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

Supporting Information: Ab initio Insights into the Structural, Energetics, Electronic, and Stability Properties of Mixed $Ce_nZr_{15-n}O_{30}$ Nanoclusters

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This document contains the self-consistent scheme to determine the cutoff radius and, consequently, the average bond length, the coordination number, and the chemical order parameter.

Analyses

The structural trends between $Ce_{15}O_{30}$ and $Zr_{15}O_{30}$ oxide clusters and also their relative compositions were evaluated by quantifying different structural properties such as the average distance (d_{av}), the coordination number (CN), the chemical order parameter (σ), the effective coordination number (ECN), and the average radius (R_{av}). The average distance between an atom i and the nearest atom j is given by the following equation:

$$d_{av}^{i} = \frac{\sum_i d_{ij}}{n} < R_{cut}^{i} \tag{1}$$

where d_{ij} is the distance between the atom i and each one of the n surrounding atom j, and $R_{cut}^{i} = \frac{1}{2}(R^i - R^j)$ where i corresponds to a centralized atom.

Hence, the coordination number can be obtained using a self-consistent strategy:

$$\mid d_{\min} \; - \; d_{\max} \mid \; \leq \; \frac{1}{2} \, (R_i^{\text{cut}} \; + \; R_j^{\text{cut}}) \tag{2}$$

where the minimum and the maximum distance from the central atom radius R_i^{cut} is given by $d_{\min}$ and $d_{\max}$, respectively. R_j^{cut} is the radius of the nearest atom.

For a better comprehension of the intrinsic interactions within $Ce_{15}O_{30}$ and $Zr_{15}O_{30}$ clusters atoms, the chemical order parameter σ parameter was considered regarding the Ce−O and Zr−O interaction for ceria and zirconia clusters, respectively. The strategy used to calculate the σ parameter is given by the following equation:

$$\sigma = \frac{N^{X-X} + N^{O-O} - N^{X-O}}{N^{X-X} + N^{O-O} + N^{X-O}} \tag{3}$$

where X is Ce or Zr atom and N^{X-X}, N^{O-O} and N^{X-O} are the weight of X−X, O−O and X−O interactions, respectively, into the cluster structure.

In view of the clusters non-spherical symmetry, the following approximation was used to verify the cluster average radius.

$$R = \frac{(R_1 + \frac{R_2}{2})}{2} \tag{4}$$

where R is the average distance, R_1 is the distance between the nearest and the farthest atom relative to the center of gravity and R_2 is the distance between the two most distant atoms inside the structure.

The effective coordination number (ECN) was employed in the correlation analysis instead of CN, since the former one takes into account the partial coordination, which is a important feature to measure the differences between atomic sites with the same CN. For instance, two atomic sites A and B can present $CN = 3$, however, if A present almost 4 neighbors we can observe that $ECN^{\mathrm{A}} > ECN^{\mathrm{B}}$, than it allows to extract more information from each atom. However, both ECN and CN present the same trends, as can be observed in the Figure S1. The ECN analysis consider the self-consistence convergence of d^i_{av} and the ECN^i, defined as follows:

$$ECN^i = \sum_j P_{ij} \tag{5}$$

where P_{ij}, are the weight for each possible correlation between i and j,

$$P_{ij} = \mathrm{EXP}\left[\left(1 - \frac{2d_{ij}}{d^i_{av} + d^j_{av}}\right)^6\right] \tag{6}$$

Note that, P_{ij} is 1 if the atoms are perfectly bounded ($d_{ij} = (d^i_{av} + d^j_{av})/2$) and approach 0 if they are distant ($d_{ij} >> (d^i_{av} + d^j_{av})/2$).

To verify if the atomic site are exposed to the vacuum or in core region, we employed an algorithm that consider the atoms as ridge spheres of radius r_i. The r_i values were obtaining minimizing $\sum_{i,j\neq i}\left[(d_{ij} - (r^i + r^j))^2 P_{ij}\right]$, within the self-consistency of ECN analysis. The

atoms exposed to the vacuum are defined as the atoms which could be in contact with an dummy adatom of radius $rd = 1.5\,\text{Å}$ which adsorb on the frozen cluster structure without overlap with any other atom. To verify if the cluster atoms were in contact with dummy atom, 1000 dummy atom positions were sampled around each atom of the cluster, at a contact distance of $r_i + Rd$. For an efficient sample, we employed the almost uniform distribution of points over a sphere surface by Markus Deserno (for details see the article "How to generate equidistributed points on the surface of a sphere", 2004).

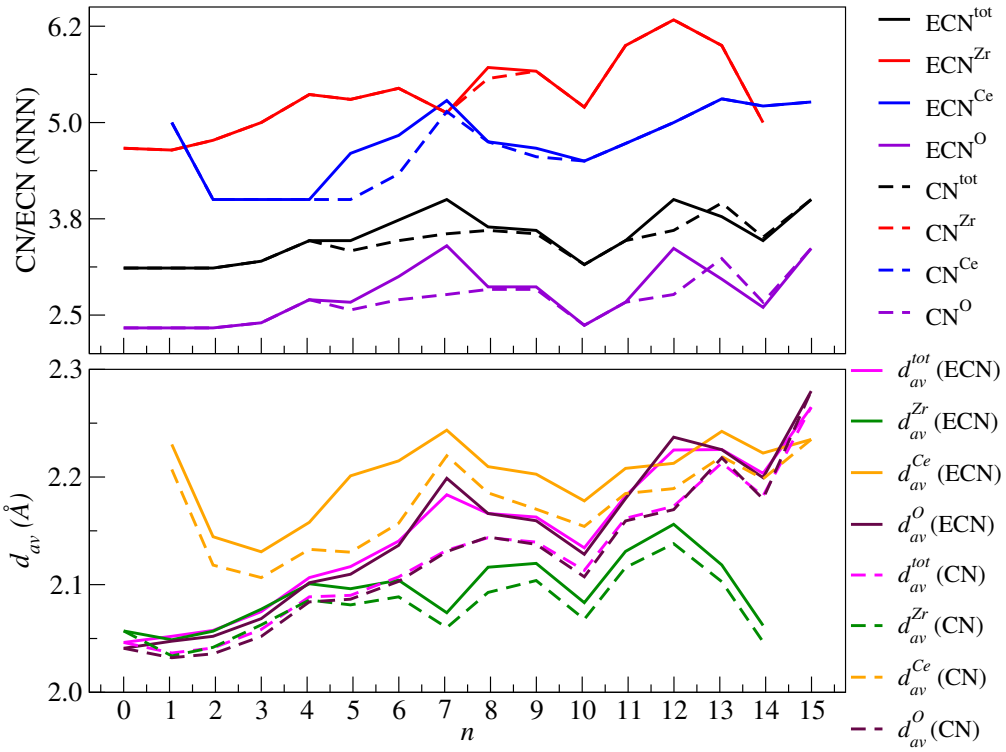

Figure S1: The difference of the coordination number and effective coordination number.

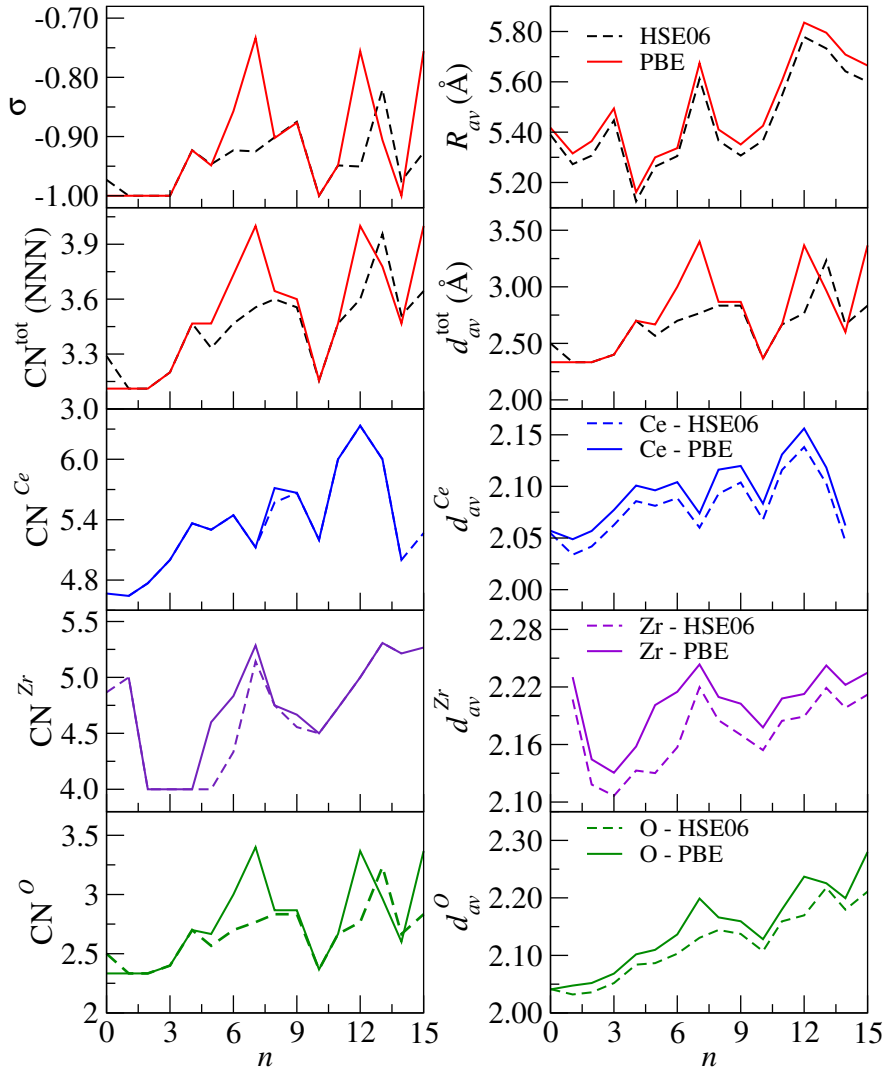

Figure S2: Structural parameters for $Ce_nZr_{15-n}O_{30}$ clusters: average bond length, d_{av}, coordination number, CN (in next near neighbors – NNN), chemical order parameter, σ, and cluster radius R_{av}, using PBE and HSE06.

Correlation Analysis

To analyse the correlation in data, we performed three correlation analysis of Pearson (ρ), Spearman (r_s), and Kendall (τ), which were calculated as

$$\rho = \frac{\mathrm{cov}(x, y)}{\sigma_x \sigma_y} \ , \tag{7}$$

$$r_s = \frac{\mathrm{cov}(\mathrm{rg}_x, \mathrm{rg}_y)}{\sigma_{\mathrm{rg}_x} \sigma_{\mathrm{rg}_y}} \ , \tag{8}$$

$$\tau = \frac{2}{n(n-1))} \sum_{i<j} \mathrm{sgn}(x_i - x_j)\mathrm{sgn}(y_i - y_j) \ , \tag{9}$$

where sgn, cov, and σ are respectively the signal, covariance, and standard deviation functions, while rg_u is the rank values for the observations u. The analysis Spearman, Parson, and Kendall correlation analysis are presented in figures S3, S5, and S4, respectively. The same results and conclusions could be draw for each one of then, however they present few differences considering the magnitude of the correlations. For instance, for the plotted data the quantity of correlations bigger than 0.25 is smaller for Kendall (87) then Spearman (137) and Pearson (136), which may indicate that Spearman and Pearson capture better the relations in data then Kendall. Thus, we selected the Spearman correlation ratter then Pearson or Kendall, because of Spearman capture better the correlation then Kendall and is less affected by outliers then Pearson.

