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## Supplemental Information

# Spontaneous Non-stoichiometry and Ordering in Degenerate but Gapped Transparent Conductors

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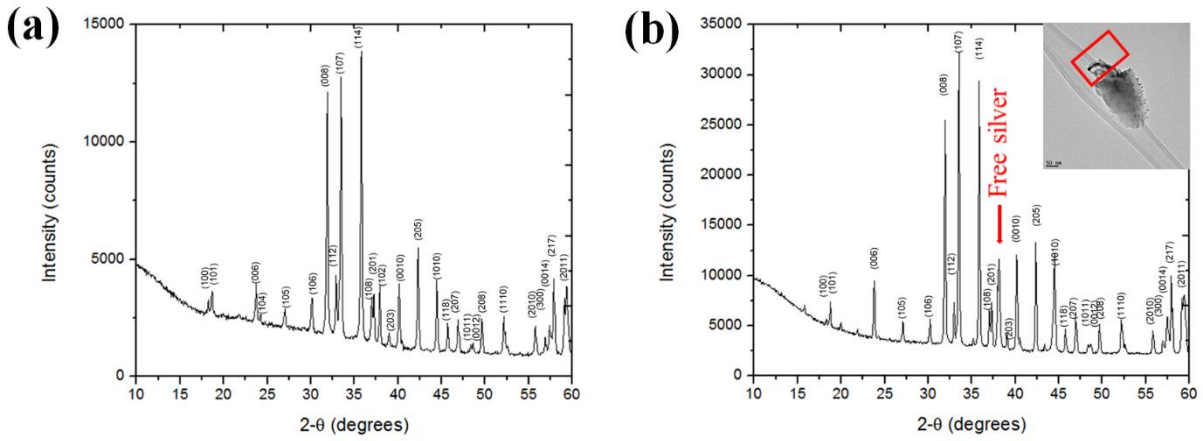
**Supplementary Note I: Experimental observation of Ag formation in $Ag_3Al_{22}O_{34+x}$ under reduced atmosphere**

$Ag_3Al_{22}O_{34}$ was predicted to be a transparent conducting oxide with a periodic 2-dimensional electron gas.[1] This composition is unusual for β-aluminas in two ways, notably the high monovalent cation loading and the partial reduced silver species, and thus an alternative synthetic route was needed. The typical sodium (or any other cation) loading in unstabilized sodium β-aluminas has been traditionally limited to about $Na_{2-2.5}Al_{22}O_{34+\delta}$.[2] This cap is a culmination of two factors: (1) the high ionic mobility of sodium and (2) the high volatility of $Na_2O$ at synthesis temperatures. To get around this, we sintered $Ba_{1.5}Al_{22}O_{34.5}$ at high temperatures as the precursor, as the divalent barium is far less mobile at high temperatures than sodium. The divalent barium is then ion exchanged at the relatively low temperature of 980°C in molten sodium chloride, preventing the volatilization of $Na_2O$ seen at sintering temperatures. From there, the highly non-stoichiometric sodium β-alumina can be ion exchanged to yield the desired the highly non-stoichiometric silver β-alumina $Ag_3Al_{22}O_{34.5}$

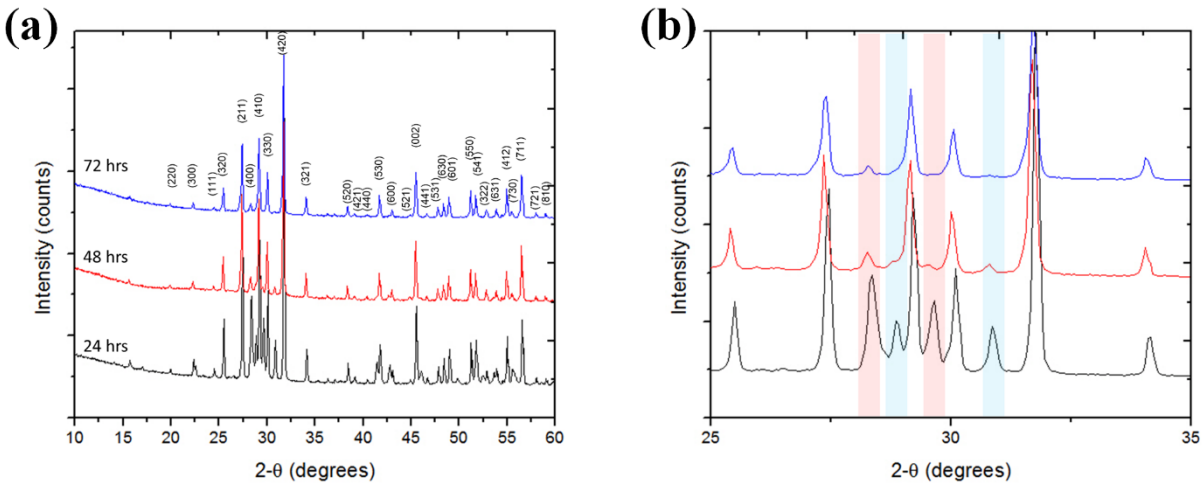
Powder X-ray diffraction confirms the synthesis of $Ag_3Al_{22}O_{34.5}$, and the peaks can be indexed to the JCPDS reference pattern #01-084-0514 (Supplementary Fig. 1a), corresponding with the phase "$Ag_3Al_{22}O_{34}$" identified by Tofield *et.al*.[3] $Ag_3Al_{22}O_{34.5}$, $Ag_3Al_{22}O_{34}$, and $Ag_{2.5}Al_{22}O_{34.25}$ all crystallize in the same space group of $P6_3/mmc$; the primary difference between all three being occupancy. The lack of conductivity is attributed to the presence of 0.5 moles interstitial oxygen, which has been found in other non-stoichiometric β-aluminas.[4, 5] Heating the compound to 700 °C so that the compound may auto-reduce and liberate both oxygen and free carriers instead resulted in the formation of free metallic silver (Supplementary Fig. 1b) and the decomposition from $Ag_3Al_{22}O_{34.5}$ to $Ag_{2.5}Al_{22}O_{34.25}$. While the presence of free silver is clear from the powder X-ray diffraction (and the fact that the formerly white compound turns a red hue from the formation of silver particles), the formation $Ag_{2.5}Al_{22}O_{34.25}$ is subtle but can be identified by two key markers: the increase in intensity of the (101) peak, and the presence of the (104) peak. Silver β-alumina have been used as fast ion conductors at elevated temperatures at varying oxygen partial pressures.[2, 6] Furthermore, any attempts to mildly reduce the compounds and raise the carrier concentration results immediately in the compensation and cation vacancy formation/silver precipitation.




**Supplementary Figure 1.** Ag formation in $Ag_3Al_{22}O_{34+x}$ under reduced atmosphere. (a) The powder X-ray diffraction of $Ag_3Al_{22}O_{34.5}$ can be indexed to the JCPDS reference pattern #01-084-0514, corresponding with the phase "$Ag_3Al_{22}O_{34}$" identified by Tofield *et al.*[3] (b) Any attempts to reduce $Ag_3Al_{22}O_{34.5}$ and introduce carriers results in the precipitation of free metallic silver and the possible formation of $Ag_{2.5}Al_{22}O_{34.25}$.

## Supplementary Note II: Synthesis of $Ba_3Nb_5O_{15}$

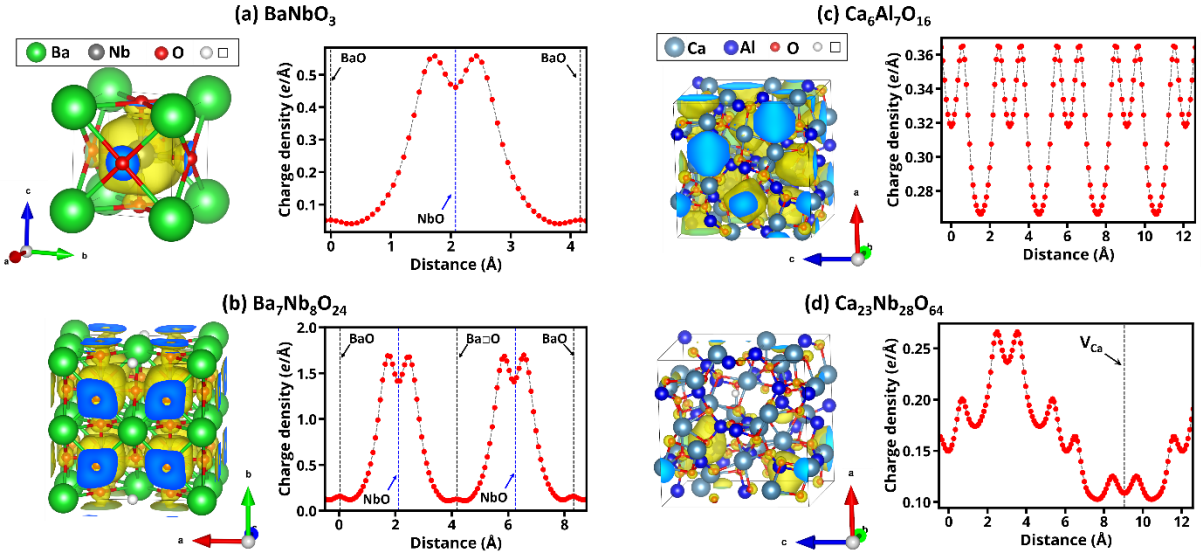
Our procedure was developed taking into consideration of all other synthetic routes, which showed that for polycrystalline compacts, long (> 40 hrs) sintering durations, multiple intermittent regrinding, and low partial oxygen pressure atmospheres were needed to prepare phase pure towards $Ba_3Nb_5O_{15}$/$Ba_6Nb_{10}O_{30}$. In our work, we have found that the targeted $Ba_3Nb_5O_{15}$ can be prepared after 72 hours of heating with intermittent grinding (Supplementary Fig. 2a). The oxygen partial pressure was kept low with a 5% $H_2$/balance argon atmosphere. The progress was monitored with pXRD at 24 hour intervals, and we can confirm the presence of two secondary phases (OVCs identified in our theoretical calculations, see Fig. 2a and 6a in the main text): $Ba_5Nb_4O_{15}$ and $BaNb_2O_6$. Given the tiny range of chemical potentials under which $Ba_3Nb_5O_{15}$ is stable, it is not surprising to find these more stable secondary phases on the way to $Ba_3Nb_5O_{15}$. These secondary phases react and disappear with further heating, and completely disappear by 72 hours of heating (Supplementary Fig. 2b).




