

Oxygen Vacancies in Self-Assemblies of Ceria Nanoparticles

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Supporting Information

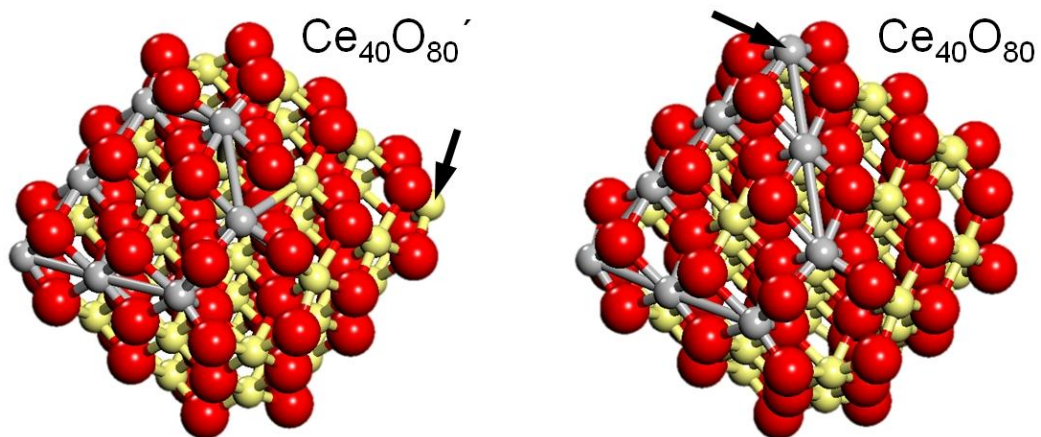


Fig. S1. Sketches of the stoichiometric ceria nanoparticles $\text{Ce}_{40}\text{O}_{80}'$ and $\text{Ce}_{40}\text{O}_{80}$. Corner Ce atoms that make these nanoparticles different are marked by arrows. O^{2-} anions – red spheres, Ce^{4+} cations – light beige spheres, those on edges of one $\{111\}$ facet – grey spheres.