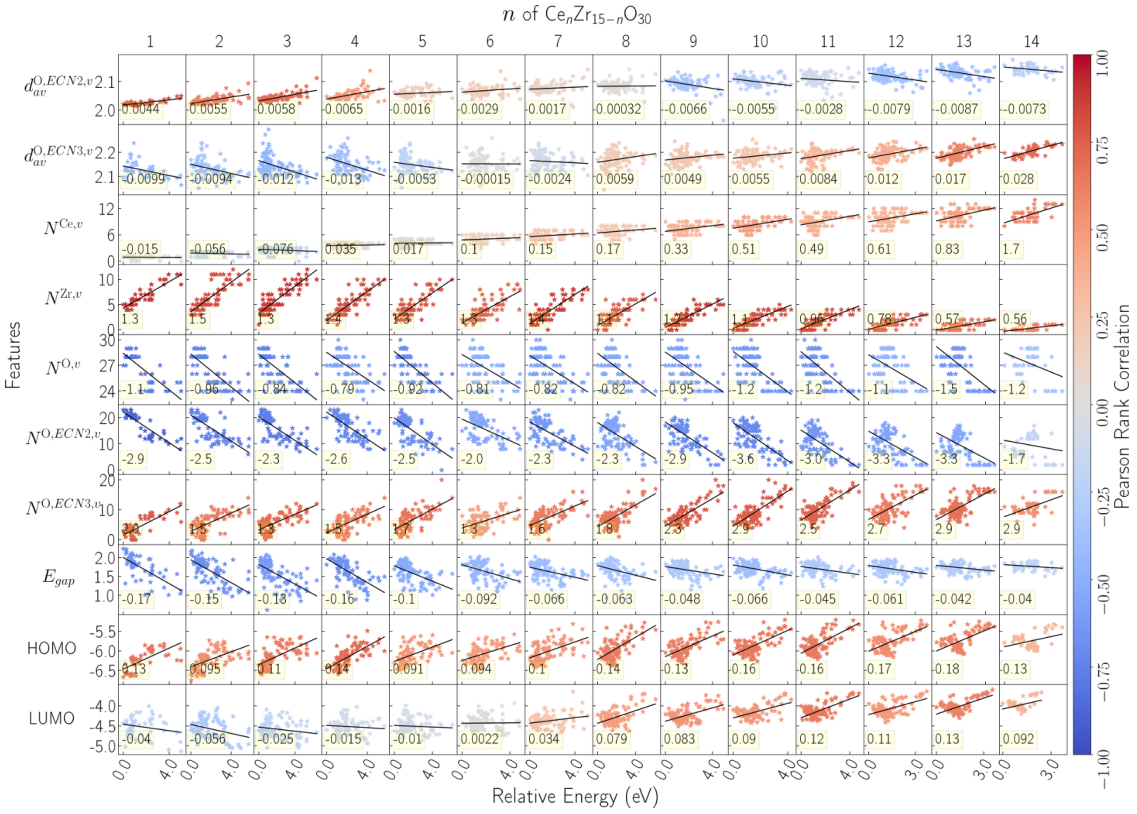

Figure S3: A scatter plots matrix of the cluster formation energies (horizontal) against their electronic and structural features (vertical), where the different cluster properties and chemical compositions run over the rows and columns, respectively. Pearson's correlation are indicated in colors and a data linear fitting model with the respective angular coefficient are shown in the cells. We only considered structures with relative energy smaller than 5 eV.

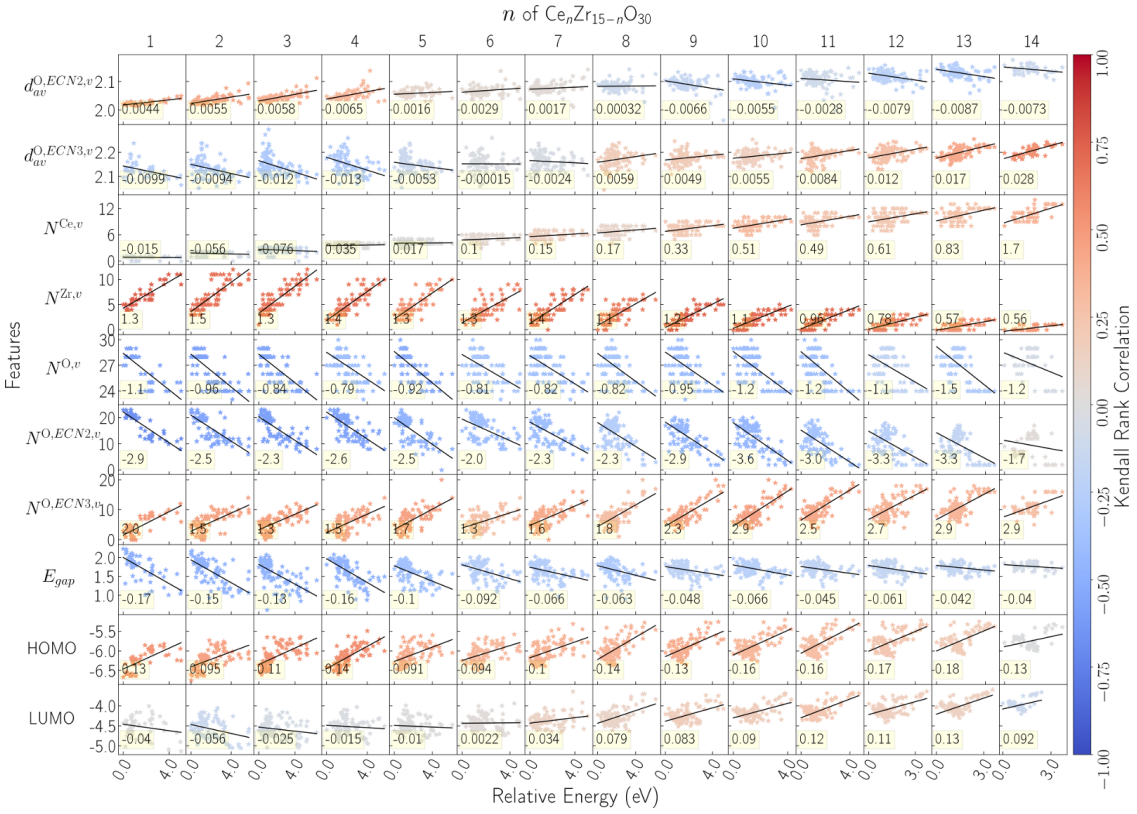

Figure S4: A scatter plots matrix of the cluster formation energies (horizontal) against their electronic and structural features (vertical), where the different cluster properties and chemical compositions run over the rows and columns, respectively. Kendall's correlation are indicated in colors and a data linear fitting model with the respective angular coefficient are shown in the cells. We only considered structures with relative energy smaller than 5 eV.

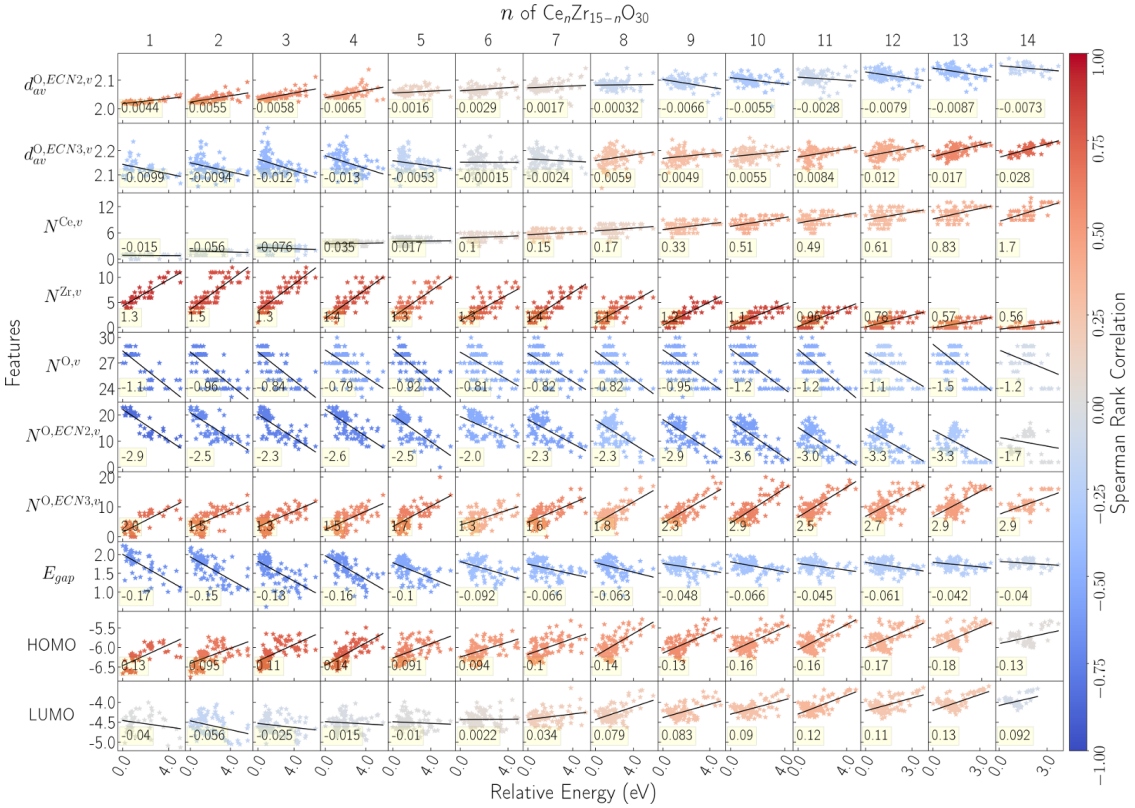

Figure S5: A scatter plots matrix of the cluster formation energies (horizontal) against their electronic and structural features (vertical), where the different cluster properties and chemical compositions run over the rows and columns, respectively. Spearman's correlation are indicated in colors and a data linear fitting model with the respective angular coefficient are shown in the cells. We only considered structures with relative energy smaller than 5 eV.

Geometry Structure

Initial Structures for CeO_2 and ZrO_2

Table S1: Parent structures for $Ce_nZr_{15-n}O_{30}$ pGMCs, in which pGMC-Zr and pGMC-Ce indicate the putative global minimum configuration for zirconia and ceria, respectively, whereas Frag. indicates the fragment bulk-like structures, i.e, monoclinic baddeleyite (ZrO_2)-bulk and fluorite (CeO_2)-bulk. The total relative energy ΔE_{tot} is given in respect to the pGMCs.

