	-5.46567880	24.12479300	12.30047242
Pt	-8.31130967	14.49346782	12.36592377
Pt	-6.93553405	16.86555637	12.29813989
Pt	-5.55506674	19.27582291	12.39500619
Pt	-4.07039802	21.69939154	12.27568044
Pt	-6.90687795	12.09327137	12.30940374
Pt	-5.53366025	14.48336376	12.32216953
Pt	-4.16389842	16.88338490	12.33853762
Pt	-2.77233153	19.28646081	12.33748304
Pt	-5.47988658	9.71536175	12.36492979
Pt	-4.12158031	12.09289516	12.29768911
Pt	-2.76491617	14.49155046	12.36562465
Pt	-1.39097114	16.86995688	12.29057016
Pt	-4.09242269	7.28059770	12.35899634
Pt	-2.71169599	9.68541385	12.30949340
Pt	-1.35975897	12.08858093	12.30395164
Pt	0.00924137	14.48549877	12.31792005
Pt	-2.72111678	4.92027803	12.36595717
Pt	-1.33867861	7.28341617	12.37412146
Pt	0.06007200	9.70285695	12.37513166
Pt	-1.39238971	2.48879291	12.40851671
Pt	0.03125892	4.91077154	12.43440383
Pt	-0.01014941	0.08477431	12.33351928
O	-6.83679614	28.19082633	15.42157539
O	-5.50159574	12.90033886	15.43961686
O	-6.40573744	22.04556223	14.54629780
O	-3.73892580	23.59395751	15.36956327
O	-5.35310357	9.85042047	14.52745409
O	-2.66663108	11.39992200	15.39493780
O	-5.68039006	15.98957657	15.44241524
O	-2.97185694	17.49515054	15.47420676
O	-3.40747198	20.58813403	15.41613241
O	-2.14359742	5.25853564	15.29650279
O	-2.80238696	14.45724414	14.53656718
O	-0.13493219	16.01104632	15.42364541
O	-0.34530914	19.09535002	14.55416478
O	-8.89414668	20.55566051	15.63812700
O	-2.45697862	8.37017252	15.47707557
O	0.18018132	9.82481937	14.53003553
O	0.04200261	12.91010299	15.43331902
O	-8.34880773	14.45555854	14.53929784
O	0.47604682	6.84518576	15.42337810
O	-6.58900752	25.14839199	15.43865837
O	-8.51610626	17.50400192	15.46940618
O	-5.87924023	19.07082830	14.56402081
Zn	-6.45445831	11.40666426	14.86265657
Zn	-6.44362365	14.39052205	14.86315660
Zn	-4.48370088	21.97679802	14.80713338
Zn	-4.84484026	24.97576272	14.87129561
Zn	-3.44451976	9.79718117	14.84079186
Zn	-3.74890314	12.79463097	14.85224846
Zn	-3.91332184	15.99977724	14.87144608
Zn	-3.99059521	18.91629521	14.87762220
Zn	-1.65588262	20.52539503	14.77102756

Zn	-3.28001221	6.72160243	15.19093096
Zn	-0.89711671	14.40430469	14.86218452
Zn	-1.23170791	17.38809893	14.84099612
Zn	0.12116207	2.13964523	14.98373568
Zn	-0.29779176	5.16804156	15.12108796
Zn	-0.72446203	8.13885731	14.89060514
Zn	-0.89221816	11.40316767	14.85746866
Zn	-7.90374028	29.59391779	14.85818901
Zn	-8.06740356	32.81176154	14.85726255
Zn	-7.47341131	23.61890475	14.85626258
Zn	-7.61372710	26.58910693	14.86456423
Zn	-6.77033240	17.36307153	14.85071419
Zn	-7.26499874	20.36011618	14.81435178

18/27 Cu

144

Lattice="-14.0396051405 -2.2106644929 0.0 -15.3159328805 -13.2639869572 0.0 0.0 0.0 20.4908976028"

Cu	-25.52655480	-13.26398696	5.50000000
Cu	-22.97389932	-13.26398696	5.50000000
Cu	-21.69757158	-11.05332246	5.50000000
Cu	-20.42124384	-8.84265797	5.50000000
Cu	-20.42124384	-13.26398696	5.50000000
Cu	-19.14491610	-11.05332246	5.50000000
Cu	-17.86858836	-8.84265797	5.50000000
Cu	-16.59226062	-6.63199348	5.50000000
Cu	-15.31593288	-4.42132899	5.50000000
Cu	-17.86858836	-13.26398696	5.50000000
Cu	-16.59226062	-11.05332246	5.50000000
Cu	-15.31593288	-8.84265797	5.50000000
Cu	-14.03960514	-6.63199348	5.50000000
Cu	-12.76327740	-4.42132899	5.50000000
Cu	-11.48694966	-2.21066449	5.50000000
Cu	-14.03960514	-11.05332246	5.50000000
Cu	-12.76327740	-8.84265797	5.50000000
Cu	-11.48694966	-6.63199348	5.50000000
Cu	-10.21062192	-4.42132899	5.50000000
Cu	-8.93429418	-2.21066449	5.50000000
Cu	-10.21062192	-8.84265797	5.50000000
Cu	-8.93429418	-6.63199348	5.50000000
Cu	-7.65796644	-4.42132899	5.50000000
Cu	-6.38163870	-2.21066449	5.50000000
Cu	-5.10531096	-4.42132899	5.50000000
Cu	-3.82898322	-2.21066449	5.50000000
Cu	0.00000000	0.00000000	5.50000000
Cu	-24.24144761	-12.50090960	7.56057806
Cu	-21.69376314	-12.50531568	7.55381972
Cu	-20.42326789	-10.29062235	7.57958765
Cu	-19.14233607	-8.09015046	7.56879478
Cu	-19.14476758	-12.49634050	7.54340916
Cu	-17.86851675	-10.28726756	7.55349740
Cu	-16.57772728	-8.08628576	7.55052979
Cu	-15.29066784	-5.87693693	7.55832450
Cu	-14.01786699	-3.66930277	7.57504170
Cu	-16.57647132	-12.51629468	7.55625427
Cu	-15.29726283	-10.30301964	7.55072297
Cu	-14.01057014	-8.08048292	7.56846647
Cu	-12.74140265	-5.87834134	7.61412481
Cu	-11.48120600	-3.68433570	7.60414698
Cu	-25.52259256	-14.74139461	7.55644492
Cu	-12.74299177	-10.29765836	7.55807590
Cu	-11.47091439	-8.08110597	7.59001170
Cu	-10.20319826	-5.88015423	7.60466999
Cu	-8.93148301	-3.68784469	7.57479371