**Supplementary Figure 2.** Synthesis of $Ba_3Nb_5O_{15}$. (a) Monitoring the progress on the formation of $Ba_3Nb_5O_{15}$ monitored through powder X-ray diffraction of $Ba_3Nb_5O_{15}$. (b) The peak intensities for phases $Ba_5Nb_4O_{15}$ (light blue) and $BaNb_2O_6$ (light red) decrease with increasing heating duration, resulting in phase pure $Ba_3Nb_5O_{15}$ after 72 hours of heating.

**Supplementary Note III: The delocalized nature of the conducting electrons in degenerate insulators**

For Ba-Nb-O degenerate insulators, the conducting electrons are localized near Nb atoms. Specifically, for the 1:1:3 cubic perovskite compound, the charge density in the NbO plane is about 9 times larger than that in the BaO plane. The vacancy formation does not significantly change the nature of the charge distribution (Supplementary Figs. 3a, b). For Ca-Al-O degenerate insulators, the conduction band electrons reside within the cavity of well-defined cage-like blocks (Supplementary Figs. 3c, d). Because of this, the formation of Ca vacancy destroys the surrounding cage-like blocks and reduces the carrier concentration within the vacancy region. Despite this, both 6:7:24 and its 23:28:64 OVC have clearly defined 0-dimensional charge carrier density localization which implies that the compounds are not only degenerate insulators but also stable inorganic electrides.




**Supplementary Figure 3.** Delocalization nature of conducting electrons in degenerate insulators. Real space partial electron density of conducting electrons in (a) $BaNbO_3$, (b) $Ba_7Nb_8O_{28}$, (c) $Ca_6Al_7O_{16}$, and (d) $Ca_{23}Al_{28}O_{64}$ and its projection on the direction *a*. The isosurfaces are set at 0.001 *e*/bohr$^3$ and 0.0005 *e*/bohr$^3$ for Ba-Nb-O and Ca-Al-O systems, respectively.

**Supplementary Data I: Ground state compounds in Ba-Nb-O system**

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Nb

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| O | O28 | 1 | 0.006125 | 0.108100 | 0.638169 | 1 |
| O | O29 | 1 | 0.256071 | 0.862216 | 0.111769 | 1 |
| O | O30 | 1 | 0.255937 | 0.134902 | 0.892191 | 1 |
| O | O31 | 1 | 0.506085 | 0.388753 | 0.865734 | 1 |
| O | O32 | 1 | 0.505954 | 0.608185 | 0.138238 | 1 |
| O | O33 | 1 | 0.236968 | 0.362047 | 0.111990 | 1 |
| O | O34 | 1 | 0.236980 | 0.634862 | 0.892207 | 1 |
| O | O35 | 1 | 0.487004 | 0.388982 | 0.365957 | 1 |
| O | O36 | 1 | 0.486886 | 0.608057 | 0.638125 | 1 |
| O | O37 | 1 | 0.736760 | 0.862152 | 0.611815 | 1 |
| O | O38 | 1 | 0.736735 | 0.134877 | 0.392233 | 1 |
| O | O39 | 1 | 0.986987 | 0.888783 | 0.865719 | 1 |
| O | O40 | 1 | 0.986995 | 0.108172 | 0.138254 | 1 |
| O | O41 | 1 | 0.501930 | 0.099700 | 0.153588 | 1 |
| O | O42 | 1 | 0.501896 | 0.897331 | 0.850414 | 1 |
| O | O43 | 1 | 0.751882 | 0.346835 | 0.103318 | 1 |
| O | O44 | 1 | 0.751779 | 0.650199 | 0.900709 | 1 |
| O | O45 | 1 | 0.001783 | 0.599713 | 0.653569 | 1 |
| O | O46 | 1 | 0.001784 | 0.397365 | 0.350534 | 1 |
| O | O47 | 1 | 0.251897 | 0.846721 | 0.603355 | 1 |
| O | O48 | 1 | 0.251917 | 0.150367 | 0.400629 | 1 |

NbO

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_cell_angle_beta   90.02487418
_cell_angle_gamma   89.97714155
_symmetry_Int_Tables_number   1
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_cell_volume   78.57824324
_cell_formula_units_Z   3
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loop_
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 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
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  Nb  Nb2  1  0.505847  0.494398  0.000883  1
  Nb  Nb3  1  0.005871  0.494443  0.501004  1
  O  O4  1  0.005984  0.994384  0.501149  1
  O  O5  1  0.506078  0.994360  0.001096  1
  O  O6  1  0.005938  0.493956  0.001060  1
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$Nb_2O_5$

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_cell_length_c   20.82946079
_cell_angle_alpha   64.37219889
_cell_angle_beta   90.00103500
_cell_angle_gamma   90.00214144
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Nb2O5
_chemical_formula_sum   'Nb28 O70'
_cell_volume   1446.69434171
_cell_formula_units_Z   14
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loop_
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 _atom_site_label
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 _atom_site_fract_x
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 _atom_site_fract_z
 _atom_site_occupancy
  Nb  Nb1  1  0.989629  0.160998  0.834128  1
  Nb  Nb2  1  0.498987  0.421155  0.703005  1
  Nb  Nb3  1  0.005453  0.004647  0.763546  1
  Nb  Nb4  1  0.984459  0.156122  0.566579  1
  Nb  Nb5  1  0.001231  0.693061  0.628814  1
  Nb  Nb6  1  0.004717  0.995881  0.235761  1
  Nb  Nb7  1  0.998223  0.152055  0.302579  1
  Nb  Nb8  1  0.498459  0.734115  0.839873  1
  Nb  Nb9  1  0.999145  0.316040  0.638360  1
  Nb  Nb10  1  0.999282  0.684483  0.360997  1
  Nb  Nb11  1  0.998396  0.848526  0.696649  1
  Nb  Nb12  1  0.998945  0.531305  0.562205  1
  Nb  Nb13  1  0.509791  0.110158  0.093378  1
  Nb  Nb14  1  0.499428  0.580409  0.770062  1
  Nb  Nb15  1  0.494823  0.264543  0.898402  1
  Nb  Nb16  1  0.524979  0.424311  0.964523  1
  Nb  Nb17  1  0.498679  0.579400  0.296328  1
  Nb  Nb18  1  0.026399  0.000297  0.499620  1
  Nb  Nb19  1  0.230222  0.000228  0.999650  1
  Nb  Nb20  1  0.510444  0.890377  0.905938  1
  Nb  Nb21  1  0.998776  0.469211  0.437128  1
  Nb  Nb22  1  0.984298  0.844413  0.432737  1
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Nb Nb23 1 0.499141 0.420155 0.229248 1
Nb Nb24 1 0.497758 0.266458 0.159396 1
Nb Nb25 1 0.989352 0.839513 0.165228 1
Nb Nb26 1 0.000436 0.307464 0.370488 1
Nb Nb27 1 0.524589 0.576263 0.034796 1
Nb Nb28 1 0.495010 0.736011 0.100934 1
O O29 1 0.500450 0.182188 0.131228 1
O O30 1 0.499135 0.339419 0.066171 1
O O31 1 0.999335 0.755514 0.812460 1
O O32 1 0.998864 0.576999 0.461025 1
O O33 1 0.992455 0.087884 0.938351 1
O O34 1 0.503197 0.014132 0.205145 1
O O35 1 0.999371 0.405337 0.258987 1
O O36 1 0.995124 0.079776 0.535933 1
O O37 1 0.998870 0.423526 0.538308 1
O O38 1 0.498638 0.165543 0.573157 1
O O39 1 0.499170 0.341437 0.200835 1
O O40 1 0.500302 0.501212 0.861213 1
O O41 1 0.998983 0.426534 0.670082 1
O O42 1 0.498768 0.834985 0.426159 1
O O43 1 0.999859 0.595180 0.740331 1
O O44 1 0.497716 0.340879 0.791309 1
O O45 1 0.500445 0.664588 0.653052 1
O O46 1 0.498947 0.503910 0.585329 1
O O47 1 0.004371 0.416485 0.962484 1
O O48 1 0.499881 0.659189 0.798373 1
O O49 1 0.005030 0.917931 0.326127 1
O O50 1 0.998360 0.247300 0.736605 1
O O51 1 0.498978 0.344085 0.645187 1
O O52 1 0.000246 0.076289 0.263778 1
O O53 1 0.493981 0.819475 0.152970 1
O O54 1 0.001779 0.238788 0.465502 1
O O55 1 0.498743 0.496613 0.414003 1
O O56 1 0.999883 0.762388 0.668414 1
O O57 1 0.999206 0.607237 0.588940 1
O O58 1 0.499278 0.826105 0.723656 1
O O59 1 0.500978 0.818335 0.868084 1
O O60 1 0.503524 0.000369 0.499557 1
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O O62 1 0.998797 0.574000 0.329268 1
O O63 1 0.992493 0.912587 0.060993 1
O O64 1 0.500589 0.181444 0.996455 1
O O65 1 0.005363 0.082609 0.673189 1
O O66 1 0.500503 0.499420 0.138138 1
O O67 1 0.004260 0.584135 0.036838 1
O O68 1 0.999812 0.919131 0.602532 1
O O69 1 0.497501 0.659680 0.208037 1

O O70 1 0.995534 0.914039 0.195169 1
O O71 1 0.996472 0.086485 0.804171 1
O O72 1 0.498953 0.501014 0.272165 1
O O73 1 0.999177 0.238140 0.330897 1
O O74 1 0.998709 0.245084 0.186783 1
O O75 1 0.999122 0.253805 0.596298 1
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O O83 1 0.497711 0.339438 0.926887 1
O O84 1 0.499784 0.335921 0.346243 1
O O85 1 0.500934 0.819088 0.002857 1
O O86 1 0.499654 0.499536 0.727169 1
O O87 1 0.506676 0.974165 0.940576 1
O O88 1 0.998890 0.393299 0.410366 1
O O89 1 0.995062 0.920773 0.463384 1
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O O91 1 0.504492 0.500237 0.999727 1
O O92 1 0.004738 0.084364 0.117765 1
O O93 1 0.000968 0.924281 0.735478 1
O O94 1 0.499509 0.661092 0.933077 1
O O95 1 0.995599 0.247686 0.884518 1
O O96 1 0.497806 0.661120 0.072462 1
O O97 1 0.995697 0.752869 0.114818 1
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$BaNbO_3$

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  Nb  Nb2  1  0.500000  0.496597  0.495748  1
  O  O3  1  0.500000  0.996596  0.495700  1
  O  O4  1  0.000000  0.496811  0.495554  1
  O  O5  1  0.500000  0.496409  0.995686  1
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$Ba_7Nb_8O_{24}$