	ΔE_{tot} (meV/$f.u$)	Structures		ΔE_{tot} (meV/$f.u$)	Structures
$Ce_0Zr_{15}O_{30}$	16	Frag.-Zr	$Ce_{08}Zr_7O_{30}$	0	pGMC-Ce
$Ce_0Zr_{15}O_{30}$	0	pGMC-Zr	$Ce_{09}Zr_6O_{30}$	0	Frag.-Zr
$Ce_{01}Zr_{14}O_{30}$	0	pGMC-Zr	$Ce_{10}Zr_5O_{30}$	0	pGMC-Zr
$Ce_{02}Zr_{13}O_{30}$	0	pGMC-Zr	$Ce_{11}Zr_4O_{30}$	0	pGMC-Ce
$Ce_{03}Zr_{12}O_{30}$	0	pGMC-Zr	$Ce_{12}Zr_3O_{30}$	0	pGMC-Ce
$Ce_{04}Zr_{11}O_{30}$	0	Frag.-Zr	$Ce_{13}Zr_2O_{30}$	0	pGMC-Ce
$Ce_{05}Zr_{10}O_{30}$	0	Frag.-Zr	$Ce_{14}Zr_1O_{30}$	0	pGMC-Zr
$Ce_{06}Zr_9O_{30}$	0	Frag.-Zr	$Ce_{15}Zr_0O_{30}$	0	pGMC-Ce
$Ce_{07}Zr_8O_{30}$	0	pGMC-Ce	$Ce_{15}Zr_0O_{30}$	59	Frag.-Ce

ZrO_2 - pGMC, $E_{tot} = -1\,543\,267.463\,961\,89\,\mathrm{eV}$, $\Delta E_{tot} = 0.0000\,\mathrm{meV}/f.u.$

Zr	0.1013250000000000	−2.5933500000000000	4.1777670000000002
O	−1.6922029999999999	−1.8510139999999999	4.0707459999999998
O	1.8416010000000000	−1.7191639999999999	4.5855660000000000
Zr	0.7740780000000000	−3.3582529999999999	1.2724359999999999
O	0.0944280000000000	−4.3661479999999999	−0.3313400000000000
O	0.3109710000000000	−4.1771830000000003	3.0374349999999999
Zr	−2.2946160000000000	−1.5693550000000001	−3.7287840000000001
O	−1.6435599999999999	−3.2779370000000001	−2.9729480000000001
O	−4.0775420000000002	−0.9883090000000000	−3.1864129999999999
Zr	−4.6423009999999998	0.6487930000000000	1.3210880000000000
O	−3.6875309999999999	2.3212590000000000	1.3230750000000000
O	−5.3907410000000002	0.4506670000000000	−0.5229320000000000
Zr	−2.0511689999999998	−1.0834550000000001	2.2251319999999999
O	−1.6089140000000000	−2.5461680000000002	0.8046010000000000
O	−4.0084020000000002	−0.6841550000000000	2.6149610000000001
Zr	−3.7202829999999998	0.1802480000000000	−1.5745229999999999
Zr	−0.9642200000000000	−2.8870960000000001	−1.0864879999999999
O	−2.9864910000000000	−0.0806590000000000	0.3148170000000000
O	−1.7104710000000001	−0.8411950000000000	−1.9476450000000001
O	0.3908390000000000	−1.5953580000000001	2.4080930000000000
O	−1.3646430000000001	0.0499910000000000	−4.4311650000000000
Zr	−0.8219410000000000	1.2118340000000001	−2.9079199999999998
O	0.7266240000000000	−1.8502650000000000	−0.6236760000000000
O	0.0537970000000000	2.8219759999999998	−3.6132640000000000
Zr	−1.7889120000000001	1.9255720000000001	0.6432840000000000
O	−0.6993230000000000	3.5427230000000001	1.0157780000000001
O	−2.5131709999999998	1.7755190000000001	−1.7401290000000000
Zr	2.5184150000000001	−1.1495460000000000	2.7799649999999998
O	−1.2555980000000000	0.7404640000000000	2.1054390000000001
O	2.6724800000000002	−2.7841339999999999	1.6870390000000000
Zr	3.7159300000000002	1.5060260000000001	1.4713600000000000
O	2.1924950000000001	0.1744310000000000	1.1197910000000000
O	3.9818490000000000	0.2553650000000000	2.9675880000000001
Zr	4.4298219999999997	1.2459000000000000	−1.6821870000000001
Zr	1.6828190000000001	−0.1355510000000000	−0.8682360000000000
Zr	1.8483719999999999	2.7446990000000002	−2.7104949999999999
Zr	1.0986460000000000	3.1656930000000001	0.3228530000000000
O	5.2095419999999999	1.5831329999999999	0.1002440000000000
O	3.5553490000000001	−0.4788320000000000	−1.5921580000000000
O	3.7782079999999998	2.4023059999999998	−3.1896779999999998
O	2.6994389999999999	1.8943850000000000	−0.8166099999999999
O	1.1690970000000001	0.6788790000000000	−2.6952470000000002
O	1.4593320000000001	4.1368340000000003	−1.3547240000000000
O	0.0663640000000000	1.4881690000000001	−0.5106889999999999
O	2.5502099999999999	3.0722559999999999	1.7181900000000001

ZrO_2 - Fragment, $E_{tot} = -1\,543\,267.231\,353\,84\,\mathrm{eV}$, $\Delta E_{tot} = 15.5072\,\mathrm{meV}/f.u.$

Zr	6.6553209999999998	7.7130179999999999	3.7693360000000000
Zr	4.3956809999999997	6.3389110000000004	8.6709920000000000
Zr	11.5788580000000003	8.0557099999999995	7.6984260000000004
Zr	7.9406960000000000	4.9134779999999996	4.3077620000000003
Zr	7.2396989999999999	10.6881730000000008	4.7215480000000003
Zr	7.4536470000000001	4.7646439999999997	9.0733689999999996
Zr	9.0298569999999998	9.9495930000000001	9.5241959999999999
Zr	7.5838169999999998	8.0055289999999992	7.0350070000000002
Zr	6.7186859999999999	8.3745469999999997	11.0597390000000004
Zr	5.2889960000000000	5.6109939999999998	5.9213959999999997
Zr	9.9082249999999998	5.3955719999999996	7.2002100000000002
Zr	6.7746320000000004	11.1861390000000007	7.7291949999999998
Zr	9.9690069999999995	9.6263649999999998	5.6097180000000000
Zr	5.5953840000000001	5.4696660000000001	11.5689609999999998
Zr	3.9436110000000002	10.0030079999999995	9.7310370000000006
O	5.0003250000000001	6.8696750000000000	4.3603870000000002
O	9.6272760000000002	4.7071490000000002	5.3400809999999996
O	9.2136030000000009	11.0560939999999999	4.4866469999999996
O	3.9668610000000002	5.4515479999999998	10.4916850000000004
O	8.3750710000000002	6.4074200000000001	8.2218929999999997
O	8.1892270000000007	8.7076870000000000	4.9303290000000004
O	10.8577949999999994	9.0764840000000007	9.1920929999999998
O	9.1072319999999998	3.9470239999999999	8.3022270000000002
O	8.8819929999999996	10.0240179999999999	7.2386140000000001
O	8.4560089999999999	9.2357999999999993	11.3149060000000006
O	3.5948690000000001	5.6293220000000002	7.0400939999999999
O	9.8980519999999999	7.6350249999999997	6.6399429999999997
O	6.2701520000000004	4.1074419999999998	4.8740059999999996
O	6.4038380000000004	9.6767769999999995	6.3766619999999996
O	6.9177970000000002	4.1757720000000003	10.9634060000000009
O	3.6429950000000000	8.2690619999999999	9.0555020000000006
O	7.6468780000000001	6.2459470000000001	2.8407420000000001
O	5.7210580000000002	7.2052750000000003	7.2978480000000001
O	11.6965210000000006	6.0649759999999997	7.8182140000000002
O	8.1287420000000008	11.6618270000000006	9.1897900000000003
O	6.1954079999999996	7.1141379999999996	12.5278960000000001
O	7.3461439999999998	6.4215049999999998	5.5072609999999997
O	6.8471320000000002	12.1986969999999992	6.0693739999999998
O	6.2923270000000002	6.5808600000000004	9.9885380000000001
O	4.8792320000000000	11.1589069999999992	8.5482019999999999
O	6.3254720000000004	9.6575410000000002	3.2844920000000002
O	5.9005260000000002	4.6730749999999999	7.9323740000000003
O	7.2870189999999999	8.9896279999999997	8.9685199999999998
O	11.8732170000000004	9.3549530000000001	6.2129190000000003
O	5.1886799999999997	9.6942930000000000	11.1401850000000007

CeO_2 - pGMC, $E_{tot} = -3\,744\,347.924\,233\,74\,\mathrm{eV}$, $\Delta E_{tot} = 0.0000\,\mathrm{meV}/f.u.$

Ce	3.7844389999999999	−1.2553540000000001	−3.9716010000000002
O	4.8090669999999998	−1.7295229999999999	−2.2834940000000001
O	2.2162500000000001	−2.7740309999999999	−3.5936119999999998
Ce	0.4092460000000000	−2.5432809999999999	−2.6389819999999999
O	2.3153269999999999	−0.0091290000000000	−4.6210269999999998
O	0.4368600000000000	−2.7444510000000002	−0.4247720000000000
Ce	−3.1500020000000002	−2.4768469999999998	−2.7094109999999998
O	−1.5517250000000000	−3.7811100000000000	−2.0275500000000002
O	−3.9380869999999999	−0.6055890000000000	−2.3864169999999998
Ce	−4.6796620000000004	0.8862650000000000	3.0520410000000000
O	−3.7276620000000000	2.5842440000000000	2.4745279999999998
O	−5.5808280000000003	0.0945930000000000	1.2787839999999999
Ce	−1.7310490000000001	−1.0094939999999999	3.4568840000000001
O	−2.0252859999999999	−2.8638479999999999	2.1708569999999998
O	−3.6715409999999999	−0.3815020000000000	4.3251359999999996
Ce	−4.0632099999999998	−0.4364290000000000	−0.1206030000000000
Ce	−1.6231810000000000	−3.2005089999999998	0.2185720000000000
O	−2.9597570000000002	0.0567110000000000	1.8043620000000000
O	−3.7934139999999998	−2.7504010000000001	−0.6550920000000000
O	−0.2138020000000000	−0.6984410000000000	4.9095950000000004
O	−1.4333400000000001	−1.5012520000000000	−3.4853269999999998
Ce	−1.4118409999999999	0.5758880000000000	−2.0924000000000000
O	−1.7980259999999999	−1.1683140000000001	−0.6685980000000000
O	−0.3016030000000000	1.7388560000000000	−3.2920590000000001
Ce	−1.8370240000000000	2.1631429999999998	1.3326680000000000
O	−0.3996280000000000	3.6976270000000002	1.0672310000000000
O	−2.9482870000000001	1.4129339999999999	−0.5950040000000000
Ce	1.0559050000000001	0.6192780000000000	3.8133360000000001
O	−0.9266100000000000	1.2895410000000000	3.1863190000000001
O	0.3250290000000000	−0.9697130000000000	2.2990490000000001
Ce	3.9648639999999999	2.0230429999999999	2.3894289999999998
O	1.9167240000000001	1.2789520000000001	1.8404670000000001
O	3.0804689999999999	1.3364769999999999	4.2011830000000003
Ce	4.4875530000000001	−0.0773610000000000	−0.7716390000000000
Ce	1.1803150000000000	−0.5520060000000000	0.3326280000000000
Ce	1.9073850000000001	1.4776959999999999	−2.9582350000000002
Ce	1.4351290000000001	3.0326040000000001	0.1632050000000000
O	5.1726349999999996	0.9972470000000000	1.0025940000000000
O	3.1640769999999998	−1.2883070000000001	0.2897220000000000
O	4.0639260000000004	0.6753510000000000	−2.8432569999999999
O	2.5459290000000001	1.0961160000000001	−0.7410780000000000
O	0.7726400000000000	−0.4736020000000000	−2.0502829999999999
O	1.7491630000000000	3.3333889999999999	−1.9223790000000001
O	−0.2161320000000000	1.2937440000000000	−0.1287530000000000
O	3.1887660000000002	3.6267960000000001	1.3729890000000000