Cu	-7.65303158	-1.47167271	7.54172879
Cu	-22.96644604	-10.28247101	7.60499809
Cu	-7.66074664	-5.88941764	7.61806759
Cu	-6.38197477	-3.69348071	7.56440915
Cu	-5.09940034	-1.46512821	7.53391355
Cu	-17.84489097	-5.88006542	7.55176491
Cu	-2.52402395	-1.45593913	7.55609994
Cu	-28.06364046	-14.72698164	7.56184912
Cu	-11.47877033	-9.56121005	9.63344848
Cu	-22.96248459	-11.77165009	9.61292104
Cu	-21.67279966	-9.58442726	9.71602976
Cu	-6.36167866	-5.17606024	9.66240454
Cu	-20.42682261	-11.77165646	9.61429039
Cu	-19.14055586	-9.56070242	9.63219802
Cu	-17.84547874	-7.35428807	9.59984492
Cu	-16.55103248	-5.13305053	9.60773052
Cu	-1.23575880	-0.71616069	9.64673127
Cu	-17.85746272	-11.76721461	9.55553466
Cu	-16.56910583	-9.55831989	9.56819493
Cu	-15.29689123	-7.34196857	9.59039534
Cu	-14.03766192	-5.12085395	9.64221144
Cu	-12.75829022	-2.91537319	9.64759834
Cu	-26.77940649	-13.98815130	9.59232806
Cu	-14.01646089	-9.55832328	9.59410045
Cu	-12.73557598	-7.35491785	9.67983094
Cu	-11.46140543	-5.15112718	9.72193660
Cu	-10.19047284	-2.95514669	9.64198941
Cu	-24.24324607	-13.99752971	9.55868865
Cu	-10.21213257	-7.34211523	9.69284809
Cu	-8.93470403	-5.14763071	9.69341062
Cu	-7.64662110	-2.95725002	9.60290394
Cu	-21.68728200	-14.00379828	9.56217193
Cu	-5.08738783	-2.95446701	9.55500754
Cu	-3.81790440	-0.72067096	9.53171132
Cu	-15.29589966	-11.78012421	9.60149649
Cu	-25.50025701	-13.26219684	11.65925119
Cu	-22.94611696	-13.29114957	11.56528178
Cu	-21.68881120	-11.10474965	11.77182915
Cu	-20.35691812	-8.83201335	11.82208956
Cu	-20.39282164	-13.28994779	11.60427259
Cu	-19.11328154	-11.06536691	11.62934982
Cu	-17.81596463	-8.82819606	11.63260761
Cu	-16.56923417	-6.59885306	11.66470487
Cu	-15.33671560	-4.35044951	11.80847946
Cu	-17.89529980	-13.21206269	11.55710985
Cu	-16.59875055	-11.00339585	11.59688227
Cu	-15.31449145	-8.78966971	11.61922309
Cu	-14.06958926	-6.56876953	11.64684953
Cu	-12.79290273	-4.34896371	11.67818165
Cu	-11.46442573	-2.15689083	11.66032199
Cu	-14.00235400	-11.02547196	11.61164192
Cu	-12.76520252	-8.85875825	11.72588358
Cu	-11.48823943	-6.62692867	11.83969089
Cu	-10.16016791	-4.36820020	11.81497384
Cu	-8.86068519	-2.18126823	11.62835202
Cu	-24.23843154	-11.07530392	11.69221676
Cu	-8.89655269	-6.63808440	11.73920600
Cu	-7.58537100	-4.41333011	11.70469595
Cu	-6.31976479	-2.21925807	11.62223978
Cu	-5.04452351	-4.37536647	11.65659035
Cu	-3.82583373	-2.16573474	11.54754178
Cu	-15.29889535	-13.17912283	11.79249033
O	-21.74259268	-11.68960297	13.91650493

O	-8.88318198	-6.68652709	15.08959207
O	-19.88826497	-9.03557586	13.97748937
O	-7.05507251	-3.97515099	14.92113846
O	-13.57894874	-9.48716776	13.94794090
O	-14.86815686	-6.67059255	14.90674130
O	-17.96044770	-6.42887208	14.15981787
O	-5.18449052	-1.31579924	14.74991524
O	-11.81251126	-6.71795556	13.95261867
O	-13.05086082	-3.94631292	15.11119057
O	-2.00387753	-1.61548085	13.98302776
O	-18.62294291	-11.94002070	14.64318364
O	-10.08711019	-3.94904653	13.91394893
O	-26.52300316	-14.46564534	15.13175037
O	-23.59404512	-14.45368743	13.84656038
O	-24.68833023	-11.70041366	15.11148067
O	-15.44476509	-12.25727592	13.94640852
O	-16.71531318	-9.35809031	14.61238609
Zn	-21.60278653	-9.81423747	14.14001906
Zn	-10.42276197	-7.68329644	14.79814220
Zn	-19.67865152	-7.16498643	14.20438965
Zn	-8.63761227	-4.89378957	14.65916719
Zn	-13.52590909	-7.59188031	13.98742123
Zn	-16.46309218	-7.52374894	14.44497313
Zn	-3.75079310	-2.34747867	14.14391076
Zn	-6.79828738	-2.18990373	14.44009853
Zn	-11.77762326	-4.81679530	14.05031050
Zn	-14.61812977	-4.85022327	14.67798221
Zn	-17.19625402	-12.97711273	14.04049436
Zn	-20.25148528	-12.78602527	14.32857317
Zn	-10.01548612	-2.01153454	13.91128379
Zn	-12.78049280	-2.13138192	14.82788851
Zn	-23.47965189	-12.53434154	13.92384219
Zn	-12.21999715	-10.44442863	14.83663116
Zn	-15.30334891	-10.33250390	13.83070908
Zn	-18.34559892	-10.14970253	14.16245918