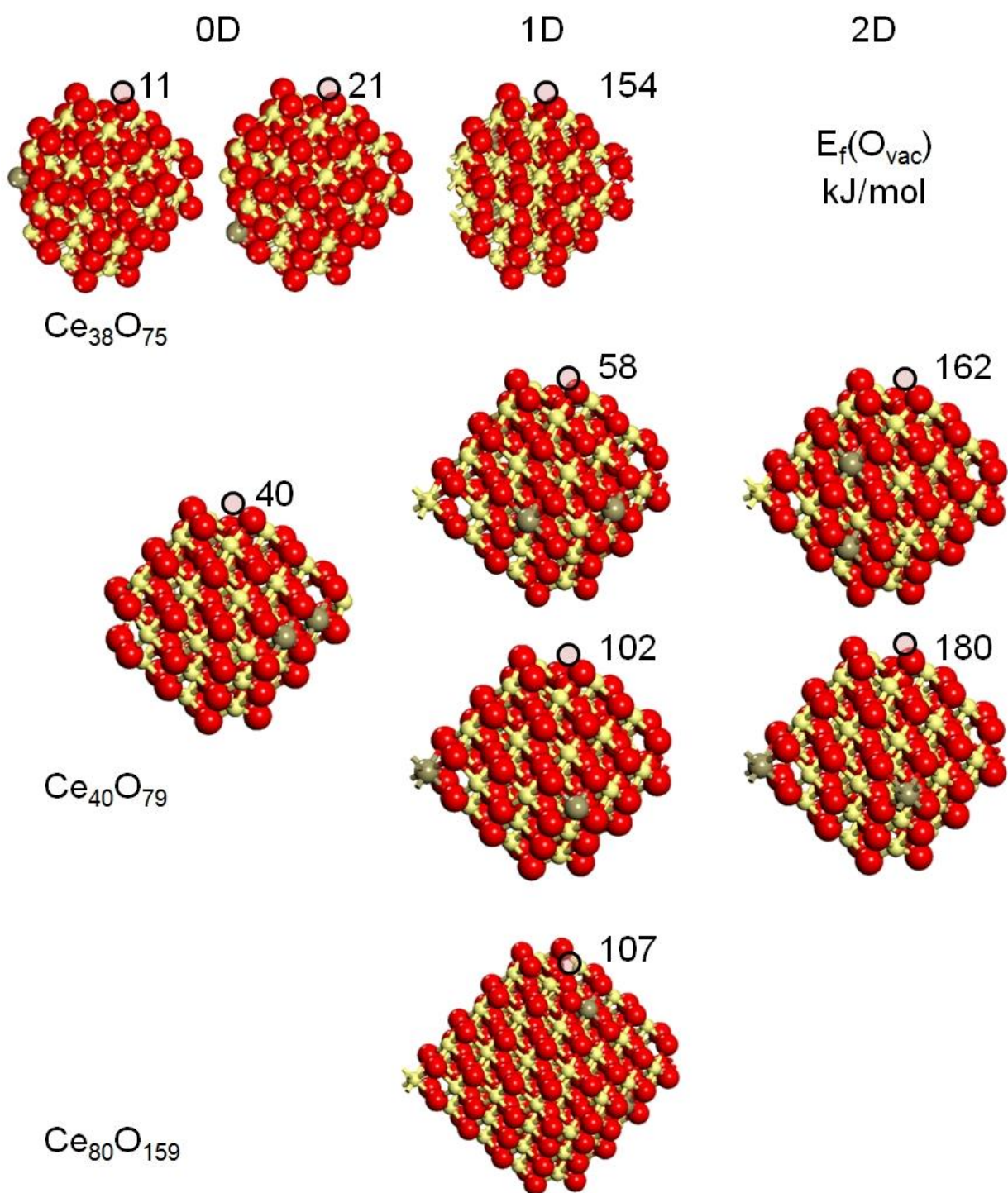


Fig. S2. Oxygen defective NPs for the 0D, 1D and 2D structures displayed in Fig. 1 containing one per NP most easily formed O_{2c} vacancy at the top O_4 sites with the corresponding oxygen vacancy formation energies $E_f(\text{O}_{\text{vac}})$ [kJ/mol] calculated vs. $\frac{1}{2} \text{O}_2$ triplet state energy. The depicted Ce^{3+} configurations result in $E_f(\text{O}_{\text{vac}})$ [kJ/mol] values, which are larger than the lowest energy values reported in Fig. 3. Ce^{4+} cations – light beige spheres, Ce^{3+} cations – dark beige spheres, O^{2-} anions – red spheres, position of O_{vac} – black circles. As a result of the adopted orientation, only one Ce^{3+} cation is visible for 1D $\text{Ce}_{80}\text{O}_{159}$.