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  Ba  Ba3  1  0.502175  0.499874  0.505554  1
  Ba  Ba4  1  0.002197  0.999847  0.005519  1
  Ba  Ba5  1  0.002158  0.999846  0.505526  1
  Ba  Ba6  1  0.002163  0.499840  0.005521  1
  Ba  Ba7  1  0.002178  0.499857  0.505530  1
  Nb  Nb8  1  0.255044  0.246978  0.252681  1
  Nb  Nb9  1  0.255037  0.246976  0.758411  1
  Nb  Nb10  1  0.255055  0.752701  0.252653  1
  Nb  Nb11  1  0.255044  0.752699  0.758392  1
  Nb  Nb12  1  0.749323  0.246985  0.252662  1
  Nb  Nb13  1  0.749309  0.246996  0.758398  1
  Nb  Nb14  1  0.749317  0.752718  0.252643  1
  Nb  Nb15  1  0.749306  0.752730  0.758385  1
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  O  O17  1  0.502169  0.253512  0.751698  1
  O  O18  1  0.502183  0.746027  0.259201  1
  O  O19  1  0.502174  0.746178  0.751855  1
  O  O20  1  0.002184  0.249551  0.255182  1
  O  O21  1  0.002181  0.249704  0.755858  1
  O  O22  1  0.002177  0.750131  0.255341  1
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| | | | | | | |
|---|---|---|---|---|---|---|
| O | O23 | 1 | 0.002169 | 0.749996 | 0.755711 | 1 |
| O | O24 | 1 | 0.248539 | 0.253625 | 0.005544 | 1 |
| O | O25 | 1 | 0.252281 | 0.249588 | 0.505538 | 1 |
| O | O26 | 1 | 0.248412 | 0.746074 | 0.005525 | 1 |
| O | O27 | 1 | 0.252495 | 0.750109 | 0.505533 | 1 |
| O | O28 | 1 | 0.755781 | 0.253719 | 0.005523 | 1 |
| O | O29 | 1 | 0.752092 | 0.249495 | 0.505519 | 1 |
| O | O30 | 1 | 0.755963 | 0.745978 | 0.005511 | 1 |
| O | O31 | 1 | 0.751916 | 0.750231 | 0.505515 | 1 |
| O | O32 | 1 | 0.248574 | 0.999833 | 0.259258 | 1 |
| O | O33 | 1 | 0.248346 | 0.999841 | 0.751818 | 1 |
| O | O34 | 1 | 0.252332 | 0.499831 | 0.255349 | 1 |
| O | O35 | 1 | 0.252496 | 0.499844 | 0.755727 | 1 |
| O | O36 | 1 | 0.755836 | 0.999850 | 0.259113 | 1 |
| O | O37 | 1 | 0.756002 | 0.999863 | 0.751929 | 1 |
| O | O38 | 1 | 0.752092 | 0.499853 | 0.255439 | 1 |
| O | O39 | 1 | 0.751881 | 0.499858 | 0.755621 | 1 |

$Ba_{26}Nb_{27}O_{81}$

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  Ba  Ba3  1  0.332409  0.328832  0.003214  1
  Ba  Ba4  1  0.332438  0.333550  0.335849  1
  Ba  Ba5  1  0.332417  0.333592  0.670576  1
  Ba  Ba6  1  0.332436  0.672975  0.003174  1
  Ba  Ba7  1  0.332458  0.668256  0.335827  1
  Ba  Ba8  1  0.332438  0.668289  0.670551  1
  Ba  Ba9  1  0.660345  0.000894  0.003124  1
  Ba  Ba10  1  0.665071  0.000894  0.335761  1
  Ba  Ba11  1  0.665073  0.000924  0.670505  1
  Ba  Ba12  1  0.665028  0.333537  0.003172  1
  Ba  Ba13  1  0.664992  0.333471  0.335733  1
  Ba  Ba14  1  0.664990  0.333511  0.670606  1
  Ba  Ba15  1  0.665066  0.668262  0.003139  1
  Ba  Ba16  1  0.665027  0.668316  0.335710  1
  Ba  Ba17  1  0.665022  0.668341  0.670576  1
  Ba  Ba18  1  0.004493  0.000904  0.003189  1
  Ba  Ba19  1  0.999792  0.000900  0.335823  1
  Ba  Ba20  1  0.999795  0.000929  0.670566  1
  Ba  Ba21  1  0.999773  0.333554  0.003220  1
  Ba  Ba22  1  0.999849  0.333488  0.335792  1
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Ba Ba25 1 0.999880 0.668330 0.335765 1
Ba Ba26 1 0.999880 0.668363 0.670635 1
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Nb Nb28 1 0.166087 0.167244 0.503226 1
Nb Nb29 1 0.167672 0.165660 0.838491 1
Nb Nb30 1 0.166090 0.500900 0.169551 1
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Nb Nb32 1 0.166084 0.500933 0.836905 1
Nb Nb33 1 0.167710 0.836185 0.167920 1
Nb Nb34 1 0.166112 0.834610 0.503203 1
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Nb Nb38 1 0.497137 0.165642 0.838435 1
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O O69 1 0.665657 0.834294 0.169723 1

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O O103 1 0.832454 0.500890 0.336578 1
O O104 1 0.832453 0.500926 0.669791 1
O O105 1 0.832451 0.834090 0.003144 1
O O106 1 0.832469 0.834205 0.336432 1
O O107 1 0.832467 0.834220 0.669865 1
O O108 1 0.162908 0.000898 0.172755 1
O O109 1 0.165632 0.000922 0.503229 1
O O110 1 0.162913 0.000932 0.833693 1
O O111 1 0.165800 0.334134 0.169839 1
O O112 1 0.165707 0.334223 0.503242 1
O O113 1 0.165792 0.334165 0.836643 1
O O114 1 0.165811 0.667673 0.169804 1
O O115 1 0.165723 0.667633 0.503229 1
O O116 1 0.165816 0.667711 0.836620 1

O O117 1 0.501951 0.000884 0.172673 1
O O118 1 0.499254 0.000913 0.503163 1
O O119 1 0.501973 0.000920 0.833592 1
O O120 1 0.499018 0.334114 0.169756 1
O O121 1 0.499150 0.334211 0.503169 1
O O122 1 0.499014 0.334154 0.836580 1
O O123 1 0.499046 0.667658 0.169738 1
O O124 1 0.499176 0.667616 0.503157 1
O O125 1 0.499038 0.667688 0.836537 1
O O126 1 0.832440 0.000891 0.169942 1
O O127 1 0.832453 0.000918 0.503168 1
O O128 1 0.832429 0.000919 0.836349 1
O O129 1 0.832423 0.334181 0.169897 1
O O130 1 0.832452 0.334320 0.503190 1
O O131 1 0.832426 0.334217 0.836461 1
O O132 1 0.832459 0.667600 0.169876 1
O O133 1 0.832474 0.667510 0.503171 1
O O134 1 0.832454 0.667630 0.836433 1

$Ba_9Nb_{10}O_{30}$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   9.26754274
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_cell_length_c   9.26830481
_cell_angle_alpha   113.60161535
_cell_angle_beta   101.52578376
_cell_angle_gamma   89.98263001
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ba9Nb10O30
_chemical_formula_sum   'Ba9 Nb10 O30'
_cell_volume   712.27721602
_cell_formula_units_Z   1
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ba  Ba1  1  0.802277  0.605618  0.000570  1
  Ba  Ba2  1  0.605397  0.197384  0.999818  1
  Ba  Ba3  1  0.393799  0.802596  0.999722  1
  Ba  Ba4  1  0.901395  0.802192  0.506365  1
  Ba  Ba5  1  0.196897  0.394382  0.998966  1
  Ba  Ba6  1  0.699577  0.399063  0.499898  1
  Ba  Ba7  1  0.499583  0.999961  0.499781  1
  Ba  Ba8  1  0.299590  0.600892  0.499695  1
  Ba  Ba9  1  0.097836  0.197827  0.493342  1
  Nb  Nb10  1  0.950641  0.396241  0.247232  1
  Nb  Nb11  1  0.752018  0.000306  0.247542  1
  Nb  Nb12  1  0.851909  0.198030  0.752319  1
  Nb  Nb13  1  0.653416  0.802889  0.753474  1
  Nb  Nb14  1  0.549860  0.599991  0.249887  1
  Nb  Nb15  1  0.345717  0.197067  0.246070  1
  Nb  Nb16  1  0.449344  0.399991  0.749689  1
  Nb  Nb17  1  0.147265  0.801941  0.247221  1
  Nb  Nb18  1  0.247186  0.999672  0.752042  1
  Nb  Nb19  1  0.048544  0.603733  0.752343  1
  O  O20  1  0.898397  0.305855  0.999813  1
  O  O21  1  0.846800  0.695112  0.745935  1
  O  O22  1  0.847103  0.203609  0.253876  1
```

O O23 1 0.949491 0.399829 0.749274 1
O O24 1 0.694372 0.898841 0.000152 1
O O25 1 0.799430 0.100308 0.499949 1
O O26 1 0.649550 0.300400 0.749846 1
O O27 1 0.948548 0.898497 0.254504 1
O O28 1 0.649241 0.800126 0.250010 1
O O29 1 0.745803 0.000444 0.746212 1
O O30 1 0.599521 0.700225 0.499974 1
O O31 1 0.499722 0.499932 0.999784 1
O O32 1 0.449792 0.900031 0.749829 1
O O33 1 0.749549 0.500426 0.250001 1
O O34 1 0.449866 0.399685 0.249370 1
O O35 1 0.549318 0.600288 0.750191 1
O O36 1 0.304851 0.101130 0.999421 1
O O37 1 0.399448 0.299779 0.499587 1
O O38 1 0.249713 0.499679 0.749848 1
O O39 1 0.549381 0.099951 0.249834 1
O O40 1 0.253346 0.999511 0.253291 1
O O41 1 0.349983 0.199847 0.749609 1
O O42 1 0.100611 0.694219 0.999745 1
O O43 1 0.199869 0.899685 0.499649 1
O O44 1 0.050663 0.101495 0.745160 1
O O45 1 0.349615 0.699505 0.249469 1
O O46 1 0.049753 0.600130 0.250316 1
O O47 1 0.152045 0.796380 0.745679 1
O O48 1 0.999696 0.499919 0.499805 1
O49 1 0.152319 0.304752 0.253419 1

$Ba_2Nb_5O_9$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   4.24427900
_cell_length_b   4.24430501
_cell_length_c   12.43007201
_cell_angle_alpha   89.99971548
_cell_angle_beta   89.99578851
_cell_angle_gamma   89.99671969
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ba2Nb5O9
_chemical_formula_sum   'Ba2 Nb5 O9'
_cell_volume   223.91549800
_cell_formula_units_Z   1
loop_
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 _symmetry_equiv_pos_as_xyz
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loop_
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 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ba  Ba1  1  0.004334  0.002399  0.168067  1
  Ba  Ba2  1  0.004678  0.002242  0.831704  1
  Nb  Nb3  1  0.504344  0.501894  0.999908  1
  Nb  Nb4  1  0.504755  0.502639  0.337074  1
  Nb  Nb5  1  0.504807  0.502589  0.662686  1
  Nb  Nb6  1  0.004850  0.502827  0.499878  1
  Nb  Nb7  1  0.504851  0.002833  0.499875  1
  O  O8  1  0.504249  0.001869  0.999907  1
  O  O9  1  0.004391  0.501759  0.999903  1
  O  O10  1  0.504577  0.502014  0.161129  1
  O  O11  1  0.504494  0.501964  0.838659  1
  O  O12  1  0.504779  0.002651  0.326954  1
  O  O13  1  0.004755  0.502790  0.326954  1
  O  O14  1  0.504853  0.002597  0.672798  1
  O  O15  1  0.004837  0.002821  0.499865  1
  O  O16  1  0.004803  0.502740  0.672806  1
```

