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

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SUMMARY

D

(C)

-

in Figure 1B) and then attempting heavy doping (by Sn or Al, respectively), making it

F r 3. S n an Va an F r a n n D n ra Ga In a ra -16.4 n-28a84 283. -5.4 6.1aa.7265n n 3Ca-3.4 a6 -1256.7265n -44.7r 5.Pr8

in $Ca_6Al_7O_{16}$, and the Ag vacancy in $Ag_3Al_{22}O_{34}$, as a function of the metal chemical potential (see Experimental Procedures). The allowed stable chemical potential regions (constructed by considering possible competing phases, see Experimental Procedures) of the respective bulk compounds are shown in Figures 3B, 3D, and 3F. We see that for the degenerate gapped compounds under cation-deficient chemical potential conditions, vacancy formation energies can be extremely low (in fact, negative). Whereas $BaNbO_3$ and $Ca_6Al_7O_{16}$ have stable chemical potential (green) zones at the respective stoichiometries indicated, $Ag_3Al_{22}O_{34}$ does not. In fact, in the latter case, the Ag vacancy formation energy (Figure 3E) is so strongly negative under all chemical potential conditions, that the CB is empty and the parent degenerate $Ag_3Al_{22}O_{34}$ phase is not stable (i.e., no green zone in Figure 3F).

D Va an Can C n n n Sa OVC F r n H a S n

The negative formation energies of dilute vacancies open the possibility of vacancy condensation and long-range ordering (Figure 2B). To examine this possibility, we have calculated the T = 0 K stable phases (‘‘ground state diagram’’ or ‘‘convex

hull'') of such ternary structures. This entails searching for configuration versus composition that lies on the energy convex hull,[14] which defines the phases with energy lower than a linear combination of any competing phases at the corresponding compositions. We create candidate configurations by considering a base compound ($BaNbO_3$, $Ba_3Nb_5O_{15}$, $Ca_6Al_7O_{16}$, or $Ag_3Al_{22}O_{34}$), then create a replica of N such units of the base compound and add successively p metal vacancies, i.e., OVC = $N \times$ (base) + pV_m, searching via total energy minimization for stable and metastable configurations. We also include experimentally known reconstructed OVCs, the compounds that satisfy the OVC expression but do not have clearly defined vacancy sites (e.g., $Ba_3Nb_5O_{15}$, $BaNb_2O_6$, and $Ba_5Nb_4O_6$).

Available information on the experimental literature[15–30] is provided in Figure 4, and the theoretical results of this work are summarized in Figure 5. The key point to

and 7B) demonstrating the phases that are stabilized as the chemical potentials of the atoms being removed are continuously changed between their allowed values. Finally, we show how a window of opportunity can be determined computationally between opposing tendencies of (1) stability (Figures 2A and 7B), (2) conductivity (Figures 6B–6D and 7C), and (3) transparency (Figure 8) to design new TCs.

Stabl Phas s and OVCs for th Ba-Nb-O Syst m

Computationally, we find 25 binary and ternary ground state compounds (described in Data S1) of which $Ba_7Nb_6O_{21}$, $Ba_5Nb_4O_{15}$, $Ba_3Nb_5O_{15}$, $Ba_7Nb_8O_{24}$, $Ba_9Nb_{10}O_{30}$, $Ba_{26}Nb_{27}O_{81}$, and $BaNb_2O_6$ are OVCs (Figure 5). Here, 7:8:24, 9:10:30, and 26:27:82 phases have clearly defined vacancy sites, and 1:2:6, 3:5:15, and 5:4:15 OVCs are

excluded.''[18] Indeed, several potential experimental compositions (i.e., $Ba_{0.95}NbO_3$ and $Ba_{0.97}NbO_3$) nearly match predicted phases ($Ba_{26}Nb_{27}O_{81}$ Ba

unstable with respect to competing phases. Our experimental attempts to reduce synthesized $Ag_3Al_{22}O_{34.5}$ to $Ag_3Al_{22}O_{34}$

complexity of material synthesis. In our own work on 3:5:15 OVC, we see the preferential formation of the secondary reconstructed 1:2:6 and 5:4:15 OVCs over the targeted compound (Note S2). This reflects the narrow stability region of the 3:5:15 phase versus the reconstructed OVCs. Hence

frequency but also changes the interband transition, which is illustrated in the absorption spectra of 6:7:16 and its OVCs (see Figure 8

acceptor states. As a result, the negative electron-hole recombination energy offsets the positive energy associated with vacancy bond breaking. Our results thus explain