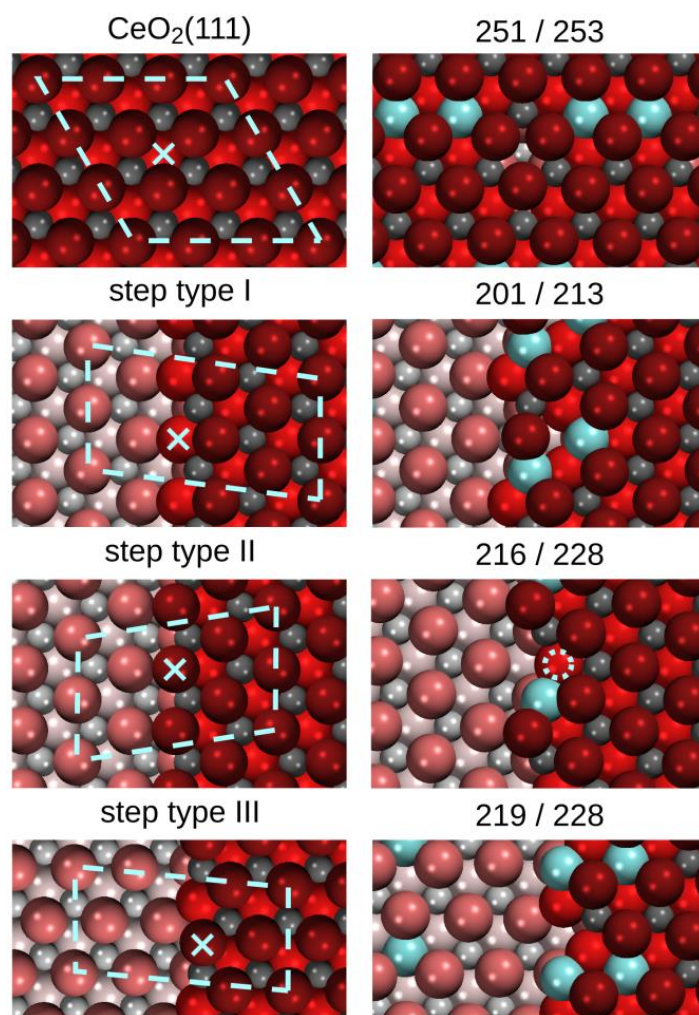


Fig. S3. Top view of the regular and three types of vicinal stepped $\text{CeO}_2(111)$ surfaces without O vacancy (left panels) and with the computed most easily formed O vacancy (right panels). The corresponding lowest oxygen vacancy formation energies $E_f(\text{O}_{\text{vac}})$ [kJ/mol] calculated vs. $\frac{1}{2} \text{O}_2$ triplet state energy obtained with PW91+4 / HSE06 are given. Ce^{4+} cations – grey spheres, surface Ce^{3+} cations – cyan spheres, subsurface Ce^{3+} cations – dotted cyan circles, O^{2-} anions – red spheres, position of O_{vac} – cyan cross. The darkest colors indicate atoms located in the uppermost surface layer. The dashed parallelogram indicates the $a \cdot b$ unit cell.

Cartesian coordinates (Å) of atoms in the PW91+4 optimized Ce_nO_{2n} nanoparticles (n=38, 40, 80, 140)

$Ce_{38}O_{76}$

Ce	14.142180	12.513730	3.826150
Ce	11.906700	12.517990	12.171840
Ce	14.376080	9.622120	12.388240
Ce	9.056830	9.802890	12.227790
Ce	14.403540	15.392500	12.394850
Ce	11.607720	7.107750	6.863330
Ce	14.721240	12.508580	9.501480
Ce	11.920860	15.189920	9.505700
Ce	11.604520	7.098500	12.130010
Ce	11.894890	9.852510	9.501260
Ce	9.055520	9.810120	6.769140
Ce	9.140420	12.530300	14.809530
Ce	16.847560	15.598160	9.508850
Ce	6.498950	12.544090	12.077870
Ce	11.622360	9.893230	4.079430
Ce	9.302970	12.533920	9.502950
Ce	6.513030	15.123490	9.504390
Ce	6.500870	12.551360	6.923900
Ce	11.617800	9.884890	14.922280
Ce	16.837390	12.500410	6.403420
Ce	14.379110	9.625110	6.614810
Ce	11.662070	17.945440	6.873900
Ce	11.657530	17.940930	12.142700
Ce	9.167220	17.839340	9.506110
Ce	9.081800	15.261980	12.235560
Ce	11.642090	15.153760	14.926510
Ce	9.145530	12.540420	4.194310
Ce	11.650310	15.162510	4.085300
Ce	14.407960	15.396140	6.621400
Ce	9.085240	15.266370	6.774720
Ce	9.113580	7.229860	9.494590
Ce	11.907440	12.523320	6.834720
Ce	16.829710	12.493880	12.605960
Ce	6.483730	9.971760	9.499310
Ce	14.136280	12.509630	15.182960
Ce	14.166590	18.189410	9.512200
Ce	14.112470	6.835520	9.498450
Ce	16.818270	9.397090	9.504720
O	13.198290	5.884170	7.906800
O	10.077310	6.061150	11.136010
O	13.233270	14.102610	16.141340

O	16.341470	13.912590	10.920240
O	16.326140	11.080730	10.920700
O	16.339000	13.917130	8.088290
O	13.153770	13.890570	5.459290
O	10.677440	13.871790	10.850700
O	7.978800	13.856560	10.821050
O	13.218270	16.627410	5.399520
O	10.098550	10.883680	15.969880
O	7.981040	13.859500	8.184600
O	13.160960	16.561340	10.881130
O	10.663250	11.179070	10.848560
O	13.224440	10.930100	2.865710
O	13.534420	13.876840	10.869490
O	7.795460	16.594250	10.900050
O	13.260630	19.150180	11.102830
O	10.493620	8.577610	8.183750
O	13.518990	11.149600	10.865870
O	7.771220	11.151640	5.443280
O	15.891230	13.920980	5.285010
O	10.508800	11.217550	5.546930
O	5.418910	14.146200	7.907980
O	13.122090	8.471800	8.125620
O	10.114830	14.165270	15.972880
O	13.175030	8.402200	13.608340
O	13.523660	11.150520	8.137220
O	13.164330	16.563210	8.135600
O	10.079810	6.065040	7.856330
O	10.123660	14.179010	3.036300
O	15.856400	8.278710	10.915630
O	10.523360	13.846420	5.551030
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O	15.856850	8.282430	8.089230
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O	5.415820	14.141820	11.091560
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O	10.358660	8.440660	13.583170
O	10.533800	16.481730	8.191920
O	13.196330	5.880480	11.087240
O	13.176040	8.408930	5.389620
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O	10.361700	8.448810	5.411410
O	13.136690	11.145160	5.454840
O	13.216570	10.921560	16.136850
O	7.964040	11.220740	10.818450
O	10.531940	16.478860	10.821680
O	13.146400	13.884760	13.552500