$BaNb_7O_9$

```
_symmetry_space_group_name_H-M   'P 1'
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_cell_length_b   4.26679901
_cell_length_c   12.63075502
_cell_angle_alpha   89.99797195
_cell_angle_beta   90.00247263
_cell_angle_gamma   90.00029533
_symmetry_Int_Tables_number   1
_chemical_formula_structural   BaNb7O9
_chemical_formula_sum   'Ba1 Nb7 O9'
_cell_volume   229.93753073
_cell_formula_units_Z   1
loop_
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 _symmetry_equiv_pos_as_xyz
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loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ba  Ba1  1  0.989408  0.005548  0.000030  1
  Nb  Nb2  1  0.489417  0.505643  0.500013  1
  Nb  Nb3  1  0.989587  0.505637  0.671313  1
  Nb  Nb4  1  0.489668  0.005550  0.671329  1
  Nb  Nb5  1  0.989328  0.505660  0.328693  1
  Nb  Nb6  1  0.489326  0.005622  0.328683  1
  Nb  Nb7  1  0.489561  0.505670  0.831492  1
  Nb  Nb8  1  0.489303  0.505740  0.168512  1
  O  O9  1  0.489273  0.005634  0.500007  1
  O  O10  1  0.989400  0.505594  0.500004  1
  O  O11  1  0.989658  0.005622  0.665531  1
  O  O12  1  0.989318  0.005649  0.334457  1
  O  O13  1  0.489613  0.005669  0.839399  1
  O  O14  1  0.989555  0.505590  0.839377  1
  O  O15  1  0.489198  0.005745  0.160607  1
  O  O16  1  0.989278  0.505772  0.160623  1
  O  O17  1  0.489587  0.506039  -0.000000  1
```

$Ba_6Nb_2O_{11}$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   6.29863509
_cell_length_b   6.31021801
_cell_length_c   20.62786560
_cell_angle_alpha   91.04383036
_cell_angle_beta   97.47155254
_cell_angle_gamma   119.74476774
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ba6Nb2O11
_chemical_formula_sum   'Ba12 Nb4 O22'
_cell_volume   702.53673442
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ba  Ba1  1  0.485520  0.800779  0.076577  1
  Ba  Ba2  1  0.833261  0.459959  0.108996  1
  Ba  Ba3  1  0.941051  0.531908  0.292260  1
  Ba  Ba4  1  0.324932  0.243323  0.386399  1
  Ba  Ba5  1  0.214523  0.166590  0.202972  1
  Ba  Ba6  1  0.395691  0.201110  0.576365  1
  Ba  Ba7  1  0.740282  0.886950  0.609426  1
  Ba  Ba8  1  0.873319  0.975637  0.792767  1
  Ba  Ba9  1  0.695159  0.929612  0.419484  1
  Ba  Ba10  1  0.252273  0.660334  0.886713  1
  Ba  Ba11  1  0.152067  0.603829  0.703660  1
  Ba  Ba12  1  0.599856  0.350647  0.919174  1
  Nb  Nb13  1  0.043004  0.000757  0.997934  1
  Nb  Nb14  1  0.580021  0.848090  0.247925  1
  Nb  Nb15  1  0.969069  0.564611  0.497962  1
  Nb  Nb16  1  0.508122  0.282790  0.747910  1
  O  O17  1  0.742330  0.728315  0.187558  1
  O  O18  1  0.243420  0.617801  0.191607  1
  O  O19  1  0.413534  0.159796  0.028977  1
  O  O20  1  0.983710  0.126453  0.075162  1
  O  O21  1  0.626412  0.123729  0.189699  1
  O  O22  1  0.921292  0.075478  0.301670  1
```

| | | | | | | |
|---|---|---|---|---|---|---|
| O | O23 | 1 | 0.021143 | 0.430605 | 0.420975 | 1 |
| O | O24 | 1 | 0.537447 | 0.577929 | 0.307767 | 1 |
| O | O25 | 1 | 0.412345 | 0.960587 | 0.308971 | 1 |
| O | O26 | 1 | 0.099975 | 0.904387 | 0.466504 | 1 |
| O | O27 | 1 | 0.220200 | 0.697095 | 0.574978 | 1 |
| O | O28 | 1 | 0.172015 | 0.168371 | 0.688279 | 1 |
| O | O29 | 1 | 0.785709 | 0.224964 | 0.529316 | 1 |
| O | O30 | 1 | 0.042949 | 0.685067 | 0.998012 | 1 |
| O | O31 | 1 | 0.653252 | 0.565702 | 0.497929 | 1 |
| O | O32 | 1 | 0.683010 | 0.550955 | 0.688012 | 1 |
| O | O33 | 1 | 0.573548 | 0.056087 | 0.692778 | 1 |
| O | O34 | 1 | 0.836076 | 0.394744 | 0.808381 | 1 |
| O | O35 | 1 | 0.672264 | 0.787503 | 0.966668 | 1 |
| O | O36 | 1 | 0.332429 | 0.003237 | 0.805878 | 1 |
| O | O37 | 1 | 0.452528 | 0.516742 | 0.804606 | 1 |
| O | O38 | 1 | 0.101950 | 0.177385 | 0.920937 | 1 |

$BaNb_5O_8$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   4.18373802
_cell_length_b   6.72819011
_cell_length_c   6.72311020
_cell_angle_alpha   89.97578764
_cell_angle_beta   90.00797859
_cell_angle_gamma   90.00314405
_symmetry_Int_Tables_number   1
_chemical_formula_structural   BaNb5O8
_chemical_formula_sum   'Ba1 Nb5 O8'
_cell_volume   189.24870779
_cell_formula_units_Z   1
loop_
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 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ba  Ba1  1  0.999130  0.000273  0.003188  1
  Nb  Nb2  1  0.499136  0.211862  0.601927  1
  Nb  Nb3  1  0.499091  0.401540  0.214950  1
  Nb  Nb4  1  0.999178  0.500264  0.503196  1
  Nb  Nb5  1  0.499251  0.598962  0.791449  1
  Nb  Nb6  1  0.499174  0.788648  0.404460  1
  O  O7  1  0.499052  0.098914  0.304240  1
  O  O8  1  0.999140  0.204599  0.617098  1
  O  O9  1  0.499132  0.301272  0.904555  1
  O  O10  1  0.999098  0.386461  0.207484  1
  O  O11  1  0.999274  0.614012  0.798938  1
  O  O12  1  0.499287  0.699209  0.101839  1
  O  O13  1  0.999187  0.795912  0.389246  1
  O  O14  1  0.499223  0.901598  0.702172  1
```

$Ba_4Nb_2O_9$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   6.10372112
_cell_length_b   10.42767657
_cell_length_c   17.19094999
_cell_angle_alpha   90.42508018
_cell_angle_beta   89.99308306
_cell_angle_gamma   89.99778826
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ba4Nb2O9
_chemical_formula_sum   'Ba16 Nb8 O36'
_cell_volume   1094.13309695
_cell_formula_units_Z   4
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ba  Ba1  1  0.991086  0.350495  0.804487  1
  Ba  Ba2  1  0.993966  0.682311  0.697795  1
  Ba  Ba3  1  0.009439  0.660322  0.432081  1
  Ba  Ba4  1  0.998764  0.322059  0.065788  1
  Ba  Ba5  1  0.501599  0.174946  0.436569  1
  Ba  Ba6  1  0.491337  0.836661  0.070255  1
  Ba  Ba7  1  0.494887  0.814647  0.304569  1
  Ba  Ba8  1  0.492024  0.146423  0.197969  1
  Ba  Ba9  1  0.505004  0.814494  0.804603  1
  Ba  Ba10  1  0.507919  0.146186  0.697976  1
  Ba  Ba11  1  0.498242  0.174883  0.936618  1
  Ba  Ba12  1  0.509157  0.836694  0.570302  1
  Ba  Ba13  1  0.001146  0.321905  0.565790  1
  Ba  Ba14  1  0.990705  0.660250  0.932121  1
  Ba  Ba15  1  0.006052  0.682333  0.197732  1
  Ba  Ba16  1  0.008635  0.350663  0.304431  1
  Nb  Nb17  1  0.012061  0.002918  0.782011  1
  Nb  Nb18  1  0.008113  0.994062  0.603459  1
  Nb  Nb19  1  0.508493  0.502840  0.398879  1
  Nb  Nb20  1  0.513000  0.493991  0.220320  1
  Nb  Nb21  1  0.486880  0.493778  0.720285  1
  Nb  Nb22  1  0.491514  0.502708  0.898854  1
```

Nb Nb23 1 0.987895 0.003063 0.281950 1
Nb Nb24 1 0.992307 0.994147 0.103379 1
O O25 1 0.957744 0.142552 0.192973 1
O O26 1 0.780111 0.908023 0.189062 1
O O27 1 0.979195 0.823745 0.555222 1
O O28 1 0.803515 0.109781 0.833571 1
O O29 1 0.694895 0.386719 0.668590 1
O O30 1 0.728087 0.407702 0.946538 1
O O31 1 0.771443 0.088994 0.555807 1
O O32 1 0.963039 0.835764 0.828335 1
O O33 1 0.720775 0.589062 0.313231 1
O O34 1 0.777096 0.935673 0.693441 1
O O35 1 0.788116 0.450342 0.172240 1
O O36 1 0.479839 0.673146 0.447160 1
O O37 1 0.712853 0.046808 0.330067 1
O O38 1 0.744083 0.070152 0.051471 1
O O39 1 0.756876 0.426625 0.450627 1
O O40 1 0.463749 0.661146 0.174059 1
O O41 1 0.456714 0.354413 0.809301 1
O O42 1 0.722195 0.560824 0.808782 1
O O43 1 0.277637 0.561008 0.308900 1
O O44 1 0.543118 0.354530 0.309232 1
O O45 1 0.536107 0.660873 0.673982 1
O O46 1 0.243209 0.426653 0.950759 1
O O47 1 0.256336 0.070180 0.551561 1
O O48 1 0.286952 0.046669 0.830163 1
O O49 1 0.211609 0.450049 0.672373 1
O O50 1 0.520457 0.673074 0.947114 1
O O51 1 0.223084 0.936033 0.193419 1
O O52 1 0.279182 0.588994 0.813295 1
O O53 1 0.228961 0.088999 0.055657 1
O O54 1 0.037243 0.835986 0.328309 1
O O55 1 0.304752 0.387079 0.168644 1
O O56 1 0.272020 0.407944 0.446673 1
O O57 1 0.196177 0.110071 0.333563 1
O O58 1 0.021339 0.823755 0.055206 1
O O59 1 0.042307 0.142375 0.693106 1
O O60 1 0.220284 0.907922 0.689057 1

$Ba_5Nb_4O_{15}$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   5.89549505
_cell_length_b   5.89549505
_cell_length_c   12.02127367
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   120.00000000
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ba5Nb4O15
_chemical_formula_sum   'Ba5 Nb4 O15'
_cell_volume   361.84424839
_cell_formula_units_Z   1
loop_
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 _symmetry_equiv_pos_as_xyz
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loop_
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 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
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  Ba  Ba2  1  0.333333  0.666667  0.430055  1
  Ba  Ba3  1  0.666667  0.333333  0.209847  1
  Ba  Ba4  1  0.333333  0.666667  0.790153  1
  Ba  Ba5  1  0.000000  0.000000  0.000000  1
  Nb  Nb6  1  0.666667  0.333333  0.895592  1
  Nb  Nb7  1  0.333333  0.666667  0.104408  1
  Nb  Nb8  1  0.000000  0.000000  0.315808  1
  Nb  Nb9  1  0.000000  0.000000  0.684192  1
  O  O10  1  0.835892  0.164108  0.387245  1
  O  O11  1  0.835892  0.671784  0.387245  1
  O  O12  1  0.328216  0.164108  0.387245  1
  O  O13  1  0.671784  0.835892  0.612755  1
  O  O14  1  0.164108  0.328216  0.612755  1
  O  O15  1  0.164108  0.835892  0.612755  1
  O  O16  1  0.831130  0.168870  0.808300  1
  O  O17  1  0.831130  0.662260  0.808300  1
  O  O18  1  0.337740  0.168870  0.808300  1
  O  O19  1  0.500000  0.000000  0.000000  1
  O  O20  1  1.000000  0.500000  0.000000  1
  O  O21  1  0.500000  0.500000  0.000000  1
  O  O22  1  0.168870  0.831130  0.191700  1
```