CeO_2 - Fragment, $E_{tot} = -3\,744\,347.039\,811\,40\,\mathrm{eV}$, $\Delta E_{tot} = 58.961\,48\,\mathrm{meV}/f.u.$

Ce	16.7637490000000007	16.7637500000000017	16.7637509999999992
Ce	11.8543780000000005	16.7559450000000005	16.6172220000000017
Ce	21.6731230000000004	16.7715539999999983	16.9102759999999996
Ce	14.2917149999999999	19.5130839999999992	16.8572179999999996
Ce	19.2357860000000009	14.0144149999999996	16.6702820000000003
Ce	14.1075149999999994	16.5505740000000010	19.3890710000000013
Ce	19.4199860000000015	16.9769250000000014	14.1384260000000008
Ce	17.0061169999999997	19.6612280000000013	19.2968739999999990
Ce	19.3564119999999988	19.6205950000000016	16.6926990000000011
Ce	14.3322540000000007	16.7054690000000008	14.0043140000000008
Ce	19.1952479999999994	16.8220320000000001	19.5231870000000001
Ce	14.1710879999999992	13.9069070000000004	16.8348019999999998
Ce	16.7473239999999990	19.4449390000000015	14.1519060000000003
Ce	16.7801760000000009	14.0825610000000001	19.3755960000000016
Ce	16.5213840000000012	13.8662720000000004	14.2306260000000009
O	20.7609150000000007	15.4869439999999994	15.4485229999999998
O	15.1914370000000005	20.5456019999999988	15.3031380000000006
O	15.1098450000000000	15.3726990000000008	20.6201730000000012
O	18.2090020000000017	12.8940099999999997	15.1654619999999998
O	12.7562660000000001	18.0949829999999992	15.3496609999999993
O	18.1367300000000000	18.3877640000000007	20.5907879999999999
O	12.6919290000000000	15.3330570000000002	18.0775289999999984
O	15.2184969999999993	12.9179680000000001	18.3955449999999985
O	15.4925850000000001	18.0475369999999984	18.4195749999999983
O	15.2812699999999992	18.2586210000000015	12.9998629999999995
O	20.8026219999999995	18.1389059999999986	18.1938330000000015
O	18.0729229999999994	15.5016230000000004	17.9493900000000011
O	18.5288019999999989	20.7509590000000017	18.2607399999999984
O	18.0349150000000016	15.4799640000000007	15.1079249999999998
O	18.3360629999999993	12.9818990000000003	18.2243619999999993
O	18.1038229999999984	18.1929030000000012	18.0063859999999991
O	15.4190280000000008	15.4226220000000005	18.0490850000000016
O	15.4545779999999997	18.0258770000000013	15.5781100000000006
O	12.7248769999999993	15.3885930000000002	15.3336649999999999
O	18.3090009999999985	20.6095320000000015	15.1319549999999996
O	12.7665849999999992	18.0405550000000012	18.0789760000000008
O	18.2462300000000006	15.2688790000000001	20.5276369999999986
O	14.9986990000000002	12.7765419999999992	15.2667599999999997
O	20.8355710000000016	18.1944429999999997	15.4499709999999997
O	15.3907699999999998	15.1397359999999992	12.9367120000000000
O	20.7712339999999998	15.4325170000000007	18.1778380000000013
O	15.3184989999999992	20.6334899999999983	18.3620389999999993
O	18.4176549999999999	18.1548009999999991	12.9073259999999994
O	18.1084740000000011	18.1048769999999983	15.4784159999999993
O	15.4236769999999996	15.3345970000000005	15.5211129999999997

pGMC Structures for $Ce_xZr_{1-x}O_2$ Mixed Oxide Clusters

$Ce_1Zr_{14}O_{30}$, $E_{tot} = -1\,690\,025.984\,542\,86$ eV

Zr	0.1419450000000000	−2.6671830000000001	3.9595989999999999
O	−1.7874060000000001	−2.2450860000000001	3.7866800000000000
O	1.7783730000000000	−1.6817640000000000	4.5601029999999998
Zr	1.2438149999999999	−3.4209909999999999	1.2244360000000001
O	0.0945770000000000	−4.3323210000000003	−0.1411760000000000
O	0.6789120000000000	−4.2584099999999996	2.9500340000000000
Zr	−2.2907760000000001	−1.8041410000000000	−3.6927020000000002
O	−1.6365660000000000	−3.4164170000000000	−2.7807559999999998
O	−4.0290609999999996	−1.1387879999999999	−3.0945900000000002
Zr	−4.6696270000000002	0.8530080000000000	1.1284790000000000
O	−3.8125049999999998	2.4784489999999999	1.7456870000000000
O	−5.2373890000000003	0.7537670000000000	−0.7666100000000000
Zr	−2.4277000000000002	−1.2293240000000001	2.1863229999999998
O	−2.1456559999999998	−2.3967440000000000	0.5558510000000000
O	−4.3504560000000003	−0.7218500000000000	2.2987780000000000
Zr	−3.5426590000000000	0.2647880000000000	−1.7288030000000001
Zr	−0.9743280000000000	−2.8746849999999999	−0.9415430000000000
O	−2.8661089999999998	0.3997750000000000	0.2941850000000000
O	−1.5957300000000001	−0.7970550000000000	−2.0963859999999999
O	0.5773390000000000	−1.7635689999999999	2.2315140000000002
O	−1.3018460000000001	−0.4364880000000000	−4.7866179999999998
Zr	−0.9162620000000000	1.0780700000000001	−3.5575909999999999
O	0.7337210000000000	−1.8361390000000000	−0.4458360000000000
O	0.1753790000000000	2.6466430000000001	−4.1465209999999999
Ce	−1.6415700000000000	2.1651060000000002	1.4997320000000001
O	−0.3560790000000000	3.8561350000000001	1.4833510000000001
O	−2.6226509999999998	1.6939109999999999	−2.7172920000000000
Zr	2.7170890000000001	−1.1392160000000000	2.8575830000000000
O	−1.4694460000000000	0.4741840000000000	2.6681290000000000
O	3.0813880000000000	−2.7401599999999999	1.7673280000000000
Zr	3.8637760000000001	1.4977710000000000	1.4996020000000001
O	2.3563010000000002	0.1472730000000000	1.2390770000000000
O	4.1526880000000004	0.2824430000000000	3.0437409999999998
Zr	4.2050049999999999	1.1840970000000000	−1.7198570000000000
Zr	1.4546509999999999	0.0135780000000000	−0.6259820000000000
Zr	1.6393340000000001	2.7537880000000001	−2.7857539999999998
Zr	1.2533930000000000	3.3358780000000001	0.4466960000000000
O	5.1967169999999996	1.4276519999999999	−0.0038060000000000
O	3.1973889999999998	−0.4543800000000000	−1.6070960000000001
O	3.5472389999999998	2.3280210000000001	−3.2387760000000001
O	2.6369330000000000	1.9676819999999999	−0.7522070000000000
O	0.7343400000000000	0.9058530000000000	−2.3663530000000002
O	1.2015510000000000	4.1053110000000004	−1.4159600000000001
O	0.2011580000000000	1.5921490000000000	0.2593180000000000
O	2.8108100000000000	3.1493769999999999	1.7259819999999999

$Ce_2Zr_{13}O_{30}$, $E_{tot} = -1\,836\,762.674\,374\,34\,\mathrm{eV}$

Zr	0.1195780000000000	−2.7783140000000000	3.9846870000000001
O	−1.7841450000000001	−2.2454019999999999	3.8736320000000002
O	1.7467660000000000	−1.7769379999999999	4.5359319999999999
Zr	1.1224419999999999	−3.4322970000000002	1.1740290000000000
O	0.0137600000000000	−4.2794010000000000	−0.2424070000000000
O	0.6198460000000000	−4.3315500000000000	2.8975890000000000
Ce	−2.4645299999999999	−2.0164979999999999	−3.9802219999999999
O	−1.8041970000000001	−3.5034310000000000	−2.7415639999999999
O	−4.1008579999999997	−1.1110949999999999	−3.0894260000000000
Zr	−4.4686469999999998	0.9460040000000000	1.1468879999999999
O	−3.5100929999999999	2.5453030000000001	1.6914560000000001
O	−5.1037169999999996	0.7638540000000000	−0.7092020000000000
Zr	−2.2415120000000002	−1.1709030000000000	2.2554080000000001
O	−2.1458849999999998	−2.3331360000000001	0.5822290000000000
O	−4.1496529999999998	−0.6023450000000000	2.3384060000000000
Zr	−3.4469150000000002	0.2343160000000000	−1.7351749999999999
Zr	−1.0552210000000000	−2.7656879999999999	−0.9760080000000000
O	−2.6699830000000002	0.4775120000000000	0.2677440000000000
O	−1.5997840000000001	−0.8784740000000000	−2.1958850000000001
O	0.4170620000000000	−1.8176620000000001	2.2472219999999998
O	−1.3190780000000000	−0.4706680000000000	−4.8852890000000002
Zr	−0.8761450000000000	0.9549440000000000	−3.5615839999999999
O	0.6882280000000000	−1.7866190000000000	−0.4345550000000000
O	0.1622210000000000	2.5650400000000002	−4.1496829999999996
Zr	−1.5504110000000000	2.0123430000000000	1.4307209999999999
O	−0.4555140000000000	3.6907489999999998	1.5606370000000001
O	−2.5701790000000000	1.6421349999999999	−2.7691789999999998
Zr	2.6389230000000001	−1.1707390000000000	2.8227210000000000
O	−1.3214300000000001	0.5736360000000000	2.7086299999999999
O	2.9617779999999998	−2.7280970000000000	1.6642180000000000
Ce	4.0014539999999998	1.6802809999999999	1.6876610000000001
O	2.2571780000000001	0.2463430000000000	1.3763980000000000
O	4.1758850000000001	0.1115310000000000	3.0975510000000002
Zr	4.1887990000000004	1.2774300000000001	−1.6845810000000001
Zr	1.4945489999999999	0.0322790000000000	−0.5485780000000000
Zr	1.5803840000000000	2.7384750000000002	−2.7643179999999998
Zr	1.1260889999999999	3.3242940000000001	0.4494800000000000
O	5.2711750000000004	1.6164870000000000	−0.0544990000000000
O	3.2720739999999999	−0.4099680000000000	−1.4748349999999999
O	3.4989550000000000	2.3762379999999999	−3.2218659999999999
O	2.6074410000000001	2.0184310000000001	−0.7081090000000000
O	0.7935680000000001	0.8335790000000000	−2.3693350000000000
O	1.0628540000000000	4.0889490000000004	−1.4032849999999999
O	0.1070840000000000	1.5560300000000000	0.1720560000000000
O	2.7098049999999998	3.3030409999999999	1.7342820000000001