O	13.121240	8.469160	10.871880
O	7.754690	8.488290	8.102030
O	5.398800	10.961930	11.090300
O	7.787310	13.941280	5.447070
O	13.262340	19.152130	7.921390
O	5.401490	10.964010	7.906900
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O	10.505910	11.209500	13.454920
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O	13.212520	16.620560	13.617850
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O	13.241410	14.111080	2.871020
O	10.492510	8.574890	10.813070
O	15.897430	16.721080	10.923450
O	13.133780	11.139400	13.549260
O	10.106390	10.897790	3.031290

Ce₄₀O₈₀

Ce	13.519630	9.491950	4.044180
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Ce	8.309480	6.734180	12.275380
Ce	13.666430	12.259660	12.282400
Ce	10.961220	4.101950	6.876860
Ce	13.607280	9.485130	9.506040
Ce	11.001300	12.158570	9.504990
Ce	10.960000	4.097100	12.116340
Ce	10.975190	6.838250	9.500460
Ce	8.312430	6.739880	6.721460
Ce	8.462010	9.508070	14.967710
Ce	16.159580	12.230170	9.509560
Ce	5.830530	9.521970	12.258700
Ce	10.982790	6.885560	4.103290
Ce	8.367680	9.511880	9.501550
Ce	5.842480	12.281410	9.501430
Ce	5.833110	9.524900	6.742920
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Ce	16.148820	9.475710	6.753660
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Ce	5.817400	6.768440	9.498260
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O	12.333960	13.481880	10.840070
O	9.611490	8.146820	10.858550
O	12.565440	7.898610	2.988560
O	12.362140	10.848150	10.862260
O	6.913650	13.584830	10.888680
O	12.598230	16.005920	11.109720
O	9.643020	5.517150	8.164780
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O	12.579930	11.100510	2.994050
O	9.641510	5.514480	10.831200
O	15.103430	13.544350	10.896220
O	12.302920	8.155130	13.494030
O	9.411080	7.912550	2.984770

Ce₄₀O₈₀

Ce	15.092520	12.486140	7.080280
Ce	12.445610	9.915520	12.437830
Ce	9.793190	9.770790	9.660550
Ce	9.935490	12.499730	17.942440
Ce	17.950130	15.026550	12.444160
Ce	7.266830	12.525940	15.204340
Ce	12.508480	9.923170	7.078540
Ce	9.817210	12.550430	12.441260
Ce	7.222070	15.237060	12.445030
Ce	7.268500	12.532690	9.676750
Ce	12.504230	9.908840	17.798140
Ce	12.456680	12.548560	15.104960
Ce	17.837090	12.474800	9.839270
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Ce	12.522620	17.747720	9.684500
Ce	12.516710	17.742950	15.214300
Ce	9.812930	17.811780	12.451150
Ce	9.774600	15.253280	15.265820
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Ce	9.937620	12.509970	6.944910
Ce	12.521800	15.077000	6.946740
Ce	15.193630	9.790330	15.175620
Ce	15.266420	15.202070	9.668260
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Ce	15.262560	15.194290	15.226460
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O	11.111780	11.226610	16.434080
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O	13.789820	13.963100	11.085730
O	8.384210	16.662630	11.096250
O	16.508080	11.154020	8.363670

O	16.510360	13.941790	16.512260
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O	16.532930	16.657410	11.053510
O	11.040990	11.235170	11.079850
O	16.506130	11.148750	16.517800
O	18.981730	14.089580	10.854070
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O	13.845800	16.675590	16.521960
O	8.320950	8.505510	13.829330
O	14.064000	14.131460	5.916820
O	11.105320	8.580700	13.771960
O	16.529320	16.656800	13.840650
O	13.767750	11.222780	16.401180
O	10.872830	10.965030	5.912370
O	14.042720	6.084260	10.826840
O	10.874500	6.033570	14.018890
O	14.059460	14.118310	18.973560
O	16.435530	13.871860	13.780380
O	16.389960	11.216750	13.767840
O	16.436740	13.873660	11.110260
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O	11.060990	13.959560	13.803280
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O	13.851880	16.690720	8.373450
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O	14.071390	10.933300	5.969650
O	13.788380	13.958270	13.805240
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O	18.910310	10.914690	14.051460
O	11.107470	8.583790	11.101850
O	13.762790	11.233500	13.793580
O	8.317080	11.194340	8.364090
O	13.858190	19.273940	13.839230
O	16.513790	13.949030	8.378400
O	11.115540	11.237710	8.446990
O	5.765700	13.959770	11.085000
O	13.760970	8.608280	11.110190
O	10.898420	14.112520	19.009050
O	13.827700	8.484530	16.512880
O	13.763040	11.237620	11.089020
O	13.822840	16.590220	11.095180
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O	10.905650	14.123380	5.879950