24/28 Ag

160

Lattice="-20.2444671454 0.0 0.0 -17.3524004103 -10.018413048 0.0 0.0 0.0 21.3222819904"

Ag	-30.36670072	-7.51380979	5.50000000
Ag	-27.47463398	-7.51380979	5.50000000
Ag	-26.02860061	-5.00920652	5.50000000
Ag	-24.58256725	-7.51380979	5.50000000
Ag	-23.13653388	-5.00920652	5.50000000
Ag	-21.69050051	-2.50460326	5.50000000
Ag	-21.69050051	-7.51380979	5.50000000
Ag	-20.24446714	-5.00920652	5.50000000
Ag	-18.79843378	-2.50460326	5.50000000
Ag	-17.35240041	0.00000000	5.50000000
Ag	-18.79843378	-7.51380979	5.50000000
Ag	-17.35240041	-5.00920652	5.50000000
Ag	-15.90636704	-2.50460326	5.50000000
Ag	-14.46033368	0.00000000	5.50000000
Ag	-15.90636704	-7.51380979	5.50000000
Ag	-14.46033367	-5.00920652	5.50000000
Ag	-13.01430031	-2.50460326	5.50000000
Ag	-11.56826694	0.00000000	5.50000000
Ag	-13.01430031	-7.51380979	5.50000000
Ag	-11.56826694	-5.00920652	5.50000000
Ag	-10.12223357	-2.50460326	5.50000000
Ag	-8.67620021	0.00000000	5.50000000
Ag	-8.67620021	-5.00920652	5.50000000
Ag	-7.23016684	-2.50460326	5.50000000

Ag	-5.78413347	0.00000000	5.50000000
Ag	-4.33810010	-2.50460326	5.50000000
Ag	-2.89206674	0.00000000	5.50000000
Ag	0.00000000	0.00000000	5.50000000
Ag	-28.92561447	-6.71443959	7.85643565
Ag	-26.03525020	-6.72334166	7.85547940
Ag	-24.57826602	-4.20614336	7.83987461
Ag	-23.12503909	-6.72111335	7.85695294
Ag	-21.67990270	-4.20663075	7.85100434
Ag	-20.25151768	-1.70164709	7.86756619
Ag	-20.22713189	-6.71083538	7.86476231
Ag	-18.78403073	-4.19167021	7.87022408
Ag	-17.34941642	-1.69312425	7.87381172
Ag	-33.25492734	-9.21694621	7.86601326
Ag	-17.35285451	-6.69835820	7.86410495
Ag	-15.89668103	-4.18946904	7.86918473
Ag	-14.45684351	-1.69551482	7.87165856
Ag	-30.36419223	-9.21197530	7.88326765
Ag	-14.46363598	-6.70806409	7.86228879
Ag	-13.01723269	-4.20860433	7.86481560
Ag	-11.56692588	-1.69663254	7.85889602
Ag	-27.47812316	-9.20738948	7.89183815
Ag	-31.81732638	-6.71379702	7.86183868
Ag	-10.12123262	-4.20782014	7.85365188
Ag	-8.67211332	-1.68885712	7.85740760
Ag	-24.58965612	-9.20203218	7.89554153
Ag	-27.47336292	-4.20870281	7.84912844
Ag	-5.78397023	-1.68182517	7.86001419
Ag	-21.69986076	-9.20655934	7.87824984
Ag	-23.14534492	-1.69326165	7.86447338
Ag	-18.81300798	-9.22009405	7.84717512
Ag	-36.15885145	-9.21491691	7.84294915
Ag	-30.36221711	-5.90215707	10.19338842
Ag	-27.47071457	-5.90221964	10.17801045
Ag	-26.00391958	-3.36224154	10.14457199
Ag	-24.57086388	-5.91715156	10.14344960
Ag	-23.11385814	-3.38978147	10.16107764
Ag	-21.69597602	-0.87471677	10.20830706
Ag	-21.66136096	-5.90435196	10.17593600
Ag	-20.23019030	-3.39300832	10.20444122
Ag	-18.80394486	-0.87613074	10.19227382
Ag	-34.72873152	-8.41738693	10.17410418
Ag	-18.78307580	-5.85484788	10.21290955
Ag	-17.32705195	-3.37130124	10.23093777
Ag	-15.88989168	-0.88097589	10.22055922
Ag	-31.81918649	-8.39886903	10.22473875
Ag	-15.90381791	-5.85142664	10.18391169
Ag	-14.42320472	-3.38459306	10.22270728
Ag	-13.00107502	-0.88068707	10.21196142
Ag	-28.91973461	-8.36829950	10.24850635
Ag	-13.01542329	-5.91183452	10.20799459
Ag	-11.54921550	-3.39367847	10.17499689
Ag	-10.12295579	-0.88012132	10.20533411
Ag	-26.04036309	-8.38103900	10.27685314
Ag	-8.65479085	-3.37332046	10.15946940
Ag	-7.23310431	-0.86724562	10.22522500
Ag	-23.14279271	-8.39393566	10.26279810
Ag	-4.33521834	-0.86337788	10.23192308
Ag	-20.24905654	-8.39476636	10.21363371
Ag	-17.38573821	-8.39797331	10.15498906
Ag	-30.41400476	-7.57302430	12.57656472
Ag	-27.48876034	-7.52586007	12.67988935
Ag	-25.98639399	-5.03914687	12.41504706