O O23 1 0.168870 0.337740 0.191700 1
O O24 1 0.662260 0.831130 0.191700 1

$BaNb_4O_6$

```
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_cell_length_c   8.34068503
_cell_angle_alpha   89.99554072
_cell_angle_beta   90.00262671
_cell_angle_gamma   90.00480550
_symmetry_Int_Tables_number   1
_chemical_formula_structural   BaNb4O6
_chemical_formula_sum   'Ba1 Nb4 O6'
_cell_volume   151.14256274
_cell_formula_units_Z   1
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 _symmetry_equiv_pos_as_xyz
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loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ba  Ba1  1  0.991840  0.001874  0.999936  1
  Nb  Nb2  1  0.491972  0.001707  0.499924  1
  Nb  Nb3  1  0.991914  0.501690  0.499878  1
  Nb  Nb4  1  0.491783  0.501724  0.253829  1
  Nb  Nb5  1  0.492007  0.501632  0.745978  1
  O  O6  1  0.491985  0.501516  0.999908  1
  O  O7  1  0.491612  0.001715  0.242629  1
  O  O8  1  0.991754  0.501785  0.242568  1
  O  O9  1  0.491863  0.001594  0.757212  1
  O  O10  1  0.992039  0.501648  0.757176  1
  O  O11  1  0.991961  0.001685  0.499875  1
```

$Ba_7Nb_6O_{21}$

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_cell_length_b   17.17666038
_cell_length_c   17.17666048
_cell_angle_alpha   19.75304374
_cell_angle_beta   19.75304374
_cell_angle_gamma   19.75304487
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ba7Nb6O21
_chemical_formula_sum   'Ba7 Nb6 O21'
_cell_volume   506.26041811
_cell_formula_units_Z   1
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 _symmetry_equiv_pos_as_xyz
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 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ba  Ba1  1  0.000000  0.000000  0.000000  1
  Ba  Ba2  1  0.849975  0.849975  0.849975  1
  Ba  Ba3  1  0.150025  0.150025  0.150025  1
  Ba  Ba4  1  0.764830  0.764830  0.764830  1
  Ba  Ba5  1  0.235170  0.235170  0.235170  1
  Ba  Ba6  1  0.617918  0.617918  0.617918  1
  Ba  Ba7  1  0.382082  0.382082  0.382082  1
  Nb  Nb8  1  0.927947  0.927947  0.927947  1
  Nb  Nb9  1  0.072053  0.072053  0.072053  1
  Nb  Nb10  1  0.690249  0.690249  0.690249  1
  Nb  Nb11  1  0.309751  0.309751  0.309751  1
  Nb  Nb12  1  0.544082  0.544082  0.544082  1
  Nb  Nb13  1  0.455918  0.455918  0.455918  1
  O  O14  1  0.500000  0.500000  0.000000  1
  O  O15  1  0.000000  0.500000  0.500000  1
  O  O16  1  0.500000  0.000000  0.500000  1
  O  O17  1  0.118760  0.118760  0.622206  1
  O  O18  1  0.622206  0.118760  0.118760  1
  O  O19  1  0.118760  0.622206  0.118760  1
  O  O20  1  0.881240  0.881240  0.377794  1
  O  O21  1  0.377794  0.881240  0.881240  1
  O  O22  1  0.881240  0.377794  0.881240  1
```

| | | | | | | |
|---|---|---|---|---|---|---|
| O | O23 | 1 | 0.237946 | 0.741484 | 0.741484 | 1 |
| O | O24 | 1 | 0.741484 | 0.237946 | 0.741484 | 1 |
| O | O25 | 1 | 0.741484 | 0.741484 | 0.237946 | 1 |
| O | O26 | 1 | 0.762054 | 0.258516 | 0.258516 | 1 |
| O | O27 | 1 | 0.258516 | 0.762054 | 0.258516 | 1 |
| O | O28 | 1 | 0.258516 | 0.258516 | 0.762054 | 1 |
| O | O29 | 1 | 0.362798 | 0.855068 | 0.362798 | 1 |
| O | O30 | 1 | 0.362798 | 0.362798 | 0.855068 | 1 |
| O | O31 | 1 | 0.855068 | 0.362798 | 0.362798 | 1 |
| O | O32 | 1 | 0.637202 | 0.144932 | 0.637202 | 1 |
| O | O33 | 1 | 0.637202 | 0.637202 | 0.144932 | 1 |
| O | O34 | 1 | 0.144932 | 0.637202 | 0.637202 | 1 |

$Ba_2Nb_{15}O_{32}$

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_cell_length_b   7.92024685
_cell_length_c   36.45514839
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_cell_angle_beta   89.86379007
_cell_angle_gamma   119.87761907
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ba2Nb15O32
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_cell_volume   1983.66548680
_cell_formula_units_Z   3
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 _atom_site_fract_x
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 _atom_site_occupancy
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  Ba  Ba2  1  0.993057  0.995908  0.360595  1
  Ba  Ba3  1  0.673598  0.337301  0.972750  1
  Ba  Ba4  1  0.659814  0.329503  0.693910  1
  Ba  Ba5  1  0.340231  0.670687  0.306082  1
  Ba  Ba6  1  0.326336  0.662636  0.027251  1
  Nb  Nb7  1  0.999973  0.999975  0.999997  1
  Nb  Nb8  1  0.666662  0.333298  0.333343  1
  Nb  Nb9  1  0.333362  0.666733  0.666659  1
  Nb  Nb10  1  0.070507  0.262322  0.733675  1
  Nb  Nb11  1  0.187155  0.923302  0.734462  1
  Nb  Nb12  1  0.734449  0.804640  0.733796  1
  Nb  Nb13  1  0.929495  0.737724  0.266318  1
  Nb  Nb14  1  0.812859  0.076754  0.265540  1
  Nb  Nb15  1  0.265562  0.195406  0.266208  1
  Nb  Nb16  1  0.737089  0.595495  0.067022  1
  Nb  Nb17  1  0.853737  0.256472  0.067810  1
  Nb  Nb18  1  0.401045  0.137800  0.067142  1
  Nb  Nb19  1  0.596244  0.071131  0.599643  1
  Nb  Nb20  1  0.479570  0.410134  0.598863  1
  Nb  Nb21  1  0.932257  0.528782  0.599528  1
  Nb  Nb22  1  0.403810  0.928866  0.400365  1
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Nb Nb25 1 0.262861 0.404462 0.932976 1
Nb Nb26 1 0.146227 0.743499 0.932184 1
Nb Nb27 1 0.598914 0.862175 0.932854 1
Nb Nb28 1 0.023545 0.218597 0.532753 1
Nb Nb29 1 0.194961 0.978537 0.532653 1
Nb Nb30 1 0.783814 0.807006 0.532678 1
Nb Nb31 1 0.976506 0.781398 0.467252 1
Nb Nb32 1 0.805096 0.021453 0.467353 1
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O O83 1 0.501457 0.595891 0.833479 1
O O84 1 0.094055 0.498922 0.833272 1
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O O145 1 0.118435 0.459768 0.699798 1
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$BaNb_8O_{14}$

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  Ba  Ba8  1  0.508574  0.484887  0.136455  1
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Nb Nb69 1 0.375768 0.923952 0.817082 1

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O O74 1 0.992806 0.253501 0.436616 1
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O O76 1 0.007194 0.246499 0.936616 1
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$Ba_4Nb_{14}O_{23}$

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  Ba  Ba6  1  0.998248  0.828997  0.602159  1
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O O62 1 0.998201 0.665025 0.695994 1
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O O65 1 0.498379 0.831775 0.698563 1
O O66 1 0.498346 0.166470 0.301597 1
O O67 1 0.498405 0.164545 0.698074 1
O O68 1 0.498334 0.833730 0.302152 1
O O69 1 0.498133 0.331616 0.198601 1

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| O | O71 | 1 | 0.498105 | 0.664369 | 0.198059 | 1 |
| O | O72 | 1 | 0.498238 | 0.333700 | 0.802139 | 1 |
| O | O73 | 1 | 0.498468 | 0.997286 | 0.595980 | 1 |
| O | O74 | 1 | 0.498475 | 0.001069 | 0.404219 | 1 |
| O | O75 | 1 | 0.498016 | 0.497162 | 0.095988 | 1 |
| O | O76 | 1 | 0.498049 | 0.500795 | 0.904221 | 1 |
| O | O77 | 1 | 0.998470 | 0.999134 | 0.500099 | 1 |
| O | O78 | 1 | 0.998051 | 0.498995 | 0.000107 | 1 |
| O | O79 | 1 | 0.498341 | 0.837641 | 0.499571 | 1 |
| O | O80 | 1 | 0.498329 | 0.160664 | 0.500632 | 1 |
| O | O81 | 1 | 0.498151 | 0.337487 | 0.999636 | 1 |
| O | O82 | 1 | 0.498159 | 0.660504 | 0.000563 | 1 |

$Ba_3Nb_{16}O_{23}$

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  Ba  Ba3  1  0.997041  0.000301  0.201349  1
  Ba  Ba4  1  0.997601  0.000231  0.798534  1
  Ba  Ba5  1  0.997651  0.500464  0.701363  1
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  Nb  Nb12  1  0.996678  0.671085  0.898411  1
  Nb  Nb13  1  0.996320  0.671150  0.101449  1
  Nb  Nb14  1  0.996719  0.328996  0.898416  1
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  Nb  Nb18  1  0.997933  0.829638  0.398422  1
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| O | O71 | 1 | 0.997678 | 0.840783 | 0.300499 | 1 |
| O | O72 | 1 | 0.998186 | 0.160411 | 0.699397 | 1 |
| O | O73 | 1 | 0.996954 | 0.659935 | 0.800494 | 1 |
| O | O74 | 1 | 0.996544 | 0.340343 | 0.199395 | 1 |
| O | O75 | 1 | 0.996955 | 0.340244 | 0.800508 | 1 |
| O | O76 | 1 | 0.996453 | 0.660057 | 0.199370 | 1 |
| O | O77 | 1 | 0.496338 | 0.500259 | 0.201067 | 1 |
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| O | O79 | 1 | 0.498326 | 0.000494 | 0.701073 | 1 |
| O | O80 | 1 | 0.497860 | 0.000585 | 0.298822 | 1 |
| O | O81 | 1 | 0.496263 | 0.000122 | 0.103115 | 1 |
| O | O82 | 1 | 0.496696 | 0.000053 | 0.896717 | 1 |
| O | O83 | 1 | 0.498494 | 0.500621 | 0.603133 | 1 |
| O | O84 | 1 | 0.497931 | 0.500669 | 0.396786 | 1 |

$BaNb_2O_6$

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  Ba  Ba4  1  0.473271  0.248626  0.034166  1
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  Nb  Nb6  1  0.033516  0.980702  0.854702  1
  Nb  Nb7  1  0.473628  0.980832  0.354751  1
  Nb  Nb8  1  0.973661  0.017014  0.144484  1
  Nb  Nb9  1  0.967262  0.522466  0.143142  1
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  Nb  Nb11  1  0.039928  0.475216  0.856186  1
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| O | O24 | 1 | 0.651083 | 0.030475 | 0.212108 | 1 |
| O | O25 | 1 | 0.654909 | 0.464715 | 0.213837 | 1 |
| O | O26 | 1 | 0.154757 | 0.532969 | 0.285507 | 1 |
| O | O27 | 1 | 0.352448 | 0.533061 | 0.785473 | 1 |
| O | O28 | 1 | 0.852428 | 0.464696 | 0.713819 | 1 |
| O | O29 | 1 | 0.494506 | 0.249297 | 0.647454 | 1 |
| O | O30 | 1 | 0.994630 | 0.748378 | 0.851843 | 1 |
| O | O31 | 1 | 0.512485 | 0.748482 | 0.351825 | 1 |
| O | O32 | 1 | 0.012747 | 0.249300 | 0.147375 | 1 |
| O | O33 | 1 | 0.613995 | 0.749793 | 0.637868 | 1 |
| O | O34 | 1 | 0.113981 | 0.247912 | 0.861271 | 1 |
| O | O35 | 1 | 0.393155 | 0.247999 | 0.361240 | 1 |
| O | O36 | 1 | 0.893360 | 0.749807 | 0.138018 | 1 |

$Ba_3Nb_5O_{15}$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   4.05161200
_cell_length_b   12.85274900
_cell_length_c   12.85647601
_cell_angle_alpha   90.00058404
_cell_angle_beta   89.99766312
_cell_angle_gamma   90.00188315
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ba3Nb5O15
_chemical_formula_sum   'Ba6 Nb10 O30'
_cell_volume   669.49265749
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ba  Ba1  1  0.997266  0.498912  0.499286  1
  Ba  Ba2  1  0.997152  0.998922  0.999326  1
  Ba  Ba3  1  0.998406  0.326327  0.836083  1
  Ba  Ba4  1  0.998052  0.671701  0.162551  1
  Ba  Ba5  1  0.996608  0.826648  0.662972  1
  Ba  Ba6  1  0.997047  0.171843  0.336332  1
  Nb  Nb7  1  0.499996  0.498922  0.999267  1
  Nb  Nb8  1  0.496011  0.998864  0.499275  1
  Nb  Nb9  1  0.497430  0.422084  0.286386  1
  Nb  Nb10  1  0.496941  0.575868  0.712192  1
  Nb  Nb11  1  0.497211  0.922169  0.212254  1
  Nb  Nb12  1  0.497340  0.075769  0.786397  1
  Nb  Nb13  1  0.497348  0.711127  0.421121  1
  Nb  Nb14  1  0.497435  0.286755  0.577561  1
  Nb  Nb15  1  0.496923  0.786721  0.921193  1
  Nb  Nb16  1  0.497330  0.211144  0.077479  1
  O  O17  1  0.997869  0.498929  0.999258  1
  O  O18  1  0.996904  0.998808  0.499258  1
  O  O19  1  0.497348  0.219703  0.719867  1
  O  O20  1  0.497282  0.778203  0.278806  1
  O  O21  1  0.496997  0.719749  0.778781  1
  O  O22  1  0.497418  0.278112  0.219785  1
```