$Ce_3Zr_{12}O_{30}$, $E_{tot} = -1\,983\,498.942\,747\,88\,\mathrm{eV}$

Ce	−0.0199960000000000	−2.5571860000000002	4.6912469999999997
O	−1.7404530000000000	−1.6658820000000001	4.2215639999999999
O	1.9363889999999999	−1.8529240000000000	4.6672169999999999
Zr	0.4608880000000000	−3.4647640000000002	1.5470910000000000
O	0.0695480000000000	−4.3384169999999997	−0.2119800000000000
O	−0.0180660000000000	−4.1970939999999999	3.3076310000000002
Ce	−2.3268629999999999	−1.6747259999999999	−3.9812110000000001
O	−1.5687570000000000	−3.3501500000000002	−3.0084780000000002
O	−4.1305740000000002	−0.9199850000000001	−3.2505359999999999
Zr	−4.5942829999999999	0.5513830000000000	1.3707440000000000
O	−3.7402000000000002	2.2939669999999999	1.3124790000000000
O	−5.3443600000000000	0.1834810000000000	−0.4374170000000000
Zr	−1.8764130000000001	−0.9426040000000000	2.2439860000000000
O	−1.3172509999999999	−2.3791229999999999	0.8076340000000000
O	−3.8720050000000001	−0.6812880000000000	2.6945830000000002
Zr	−3.6778369999999998	0.0627320000000000	−1.5525789999999999
Zr	−0.7938130000000000	−2.8327950000000000	−1.1844760000000001
O	−2.8899610000000000	−0.0862820000000000	0.3899050000000000
O	−1.8330830000000000	−0.9600880000000001	−1.9345850000000000
O	0.3231660000000000	−1.5556490000000001	2.6264040000000000
O	−1.4010940000000001	0.1729820000000000	−4.3608349999999998
Zr	−0.8172850000000000	1.2857820000000000	−2.8013119999999998
O	0.8823420000000000	−1.8437950000000001	−1.3437140000000001
O	−0.0290250000000000	2.9297430000000002	−3.4881310000000001
Zr	−1.8591110000000000	1.9794940000000001	0.5885170000000000
O	−0.7598840000000000	3.5969630000000001	0.9212070000000000
O	−2.5598079999999999	1.7474670000000001	−1.6543079999999999
Zr	2.3936050000000000	−1.2815580000000000	2.7640389999999999
O	−1.1728840000000000	0.8836330000000000	2.1011679999999999
O	2.4155270000000000	−2.9597639999999998	1.7554719999999999
Zr	3.5956030000000001	1.3607530000000001	1.4082600000000001
O	2.2057090000000001	−0.0636500000000000	0.9266930000000000
O	3.8339219999999998	0.1634690000000000	2.9388070000000002
Ce	4.7593189999999996	1.4558489999999999	−1.8158710000000000
Zr	1.8976059999999999	−0.1745910000000000	−1.1238020000000000
Zr	1.8387089999999999	2.8248940000000000	−2.6936770000000001
Zr	1.0427780000000000	3.1341340000000000	0.2937270000000000
O	5.2296310000000004	1.5871759999999999	0.1916970000000000
O	3.7749069999999998	−0.3768700000000000	−1.7930560000000000
O	3.7757610000000001	2.6427589999999999	−3.2611059999999998
O	2.7367119999999998	1.9027510000000001	−0.8752840000000000
O	1.2214110000000000	0.7839380000000000	−2.8094269999999999
O	1.4974090000000000	4.1918259999999998	−1.3070839999999999
O	0.0258760000000000	1.5244810000000000	−0.6181820000000000
O	2.4261889999999999	2.8995270000000000	1.7369800000000000

$Ce_4Zr_{11}O_{30}$, $E_{tot} = -2\,130\,236.105\,454\,48\,\mathrm{eV}$

Zr	6.5362030000000004	7.7091839999999996	3.8298380000000001
Zr	4.2538159999999996	6.0959950000000003	8.7987339999999996
Ce	12.0447039999999994	8.1549619999999994	7.7895079999999997
Ce	7.8634089999999999	4.6959099999999996	4.2753829999999997
Zr	7.2849430000000002	10.6691170000000000	4.7163370000000002
Zr	7.4787929999999996	5.0322209999999998	9.0711139999999997
Zr	9.0146639999999998	9.8216680000000007	9.5283519999999999
Zr	7.3119310000000004	8.0784889999999994	7.0407999999999999
Zr	6.5937419999999998	8.3380080000000003	11.1287800000000008
Zr	5.1140499999999998	5.6500170000000001	5.9378229999999999
Zr	9.9668500000000009	5.6236639999999998	7.1709480000000001
Zr	7.0436090000000000	11.4497450000000001	7.7157080000000002
Zr	10.0156720000000004	9.5417480000000001	5.7011310000000002
Ce	5.5687009999999999	5.2297459999999996	11.8587840000000000
Ce	4.5689359999999999	9.4889130000000002	8.7032159999999994
O	4.8270090000000003	6.9559259999999998	4.4247360000000002
O	9.6403219999999994	4.7820029999999996	5.3619719999999997
O	9.2543810000000004	10.8284190000000002	4.3957020000000000
O	3.9860069999999999	5.0617089999999996	10.5450649999999992
O	8.4488959999999995	6.7302470000000003	8.1857450000000007
O	8.0133690000000009	8.6637260000000005	5.0723130000000003
O	10.9062640000000002	9.0735419999999998	9.2320150000000005
O	9.0921199999999995	4.2071449999999997	8.2722630000000006
O	8.8362789999999993	9.8681730000000005	7.2820010000000002
O	8.4070499999999999	9.1466729999999998	11.2899480000000008
O	3.4968560000000002	5.4498780000000000	7.0943509999999996
O	10.3365220000000004	7.6007350000000002	6.3751480000000003
O	5.9857870000000002	4.1166929999999997	4.8805410000000000
O	6.2846330000000004	9.8893989999999992	6.4966840000000001
O	7.1122439999999996	4.2294590000000003	10.8987850000000002
O	3.3456130000000002	7.8605359999999997	9.1024220000000007
O	7.5007010000000003	6.2615200000000000	2.8730910000000001
O	5.4113559999999996	7.4356260000000001	7.4178620000000004
O	11.7569940000000006	6.0781510000000001	7.9683270000000004
O	8.4292949999999998	11.6511490000000002	9.2230349999999994
O	6.1448320000000001	7.0560499999999999	12.6514989999999994
O	7.1420560000000002	6.4032530000000003	5.6054349999999999
O	7.1718019999999996	12.2989280000000001	5.9579779999999998
O	6.1683909999999997	6.5872050000000000	10.0526280000000003
O	5.2123960000000000	11.4765759999999997	8.4871370000000006
O	6.2883550000000001	9.6568939999999994	3.3170730000000002
O	5.9458110000000000	4.8448060000000002	7.8913219999999997
O	7.0598720000000004	9.1025419999999997	8.9726330000000001
O	11.8822960000000002	9.7355750000000008	6.3876949999999999
O	5.0600319999999996	9.4613449999999997	10.7938589999999994

$Ce_5Zr_{10}O_{30}$, $E_{tot} = -2\,276\,971.921\,262\,41$ eV

Zr	6.4884399999999998	7.7485609999999996	3.8020800000000001
Zr	4.2473190000000001	6.0849310000000001	8.8060329999999993
Ce	12.0995039999999996	8.0515770000000000	7.7899870000000000
Zr	7.8462850000000000	4.9784800000000002	4.4019180000000002
Zr	7.1608489999999998	10.6969349999999999	4.7497299999999996
Zr	7.4582769999999998	5.0547839999999997	9.1318190000000001
Zr	9.0946590000000000	9.8210119999999996	9.4319849999999992
Zr	7.3699479999999999	8.1329110000000000	7.0532690000000002
Ce	6.5762099999999997	8.4642149999999994	11.3326499999999992
Zr	5.1791900000000002	5.5984710000000000	5.9756450000000001
Zr	9.9331709999999998	5.5819580000000002	7.1881219999999999
Zr	7.0503210000000003	11.4276160000000004	7.7661400000000000
Ce	10.1680100000000007	9.5440579999999997	5.4170769999999999
Ce	5.4729520000000003	5.1389649999999998	11.8461529999999993
Ce	4.5642880000000003	9.4559840000000008	8.5850519999999992
O	4.8568840000000000	6.9256789999999997	4.4563660000000000
O	9.5628100000000007	4.7802220000000002	5.3806680000000000
O	9.1281250000000007	10.9623249999999999	4.3278140000000000
O	3.8881730000000001	5.0270919999999997	10.5050059999999998
O	8.4373260000000005	6.7499279999999997	8.2156640000000003
O	7.9438680000000002	8.7217920000000007	5.0164350000000004
O	10.9991149999999998	9.1074230000000007	9.1661129999999993
O	9.0926580000000001	4.2274289999999999	8.3604950000000002
O	8.8168460000000000	9.8399450000000002	7.2319269999999998
O	8.5740350000000003	9.1395049999999998	11.2336320000000001
O	3.5414500000000002	5.4117350000000002	7.0718100000000002
O	10.3455259999999996	7.5985420000000001	6.4377030000000000
O	6.1551729999999996	4.1445489999999996	4.8978460000000004
O	6.2153669999999996	9.8925809999999998	6.5070139999999999
O	7.0655890000000001	4.1775099999999998	10.9097969999999993
O	3.3155359999999998	7.8493729999999999	9.0045610000000007
O	7.5574690000000002	6.2933760000000003	2.9254780000000000
O	5.4694750000000001	7.4276119999999999	7.4368829999999999
O	11.7612970000000008	5.9855169999999998	7.9386700000000001
O	8.5052669999999999	11.6605779999999992	9.2060870000000001
O	6.0256259999999999	6.8874880000000003	12.7799840000000007
O	7.2046289999999997	6.4512299999999998	5.6242440000000000
O	7.1139029999999996	12.3009839999999997	6.0059620000000002
O	6.0879560000000001	6.5375030000000001	10.1126600000000000
O	5.2180720000000003	11.4628460000000008	8.5223990000000001
O	6.1659230000000003	9.6934120000000004	3.3298559999999999
O	5.9658179999999996	4.8377100000000004	7.9055190000000000
O	7.0576790000000003	9.2069449999999993	8.9616819999999997
O	12.1090630000000008	9.5567240000000009	6.2949500000000000
O	4.9174850000000001	9.4552510000000005	10.7308350000000008