Ag	-24.60448040	-7.59971504	12.67108307
Ag	-23.13541024	-5.11108470	12.43166888
Ag	-21.66264077	-2.56683504	12.54374504
Ag	-21.71560704	-7.58151587	12.60964387
Ag	-20.27049716	-5.07289735	12.58993289
Ag	-18.79777897	-2.55588299	12.56611400
Ag	-17.35647879	-0.13121302	12.56599370
Ag	-18.84157269	-7.49137184	12.53385921
Ag	-17.34528811	-5.03704325	12.63495016
Ag	-15.83659933	-2.57464194	12.57275612
Ag	-14.44320733	-0.08542902	12.58852343
Ag	-15.98826773	-7.52421293	12.42083885
Ag	-14.43913120	-5.11003379	12.58982759
Ag	-12.92669005	-2.58481153	12.54269605
Ag	-11.58274986	-0.01127339	12.56103737
Ag	-33.34633016	-7.63861229	12.52100310
Ag	-11.56618180	-5.09827748	12.53532500
Ag	-10.07521715	-2.59837556	12.50444929
Ag	-8.72672084	-0.04671430	12.59352069
Ag	-28.90211274	-5.03185703	12.49994582
Ag	-7.16742187	-2.58957454	12.52151486
Ag	-5.79823672	-0.08068832	12.59340985
Ag	-24.50224120	-2.58707476	12.52038251
Ag	-2.86847177	-0.03559186	12.56110815
Ag	-20.23502719	-0.04590548	12.52955933
O	-33.90385197	-8.06309280	14.92001653
O	-12.84071940	-5.17120752	15.87738600
O	-30.77815891	-7.31813211	15.01114937
O	-9.72046896	-4.35584086	15.68441873
O	-27.65402211	-6.61419614	15.10560508
O	-6.62181817	-3.55343013	15.47559784
O	-24.53640193	-5.71967616	15.11105363
O	-23.75041965	-2.71568729	15.62228700
O	-21.40281130	-4.82123826	15.05265294
O	-20.58956446	-1.84480653	15.81479884
O	-18.28423364	-4.01009701	15.29897710
O	-17.43467872	-0.97609630	15.72219600
O	-15.18446771	-3.16170756	15.12218000
O	-14.32640648	-0.17555667	15.80148129
O	-12.06611497	-2.26173886	14.96392986
O	-28.54266785	-9.43734932	16.02643332
O	-8.89794544	-1.35488796	15.03825757
O	-25.35919548	-8.55926579	16.20753405
O	-5.76324375	-0.53676876	15.04551212
O	-22.21535905	-7.70129162	16.06654103
O	-19.99128796	-9.81380400	14.98046697
O	-19.11523611	-6.95795261	15.92163606
O	-16.82725428	-8.97563951	14.88913589
O	-15.96450512	-6.12353826	15.93660592
Zn	-12.31292668	-6.77922857	15.13423544
Zn	-14.64615341	-4.87606858	15.60196393
Zn	-29.42373113	-6.03003134	15.11012915
Zn	-11.50358976	-3.98944788	15.36706691
Zn	-26.34496763	-5.28551549	15.05453384
Zn	-8.40439363	-3.15224060	15.17920898
Zn	-23.22555291	-4.39867029	15.02843682
Zn	-5.26225281	-2.33754545	15.18411034
Zn	-20.07257839	-3.53098844	15.22766586
Zn	-22.35021935	-1.54697982	15.36698144
Zn	-16.98566779	-2.70043415	15.20309564
Zn	-19.21701843	-0.69333860	15.36502525
Zn	-13.87350618	-1.85363396	15.17088896
Zn	-33.42152805	-9.81515893	15.33453173

Zn	-10.72131864	-0.97146054	15.10825628
Zn	-30.26689847	-9.03610607	15.52195766
Zn	-7.55007130	-0.10862937	15.32226560
Zn	-27.13678005	-8.26196552	15.81982229
Zn	-21.75023966	-9.31305617	15.30271109
Zn	-24.00887044	-7.35651746	15.79134593
Zn	-18.62587831	-8.53926740	15.09766441
Zn	-20.87226987	-6.52309567	15.55748639
Zn	-15.48107251	-7.67900272	15.04356548
Zn	-17.74831632	-5.74943956	15.64851560

24/28 Au

160

Lattice="20.1949696707 0.0 0.0 17.3099740034 9.9939181506 0.0 0.0 0.0 21.3049614823"

Au	0.00000000	0.00000000	5.50000000
Au	2.88499567	0.00000000	5.50000000
Au	4.32749350	2.49847954	5.50000000
Au	5.76999133	0.00000000	5.50000000
Au	7.21248917	2.49847954	5.50000000
Au	8.65498700	4.99695908	5.50000000
Au	8.65498700	0.00000000	5.50000000
Au	10.09748484	2.49847954	5.50000000
Au	11.53998267	4.99695908	5.50000000
Au	12.98248050	7.49543861	5.50000000
Au	11.53998267	0.00000000	5.50000000
Au	12.98248050	2.49847954	5.50000000
Au	14.42497834	4.99695908	5.50000000
Au	15.86747617	7.49543861	5.50000000
Au	14.42497834	0.00000000	5.50000000
Au	15.86747617	2.49847954	5.50000000
Au	17.30997400	4.99695908	5.50000000
Au	18.75247184	7.49543861	5.50000000
Au	17.30997400	0.00000000	5.50000000
Au	18.75247184	2.49847954	5.50000000
Au	20.19496967	4.99695908	5.50000000
Au	21.63746750	7.49543861	5.50000000
Au	21.63746750	2.49847954	5.50000000
Au	23.07996534	4.99695908	5.50000000
Au	24.52246317	7.49543861	5.50000000
Au	25.96496100	4.99695908	5.50000000
Au	27.40745884	7.49543861	5.50000000
Au	30.29245451	7.49543861	5.50000000
Au	1.42667277	0.67360952	7.95859507
Au	4.31033960	0.67313162	7.95609716
Au	5.76347528	3.17650000	7.93093311
Au	7.20281472	0.68476791	7.95998365
Au	8.66043714	3.18874748	7.93914139
Au	10.08552841	5.69823764	7.97020099
Au	10.10093745	0.68940935	7.98370748
Au	11.54823461	3.18682381	7.96698688
Au	12.96489281	5.67533465	7.93794390
Au	14.40653648	8.20385802	7.91829379
Au	12.98531327	0.69582033	7.98900645
Au	14.42841989	3.19726420	8.00215842
Au	15.86965934	5.67764153	7.93177973
Au	17.31200252	8.18671903	7.93313824
Au	15.84908088	0.71879898	7.97020409
Au	17.31088967	3.21365835	7.99557099
Au	18.79184082	5.66550925	7.95273199
Au	20.20378856	8.16852028	7.98785938
Au	18.73412539	0.70425439	7.94640966
Au	20.18681541	3.16859955	7.99495786
Au	21.65145859	5.67562217	7.97839868