40 × 40 × 40, 20 × 20 × 20, 20 × 20 × 20, 8 × 24 × 8, 16 × 12 × 8, 20 × 20 × 20, 8 × 8 × 8, and 8 × 8 × 8 Γ-centered k-point grids were used for $BaNbO_3$, $Ba_7Nb_8O_{24}$, $Ba_7Nb_6O_{21}$, $Ba_3Nb_5O_{15}$, $BaNb_2O_6$, $Ca_6Al_7O_{16}$, $Ca_{23}Al_{28}O_{64}$, and $Ca_{11}Al_{14}O_{32}$, respectively. The Drude contribution to optical properties was included by utilizing kram code[48] with plasma frequencies calculated from first-principles calculations and the damping coefficient of 0.2 eV, which is analogous to traditional TCs.[49]

D Ca a n

Supercells with 116, 135, and 236 atoms were used to calculate defect energetics in $Ca_6Al_7O_{16}$, $BaNbO_3$, and $Ag_3Al_{22}O_{34}$ systems, respectively. The defect formation energies (Figures 3A, 3C, and 3E) and finite size corrections were computed within the framework described by Lany and Zunger[50,51] and implemented in the pyladadefects code.[52] For the defect calculations, the ranges of chemical potentials were determined using only experimentally known stoichiometric crystal structures as described above. It should be noted that unlike conventional insulators where the Fermi energy can span the full range of the gap (Figure 1B), thus controlling the balance between different charges, if the Fermi energy resides inside a continuum band, as is the case in Figure 1A, it represents the energy to add or remove an electron from the host system, not from point defects in the gap. Thus, the conventional calculation of charged defects versus E_F is not meaningful in degenerate gapped materials.

DATA AND SOFTWARE AVAILABILITY

All data needed to evaluate the conclusions in the paper are present in the paper and the Supplemental Information. Additional data related to this paper may be requested from the authors.

SUPPLEMENTAL INFORMATION

Supplemental Information can be found online at https://doi.org/10.1016/j.matt.2019.05.014.

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AUTHOR CONTRIBUTIONS

O.I.M. carried out the theoretical calculations. M.T.Y. fabricated the samples and carried out structure analysis by X-ray powder diffraction. A.Z. directed the design of the research, analysis of the results, and writing of the paper. O.I.M. contributed most to writing of the paper, with contributions from all co-authors. K.R.P. supervised the experimental work. C.P. and A.Z. supervised all theoretical studies.

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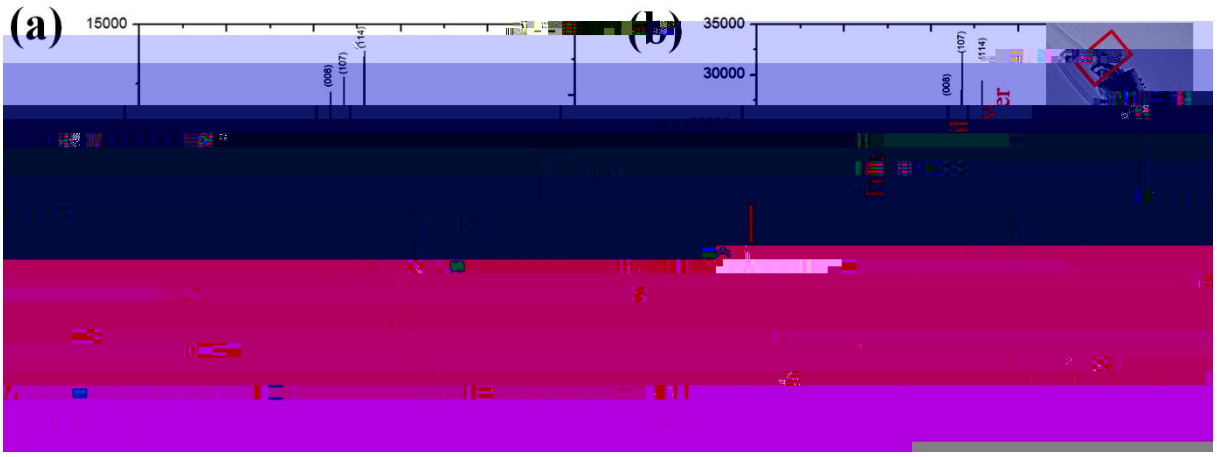