| | | | | | | |
|---|---|---|---|---|---|---|
| O | O23 | 1 | 0.997501 | 0.419816 | 0.291393 | 1 |
| O | O24 | 1 | 0.997132 | 0.578012 | 0.707260 | 1 |
| O | O25 | 1 | 0.997154 | 0.919949 | 0.207318 | 1 |
| O | O26 | 1 | 0.997166 | 0.077862 | 0.791314 | 1 |
| O | O27 | 1 | 0.997238 | 0.706926 | 0.421387 | 1 |
| O | O28 | 1 | 0.997263 | 0.290879 | 0.577142 | 1 |
| O | O29 | 1 | 0.997104 | 0.790851 | 0.921522 | 1 |
| O | O30 | 1 | 0.997414 | 0.207053 | 0.077013 | 1 |
| O | O31 | 1 | 0.497021 | 0.155502 | 0.493289 | 1 |
| O | O32 | 1 | 0.497140 | 0.842203 | 0.505577 | 1 |
| O | O33 | 1 | 0.497591 | 0.655573 | 0.005535 | 1 |
| O | O34 | 1 | 0.497728 | 0.342296 | 0.993048 | 1 |
| O | O35 | 1 | 0.497858 | 0.506942 | 0.156183 | 1 |
| O | O36 | 1 | 0.497501 | 0.490870 | 0.842358 | 1 |
| O | O37 | 1 | 0.496845 | 0.990820 | 0.656203 | 1 |
| O | O38 | 1 | 0.496997 | 0.007153 | 0.342385 | 1 |
| O | O39 | 1 | 0.497493 | 0.357962 | 0.430800 | 1 |
| O | O40 | 1 | 0.497321 | 0.639601 | 0.567695 | 1 |
| O | O41 | 1 | 0.496963 | 0.858115 | 0.067794 | 1 |
| O | O42 | 1 | 0.497166 | 0.139711 | 0.930815 | 1 |
| O | O43 | 1 | 0.497235 | 0.565948 | 0.360726 | 1 |
| O | O44 | 1 | 0.497034 | 0.431857 | 0.637847 | 1 |
| O | O45 | 1 | 0.497229 | 0.931814 | 0.860726 | 1 |
| O | O46 | 1 | 0.497357 | 0.065997 | 0.137775 | 1 |

**Supplementary Data II: Ground state compounds in Ca-Al-O system**

$Ca_8Al_3$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   9.45444800
_cell_length_b   9.52417724
_cell_length_c   9.61302941
_cell_angle_alpha   98.99568942
_cell_angle_beta   101.05673721
_cell_angle_gamma   119.71752218
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ca8Al3
_chemical_formula_sum   'Ca16 Al6'
_cell_volume   704.98265563
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ca  Ca1  1  0.531993  0.701328  0.649456  1
  Ca  Ca2  1  0.468007  0.298672  0.350544  1
  Ca  Ca3  1  0.079721  0.230386  0.106950  1
  Ca  Ca4  1  0.920279  0.769614  0.893050  1
  Ca  Ca5  1  0.878513  0.400728  0.648007  1
  Ca  Ca6  1  0.121487  0.599272  0.351993  1
  Ca  Ca7  1  0.332551  0.878966  0.110265  1
  Ca  Ca8  1  0.667449  0.121034  0.889735  1
  Ca  Ca9  1  0.960279  0.060756  0.669722  1
  Ca  Ca10  1  0.039721  0.939244  0.330278  1
  Ca  Ca11  1  0.701537  0.497909  0.110530  1
  Ca  Ca12  1  0.298463  0.502091  0.889470  1
  Ca  Ca13  1  0.774152  0.152828  0.298912  1
  Ca  Ca14  1  0.225848  0.847172  0.701088  1
  Ca  Ca15  1  0.544172  0.710658  0.296785  1
  Ca  Ca16  1  0.455828  0.289342  0.703215  1
  Al  Al17  1  -0.000000  0.500000  0.000000  1
  Al  Al18  1  0.500000  -0.000000  0.500000  1
  Al  Al19  1  0.172695  0.337461  0.500337  1
  Al  Al20  1  0.827305  0.662539  0.499663  1
```

Al Al21 1 0.676291 0.839839 0.025977 1
Al Al22 1 0.323709 0.160161 0.974023 1

$CaO_2$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   3.87428343
_cell_length_b   3.87428343
_cell_length_c   7.03166330
_cell_angle_alpha   65.78303287
_cell_angle_beta   65.78303287
_cell_angle_gamma   56.73067843
_symmetry_Int_Tables_number   1
_chemical_formula_structural   CaO2
_chemical_formula_sum   'Ca2 O4'
_cell_volume   78.07200303
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ca  Ca1  1  0.640785  0.359215  0.750000  1
  Ca  Ca2  1  0.359215  0.640785  0.250000  1
  O  O3  1  0.885628  0.604588  0.911486  1
  O  O4  1  0.395412  0.114372  0.588514  1
  O  O5  1  0.114372  0.395412  0.088514  1
  O  O6  1  0.604588  0.885628  0.411486  1
```