Au	23.07499072	8.18452656	7.99047968
Au	23.06412180	3.16857902	7.95280600
Au	24.52555313	5.69588544	7.96323411
Au	25.95308802	8.19850178	7.98682788
Au	27.40181483	5.71228812	7.96250857
Au	28.84235042	8.19916843	7.97354197
Au	31.71984652	8.19241482	7.94270731
Au	20.15308880	1.47933796	10.35361474
Au	2.83686427	1.47379051	10.32935963
Au	24.50144094	4.00342251	10.27686814
Au	5.74199525	1.49664316	10.31945716
Au	7.20348042	3.99882328	10.27291693
Au	28.84796262	6.50060759	10.36147494
Au	8.64300606	1.48248237	10.31624929
Au	10.10799553	3.99590174	10.31054415
Au	11.55877895	6.49342931	10.32492005
Au	33.15411652	9.02782467	10.29326748
Au	11.54629692	1.50063801	10.35650626
Au	13.00913156	4.00611156	10.38886059
Au	14.42877820	6.47383379	10.24285536
Au	15.83595641	8.98124191	10.27597713
Au	14.43019482	1.55178926	10.39670482
Au	15.89032895	4.03331760	10.44959039
Au	17.36704761	6.46223779	10.24887456
Au	18.73811895	8.95158367	10.33405822
Au	17.29460646	1.56350980	10.32998694
Au	18.76470866	4.01618716	10.43542034
Au	20.24685460	6.47965793	10.39004099
Au	21.64440041	8.98341363	10.37965878
Au	21.62564398	3.99396214	10.34377948
Au	23.10301748	6.52347108	10.37761221
Au	24.53061216	8.99244231	10.38810944
Au	25.96177732	6.51057976	10.37583820
Au	27.40844495	8.98205848	10.37862659
Au	30.29085881	9.00619354	10.34890596
Au	17.25650719	9.78734485	12.67568594
Au	20.16512756	9.76298055	12.68317932
Au	4.24189836	2.32551670	12.67563816
Au	23.09848668	9.79965103	12.74211706
Au	7.18768513	2.31163096	12.68727546
Au	8.63723772	4.77731661	12.71751732
Au	25.97920455	9.75362330	12.82503073
Au	10.05239037	2.32237195	12.71351454
Au	11.52865084	4.83376036	12.78225686
Au	13.08614390	7.35253800	12.62193880
Au	28.81247208	9.78970711	12.80796787
Au	12.91377165	2.34455820	12.82031847
Au	14.38901584	4.80364409	13.00889034
Au	15.94020572	7.17859133	12.55472345
Au	31.69621924	9.87613479	12.74857008
Au	15.80622338	2.34592722	12.95906591
Au	17.26794542	4.76347892	13.06442319
Au	18.76511612	7.19400771	12.79379600
Au	34.60052677	9.90783851	12.65149280
Au	18.70223725	2.34629149	12.87760270
Au	20.18568197	4.80274460	12.92740072
Au	21.63829751	7.27947876	12.95207542
Au	21.55743220	2.32750792	12.76588793
Au	23.05457119	4.83769154	12.72333322
Au	24.49779987	7.29889815	12.99893829
Au	25.91660670	4.77772905	12.69944223
Au	27.38226581	7.26850181	12.84229035
Au	30.33181612	7.34509198	12.68685082

O	33.89788196	7.93708953	15.01625582
O	12.82806830	5.17448169	16.19030909
O	30.73579700	7.20612489	15.09388006
O	9.77725590	4.30814514	15.91840340
O	27.61554148	6.52811650	15.32196704
O	6.65302106	3.48901620	15.67704149
O	24.52179017	5.60901864	15.79285359
O	23.74848885	2.61253519	15.51353082
O	21.41588014	4.76267154	15.70643603
O	20.60529168	1.76231463	15.91860940
O	18.28423744	3.93083967	15.89018497
O	17.43371121	0.89844155	15.84725969
O	15.18394657	3.09511282	16.28009120
O	14.37411243	0.07436057	15.69578422
O	12.16639870	2.21482177	15.30219606
O	28.56326707	9.33815355	16.19609068
O	8.98817014	1.33979357	15.42582730
O	25.37069783	8.53862785	16.41547428
O	5.83602598	0.45392331	15.16737174
O	22.21018705	7.73056298	16.47092161
O	20.01344497	9.68172081	15.09048878
O	19.10998315	6.92666563	16.29396459
O	16.87332546	8.90482867	15.03077038
O	15.97302840	6.14821704	16.22681089
Zn	12.32843339	6.70798861	15.30400076
Zn	14.65165994	4.86413335	16.16627603
Zn	29.37228738	5.92482143	15.27258817
Zn	11.56419015	3.94543558	15.61222287
Zn	26.26692478	5.22981848	15.34441387
Zn	8.44319955	3.10417884	15.48703096
Zn	23.19590163	4.39250522	15.36977216
Zn	5.34606914	2.27031985	15.22507916
Zn	20.05710968	3.51715805	15.58964705
Zn	22.31811745	1.46498988	15.33382439
Zn	16.92532844	2.68745923	15.81974471
Zn	19.20943198	0.64136043	15.49779219
Zn	13.95841025	1.87806436	15.68471199
Zn	33.44357457	9.74182542	15.22512126
Zn	10.79638466	0.94581156	15.34462266
Zn	30.23692177	8.94671792	15.56124802
Zn	7.64422057	0.06702910	15.43303761
Zn	27.12736561	8.19627382	16.00909917
Zn	21.77299125	9.23482295	15.51076470
Zn	23.99322835	7.31781498	16.21781726
Zn	18.65097589	8.39886598	15.29185732
Zn	20.88925697	6.48237645	16.08095063
Zn	15.54099215	7.56966634	15.11612016
Zn	17.75314855	5.68748204	16.07906246