O	16.490880	8.484910	13.830820
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O	11.061850	13.965890	11.085300
O	16.491920	8.486440	11.045090
O	11.068290	16.674630	8.400610
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O	11.064960	16.665260	16.497230
O	11.030450	8.503910	16.503080
O	11.119680	16.606370	11.095420
O	14.041340	6.080720	14.039380
O	13.828910	8.494930	8.360960
O	18.982670	14.083890	14.028630
O	11.034580	8.514010	8.368630
O	13.770950	11.234830	8.479320
O	14.065160	10.917660	18.908420
O	8.412190	11.217950	13.792210
O	11.115620	16.600170	13.803780
O	13.787780	13.878310	16.439450
O	13.759870	8.605390	13.762730
O	8.323780	8.509110	11.041750
O	5.726590	11.200510	13.822480
O	8.354440	13.977980	8.396710
O	18.911070	10.920850	10.835380
O	5.728910	11.204020	11.048770

Ce₈₀O₁₆₀

Ce	17.614970	12.500050	20.548450
Ce	15.041810	15.094610	20.578650
Ce	15.041880	9.905390	20.578680
Ce	17.614970	12.500050	4.451550
Ce	12.478180	12.500010	20.647550
Ce	15.041880	9.905390	4.421320
Ce	15.041810	15.094610	4.421350
Ce	12.478180	12.500010	4.352450
Ce	15.010410	12.499930	17.820550
Ce	15.010410	12.499930	7.179450
Ce	20.329340	12.500010	17.811470
Ce	15.024960	17.830390	17.830410
Ce	15.025090	7.169600	17.830370
Ce	20.329340	12.500010	7.188530
Ce	9.781870	12.499980	17.946180
Ce	15.025090	7.169600	7.169630
Ce	15.024960	17.830390	7.169590
Ce	9.781870	12.499980	7.053820
Ce	17.749690	15.239930	17.939840
Ce	12.312160	9.748870	17.975490
Ce	17.749690	15.239930	7.060160
Ce	12.312160	9.748870	7.024510
Ce	17.749720	9.760110	17.939830
Ce	12.312120	15.251050	17.975450
Ce	17.749720	9.760110	7.060170
Ce	12.312120	15.251050	7.024550
Ce	20.440310	15.236580	15.236640
Ce	17.749750	17.939860	15.239910
Ce	12.312070	7.024660	15.251220
Ce	20.440310	15.236580	9.763360
Ce	9.641510	9.719960	15.280040
Ce	12.312070	7.024660	9.748780
Ce	17.749750	17.939860	9.760090
Ce	9.641510	9.719960	9.719960
Ce	20.440310	9.763440	15.236590
Ce	12.312190	17.975470	15.251120
Ce	17.749750	7.060190	15.239880
Ce	20.440310	9.763440	9.763410
Ce	9.641590	15.280090	15.280080
Ce	17.749750	7.060190	9.760120
Ce	12.312190	17.975470	9.748880
Ce	9.641590	15.280090	9.719920
Ce	17.689980	12.499990	15.194520
Ce	15.008350	15.194440	15.194440
Ce	15.008320	9.805560	15.194460
Ce	17.689980	12.499990	9.805480

Ce	12.325140	12.499980	15.204890
Ce	15.008320	9.805560	9.805540
Ce	15.008350	15.194440	9.805560
Ce	12.325140	12.499980	9.795110
Ce	23.053210	12.500070	15.083280
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Ce	15.041840	4.421380	15.094620
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Ce	15.041840	4.421380	9.905380
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Ce	20.329350	7.188500	12.500000
Ce	9.782050	17.946250	12.500000
Ce	4.750870	12.499930	12.500000
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Ce	12.325160	9.795090	12.500000
Ce	17.690120	9.805430	12.500000
Ce	12.325150	15.204830	12.500000
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O	16.379870	16.610900	5.765910
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O	13.599190	16.592490	19.230820
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O	19.091860	11.110680	5.770610
O	10.892240	13.883400	19.257000
O	16.379960	8.389090	5.765940
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O	16.333620	13.832390	19.134550
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O	16.333680	11.167590	19.134560
O	13.675400	13.832980	19.160220
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O	19.040050	13.852810	16.549090
O	16.345310	16.551420	16.551420
O	13.642160	8.443170	16.556870
O	19.040050	13.852810	8.450910
O	10.933170	11.145630	16.575720
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O	16.345310	16.551420	8.448580
O	10.933170	11.145630	8.424280
O	19.092630	8.390510	16.609530
O	10.866270	16.597550	16.597560
O	19.092630	8.390510	8.390470
O	10.866270	16.597550	8.402440
O	16.365800	13.882090	16.520640
O	13.602690	11.119090	16.530670
O	16.365800	13.882090	8.479360
O	13.602690	11.119090	8.469330
O	21.720170	13.889590	16.599080
O	16.379900	19.234110	16.610880
O	13.599230	5.769230	16.592530
O	21.720170	13.889590	8.400920
O	8.210200	11.119930	16.581390
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O	16.379900	19.234110	8.389120
O	8.210200	11.119930	8.418610
O	19.092550	16.609530	16.609520
O	10.866290	8.402410	16.597580
O	19.092550	16.609530	8.390480
O	10.866290	8.402410	8.402420
O	19.040040	11.147220	16.549090
O	13.642110	16.556830	16.556850