Ag formation in $Ag_3Al_{22}O_{34+x}$ under reduced atmosphere. (a) The powder X-ray diffrfacion of $Ag_3Al_{22}O_{34.5}$ can be indexed to the JCPDS reference pattern #01-084-0514, corresponding with the phase "$Ag_3Al_{22}O_{34}$" identified by Tofield .[3] (b) Any attempts to reduce $Ag_3Al_{22}O_{34.5}$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

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BaO_2

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Nb

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$Nb_{12}O_{29}$

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O O26 1 0.538262 0.452974 0.750090 1
O O27 1 0.832029 0.161325 0.250066 1
O O28 1 0.161138 0.830145 0.750093 1
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NbO_2

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NbO

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Nb_2O_5

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$Ba_9Nb_{10}O_{30}$

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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_
 _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  0.004334  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
```

$BaNb_7O_9$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   4.26656500
_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_
 _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  0.989408  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
```

$Ba_6Nb_2O_{11}$

```
_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_
```

$BaNb_5O_8$

```
_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_
 _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  0.999130  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_
```

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

$Ba_7Nb_6O_{21}$

_symmetry_space_group_name_H-M 'P 1'
_cell_length_a 17.17666038
_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

$Ba_2Nb_{15}O_{32}$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   7.92360186
_cell_length_b   7.92024685
_cell_length_c   36.45514839
_cell_angle_alpha   90.48688439
_cell_angle_beta   89.86379007
_cell_angle_gamma   119.87761907
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ba2Nb15O32
_chemical_formula_sum   'Ba6 Nb45 O96'
_cell_volume   1983.66548680
_cell_formula_units_Z   3
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
```

$BaNb_8O$

Nb Nb23 1 0.375709 0.421362 0.433591 1
Nb Nb24 1 0.875709 0.578638 0.066409 1
Nb Nb25 1 0.377054 0.927082 0.182378 1
Nb Nb26 1 0.877054 0.072918 0.317622 1
Nb Nb27 1 0.622946 0.572918 0.682378 1
Nb Nb28 1 0.122946 0.427082 0.817622 1
Nb Nb29 1 0.622946 0.072918 0.817622 1
Nb Nb30 1 0.122946 0.927082 0.682378 1
Nb Nb31 1 0.377054 0.427082 0.317622 1
Nb Nb32 1 0.877054 0.572918 0.182378 1
Nb Nb33 1 0.381809 0.161385 0.120165 1
Nb Nb34 1 0.881809 0.838615 0.379835 1
Nb Nb35 1 0.618191 0.338615 0.620165 1