30/14 Sn

144

Lattice="-4.5891230099 15.8971884307 0.0 -18.3564920396 7.9485942153 0.0 0.0 0.0 22.6689514933"

Sn	-20.65105355	19.87148554	5.50000000
Sn	-18.35649204	15.89718843	5.50000000
Sn	-16.06193054	19.87148554	5.50000000
Sn	-16.06193053	11.92289132	5.50000000
Sn	-13.76736903	15.89718843	5.50000000
Sn	-13.76736903	7.94859422	5.50000000
Sn	-11.47280752	11.92289132	5.50000000
Sn	-9.17824602	15.89718843	5.50000000
Sn	-9.17824602	7.94859422	5.50000000
Sn	-6.88368452	11.92289132	5.50000000
Sn	-6.88368451	3.97429711	5.50000000

Sn	-4.58912301	7.94859422	5.50000000
Sn	-2.29456150	3.97429711	5.50000000
Sn	0.00000000	0.00000000	5.50000000
Sn	-18.36418399	21.19350184	6.50390787
Sn	-16.07344207	17.20583733	6.59598706
Sn	-9.18117689	5.29509915	6.52229210
Sn	-13.77077637	13.23903938	6.56306414
Sn	-11.46943304	17.21848153	6.53230923
Sn	-11.47762458	9.27428277	6.49669257
Sn	-9.18009493	13.24534419	6.59615492
Sn	-2.30222561	1.31840783	6.49990314
Sn	-6.88850917	9.27179170	6.47084071
Sn	-4.59454149	13.23723436	6.54639101
Sn	-4.58867512	5.30214073	6.39414640
Sn	-20.65428414	17.22542531	6.55608993
Sn	-18.35771964	13.24661281	6.51171549
Sn	-16.06454993	9.26602009	6.50264978
Sn	-18.27634798	20.96106696	9.40497208
Sn	-15.98673729	17.08857953	9.51731903
Sn	-9.21382906	5.01586294	9.41437688
Sn	-13.67321694	13.08583313	9.47083564
Sn	-11.59961236	16.98602879	9.44869558
Sn	-11.43091185	9.07072708	9.36691364
Sn	-9.10366640	13.18897257	9.51764899
Sn	-2.14979095	1.02799305	9.40747150
Sn	-6.82134385	9.15951143	9.35864012
Sn	-4.66086867	13.07900364	9.46392835
Sn	-4.48484723	5.17793770	9.26363788
Sn	-20.57303541	17.12968419	9.45887895
Sn	-18.20962079	13.04536796	9.39597320
Sn	-16.06677273	9.11066095	9.40415878
Sn	-20.62069752	22.30547579	10.25820485
Sn	-18.29264672	18.37360160	10.60009346
Sn	-11.44069654	6.44277432	10.42894545
Sn	-15.97492490	14.41353490	10.47920542
Sn	-13.73859861	18.38272867	10.72794353
Sn	-13.73192403	10.39197640	10.35142089
Sn	-11.43132654	14.39779329	10.63709487
Sn	-4.56120221	2.42669816	9.91190103
Sn	-9.15370376	10.46457532	10.30640179
Sn	-6.83134940	14.39353447	10.77567460
Sn	-6.87556661	6.43717327	10.10306109
Sn	-4.55054115	10.44311729	10.50388285
Sn	-2.16686725	6.46975653	10.26862731
Sn	-18.32984035	10.42867815	10.51355490
Sn	-20.31879641	22.42515638	13.11298751
Sn	-18.12364150	18.25834207	13.52596053
Sn	-11.57153927	6.36145832	13.31380206
Sn	-16.19401288	14.35952610	13.35766747
Sn	-13.75486526	18.58235919	13.68691473
Sn	-13.74448070	10.39668857	13.23114918
Sn	-11.48919248	14.35808520	13.59580416
Sn	-4.28769019	2.67319460	12.71784511
Sn	-9.49331373	10.22136697	13.15553147
Sn	-6.88746798	14.34860299	13.78590293
Sn	-6.90699103	6.69529991	12.94360320
Sn	-4.60094610	10.37058352	13.42440655
Sn	-2.10853115	6.40904841	13.13492869
Sn	-18.28745681	10.49372700	13.43318593
Sn	-20.55588731	19.74378219	14.05735981
Sn	-18.40974510	15.63766763	14.61166949
Sn	-16.09847206	19.83233737	14.83385640
Sn	-15.92105644	11.73228251	14.41564837