$Ce_6Zr_9O_{30}$, $E_{tot} = -2\,423\,708.456\,937\,85$ eV

Zr	6.5634920000000001	7.6775849999999997	3.7613319999999999
Zr	4.2124949999999997	6.1151809999999998	8.7779559999999996
Ce	12.1904480000000000	8.0989430000000002	7.6130860000000000
Zr	7.9158660000000003	4.9240290000000000	4.4621380000000004
Ce	6.9486990000000004	10.9193750000000005	4.6336740000000001
Zr	7.4730829999999999	5.2071829999999997	9.1812570000000004
Zr	9.1343490000000003	9.5056519999999995	9.3973410000000008
Zr	7.2692050000000004	8.1667939999999994	7.0026260000000002
Ce	6.4933500000000004	8.4955449999999999	11.3697789999999994
Zr	5.2234800000000003	5.5586820000000001	5.9892609999999999
Zr	9.9501620000000006	5.6849759999999998	7.1947559999999999
Zr	7.1347569999999996	11.3279239999999994	7.9301589999999997
Ce	10.0764750000000003	9.5991309999999999	5.3807169999999998
Ce	5.4028090000000004	5.1731840000000000	11.8374439999999996
Ce	4.5405689999999996	9.5086530000000007	8.6110629999999997
O	4.9389859999999999	6.8609830000000001	4.4337640000000000
O	9.6250540000000004	4.7488970000000004	5.4479800000000003
O	9.1219940000000008	11.0021540000000009	4.2483019999999998
O	3.8471750000000000	5.0424749999999996	10.4712820000000004
O	8.4645600000000005	6.9366760000000003	8.2415269999999996
O	7.8585130000000003	8.7555870000000002	4.9998740000000002
O	11.0777850000000004	8.9950320000000001	9.0993279999999999
O	9.1142140000000005	4.3884439999999998	8.4371489999999998
O	8.7645990000000005	9.7735710000000005	7.2470270000000001
O	8.5731619999999999	8.7661800000000003	11.1647239999999996
O	3.5630639999999998	5.3659210000000002	7.0506929999999999
O	10.4026580000000006	7.6277790000000003	6.3272620000000002
O	6.2200069999999998	4.0912470000000001	4.9547790000000003
O	6.1129059999999997	9.9561829999999993	6.5662149999999997
O	7.0612769999999996	4.2938609999999997	10.9309689999999993
O	3.2836210000000001	7.8793319999999998	8.9653379999999991
O	7.6636839999999999	6.2058340000000003	2.9506250000000001
O	5.4127330000000002	7.4190170000000002	7.3913650000000004
O	11.8072879999999998	6.0469900000000001	7.8632540000000004
O	8.6013570000000001	11.3835420000000003	9.3693170000000006
O	5.9019550000000001	6.9173080000000002	12.7992819999999998
O	7.2747560000000000	6.4149880000000001	5.6605160000000003
O	7.2858929999999997	12.3104490000000002	6.1856939999999998
O	6.0079060000000002	6.6167379999999998	10.1249629999999993
O	5.2968970000000004	11.5017619999999994	8.6429270000000002
O	6.1496209999999998	9.5758650000000003	3.1834319999999998
O	6.0078149999999999	4.8950329999999997	7.9409029999999996
O	6.9423149999999998	9.2095120000000001	8.9587599999999998
O	12.0639099999999999	9.6632210000000001	6.2122599999999997
O	4.8326219999999998	9.4858510000000003	10.7636240000000001

$Ce_7Zr_8O_{30}$, $E_{tot} = -2\,570\,444.279\,805\,39\,\mathrm{eV}$

Ce	3.9415650000000002	−1.1039850000000000	−3.6749120000000000
O	5.1790529999999997	−1.2412810000000001	−2.0656620000000001
O	2.3848870000000000	−2.5849449999999998	−3.4208289999999999
Ce	0.4634930000000000	−2.4927380000000001	−2.5709089999999999
O	2.5910899999999999	0.1408800000000000	−4.7281139999999997
O	0.6303020000000000	−2.6079590000000001	−0.4314790000000000
Ce	−3.0864880000000001	−2.4395199999999999	−2.4510130000000001
O	−1.5160380000000000	−3.6795450000000001	−1.7282450000000000
O	−3.7496900000000002	−0.3901260000000000	−2.3616649999999999
Zr	−4.1219830000000002	0.8945480000000000	2.9519259999999998
O	−3.2586569999999999	2.5620090000000002	2.4600240000000002
O	−5.3913460000000004	0.3215240000000000	1.5291470000000000
Zr	−1.5967650000000000	−0.9969270000000000	3.2938589999999999
O	−2.1394350000000002	−2.8045270000000002	2.5176140000000000
O	−3.2027739999999998	−0.2420830000000000	4.2840389999999999
Ce	−4.1330359999999997	−0.2607610000000000	−0.1284400000000000
Ce	−1.3584579999999999	−2.8833270000000000	0.5765280000000000
O	−2.7607080000000002	0.0269280000000000	1.7223170000000001
O	−4.0995270000000001	−2.4210799999999999	−0.5865430000000000
O	0.0087270000000000	−0.9244570000000000	4.5103569999999999
O	−1.3440710000000000	−1.5279170000000000	−3.4078059999999999
Ce	−1.4493549999999999	0.5658820000000000	−2.0968200000000001
O	−1.8709570000000000	−1.1639070000000000	−0.7360530000000000
O	−0.4226230000000000	1.6279360000000000	−3.5251169999999998
Zr	−1.6873309999999999	2.0736690000000002	1.2318800000000001
O	−0.5605990000000000	3.6052550000000001	0.7272370000000000
O	−2.7935740000000000	1.5437520000000000	−0.5000620000000000
Zr	1.0180260000000001	0.6316510000000000	3.7928130000000002
O	−0.6313440000000000	1.2447189999999999	2.9121000000000001
O	−0.2916850000000000	−1.2912889999999999	1.5732170000000001
Zr	3.3187519999999999	1.6388799999999999	1.9851479999999999
O	1.9457780000000000	0.0288640000000000	2.1538580000000001
O	2.7143640000000002	1.7002790000000001	3.9348719999999999
Zr	4.2535030000000003	−0.0162550000000000	−0.5923380000000000
Zr	1.1840820000000001	−0.6094260000000000	0.2444090000000000
Ce	1.7328290000000000	1.5217710000000000	−3.2990830000000000
Zr	1.1662990000000000	2.8825240000000001	−0.0357490000000000
O	4.9470150000000004	0.8692600000000000	1.0846330000000000
O	3.0439569999999998	−1.3995590000000000	−0.0629040000000000
O	3.6335250000000001	0.7456580000000000	−2.4479060000000001
O	2.5088330000000001	1.1576450000000000	−0.0363510000000000
O	0.8153660000000000	−0.3562970000000000	−1.9960899999999999
O	1.5784039999999999	3.1681189999999999	−1.9553600000000000
O	−0.1044240000000000	1.1521410000000001	−0.0133080000000000
O	2.5110199999999998	3.3340169999999998	1.3667910000000001

$Ce_8Zr_7O_{30}$, $E_{tot} = -2\,717\,181.069\,607\,58\,\mathrm{eV}$

Ce	3.4700240000000000	−1.3914470000000001	−3.7083420000000000
O	4.3356769999999996	−1.8209990000000000	−1.8623339999999999
O	1.8687290000000001	−2.8286080000000000	−3.4257089999999999
Zr	0.3453600000000000	−2.3240880000000002	−2.3127759999999999
O	2.3321190000000001	0.0495130000000000	−4.5573730000000001
O	0.6940640000000000	−2.3587739999999999	−0.2691290000000000
Ce	−2.9366780000000001	−2.5514239999999999	−2.3229700000000002
O	−1.2528889999999999	−3.5850810000000002	−1.4976100000000001
O	−3.9720900000000001	−0.7628350000000000	−2.2390089999999998
Ce	−4.5994859999999997	0.6394600000000000	2.8902250000000000
O	−3.6330570000000000	2.3579580000000000	2.3981620000000001
O	−5.4168710000000004	0.0477620000000000	0.9927710000000000
Zr	−1.6928410000000000	−1.0531580000000000	3.2923979999999999
O	−1.8333590000000000	−2.8398279999999998	2.3804669999999999
O	−3.4856389999999999	−0.5750930000000000	4.1671160000000000
Zr	−3.8617650000000001	−0.3434640000000000	−0.1837660000000000
Zr	−1.2856280000000000	−2.4926640000000000	0.5072560000000000
O	−2.8747460000000000	−0.1234570000000000	1.6588210000000001
O	−3.4034130000000000	−2.4448449999999999	−0.1742380000000000
O	−0.0159330000000000	−1.0617890000000001	4.4502720000000000
O	−1.2962469999999999	−1.6096770000000000	−3.3674510000000000
Ce	−1.4062800000000000	0.7368080000000000	−2.2464309999999998
O	−1.6051890000000000	−0.9327000000000000	−0.8431900000000000
O	−0.2009390000000000	1.7770640000000000	−3.4453689999999999
Ce	−1.7117860000000000	1.9928330000000001	1.3193750000000000
O	−0.4333030000000000	3.6484269999999999	1.1641340000000000
O	−2.9251520000000002	1.4326909999999999	−0.6473179999999999
Ce	0.9816340000000000	0.6597250000000000	3.8953229999999999
O	−1.0260080000000000	1.1256050000000000	3.3374239999999999
O	−0.3627930000000000	−0.8592580000000000	1.5532619999999999
Zr	3.5128870000000001	1.2572800000000000	1.8053550000000000
O	1.3688549999999999	1.2207380000000001	1.7690809999999999
O	3.0968239999999998	0.8257920000000000	3.7322120000000001
Zr	4.2137079999999996	−0.0980380000000000	−0.7619190000000000
Zr	1.0528270000000000	−0.2738850000000000	0.1717680000000000
Ce	1.9984530000000000	1.6271100000000001	−2.9637270000000000
Ce	1.4406920000000001	3.2001100000000000	0.1609300000000000
O	5.1781170000000003	0.8220600000000000	0.6795570000000000
O	2.9652759999999998	−0.7032060000000000	0.7913170000000000
O	4.0251320000000002	0.6282110000000000	−2.6898659999999999
O	2.5707429999999998	1.2785540000000000	−0.6181920000000000
O	0.9963550000000000	−0.3947340000000000	−2.0223160000000000
O	1.7853040000000000	3.4676909999999999	−1.9534320000000001
O	−0.1635380000000000	1.4649680000000000	−0.4308210000000000
O	3.1628539999999998	3.1686920000000001	1.4260710000000001