Nb Nb36 1 0.118191 0.661385 0.879835 1
Nb Nb37 1 0.618191 0.838615 0.879835 1
Nb Nb38 1 0.118191 0.161385 0.620165 1
Nb Nb39 1 0.381809 0.661385 0.379835 1
Nb Nb40 1 0.881809 0.338615 0.120165 1
Nb Nb41 1 0.361827 0.185140 0.253526 1
Nb Nb42 1 0.861827 0.814860 0.246474 1
Nb Nb43 1 0.638173 0.314860 0.753526 1
Nb Nb44 1 0.138173 0.685140 0.746474 1
Nb Nb45 1 0.638173 0.814860 0.746474 1
Nb Nb46 1 0.138173 0.185140 0.753526 1
Nb Nb47 1 0.361827 0.685140 0.246474 1
Nb Nb48 1 0.861827 0.314860 0.253526 1
Nb Nb49 1 0.117159 0.159820 0.998594 1
Nb Nb50 1 0.617159 0.840180 0.501406 1
Nb Nb51 1 0.882841 0.340180 0.498594 1
Nb Nb52 1 0.382841 0.659820 0.001406 1
Nb Nb53 1 0.882841 0.840180 0.001406 1
Nb Nb54 1 0.382841 0.159820 0.498594 1
Nb Nb55 1 0.117159 0.659820 0.501406 1
Nb Nb56 1 0.617159 0.340180 0.998594 1
Nb Nb57 1 0.617001 0.834936 0.124067 1
Nb Nb58 1 0.117001 0.165064 0.375933 1
Nb Nb59 1 0.382999 0.665064 0.624067 1
Nb Nb60 1 0.882999 0.334936 0.875933 1
Nb Nb61 1 0.382999 0.165064 0.875933 1
Nb Nb62 1 0.882999 0.834936 0.624067 1
Nb Nb63 1 0.617001 0.334936 0.375933 1
Nb Nb64 1 0.117001 0.665064 0.124067 1
Nb Nb65 1 0.624232 0.076048 0.182918 1
Nb Nb66 1 0.124232 0.923952 0.317082 1
Nb Nb67 1 0.375768 0.423952 0.682918 1

Nb Nb70 1 0.875768 0.076048 0.682918 1
Nb Nb71 1 0.624232 0.576048 0.317082 1
Nb Nb72 1 0.124232 0.423952 0.182918 1
O O73 1 0.492806 0.746499 0.063384 1
O O74 1 0.992806 0.253501 0.436616 1
O O75 1 0.507194 0.753501 0.563384 1
O O76 1 0.007194 0.246499 0.936616 1
O O77 1 0.507194 0.253501 0.936616 1
O O78 1 0.007194 0.746499 0.563384 1
O O79 1 0.492806 0.246499 0.436616 1
O O80 1 0.992806 0.753501 0.063384 1
O O81 1 0.750463 0.910352 0.188317 1
O O82 1 0.250463 0.089648 0.311683 1
O O83 1 0.249537 0.589648 0.688317 1
O O84 1 0.749537 0.410352 0.811683 1
O O85 1 0.249537 0.089648 0.811683 1
O O86 1 0.749537 0.910352 0.688317 1
O O87 1 0.750463 0.410352 0.311683 1
O O88 1 0.250463 0.589648 0.188317 1
O O89 1 0.489415 0.751247 0.186705 1
O O90 1 0.989415 0.248753 0.313295 1
O O91 1 0.510585 0.748753 0.686705 1
O O92 1 0.010585 0.251247 0.813295 1
O O93 1 0.510585 0.248753 0.813295 1
O O94 1 0.010585 0.751247 0.686705 1
O O95 1 0.489415 0.251247 0.313295 1
O O96 1 0.989415 0.748753 0.186705 1
O O97 1 0.755704 0.912306 0.062871 1
O O98 1 0.255704 0.087694 0.437129 1
O O99 1 0.244296 0.587694 0.562871 1
O O100 1 0.744296 0.412306 0.937129 1
O O101 1 0.244296 0.087694 0.937129 1
O O102 1 0.744296 0.912306 0.562871 1
O O103 1 0.755704 0.412306 0.437129 1
O O104 1 0.255704 0.587694 0.062871 1
O O105 1 0.739808 0.153225 0.374913 1
O O106 1 0.239808 0.653225 0.874913 1
O O107 1 0.760192 0.346775 0.125087 1
O O108 1 0.260192 0.846775 0.625087 1

O O117 1 0.242748 0.842372 0.875237 1
O O118 1 0.742748 0.157628 0.624763 1
O O119 1 0.757252 0.657628 0.375237 1
O O120 1 0.257252 0.342372 0.124763 1
O O121 1 0.487412 0.018593 0.247209 1
O O122 1 0.987412 0.981407 0.252791 1