O	16.345350	8.448680	16.551340
O	19.040040	11.147220	8.450910
O	10.933160	13.854300	16.575730
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O	13.642110	16.556830	8.443150
O	10.933160	13.854300	8.424270
O	16.365800	11.117920	16.520640
O	13.602730	13.880840	16.530680
O	16.365800	11.117920	8.479360
O	13.602730	13.880840	8.469320
O	21.720150	11.110470	16.599090
O	13.599220	19.230800	16.592500
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O	13.599220	19.230800	8.407500
O	8.210150	13.880050	8.418640
O	19.002040	13.880800	13.880800
O	16.365820	16.520620	13.882100
O	13.602690	8.469340	13.880900
O	19.002040	13.880800	11.119200
O	10.936940	11.117760	13.882240
O	13.602690	8.469340	11.119100
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O	19.040090	8.450930	13.852810
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O	19.040090	8.450930	11.147190
O	10.933240	16.575650	11.145650
O	24.145690	14.092690	14.092620
O	16.612560	21.647540	14.101220
O	13.438330	3.309850	14.094150
O	24.145690	14.092690	10.907380
O	5.640720	11.126410	13.873310
O	13.438330	3.309850	10.905850
O	16.612560	21.647540	10.898780
O	5.640720	11.126410	11.126690
O	19.040080	16.549110	13.852820
O	10.933160	8.424300	13.854360
O	19.040080	16.549110	11.147180
O	10.933160	8.424300	11.145640
O	19.002040	11.119150	13.880770
O	13.602740	16.530630	13.880850
O	16.365820	8.479360	13.882090
O	19.002040	11.119150	11.119230
O	10.936940	13.882210	13.882240
O	16.365820	8.479360	11.117910

O	13.602740	16.530630	11.119150
O	10.936940	13.882210	11.117760
O	24.145680	10.907410	14.092620
O	13.438310	21.690090	14.094110
O	16.612430	3.352450	14.101180
O	24.145680	10.907410	10.907380
O	5.640760	13.873170	13.873520
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O	13.438310	21.690090	10.905890
O	5.640760	13.873170	11.126480
O	16.320160	13.840650	13.840670
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O	16.320160	13.840650	11.159330
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O	21.619930	13.830160	13.830120
O	16.333670	19.134530	13.832390
O	13.675440	5.839790	13.833020
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O	8.310800	11.146990	13.853030
O	13.675440	5.839790	11.166980
O	16.333670	19.134530	11.167610
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O	21.720180	8.400930	13.889570
O	10.892240	19.256950	13.883440
O	19.091890	5.770660	13.889340
O	21.720180	8.400930	11.110430
O	8.210280	16.581400	13.880120
O	19.091890	5.770660	11.110660
O	10.892240	19.256950	11.116560
O	8.210280	16.581400	11.119880
O	16.320130	11.159310	13.840680
O	13.630200	13.842860	13.842890
O	16.320130	11.159310	11.159320
O	13.630200	13.842860	11.157110
O	21.720180	16.599110	13.889560
O	19.091850	19.229380	13.889330
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O	10.892280	5.743050	11.116570
O	19.091850	19.229380	11.110670
O	8.210200	8.418630	11.119920
O	21.619930	11.169910	13.830120
O	13.675440	19.160200	13.833010
O	16.333690	5.865470	13.832410
O	21.619930	11.169910	11.169880
O	8.310860	13.853050	13.853020
O	16.333690	5.865470	11.167590

O	13.675440	19.160200	11.166990
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Ce₁₄₀O₂₈₀