$Ce_9Zr_6O_{30}$, $E_{tot} = -2\,863\,917.064\,580\,01$ eV

Ce	6.4951410000000003	7.6717909999999998	3.4892900000000000
Ce	3.9411900000000002	6.0282520000000002	8.8349039999999999
Ce	12.3018219999999996	8.3118330000000000	7.7727789999999999
Ce	7.8991480000000003	4.5635009999999996	4.3757849999999996
Ce	7.0382379999999998	10.9747550000000000	4.6747410000000000
Zr	7.3909700000000003	5.1865829999999997	9.0755020000000002
Zr	9.0781060000000000	9.4815140000000007	9.4466049999999999
Zr	7.2154819999999997	8.1264339999999997	6.9272499999999999
Zr	6.4913699999999999	8.3240700000000007	11.1375299999999999
Zr	5.1507649999999998	5.6248560000000003	5.9391090000000002
Ce	10.1586990000000004	5.6329690000000001	7.2234080000000001
Zr	7.1494010000000001	11.3219849999999997	7.9384800000000002
Ce	10.1097850000000005	9.6024229999999999	5.4479610000000003
Ce	5.5892609999999996	5.2253069999999999	11.9569960000000002
Ce	4.5501060000000004	9.5671490000000006	8.7035669999999996
O	4.8178710000000002	6.7920550000000004	4.3101599999999998
O	9.7284140000000008	4.6379299999999999	5.3295940000000002
O	9.2154790000000002	11.0362890000000000	4.3038850000000002
O	3.8974959999999998	5.0203699999999998	10.8333999999999993
O	8.3897349999999999	6.8925799999999997	8.2312139999999996
O	7.9006470000000002	8.7687340000000003	4.9523799999999998
O	11.0393299999999996	9.0216899999999995	9.2383270000000000
O	9.0319830000000003	4.2866739999999997	8.3471609999999998
O	8.7689140000000005	9.7012760000000000	7.2726920000000002
O	8.4127360000000007	8.8200760000000002	11.1954999999999991
O	3.4168289999999999	5.3784789999999996	6.9283950000000001
O	10.6509239999999998	7.6373629999999997	6.3331660000000003
O	6.0026320000000002	4.0317100000000003	4.9708439999999996
O	6.1526310000000004	9.9824710000000003	6.5455069999999997
O	7.1420849999999998	4.3363680000000002	10.8972599999999993
O	3.1719240000000002	8.0048040000000000	8.9909610000000004
O	7.6581000000000001	6.0186830000000002	2.8361310000000000
O	5.3313350000000002	7.4190719999999999	7.2996610000000004
O	12.0692649999999997	6.2751370000000000	8.0835159999999995
O	8.5908689999999996	11.3650350000000007	9.3740679999999994
O	6.0807029999999997	7.0961879999999997	12.7057620000000000
O	7.2041750000000002	6.3472309999999998	5.6131440000000001
O	7.3572059999999997	12.3531600000000008	6.2438580000000004
O	6.0252990000000004	6.6061319999999997	10.1011410000000001
O	5.3149730000000002	11.5409980000000001	8.6489220000000007
O	6.1234130000000002	9.7755030000000005	3.1825760000000001
O	5.8616159999999997	4.8161800000000001	7.9299390000000001
O	6.8993560000000000	9.1390630000000002	8.9354580000000006
O	12.0358239999999999	9.8748819999999995	6.3970300000000000
O	4.9563139999999999	9.4737130000000001	10.8001609999999992

$Ce_{10}Zr_5O_{30}$, $E_{tot} = -3\,010\,653.012\,945\,60\,\mathrm{eV}$

Ce	0.0799940000000000	−3.0261580000000001	4.2607540000000004
O	−1.8541559999999999	−2.4818410000000002	3.7899829999999999
O	1.7152689999999999	−1.7772800000000000	4.7004669999999997
Ce	1.3004249999999999	−3.5807050000000000	1.0774210000000000
O	−0.2204230000000000	−4.2367369999999998	−0.1582770000000000
O	0.7392320000000000	−4.4977239999999998	2.9391820000000002
Ce	−2.3099690000000002	−2.0886060000000000	−4.2570329999999998
O	−1.4609399999999999	−3.5429610000000000	−3.0276920000000000
O	−3.9655070000000001	−1.4813890000000001	−3.2198169999999999
Ce	−4.8602049999999997	1.0934809999999999	1.4642610000000000
O	−3.7334239999999999	2.7269420000000002	1.9869150000000000
O	−5.2543550000000003	0.4761730000000000	−0.4801600000000000
Ce	−2.1819660000000001	−1.1440189999999999	2.1083780000000001
O	−2.4705360000000001	−2.0061330000000002	−0.1151180000000000
O	−4.2226450000000000	−0.5962750000000000	2.4936989999999999
Ce	−3.4545189999999999	−0.2010840000000000	−1.4910030000000001
Zr	−0.9965640000000000	−2.7019739999999999	−1.2324690000000000
O	−2.7915790000000000	0.6621310000000000	0.5660570000000000
O	−1.4076450000000000	−0.9632140000000000	−2.4913080000000001
O	0.4562540000000000	−1.9241889999999999	2.3516889999999999
O	−1.4264349999999999	−0.3739110000000000	−5.0837940000000001
Zr	−0.9821500000000000	0.9174420000000000	−3.5919349999999999
O	0.6647940000000000	−1.7132630000000000	−0.5075140000000000
O	0.1149880000000000	2.4975950000000000	−4.2326129999999997
Ce	−1.5785199999999999	2.3239649999999998	1.6010949999999999
O	−0.3660310000000000	4.0831359999999997	1.4951289999999999
O	−2.6086390000000002	1.4345840000000001	−2.6357830000000000
Zr	2.4988939999999999	−1.1141859999999999	2.9574970000000000
O	−1.3056900000000000	0.6279400000000001	2.8403470000000000
O	3.0734070000000000	−2.6419160000000002	1.9002260000000000
Ce	4.0403750000000000	1.6036210000000000	1.7596520000000000
O	2.2285930000000000	0.2897590000000000	1.4315270000000000
O	4.0572530000000002	0.1640160000000000	3.2767990000000000
Ce	4.4110959999999997	1.1598720000000000	−1.8407359999999999
Zr	1.4622569999999999	0.1733340000000000	−0.4997260000000000
Zr	1.5668500000000001	2.6496460000000002	−2.9016750000000000
Ce	1.3518380000000001	3.6922769999999998	0.3484220000000000
O	5.3310890000000004	1.4654650000000000	0.0136830000000000
O	3.2104650000000001	−0.4403510000000000	−1.3791700000000000
O	3.4695309999999999	2.2117960000000001	−3.4202089999999998
O	2.6503660000000000	2.0730040000000001	−0.8188650000000000
O	0.6905710000000000	0.8650670000000000	−2.3264170000000002
O	1.1747280000000000	4.1899210000000000	−1.7220130000000000
O	0.1667740000000000	1.7774730000000001	0.2870790000000000
O	2.9968569999999999	3.3752740000000001	1.7830610000000000

$Ce_{11}Zr_4O_{30}$, $E_{tot} = -3\,157\,389.383\,320\,83\,\mathrm{eV}$

Ce	3.4125809999999999	−1.3605419999999999	−3.9469870000000000
O	4.3644730000000003	−1.9415940000000000	−2.1574230000000001
O	1.8476889999999999	−2.7880159999999998	−3.5326029999999999
Zr	0.3773460000000000	−2.3053400000000002	−2.3371469999999999
O	2.2244199999999998	0.0939400000000000	−4.6195810000000002
O	0.7304150000000000	−2.3244660000000001	−0.2706360000000000
Ce	−2.8925580000000002	−2.6449410000000002	−2.3768090000000002
O	−1.1524770000000000	−3.6003159999999998	−1.5359799999999999
O	−4.1299970000000004	−0.9932360000000000	−2.3561440000000000
Ce	−4.5515189999999999	0.7398910000000000	3.0393789999999998
O	−3.6368710000000002	2.4441440000000001	2.3600789999999998
O	−5.5704859999999998	0.0795400000000000	1.2981009999999999
Zr	−1.6879150000000001	−1.0310470000000000	3.2362359999999999
O	−1.8243190000000000	−2.8241120000000000	2.3298169999999998
O	−3.4313929999999999	−0.5670240000000000	4.2143040000000003
Ce	−4.1169929999999999	−0.3942410000000000	−0.2147010000000000
Zr	−1.2747569999999999	−2.4832049999999999	0.4571100000000000
O	−2.9619559999999998	−0.0676070000000000	1.6764710000000000
O	−3.4099210000000002	−2.6167419999999999	−0.2581490000000000
O	−0.0419930000000000	−0.9741500000000000	4.4183100000000000
O	−1.2530920000000001	−1.6043710000000000	−3.3824010000000002
Ce	−1.3588249999999999	0.7149450000000001	−2.2332049999999999
O	−1.7406200000000001	−0.9785950000000000	−0.8975040000000000
O	−0.1707630000000000	1.8177300000000001	−3.4025569999999998
Ce	−1.7638039999999999	2.0040849999999999	1.2532390000000000
O	−0.4148990000000000	3.6312220000000002	1.1734920000000000
O	−2.9351880000000001	1.4359980000000001	−0.7394700000000000
Ce	0.8459470000000000	0.8531810000000000	4.0201770000000003
O	−1.1226280000000000	1.1808099999999999	3.3009490000000001
O	−0.4252830000000000	−0.8071250000000000	1.4625159999999999
Ce	3.6959860000000000	1.2742270000000000	2.0422129999999998
O	1.4240520000000001	1.1962310000000000	1.8621390000000000
O	2.9148260000000001	0.9442060000000000	4.0794800000000002
Ce	4.4861230000000001	−0.2560250000000000	−0.8322420000000000
Zr	1.1625930000000000	−0.2769930000000000	0.2269490000000000
Ce	2.0055960000000002	1.6296240000000000	−2.9022610000000002
Ce	1.4548900000000000	3.1527409999999998	0.2049130000000000
O	5.3658510000000001	0.8092470000000000	0.7227460000000000
O	3.0824120000000002	−0.7400500000000000	0.8579250000000000
O	4.0341570000000004	0.5570510000000000	−2.8244889999999998
O	2.6017239999999999	1.2542169999999999	−0.6161060000000000
O	0.9720190000000000	−0.3656440000000000	−1.9931200000000000
O	1.8173690000000000	3.4705960000000000	−1.9020090000000001
O	−0.1427750000000000	1.4375950000000000	−0.3869410000000000
O	3.1905640000000002	3.2241599999999999	1.4819240000000000