Sn	-13.89530221	15.77394726	14.32822462
Sn	-13.64819315	7.86057888	14.60080140
Sn	-11.52815019	11.64084756	14.56012319
Sn	-9.20685485	16.06358190	14.00876254
Sn	-9.22462205	7.62789266	14.28850050
Sn	-7.15870858	11.47139756	14.17098447
Sn	-6.57056391	3.99956102	13.81665441
Sn	-4.46486941	7.61981740	14.05363060
Sn	-2.27518011	3.84306406	14.36186528
Sn	-22.69799696	23.60985791	14.12644111
O	-15.05836693	18.66458292	18.10577337
O	-12.15379036	17.95042605	17.09142364
O	-14.20984180	15.61261603	16.61288320
O	-11.29599355	14.81900398	17.33880538
O	-9.23677715	16.99396036	16.08181735
O	-6.41566220	16.31212793	17.62016974
O	-13.29937854	12.35482699	17.47619577
O	-10.29441568	11.57493771	17.86585823
O	-8.38599077	13.92706710	17.09697015
O	-5.30446139	13.13615024	17.39252360
O	-12.43276834	9.16389104	18.14139160
O	-9.40043279	8.46217411	17.69535232
O	-7.50624907	10.87293975	16.38684948
O	-4.61946223	9.98078144	17.21365066
O	-20.77842725	20.23137997	16.25359653
O	-18.15023102	19.50277816	17.97850120
O	-11.48199948	6.01020695	18.25888394
O	-8.55952869	5.20972703	17.34751304
O	-6.65889849	7.57732753	16.58486306
O	-3.92660262	6.65192140	17.53457394
O	-20.11758397	17.07130325	17.32715914
O	-17.11709257	16.31730479	17.87212224
O	-5.75687531	4.33855090	15.89551676
O	-3.19442927	3.45451986	17.80913427
O	-19.28983696	13.85876046	17.84073387
O	-16.20170606	13.19205501	17.47711139
O	-18.34883802	10.77546374	17.31776457
O	-15.35535901	9.89213792	17.42885950
O	-17.37507570	7.63709244	16.27036285
O	-14.62972071	6.69515792	17.79616495
Zn	-13.94210554	17.43511927	17.31132193
Zn	-7.38318250	3.89227442	16.87764699
Zn	-13.02502570	14.13747554	17.15263832
Zn	-10.98319134	16.56148670	16.80404247
Zn	-8.03081459	15.73281221	16.92542623
Zn	-1.73833005	2.29651480	17.64134414
Zn	-12.09262729	10.96198324	17.83575157
Zn	-10.13979441	13.35560386	17.39716996
Zn	-7.07511781	12.63478808	17.06240504
Zn	-5.19253538	14.98047088	17.22771463
Zn	-11.12040797	7.83819961	18.09427573
Zn	-9.20807072	10.22606580	17.18402574
Zn	-6.29445657	9.36220013	16.68981332
Zn	-4.17324924	11.73882637	16.90866579
Zn	-19.66577854	18.84595994	17.15847240
Zn	-17.83830443	21.34830098	18.01466578
Zn	-10.26230697	4.63549157	17.89239636
Zn	-8.43116167	7.03839530	16.89555710
Zn	-5.32521079	6.26106261	16.32884662
Zn	-3.50042693	8.45242719	17.31411828
Zn	-18.86480794	15.65706009	17.45415145
Zn	-16.86251170	18.14842418	18.01199198
Zn	-4.18910412	3.11331250	16.20764922

Zn	-2.68839821	5.28078425	17.78397465
Zn	-17.96833717	12.59815372	17.50837873
Zn	-15.98420767	15.00136928	17.25518211
Zn	-17.06997094	9.50041655	16.88483750
Zn	-15.04493941	11.72658994	17.11485530
Zn	-20.46837265	22.21298642	16.46687898
Zn	-14.11544501	8.51635873	17.63514431

30/24 Pb

156

Lattice="-21.0010714012 0.0 0.0 -14.0007142675 -12.1249742268 0.0 0.0 0.0 22.8118456849"

Pb	-29.75151782	-9.09373067	5.50000000
Pb	-26.25133925	-9.09373067	5.50000000
Pb	-24.50124997	-6.06248711	5.50000000
Pb	-22.75116069	-3.03124356	5.50000000
Pb	-22.75116068	-9.09373067	5.50000000
Pb	-21.00107140	-6.06248711	5.50000000
Pb	-19.25098212	-3.03124356	5.50000000
Pb	-17.50089283	0.00000000	5.50000000
Pb	-19.25098212	-9.09373067	5.50000000
Pb	-17.50089283	-6.06248711	5.50000000
Pb	-15.75080355	-3.03124356	5.50000000
Pb	-14.00071427	0.00000000	5.50000000
Pb	-15.75080355	-9.09373067	5.50000000
Pb	-14.00071427	-6.06248711	5.50000000
Pb	-12.25062498	-3.03124356	5.50000000
Pb	-10.50053570	0.00000000	5.50000000
Pb	-12.25062498	-9.09373067	5.50000000
Pb	-10.50053570	-6.06248711	5.50000000
Pb	-8.75044642	-3.03124356	5.50000000
Pb	-7.00035713	0.00000000	5.50000000
Pb	-7.00035713	-6.06248711	5.50000000
Pb	-5.25026785	-3.03124356	5.50000000
Pb	-3.50017857	0.00000000	5.50000000
Pb	0.00000000	0.00000000	5.50000000
Pb	-27.97869070	-8.09140755	8.29711534
Pb	-24.48887708	-8.11072299	8.27334745
Pb	-22.71608021	-5.07495050	8.32212523
Pb	-20.96184075	-2.02731857	8.29675062
Pb	-20.99408579	-8.12981691	8.30437555
Pb	-19.24323849	-5.09418561	8.30005049
Pb	-17.48064761	-2.04875615	8.27908238
Pb	-29.72131601	-11.13836693	8.32760463
Pb	-17.49029737	-8.10633490	8.27491576
Pb	-15.75150837	-5.08588169	8.27588933
Pb	-13.99645877	-2.06652682	8.31220304
Pb	-26.24792763	-11.15918338	8.29836470
Pb	-13.98017569	-8.09831612	8.26440131
Pb	-12.23287646	-5.07629055	8.30626247
Pb	-10.49665185	-2.04871383	8.27823649
Pb	-22.75272823	-11.14836217	8.26829533
Pb	-10.46622849	-8.07724100	8.31497495
Pb	-8.72056625	-5.07055953	8.28892813
Pb	-6.98259347	-2.03668326	8.26144632
Pb	-19.23642885	-11.13529258	8.29709689
Pb	-26.20858483	-5.05478637	8.28431987
Pb	-3.46294808	-2.01550580	8.30542746
Pb	-15.71876587	-11.13193031	8.28149579
Pb	-33.20822493	-11.11732960	8.28962687
Pb	-8.82234051	-7.08795321	11.23685213
Pb	-26.32034342	-7.08710756	11.23455457
Pb	-24.57184776	-4.08558306	11.21708199
Pb	-1.80567929	-1.02719719	11.21456520