Ce	4.840740	20.033640	17.093930
Ce	3.023450	18.202750	14.510500
Ce	6.671630	21.850920	14.510500
Ce	4.840740	20.033640	11.927070
Ce	6.758770	18.115610	19.825020
Ce	4.754690	16.246490	17.252470
Ce	8.627890	20.119680	17.252470
Ce	3.007910	14.356810	14.510500
Ce	6.805430	18.068950	14.510500
Ce	10.517570	21.866470	14.510500
Ce	4.754690	16.246490	11.768530
Ce	8.627890	20.119680	11.768530
Ce	6.758770	18.115610	9.195980
Ce	8.681700	16.192680	22.544170
Ce	6.641630	14.341640	19.961610
Ce	10.532740	18.232740	19.961610
Ce	4.737060	12.437190	17.267240
Ce	8.639970	16.234410	17.218650
Ce	12.437190	20.137320	17.267240
Ce	3.007910	10.517570	14.510500
Ce	6.728760	14.323620	14.510500
Ce	10.550760	18.145620	14.510500
Ce	14.356810	21.866470	14.510500
Ce	4.737060	12.437190	11.753760
Ce	8.639970	16.234410	11.802350
Ce	12.437190	20.137320	11.753760
Ce	6.641630	14.341640	9.059390
Ce	10.532740	18.232740	9.059390
Ce	8.681700	16.192680	6.476830
Ce	3.023450	6.671630	14.510500
Ce	4.754690	8.627890	17.252470
Ce	4.754690	8.627890	11.768530
Ce	6.641630	10.532740	19.961610
Ce	6.728760	10.550760	14.510500
Ce	6.641630	10.532740	9.059390
Ce	8.567530	12.437190	22.640120
Ce	8.596060	12.437190	17.223140
Ce	8.596060	12.437190	11.797860
Ce	8.567530	12.437190	6.380880
Ce	10.612030	14.262350	25.252830
Ce	10.524820	14.349560	19.876080
Ce	10.541920	14.332460	14.510500
Ce	10.524820	14.349560	9.144920
Ce	10.612030	14.262350	3.768170
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Ce	12.437190	16.278310	17.223140

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Ce	14.341640	18.232740	19.961610
Ce	14.323620	18.145620	14.510500
Ce	14.341640	18.232740	9.059390
Ce	16.246490	20.119680	17.252470
Ce	16.246490	20.119680	11.768530
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Ce	4.840740	4.840740	11.927070
Ce	6.805430	6.805430	14.510500
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Ce	8.639970	8.639970	17.218650
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Ce	10.524820	10.524820	19.876080
Ce	10.524820	10.524820	9.144920
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Ce	10.612030	10.612030	3.768170
Ce	12.437190	12.437190	17.181110
Ce	12.437190	12.437190	11.839890
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Ce	14.332460	14.332460	14.510500
Ce	14.349560	14.349560	19.876080
Ce	14.349560	14.349560	9.144920
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Ce	14.262350	14.262350	3.768170
Ce	16.234410	16.234410	17.218650
Ce	16.234410	16.234410	11.802350
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Ce	16.278310	12.437190	11.797860
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Ce	20.119680	16.246490	11.768530
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Ce	16.234410	8.639970	17.218650
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Ce	20.137320	12.437190	17.267240
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Ce	16.234410	8.639970	11.802350
Ce	16.192680	8.681700	22.544170
O	16.192680	8.681700	6.476830
O	18.232740	10.532740	9.059390
O	20.137320	12.437190	11.753760
O	21.866470	14.356810	14.510500
O	14.341640	6.641630	9.059390
O	12.437190	4.737060	11.753760
O	10.517570	3.007910	14.510500
O	20.119680	8.627890	17.252470
O	16.246490	4.754690	17.252470
O	18.068950	6.805430	14.510500
O	18.115610	6.758770	19.825020
O	21.866470	10.517570	14.510500
O	20.119680	8.627890	11.768530
O	18.115610	6.758770	9.195980
O	14.356810	3.007910	14.510500
O	16.246490	4.754690	11.768530
O	20.033640	4.840740	17.093930
O	21.850920	6.671630	14.510500
O	18.202750	3.023450	14.510500
O	20.033640	4.840740	11.927070
O	5.206640	21.915460	16.099300
O	2.958920	19.667740	16.099300