$Ce_{12}Zr_3O_{30}$, $E_{tot} = -3\,304\,125.563\,005\,92\,\mathrm{eV}$

Ce	3.7776809999999998	−0.9657829999999999	−4.0808010000000001
O	4.9131539999999996	−1.4266310000000000	−2.4511949999999998
O	2.3360379999999998	−2.6243710000000000	−3.7406359999999999
Ce	0.6157610000000000	−2.6395110000000002	−2.6271249999999999
O	2.2636129999999999	0.2350760000000000	−4.6660539999999999
O	0.9384550000000000	−2.6313219999999999	−0.4832860000000000
Ce	−3.0043110000000000	−2.6266699999999998	−2.1283210000000001
O	−1.4529630000000000	−3.8539430000000001	−1.2776920000000000
O	−3.5377909999999999	−0.4839250000000000	−2.3223449999999999
Ce	−4.7347020000000004	1.4104340000000000	2.8522710000000000
O	−3.3067570000000002	2.7465069999999998	2.2609260000000000
O	−5.7032249999999998	0.7273790000000000	1.1419220000000001
Ce	−2.2393230000000002	−0.9121680000000000	3.6345559999999999
O	−2.1169910000000001	−2.7325729999999999	2.4191829999999999
O	−3.9720000000000000	0.1469240000000000	4.3729060000000004
Ce	−4.2287509999999999	−0.2526930000000000	−0.1722620000000000
Ce	−0.9092750000000001	−2.9122979999999998	0.7356930000000000
O	−3.2242989999999998	0.0658450000000000	1.8379970000000001
O	−4.4747579999999996	−2.3568870000000000	−0.6699720000000000
O	−0.3943790000000000	−1.0540520000000000	4.6949800000000002
O	−1.2774859999999999	−1.8235730000000001	−3.2420670000000000
Ce	−1.3851620000000000	0.4123120000000000	−2.0151219999999999
O	−1.9167600000000000	−1.3645389999999999	−0.4521660000000000
O	−0.3592200000000000	1.6175600000000001	−3.2911869999999999
Zr	−1.7096920000000000	1.8780740000000000	1.2836460000000001
O	−0.4236260000000000	3.3550570000000000	1.0859179999999999
O	−2.7683380000000000	1.4320230000000000	−0.4793360000000000
Ce	1.0214730000000001	−0.0073040000000000	3.4992030000000001
O	−0.9243180000000000	0.8864069999999999	2.9479280000000001
O	0.4682670000000000	−1.3887860000000001	1.7614520000000000
Ce	3.7663289999999998	1.9326700000000001	2.3681049999999999
O	1.8687069999999999	0.9550160000000000	1.6661760000000001
O	2.8908299999999998	0.9613510000000000	4.0589919999999999
Ce	4.5847879999999996	0.1568580000000000	−0.8917740000000000
Zr	1.4652190000000000	−0.5758680000000000	0.0605580000000000
Ce	1.8087569999999999	1.6403170000000000	−2.9390269999999998
Zr	1.2687280000000001	2.7088960000000002	0.2276350000000000
O	5.1363200000000004	1.1923729999999999	0.9744520000000000
O	3.3701949999999998	−1.1699010000000001	0.1486730000000000
O	4.0241110000000004	0.9568340000000000	−2.9066369999999999
O	2.5380470000000002	1.1448890000000000	−0.7762260000000000
O	0.9363800000000000	−0.5250430000000000	−2.0489989999999998
O	1.4131899999999999	3.3178179999999999	−1.6590510000000001
O	−0.1302260000000000	0.9939519999999999	−0.0858610000000000
O	2.7883089999999999	3.4532720000000001	1.3739760000000001

$Ce_{13}Zr_2O_{30}$, $E_{tot} = -3\,450\,861.932\,071\,65\,\mathrm{eV}$

Ce	3.3992369999999998	−1.2430129999999999	−4.0211509999999997
O	4.4661039999999996	−1.7022590000000000	−2.2694619999999999
O	1.9468790000000000	−2.8028499999999998	−3.5863010000000002
Zr	0.5101280000000000	−2.4111250000000002	−2.3246270000000000
O	2.0919310000000002	0.1103140000000000	−4.6813370000000001
O	1.0598289999999999	−2.3875700000000002	−0.3213050000000000
Ce	−2.8146770000000001	−2.6567769999999999	−2.2743199999999999
O	−1.0305070000000001	−3.7006980000000000	−1.4953890000000001
O	−3.5379770000000001	−0.6062900000000000	−2.3756230000000000
Ce	−4.9014199999999999	1.1343740000000000	2.8333339999999998
O	−3.6633730000000000	2.6668949999999998	2.3384630000000000
O	−5.7234230000000004	0.3432170000000000	1.0753839999999999
Ce	−2.2014469999999999	−0.9490840000000000	3.6633719999999999
O	−2.0841850000000002	−2.7796740000000000	2.3822410000000001
O	−4.0844420000000001	−0.1059790000000000	4.3307719999999996
Ce	−4.1337010000000003	−0.4405030000000000	−0.1967390000000000
Ce	−0.8250580000000000	−2.8032119999999998	0.7807700000000000
O	−3.1778640000000000	0.0358400000000000	1.8300650000000001
O	−4.1511909999999999	−2.6036910000000000	−0.7131820000000000
O	−0.3823340000000000	−1.1353599999999999	4.7160190000000002
O	−1.1447250000000000	−1.6458630000000001	−3.2463240000000000
Ce	−1.4017510000000000	0.5076000000000001	−2.0801020000000001
O	−1.7706450000000000	−1.2963030000000000	−0.5165790000000000
O	−0.3208440000000000	1.7139009999999999	−3.3063639999999999
Ce	−1.7784489999999999	2.0061270000000002	1.3364959999999999
O	−0.4280930000000000	3.6100650000000001	1.1291130000000000
O	−2.8816540000000002	1.3742669999999999	−0.5715770000000000
Ce	0.9535030000000000	0.1558870000000000	3.6312720000000001
O	−1.0584309999999999	1.0030239999999999	3.2695539999999998
O	0.2418780000000000	−1.1216660000000001	1.8113290000000000
Ce	3.8387129999999998	1.3607499999999999	2.0253310000000000
O	1.5861200000000000	1.2217800000000001	1.7571369999999999
O	3.0157620000000001	0.5323380000000000	3.8809269999999998
Ce	4.5994200000000003	0.0466190000000000	−1.0127299999999999
Zr	1.3794390000000001	−0.2948860000000000	0.1684240000000000
Ce	1.8531730000000000	1.6642490000000001	−2.9887410000000001
Ce	1.4481170000000001	3.1225329999999998	0.1977300000000000
O	5.4550789999999996	1.0853189999999999	0.5709050000000000
O	3.3264100000000001	−0.6144740000000000	0.7354490000000000
O	3.9785699999999999	0.7519930000000000	−3.0089020000000000
O	2.6027870000000002	1.3033079999999999	−0.7674380000000000
O	1.0173140000000001	−0.4280170000000000	−1.9976090000000000
O	1.6368140000000000	3.4806800000000000	−1.9130469999999999
O	−0.1496300000000000	1.2316020000000001	−0.2214400000000000
O	3.2386149999999998	3.2666119999999998	1.4262070000000000

$Ce_{14}Zr_1O_{30}$, $E_{tot} = -3\,597\,597.816\,549\,72\,\mathrm{eV}$

Ce	0.0820580000000000	−3.3904420000000002	4.0853339999999996
O	−1.9093130000000000	−2.8478640000000000	3.9228990000000001
O	1.0764920000000000	−1.6306300000000000	4.5088049999999997
Ce	1.3206950000000000	−3.4232130000000001	0.8178890000000000
O	−0.2948040000000000	−4.3484429999999996	−0.1161980000000000
O	1.3314520000000001	−4.4126440000000002	2.7642970000000000
Ce	−2.5051690000000000	−1.7910500000000000	−4.1180000000000003
O	−1.7756600000000000	−3.4825490000000001	−3.0410360000000001
O	−4.2252330000000002	−1.2557039999999999	−3.0651400000000000
Ce	−4.8275100000000002	0.9692990000000000	1.9196320000000000
O	−3.5576150000000002	2.5652089999999999	1.7800380000000000
O	−5.4595490000000000	0.2483070000000000	0.0705090000000000
Ce	−2.2390840000000001	−1.4370000000000001	2.2729490000000001
O	−2.6493120000000001	−2.2771110000000001	0.0516480000000000
O	−4.0805720000000001	−0.6033470000000000	3.0810379999999999
Ce	−3.7422010000000001	−0.4199450000000000	−1.1287700000000001
Zr	−1.2050479999999999	−2.8959269999999999	−1.2096819999999999
O	−2.9848270000000001	0.1941170000000000	0.8880780000000000
O	−1.6843010000000000	−0.9844490000000000	−2.1883819999999998
O	−0.0821610000000000	−2.2693219999999998	2.1354489999999999
O	−1.6745559999999999	−0.0271110000000000	−4.6561079999999997
Ce	−0.8862710000000000	1.1338539999999999	−2.8779040000000000
O	0.6436480000000000	−2.0398459999999998	−0.9319940000000000
O	0.1600610000000000	2.7345100000000002	−3.7893740000000000
Ce	−1.6380330000000001	1.9925619999999999	0.7651010000000000
O	−0.3652230000000000	3.6367799999999999	1.0423420000000001
O	−2.5995490000000001	1.4857959999999999	−1.4369630000000000
Ce	1.3259970000000001	−0.2837350000000000	2.8146840000000002
O	−0.7693190000000000	0.3850950000000000	2.3375080000000001
O	2.2965570000000000	−1.4977630000000000	1.1616320000000000
Ce	4.0100769999999999	1.9103520000000001	2.1051890000000002
O	2.0594830000000002	1.2467079999999999	1.2332190000000001
O	3.1641599999999999	0.7122130000000000	3.5528309999999999
Ce	4.9980110000000000	1.2124220000000001	−1.5907279999999999
Ce	1.8864820000000000	−0.1341070000000000	−0.8079769999999999
Ce	2.2059810000000000	2.6351230000000001	−3.2205640000000000
Ce	1.5469349999999999	3.3685079999999998	0.1350390000000000
O	5.3891669999999996	1.5169280000000001	0.4678760000000000
O	3.9104239999999999	−0.5457680000000000	−1.4219580000000001
O	4.3902510000000001	2.1460740000000000	−3.3496229999999998
O	2.9612129999999999	1.9287939999999999	−1.1545080000000001
O	1.3132930000000000	0.5490410000000000	−2.8666540000000000
O	1.7967340000000001	4.1696859999999996	−1.8166230000000001
O	0.0950650000000000	1.5447470000000001	−0.6794000000000000
O	3.1910729999999998	3.7118440000000001	1.5535980000000000