O O123 1 0.512588 0.481407 0.747209 1
O O124 1 0.012588 0.518593 0.752791 1
O O125 1 0.512588 0.981407 0.752791 1
O O126 1 0.012588 0.018593 0.747209 1
O O127 1 0.487412 0.518593 0.252791 1
O O128 1 0.987412 0.481407 0.247209 1
O O129 1 0.493081 0.238861 0.189072 1
O O130 1 0.993081 0.761139 0.310928 1
O O131 1 0.506919 0.261139 0.689072 1
O O132 1 0.006919 0.738861 0.810928 1
O O133 1 0.506919 0.761139 0.810928 1
O O134 1 0.006919 0.238861 0.689072 1
O O135 1 0.493081 0.738861 0.310928 1
O O136 1 0.993081 0.261139 0.189072 1
O O137 1 0.755456 0.161658 0.248569 1
O O138 1 0.255456 0.838342 0.251431 1
O O139 1 0.244544 0.338342 0.748569 1
O O140 1 0.744544 0.661658 0.751431 1
O O141 1 0.244544 0.838342 0.751431 1
O O142 1 0.744544 0.161658 0.748569 1
O O143 1 0.755456 0.661658 0.251431 1
O O144 1 0.255456 0.338342 0.248569 1
O O145 1 0.500000 0.000000 0.000000 1
O O146 1 0.000000 0.000000 0.500000 1
O O147 1 0.500000 0.500000 0.500000 1
O O148 1 0.000000 0.500000 0.000000 1
O O149 1 0.509289 0.253900 0.062752 1
O O150 1 0.009289 0.746100 0.437248 1
O O151 1 0.490711 0.246100 0.562752 1
O O152 1 0.990711 0.753900 0.937248 1
O O153 1 0.490711 0.746100 0.937248 1
O O154 1 0.990711 0.253900 0.562752 1
O O155 1 0.509289 0.753900 0.437248 1
O O156 1 0.009289 0.246100 0.062752 1
O O157 1 0.728666 0.181070 0.000347 1
O O158 1 0.228666 0.818930 0.499653 1
O O159 1 0.271334 0.318930 0.500347 1
O O160 1 0.771334 0.681070 0.999653 1
O O161 1 0.271334 0.818930 0.999653 1
O O162 1 0.771334 0.181070 0.500347 1
O O163 1 0.728666 0.681070 0.499653 1

O O70 1 0.498218 0.666480 0.801629 1
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

$Ba_3Nb_{16}O_{23}$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   4.23317500
_cell_length_b   12.66309700
_cell_length_c   21.30748300
_cell_angle_alpha   90.00022649
_cell_angle_beta   89.99923621
_cell_angle_gamma   89.99911484
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ba3Nb16O23
_chemical_formula_sum   'Ba6 Nb32 O46'
_cell_volume   1142.18987747
_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  0.996455  0.000016  0.999922  1
  Ba  Ba2  1  0.998217  0.500675  0.499959  1
  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
  Ba  Ba6  1  0.997053  0.500554  0.298517  1
  Nb  Nb7  1  0.496530  0.327557  0.999963  1
  Nb  Nb8  1  0.496431  0.672401  0.999930  1
  Nb  Nb9  1  0.498117  0.828310  0.499937  1
  Nb  Nb10  1  0.498101  0.173153  0.499946  1
  Nb  Nb11  1  0.996413  0.329049  0.101486  1
  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
  Nb  Nb15  1  0.998249  0.829577  0.601462  1
  Nb  Nb16  1  0.997913  0.171739  0.398416  1
  Nb  Nb17  1  0.998224  0.171674  0.601488  1
  Nb  Nb18  1  0.997933  0.829638  0.398422  1
  Nb  Nb19  1  0.496339  0.500063  0.100993  1
  Nb  Nb20  1  0.496685  0.500000  0.898893  1
  Nb  Nb21  1  0.498275  0.000672  0.601001  1
  Nb  Nb22  1  0.497889  0.000720  0.398895  1
```