O	5.206640	21.915460	12.921700
O	2.958920	19.667740	12.921700
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O	6.770360	20.066560	18.621560
O	4.924010	18.068350	15.843350
O	4.807820	18.104020	18.621560
O	8.695600	21.992460	15.895800
O	6.806030	19.950370	13.177650
O	4.924010	18.068350	13.177650
O	6.770360	20.066560	10.399440
O	8.695600	21.992460	13.125200
O	2.881910	16.178780	13.125200
O	4.807820	18.104020	10.399440
O	8.693870	18.141820	15.897480
O	8.631730	18.156230	18.579900
O	6.732550	16.180510	15.897480
O	6.718150	16.242650	18.579900
O	10.551920	20.073020	15.865050
O	10.528440	20.160090	18.623700
O	4.801360	14.322460	15.865050
O	4.714290	14.345940	18.623700
O	8.693870	18.141820	13.123520
O	8.623280	18.204880	21.289530
O	6.732550	16.180510	13.123520
O	6.669500	16.251100	21.289530
O	8.631730	18.156230	10.441100
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O	12.437190	22.021700	15.892280
O	2.852680	12.437190	15.892280
O	8.623280	18.204880	7.731470
O	6.669500	16.251100	7.731470
O	10.528440	20.160090	10.397300
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O	10.551710	16.237760	15.865580
O	10.536090	16.300700	18.586980
O	8.636620	14.322670	15.865580
O	8.573680	14.338290	18.586980
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O	6.673990	12.437190	15.899140
O	6.655690	12.437190	18.600930
O	10.551710	16.237760	13.155420
O	10.517940	16.269030	21.246430
O	8.636620	14.322670	13.155420

O	8.605350	14.356440	21.246430
O	10.536090	16.300700	10.434020
O	10.513050	16.322390	23.916480
O	12.437190	18.200390	13.121860
O	12.437190	18.250920	21.324570
O	6.623460	12.437190	21.324570
O	6.673990	12.437190	13.121860
O	8.573680	14.338290	10.434020
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O	14.322460	20.073020	15.865050
O	4.801360	10.551920	15.865050
O	14.345940	20.160090	18.623700
O	4.714290	10.528440	18.623700
O	16.178780	21.992460	15.895800
O	2.881910	8.695600	15.895800
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O	8.605350	14.356440	7.774570
O	12.437190	18.218680	10.420070
O	14.322460	20.073020	13.155950
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O	10.513050	16.322390	5.104520
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O	12.437190	18.250920	7.696430
O	6.623460	12.437190	7.696430
O	14.345940	20.160090	10.397300
O	4.714290	10.528440	10.397300
O	16.178780	21.992460	13.125200
O	2.881910	8.695600	13.125200
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O	12.437190	14.353590	18.526330
O	10.529210	12.437190	15.856820
O	10.520790	12.437190	18.526330
O	14.322670	16.237760	15.865580
O	14.338290	16.300700	18.586980
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O	8.573680	10.536090	18.586980
O	12.437190	14.345170	13.164180
O	12.437190	14.398210	21.190190
O	10.529210	12.437190	13.164180
O	10.476170	12.437190	21.190190
O	12.437190	14.353590	10.494670
O	12.437190	14.318150	23.807390
O	14.322670	16.237760	13.155420
O	14.356440	16.269030	21.246430
O	8.605350	10.517940	21.246430
O	8.636620	10.551710	13.155420
O	10.520790	12.437190	10.494670

O	10.556230	12.437190	23.807390
O	16.180510	18.141820	15.897480
O	6.732550	8.693870	15.897480
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O	6.718150	8.631730	18.579900
O	18.068350	19.950370	15.843350
O	18.104020	20.066560	18.621560
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O	12.437190	14.690410	26.327150
O	10.183970	12.437190	26.327150
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O	16.180510	18.141820	13.123520
O	14.361320	16.322390	23.916480
O	16.251100	18.204880	21.289530
O	8.573680	10.536090	10.434020
O	6.732550	8.693870	13.123520
O	8.551980	10.513050	23.916480
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O	12.437190	14.318150	5.213610
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O	2.958920	5.206640	16.099300
O	10.556230	12.437190	5.213610
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O	8.605350	10.517940	7.774570
O	16.242650	18.156230	10.441100
O	6.718150	8.631730	10.441100
O	18.068350	19.950370	13.177650
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O	21.915460	5.206640	12.921700
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O	19.950370	6.806030	15.843350
O	20.066560	6.770360	18.621560
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O	18.104020	4.807820	18.621560
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O	16.178780	2.881910	15.895800
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O	18.068350	4.924010	13.177650
O	20.066560	6.770360	10.399440
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O	22.021700	12.437190	15.892280
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O	18.204880	8.623280	7.731470
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O	16.237760	10.551710	15.865580
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O	18.200390	12.437190	15.899140
O	18.218680	12.437190	18.600930
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O	12.437190	6.655690	18.600930
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O	14.338290	8.573680	10.434020
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O	14.353590	12.437190	10.494670
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