Pb	-22.83188926	-7.09688659	11.24005203
Pb	-21.05552392	-4.03624431	11.19957377
Pb	-19.30269261	-1.03229403	11.25427343
Pb	-31.56075808	-10.15690023	11.23573690
Pb	-19.28847454	-7.06329619	11.20129653
Pb	-17.54403318	-4.02782345	11.23831807
Pb	-15.83417503	-1.03072284	11.27397550
Pb	-28.05994855	-10.09282790	11.20716761
Pb	-15.80861714	-7.06083701	11.16891545
Pb	-14.05145372	-4.02925226	11.18603425
Pb	-12.29472260	-1.00409291	11.20758035
Pb	-24.55884098	-10.08778877	11.21801452
Pb	-12.28352943	-7.07876230	11.18299452
Pb	-10.55213322	-4.05141500	11.22162691
Pb	-8.81141972	-0.99517235	11.16389781
Pb	-21.06299567	-10.08831015	11.16871676
Pb	-7.06579832	-4.02559327	11.20257334
Pb	-5.27478242	-1.01719484	11.18057262
Pb	-17.55067023	-10.11268635	11.20358895
Pb	-14.05136173	-10.09831296	11.20368965
Pb	-29.83067989	-9.09560228	14.10282673
Pb	-26.27079464	-9.12408574	14.05758116
Pb	-24.52463113	-6.07100241	14.08462868
Pb	-22.79719246	-3.03423586	14.07067346
Pb	-22.76093447	-9.14951815	14.09925948
Pb	-21.07692119	-6.06419777	13.93000717
Pb	-19.25328857	-3.07244224	14.07579252
Pb	-17.50141049	-0.02065216	14.13702194
Pb	-19.29771336	-9.15202857	13.92906046
Pb	-17.52830021	-6.09730384	13.99857028
Pb	-15.75881583	-3.10338366	14.14955618
Pb	-14.04809137	0.00302808	13.94549106
Pb	-15.84125757	-9.09296481	13.93894634
Pb	-14.03756931	-6.14919076	14.04601211
Pb	-12.29657934	-3.08740908	13.95355059
Pb	-10.52165645	-0.01558743	13.98655820
Pb	-12.31130696	-9.18207160	14.07751022
Pb	-10.56115751	-6.11484276	14.07148828
Pb	-8.82635127	-3.01855186	13.95699042
Pb	-7.04572350	-0.07549697	14.03120760
Pb	-7.00490351	-6.07372307	13.96638396
Pb	-5.29241265	-3.10568670	14.05085389
Pb	-3.56937144	-0.06680531	14.03656622
Pb	-20.99659280	-0.02086596	13.95605582
O	-19.42939651	-3.81979584	17.03481629
O	-16.67198415	-5.10889728	17.91751331
O	-14.55783089	-3.05170008	16.85052295
O	-11.70468637	-4.20699081	17.83610437
O	-9.17704750	-2.24695530	17.46518056
O	-6.33747671	-3.42794421	16.79587791
O	-4.15364235	-1.39511626	17.91600646
O	-22.39523809	-2.66777348	16.97903630
O	-19.90428262	-0.62346703	17.08055706
O	-17.17705958	-1.84600988	18.22378284
O	-24.19829037	-7.89872492	18.02241216
O	-21.49681825	-9.11380819	16.85469931
O	-18.97753450	-7.11197321	17.05675916
O	-16.10265251	-8.32009382	17.46509867
O	-13.88637248	-6.24531249	16.72301205
O	-11.20376213	-7.44604887	18.04766200
O	-8.83413716	-5.45022451	17.31292545
O	-26.99312633	-6.67812795	17.06754578
O	-24.67120352	-4.65410219	17.97576168

O	-21.82671620	-5.88141662	17.32606817
O	-28.89322880	-11.93543498	17.37760538
O	-12.05628852	-1.04496843	17.10299258
O	-23.71756691	-11.15583420	17.79600230
O	-6.90288416	-0.19190907	16.73199656
O	-18.63141455	-10.29320250	17.71705129
O	-15.74250904	-11.52345774	17.27024819
O	-13.26362738	-9.49399034	16.74877656
O	-31.69766987	-10.70570892	18.18419067
O	-29.47564988	-8.72135176	17.04054492
O	-26.50606031	-9.87730626	16.97025673
Zn	-18.42190342	-5.36436554	17.29473046
Zn	-16.16888217	-3.33125552	17.77087184
Zn	-13.34059597	-4.46133884	17.00420336
Zn	-11.00859226	-2.52937791	17.46907725
Zn	-8.17901765	-3.74535124	16.99437948
Zn	-5.80860007	-1.66474523	17.11744680
Zn	-24.11954542	-2.91532026	17.66474442
Zn	-21.74372079	-0.92182251	16.92073605
Zn	-18.84359613	-2.09462808	17.43133547
Zn	-16.61858993	-0.08414130	17.99008757
Zn	-23.17857552	-9.39293269	17.62882513
Zn	-20.81355412	-7.37621263	16.88945696
Zn	-17.93429074	-8.60898137	17.40028215
Zn	-15.65498087	-6.53581320	17.32317338
Zn	-12.80088605	-7.71944847	17.13577938
Zn	-10.60723222	-5.70229683	17.79485764
Zn	-28.83405525	-6.97235669	16.97742462
Zn	-26.35346657	-4.95297328	17.24132668
Zn	-23.59461908	-6.15581543	17.79791725
Zn	-21.27004528	-4.15294038	17.00357677
Zn	-13.88943619	-1.30290323	16.90202504
Zn	-25.48798390	-11.41588475	17.24106113
Zn	-8.68682745	-0.47846212	17.27895824
Zn	-20.31294378	-10.54754691	16.98608972
Zn	-17.53201669	-11.78588825	17.67601198
Zn	-15.11902407	-9.80920741	16.92827935
Zn	-33.31386597	-11.01116071	17.30810115
Zn	-31.15857046	-8.96685639	17.82371956
Zn	-28.34977239	-10.20952361	17.00772178
Zn	-25.90512959	-8.14856024	17.33147242