O O70 1 0.998147 0.840694 0.699380 1
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
O O78 1 0.496845 0.500159 0.798815 1
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

$BaNb_2O_6$

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   5.96810002
_cell_length_b   8.06862644
```

O	O23	1	0.151045	0.967329	0.287092	1
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/F1 12 Tf5(3)7(2 )-6( )6(1)]TJETQ0.51912 f5BT/F1 12 Tf1 0 0 1 271.61 333.65 Tm0 g0 G[ )]TJETQEMC 21q
```

Nb

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

Ca_8Al_3

_symmetry_space_group_name_H-M 'P 1'

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Al Al22 1 0.323709 0.160161 0.974023 1

Al

Al

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CaAl$_4$

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_cell_angle_alpha   140.30519444
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_cell_angle_gamma   57.39019638
_symmetry_Int_Tables_number   1
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 _atom_site_occupancy
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$CaAl_2$

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_cell_angle_alpha   60.00000000
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_symmetry_Int_Tables_number   1
_chemical_formula_structural   CaAl2
_chemical_formula_sum   'Ca2 Al4'
_cell_volume   128.50812690
_cell_formula_units_Z   2
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CaO

$CaAl_4O_7$

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_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
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 _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
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O O23 1 0.829950 0.939148 0.072687 1
O O24 1 0.060852 0.170050 0.427313 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(156871 eW*nBT6( )61 098595.32 841.92 reW*nBT/F1 12 Tf1 0 0
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

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

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_cell_angle_gamma   90.00000000
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Al Al23 1 0.250000 0.378655 0.000000 1
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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

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

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_symmetry_Int_Tables_number   1
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  Ca  Ca2  1  0.250000  0.363106  0.500000  1
  Ca  Ca3  1  0.250000  0.887496  0.500000  1
  Ca  Ca4  1  0.250000  0.111280  -0.000000  1
  Ca  Ca5  1  0.995768  0.244617  0.633740  1
  Ca  Ca6  1  0.504232  0.244617  0.366260  1
  Ca  Ca7  1  0.500027  0.250835  0.885660  1
  Ca  Ca8  1  0.999973  0.250835  0.114340  1
  Ca  Ca9  1  0.634996  0.002980  0.253318  1
  Ca  Ca10  1  0.362710  0.498329  0.250523  1
  Ca  Ca11  1  0.887005  0.498802  0.251662  1
  Ca  Ca12  1  0.112268  0.000654  0.251396  1
  Ca  Ca13  1  0.750000  0.864140  -0.000000  1
  Ca  Ca14  1  0.750000  0.389214  -0.000000  1
  Ca  Ca15  1  0.750000  0.617536  0.500000  1
  Ca  Ca16  1  0.499919  0.750962  0.136514  1
  Ca  Ca17  1  0.000081  0.750962  0.863486  1
  Ca  Ca18  1  0.998442  0.752778  0.388771  1
  Ca  Ca19  1  0.501558  0.752778  0.611229  1
  Ca  Ca20  1  0.137290  0.498329  0.749477  1
  Ca  Ca21  1  0.865004  0.002980  0.746682  1
  Ca  Ca22  1  0.387732  0.000654  0.748604  1
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O O70 1 0.056162 0.651326 0.034493 1
O O71 1 0.444027 0.354197 0.541412 1
O O72 1 0.899168 0.692227 0.214141 1
O O73 1 0.605362 0.302827 0.713907 1
O O74 1 0.894638 0.302827 0.286093 1 Tf1 0 0 1 59.52 597.34 Tm0 g0 G[O 0n./F1 12 582.65 0 0 1 59.52 69
O O75 1 0.097627 0.195947 0.282170 1
O O76 1 0.463199 0.943609 0.148553 1
O O77 1 0.461067 0.052988 0.350196 1
O O78 1 0.038933 0.052988 0.649804 1
O O79 1 0.536002 0.443321 0.350402 1
O O80 1 0.216042 0.899422 0.694462 1
O O81 1 0.00008871 0 595.32 848841.92 reO8227 0.214141 1

Ag

AlAg

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5.3 8 van Berkel, F. P. F., Zandbergen, H. W., Verschoor, G. C., and IJdo, D. J. W., (1984), The structure of barium aluminate, $BaAl_{10.79}Mg_{1.01}O_{17.25}$. Acta r, ecr198