$Al_2O_3$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   5.17748333
_cell_length_b   5.17748333
_cell_length_c   5.17748380
_cell_angle_alpha   55.30162853
_cell_angle_beta   55.30162853
_cell_angle_gamma   55.30163320
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Al2O3
_chemical_formula_sum   'Al4 O6'
_cell_volume   87.42409448
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Al  Al1  1  0.352148  0.352148  0.352148  1
  Al  Al2  1  0.147852  0.147852  0.147852  1
  Al  Al3  1  0.852148  0.852148  0.852148  1
  Al  Al4  1  0.647852  0.647852  0.647852  1
  O  O5  1  0.943816  0.250000  0.556184  1
  O  O6  1  0.750000  0.443816  0.056184  1
  O  O7  1  0.250000  0.556184  0.943816  1
  O  O8  1  0.556184  0.943816  0.250000  1
  O  O9  1  0.443816  0.056184  0.750000  1
  O  O10  1  0.056184  0.750000  0.443816  1
```

Al

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   2.85042097
_cell_length_b   2.85042097
_cell_length_c   2.85042097
_cell_angle_alpha   60.00000000
_cell_angle_beta   60.00000000
_cell_angle_gamma   60.00000000
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Al
_chemical_formula_sum   Al1
_cell_volume   16.37615790
_cell_formula_units_Z   1
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Al  Al1  1  0.000000  0.000000  0.000000  1
```

$CaAl_4$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   6.39847767
_cell_length_b   6.39847767
_cell_length_c   6.39847767
_cell_angle_alpha   140.30519444
_cell_angle_beta   140.30519444
_cell_angle_gamma   57.39019638
_symmetry_Int_Tables_number   1
_chemical_formula_structural   CaAl4
_chemical_formula_sum   'Ca1 Al4'
_cell_volume   105.95058245
_cell_formula_units_Z   1
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ca  Ca1  1  -0.000000  -0.000000  -0.000000  1
  Al  Al2  1  0.750000  0.250000  0.500000  1
  Al  Al3  1  0.386251  0.386251  -0.000000  1
  Al  Al4  1  0.613749  0.613749  0.000000  1
  Al  Al5  1  0.250000  0.750000  0.500000  1
```

$CaAl_2$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   5.66432978
_cell_length_b   5.66432978
_cell_length_c   5.66432978
_cell_angle_alpha   60.00000000
_cell_angle_beta   60.00000000
_cell_angle_gamma   60.00000000
_symmetry_Int_Tables_number   1
_chemical_formula_structural   CaAl2
_chemical_formula_sum   'Ca2 Al4'
_cell_volume   128.50812690
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ca  Ca1  1  0.250000  0.250000  0.250000  1
  Ca  Ca2  1  0.000000  0.000000  0.000000  1
  Al  Al3  1  0.625000  0.125000  0.625000  1
  Al  Al4  1  0.625000  0.625000  0.625000  1
  Al  Al5  1  0.625000  0.625000  0.125000  1
  Al  Al6  1  0.125000  0.625000  0.625000  1
```

CaO

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   3.41543748
_cell_length_b   3.41543748
_cell_length_c   3.41543748
_cell_angle_alpha   60.00000000
_cell_angle_beta   60.00000000
_cell_angle_gamma   60.00000000
_symmetry_Int_Tables_number   1
_chemical_formula_structural   CaO
_chemical_formula_sum   'Ca1 O1'
_cell_volume   28.17241132
_cell_formula_units_Z   1
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ca  Ca1  1  0.000000  0.000000  0.000000  1
  O  O2  1  0.500000  0.500000  0.500000  1
```

Ca

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   3.89902498
_cell_length_b   3.89902498
_cell_length_c   3.89902498
_cell_angle_alpha   60.00000000
_cell_angle_beta   60.00000000
_cell_angle_gamma   60.00000000
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ca
_chemical_formula_sum   Ca1
_cell_volume   41.91341557
_cell_formula_units_Z   1
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ca  Ca1  1  0.000000  0.000000  0.000000  1
```

$CaAl_4O_7$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   7.87908043
_cell_length_b   7.87908043
_cell_length_c   5.49135228
_cell_angle_alpha   76.63155928
_cell_angle_beta   76.63155928
_cell_angle_gamma   69.28149864
_symmetry_Int_Tables_number   1
_chemical_formula_structural   CaAl4O7
_chemical_formula_sum   'Ca2 Al8 O14'
_cell_volume   306.00622724
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ca  Ca1  1  0.804883  0.195117  0.250000  1
  Ca  Ca2  1  0.195117  0.804883  0.750000  1
  Al  Al3  1  0.319417  0.439886  0.243609  1
  Al  Al4  1  0.560114  0.680583  0.256391  1
  Al  Al5  1  0.680583  0.560114  0.756391  1
  Al  Al6  1  0.439886  0.319417  0.743609  1
  Al  Al7  1  0.922581  0.751201  0.305795  1
  Al  Al8  1  0.248799  0.077419  0.194205  1
  Al  Al9  1  0.077419  0.248799  0.694205  1
  Al  Al10  1  0.751201  0.922581  0.805795  1
  O  O11  1  0.251362  0.362711  0.579734  1
  O  O12  1  0.637289  0.748638  0.920266  1
  O  O13  1  0.748638  0.637289  0.420266  1
  O  O14  1  0.362711  0.251362  0.079734  1
  O  O15  1  0.135780  0.627911  0.149387  1
  O  O16  1  0.372089  0.864220  0.350613  1
  O  O17  1  0.864220  0.372089  0.850613  1
  O  O18  1  0.627911  0.135780  0.649387  1
  O  O19  1  0.939148  0.829950  0.572687  1
  O  O20  1  0.170050  0.060852  0.927313  1
  O  O21  1  0.468228  0.531772  0.750000  1
  O  O22  1  0.531772  0.468228  0.250000  1
```

O O23 1 0.829950 0.939148 0.072687 1
O O24 1 0.060852 0.170050 0.427313 1

$Ca_6Al_7O_{16}$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   10.47574813
_cell_length_b   10.47574813
_cell_length_c   10.47574813
_cell_angle_alpha   109.47122063
_cell_angle_beta   109.47122063
_cell_angle_gamma   109.47122063
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ca6Al7O16
_chemical_formula_sum   'Ca12 Al14 O32'
_cell_volume   884.97958599
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ca  Ca1  1  0.637845  0.250000  0.887845  1
  Ca  Ca2  1  0.862155  0.750000  0.612155  1
  Ca  Ca3  1  0.387845  0.750000  0.137845  1
  Ca  Ca4  1  0.112155  0.250000  0.362155  1
  Ca  Ca5  1  0.887845  0.637845  0.250000  1
  Ca  Ca6  1  0.612155  0.862155  0.750000  1
  Ca  Ca7  1  0.137845  0.387845  0.750000  1
  Ca  Ca8  1  0.362155  0.112155  0.250000  1
  Ca  Ca9  1  0.250000  0.887845  0.637845  1
  Ca  Ca10  1  0.750000  0.612155  0.862155  1
  Ca  Ca11  1  0.750000  0.137845  0.387845  1
  Ca  Ca12  1  0.250000  0.362155  0.112155  1
  Al  Al13  1  0.375000  0.250000  0.625000  1
  Al  Al14  1  0.125000  0.750000  0.875000  1
  Al  Al15  1  0.625000  0.375000  0.250000  1
  Al  Al16  1  0.875000  0.125000  0.750000  1
  Al  Al17  1  0.250000  0.625000  0.375000  1
  Al  Al18  1  0.750000  0.875000  0.125000  1
  Al  Al19  1  0.500000  0.000000  0.034143  1
  Al  Al20  1  0.034143  0.500000  0.000000  1
  Al  Al21  1  0.000000  0.034143  0.500000  1
  Al  Al22  1  0.465857  0.465857  0.465857  1
```

Al Al23 1 0.534143 0.500000 0.000000 1
Al Al24 1 0.500000 0.000000 0.534143 1
Al Al25 1 0.000000 0.534143 0.500000 1
Al Al26 1 0.965857 0.965857 0.965857 1
O O27 1 0.500000 0.000000 0.867850 1
O O28 1 0.867850 0.500000 0.000000 1
O O29 1 0.000000 0.867850 0.500000 1
O O30 1 0.632150 0.632150 0.632150 1
O O31 1 0.367850 0.500000 0.000000 1
O O32 1 0.500000 0.000000 0.367850 1
O O33 1 0.000000 0.367850 0.500000 1
O O34 1 0.132150 0.132150 0.132150 1
O O35 1 0.408850 0.094214 0.615227 1
O O36 1 0.521013 0.405786 0.814635 1
O O37 1 0.091150 0.706377 0.685365 1
O O38 1 0.978987 0.793623 0.884773 1
O O39 1 0.115227 0.594214 0.908850 1
O O40 1 0.314635 0.905786 0.021013 1
O O41 1 0.185365 0.206377 0.591150 1
O O42 1 0.384773 0.293623 0.478987 1
O O43 1 0.615227 0.408850 0.094214 1
O O44 1 0.814635 0.521013 0.405786 1
O O45 1 0.685365 0.091150 0.706377 1
O O46 1 0.884773 0.978987 0.793623 1
O O47 1 0.908850 0.115227 0.594214 1
O O48 1 0.021013 0.314635 0.905786 1
O O49 1 0.591150 0.185365 0.206377 1
O O50 1 0.478987 0.384773 0.293623 1
O O51 1 0.094214 0.615227 0.408850 1
O O52 1 0.405786 0.814635 0.521013 1
O O53 1 0.706377 0.685365 0.091150 1
O O54 1 0.793623 0.884773 0.978987 1
O O55 1 0.594214 0.908850 0.115227 1
O O56 1 0.905786 0.021013 0.314635 1
O O57 1 0.206377 0.591150 0.185365 1
O O58 1 0.293623 0.478987 0.384773 1

$Ca_{11}Al_{14}O_{32}$

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_chemical_formula_sum   'Ca22 Al28 O64'
_cell_volume   1769.50007290
_cell_formula_units_Z   2
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  Ca  Ca9  1  0.365879  0.501316  0.247622  1
  Ca  Ca10  1  0.886815  0.499388  0.250223  1
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  Ca  Ca12  1  0.750000  0.864381  0.000000  1
  Ca  Ca13  1  0.750000  0.389460  0.000000  1
  Ca  Ca14  1  0.750000  0.617908  0.500000  1
  Ca  Ca15  1  0.495267  0.745331  0.133979  1
  Ca  Ca16  1  0.004733  0.745331  0.866021  1
  Ca  Ca17  1  0.998448  0.753300  0.387150  1
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  Ca  Ca19  1  0.134121  0.501316  0.752378  1
  Ca  Ca20  1  0.866141  0.001359  0.747714  1
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```

| | | | | | | |
|---|---|---|---|---|---|---|
| Al | Al23 | 1 | 0.250000 | 0.378655 | 0.000000 | 1 |
| Al | Al24 | 1 | 0.750000 | 0.125653 | 0.000000 | 1 |
| Al | Al25 | 1 | 0.997795 | 0.249086 | 0.374848 | 1 |
| Al | Al26 | 1 | 0.001875 | 0.748966 | 0.125332 | 1 |
| Al | Al27 | 1 | 0.373889 | 0.999505 | 0.248917 | 1 |
| Al | Al28 | 1 | 0.126111 | 0.999505 | 0.751083 | 1 |
| Al | Al29 | 1 | 0.763486 | 0.266993 | 0.226260 | 1 |
| Al | Al30 | 1 | 0.236071 | 0.766877 | 0.273715 | 1 |
| Al | Al31 | 1 | 0.267560 | 0.233312 | 0.767443 | 1 |
| Al | Al32 | 1 | 0.232440 | 0.233312 | 0.232557 | 1 |
| Al | Al33 | 1 | 0.980823 | 0.016757 | 0.517770 | 1 |
| Al | Al34 | 1 | 0.019321 | 0.516697 | 0.982398 | 1 |
| Al | Al35 | 1 | 0.517159 | 0.983390 | 0.016809 | 1 |
| Al | Al36 | 1 | 0.482791 | 0.483489 | 0.483029 | 1 |
| Al | Al37 | 1 | 0.750000 | 0.878898 | 0.500000 | 1 |
| Al | Al38 | 1 | 0.250000 | 0.625649 | 0.500000 | 1 |
| Al | Al39 | 1 | 0.498125 | 0.748966 | 0.874668 | 1 |
| Al | Al40 | 1 | 0.502205 | 0.249086 | 0.625152 | 1 |
| Al | Al41 | 1 | 0.874182 | 0.499652 | 0.749039 | 1 |
| Al | Al42 | 1 | 0.625818 | 0.499652 | 0.250961 | 1 |
| Al | Al43 | 1 | 0.263929 | 0.766877 | 0.726285 | 1 |
| Al | Al44 | 1 | 0.736514 | 0.266993 | 0.773740 | 1 |
| Al | Al45 | 1 | 0.767168 | 0.733328 | 0.267470 | 1 |
| Al | Al46 | 1 | 0.732832 | 0.733328 | 0.732530 | 1 |
| Al | Al47 | 1 | 0.480679 | 0.516697 | 0.017602 | 1 |
| Al | Al48 | 1 | 0.519177 | 0.016757 | 0.482230 | 1 |
| Al | Al49 | 1 | 0.017209 | 0.483489 | 0.516971 | 1 |
| Al | Al50 | 1 | 0.982841 | 0.983390 | 0.983191 | 1 |
| O | O51 | 1 | 0.161130 | 0.685366 | 0.780854 | 1 |
| O | O52 | 1 | 0.839571 | 0.185518 | 0.719564 | 1 |
| O | O53 | 1 | 0.685089 | 0.813243 | 0.180451 | 1 |
| O | O54 | 1 | 0.314534 | 0.313191 | 0.319593 | 1 |
| O | O55 | 1 | 0.065747 | 0.935567 | 0.431598 | 1 |
| O | O56 | 1 | 0.934323 | 0.435492 | 0.068557 | 1 |
| O | O57 | 1 | 0.433580 | 0.068541 | 0.935599 | 1 |
| O | O58 | 1 | 0.066420 | 0.068541 | 0.064401 | 1 |
| O | O59 | 1 | 0.140786 | 0.448587 | 0.937383 | 1 |
| O | O60 | 1 | 0.359214 | 0.448587 | 0.062617 | 1 |
| O | O61 | 1 | 0.650831 | 0.034504 | 0.055681 | 1 |
| O | O62 | 1 | 0.349081 | 0.534514 | 0.444171 | 1 |
| O | O63 | 1 | 0.689069 | 0.217509 | 0.905388 | 1 |
| O | O64 | 1 | 0.311099 | 0.717400 | 0.594556 | 1 |
| O | O65 | 1 | 0.305280 | 0.286557 | 0.899479 | 1 |
| O | O66 | 1 | 0.194720 | 0.286557 | 0.100521 | 1 |
| O | O67 | 1 | 0.956156 | 0.150633 | 0.468739 | 1 |
| O | O68 | 1 | 0.056183 | 0.355291 | 0.456224 | 1 |
| O | O69 | 1 | 0.044061 | 0.650548 | 0.031595 | 1 |

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O O71 1 0.901791 0.694557 0.217727 1
O O72 1 0.604745 0.302382 0.714341 1
O O73 1 0.895255 0.302382 0.285659 1
O O74 1 0.097750 0.194680 0.282262 1
O O75 1 0.461331 0.942838 0.147324 1
O O76 1 0.461670 0.052852 0.349762 1
O O77 1 0.038330 0.052852 0.650238 1
O O78 1 0.538325 0.442816 0.352428 1
O O79 1 0.219001 0.904505 0.691711 1
O O80 1 0.714650 0.600334 0.307833 1
O O81 1 0.280999 0.904505 0.308289 1
O O82 1 0.285008 0.100289 0.192327 1
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O O84 1 0.338870 0.685366 0.219146 1
O O85 1 0.185466 0.313191 0.680407 1
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O O88 1 0.434253 0.935567 0.568402 1
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O O92 1 0.859242 0.948780 0.562634 1
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O O99 1 0.455939 0.650548 0.968405 1
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O O101 1 0.543844 0.150633 0.531261 1
O O102 1 0.943721 0.855165 0.043798 1
O O103 1 0.402250 0.194680 0.717738 1
O O104 1 0.104152 0.802417 0.214723 1
O O105 1 0.395848 0.802417 0.785277 1
O O106 1 0.598209 0.694557 0.782273 1
O O107 1 0.961675 0.442816 0.647572 1
O O108 1 0.961924 0.553038 0.849915 1
O O109 1 0.538076 0.553038 0.150085 1
O O110 1 0.038669 0.942838 0.852676 1
O O111 1 0.718762 0.404700 0.191564 1
O O112 1 0.214992 0.100289 0.807673 1
O O113 1 0.781238 0.404700 0.808436 1
O O114 1 0.785350 0.600334 0.692167 1

$Ca_{23}Al_{28}O_{64}$

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Al Al26 1 0.997463 0.249276 0.375104 1
Al Al27 1 0.999287 0.749649 0.125512 1
Al Al28 1 0.373887 0.999023 0.249105 1
Al Al29 1 0.126113 0.999023 0.750895 1
Al Al30 1 0.762658 0.267615 0.226974 1
Al Al31 1 0.231473 0.766349 0.267462 1
Al Al32 1 0.267937 0.233360 0.767333 1
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Al Al34 1 0.981651 0.015543 0.517447 1
Al Al35 1 0.017437 0.517947 0.982714 1
Al Al36 1 0.517600 0.983093 0.016927 1
Al Al37 1 0.483312 0.483359 0.482861 1
Al Al38 1 0.750000 0.878259 0.500000 1
Al Al39 1 0.250000 0.625058 0.500000 1
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Al Al41 1 0.502537 0.249276 0.624896 1
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Al Al43 1 0.624792 0.500453 0.250297 1
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O O87 1 0.816291 0.813567 0.818757 1
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O O91 1 0.567212 0.568003 0.564080 1
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O O93 1 0.859750 0.947987 0.562043 1
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O O95 1 0.848916 0.034128 0.945016 1
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O O112 1 0.717556 0.405348 0.191132 1
O O113 1 0.215989 0.099760 0.806152 1
O O114 1 0.782444 0.405348 0.808868 1
O O115 1 0.786755 0.600501 0.692000 1

**Supplementary Data III: Ground state compounds in Ag-Al-O system**

$AlAgO_2$

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  Al  Al2  1  0.442996  0.624743  0.498830  1
  Al  Al3  1  0.943050  0.874995  0.498485  1
  Al  Al4  1  0.063706  0.124931  0.998444  1
  Ag  Ag5  1  0.562203  0.873148  0.994550  1
  Ag  Ag6  1  0.444586  0.126781  0.494266  1
  Ag  Ag7  1  0.943984  0.372572  0.494657  1
  Ag  Ag8  1  0.062508  0.627496  0.994559  1
  O  O9  1  0.533517  0.429617  0.316149  1
  O  O10  1  0.473323  0.570297  0.816200  1
  O  O11  1  0.973130  0.929940  0.815681  1
  O  O12  1  0.033627  0.070013  0.315740  1
  O  O13  1  0.633421  0.821861  0.432252  1
  O  O14  1  0.373344  0.178036  0.932017  1
  O  O15  1  0.873444  0.322175  0.932448  1
  O  O16  1  0.133357  0.677736  0.432519  1
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$Al_2O_3$

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  Al  Al3  1  0.151165  0.142048  0.150085  1
  Al  Al4  1  0.355617  0.346310  0.354366  1
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  O  O6  1  0.947289  0.244061  0.558481  1
  O  O7  1  0.059569  0.744168  0.445995  1
  O  O8  1  0.753406  0.437975  0.058469  1
  O  O9  1  0.253415  0.550235  0.946081  1
  O  O10  1  0.559536  0.937976  0.252284  1
```

Ag

```
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Al

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 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
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$Ag_2O$

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_cell_length_c   4.87737072
_cell_angle_alpha   89.58493007
_cell_angle_beta   89.60775610
_cell_angle_gamma   89.91504569
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ag2O
_chemical_formula_sum   'Ag4 O2'
_cell_volume   115.74008401
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ag  Ag1  1  0.497228  0.502274  0.995678  1
  Ag  Ag2  1  0.997265  0.503471  0.495889  1
  Ag  Ag3  1  0.497635  0.003499  0.496859  1
  Ag  Ag4  1  0.996944  0.002850  0.997152  1
  O  O5  1  0.245733  0.251328  0.246194  1
  O  O6  1  0.749157  0.754665  0.746897  1
```

AlAg

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   5.13133469
_cell_length_b   2.94549779
_cell_length_c   4.52704701
_cell_angle_alpha   89.98839865
_cell_angle_beta   89.99772683
_cell_angle_gamma   89.70203224
_symmetry_Int_Tables_number   1
_chemical_formula_structural   AlAg
_chemical_formula_sum   'Al2 Ag2'
_cell_volume   68.42237845
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Al  Al1  1  0.663007  0.999407  0.497725  1
  Al  Al2  1  0.162749  0.497003  0.497855  1
  Ag  Ag3  1  0.329868  0.997400  0.997848  1
  Ag  Ag4  1  0.829783  0.498826  0.997624  1
```

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