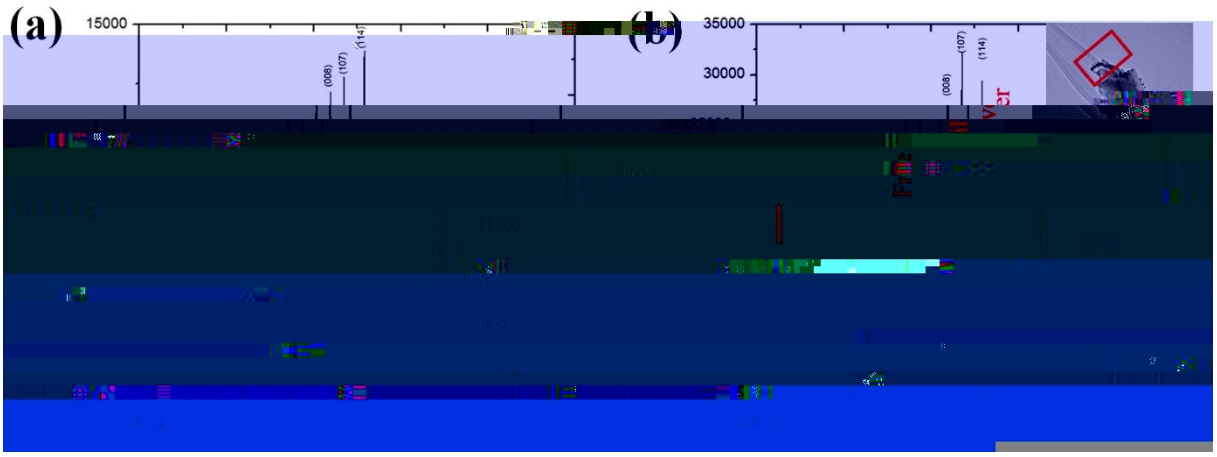

Ag formation in $Ag_3Al_{22}O_{34+x}$ under reduced atmosphere. (a) The powder X-ray diffrfacion of $Ag_3Al_{22}O_{34.5}$ can be indexed to the JCPDS reference pattern #01-084-0514, corresponding with the phase "$Ag_3Al_{22}O_{34}$" identified by Tofield .[3] (b) Any attempts to reduce $Ag_3Al_{22}O_{34.5}$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

Ba

_symmetry_space_group_name_H-M 'P 1'
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_cell_length_c 4.35636800
_cell_angle_alpha 109.47121581

BaO

_symmetry_space_group_name_H-M 'P 1'
_cell_length_a 5.61544600
_cell_length_b 5.61562200
_cell_length_c 5.61599000

BaO_2

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_cell_length_c   7.72989432
_cell_angle_alpha   64.10308353
_cell_angle_beta   64.10308353
_cell_angle_gamma   51.68671041
_symmetry_Int_Tables_number   1
_chemical_formula_structural   BaO2
_chemical_formula_sum   'Ba2 O4'
_cell_volume   104.19138075
_cell_formula_units_Z   2
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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
  Ba  Ba1  1  0.500535  0.499465  0.250000  1
  Ba  Ba2  1  0.499465  0.500535  0.750000  1
  O  O3  1  0.888579  0.895978  0.054472  1
  O  O4  1  0.104022  0.111421  0.445528  1
  O  O5  1  0.111421  0.104022  0.945528  1
  O  O6  1  0.895978  0.888579  0.554472  1
```

Nb

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   2.90286990
_cell_length_b   2.90286979
_cell_length_c   2.90286989
_cell_angle_alpha   109.47120777
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_cell_angle_gamma   109.47123504
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Nb
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 _atom_site_fract_y
 _atom_site_fract_z
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Nb_8O

```
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_cell_angle_gamma   89.99435529
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 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Nb  Nb1  1  0.502301  0.127693  0.383456  1
  Nb  Nb2  1  0.502376  0.868509  0.616799  1
  Nb  Nb3  1  0.002331  0.627667  0.116797  1
  Nb  Nb4  1  0.002086  0.368558  0.883454  1
  Nb  Nb5  1  0.502211  0.381333  0.129773  1
  Nb  Nb6  1  0.502231  0.614875  0.870486  1
  Nb  Nb7  1  0.002441  0.114851  0.629711  1
  Nb  Nb8  1  0.002202  0.881324  0.370550  1
  Nb  Nb9  1  0.501894  0.651434  0.346653  1
  Nb  Nb10  1  0.501875  0.344707  0.653627  1
  Nb  Nb11  1  0.002629  0.151361  0.153523  1
  Nb  Nb12  1  0.002765  0.844838  0.846713  1
  Nb  Nb13  1  0.502983  0.880124  0.118046  1
  Nb  Nb14  1  0.502987  0.116100  0.882237  1
  Nb  Nb15  1  0.001753  0.380053  0.382178  1
  Nb  Nb16  1  0.001461  0.616152  0.618093  1
  O  O17  1  0.501405  0.498093  0.500170  1
  O  O18  1  0.003083  0.998097  0.000129  1
```

$Nb_{12}O_{29}$

```
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_cell_length_c   29.49183109
_cell_angle_alpha   89.99362541
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Nb Nb24 1 0.352774 0.648138 0.684530 1
O O25 1 0.454811 0.538502 0.250094 1
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
O O29 1 0.649067 0.346411 0.250103 1
O O30 1 0.345526 0.646439 0.750057 1

O O70 1 0.638284 0.351434 0.679804 1
O O71 1 0.742572 0.252292 0.179970 1
O O72 1 0.252602 0.740888 0.820121 1
O O73 1 0.741039 0.250981 0.320149 1
O O74 1 0.249942 0.738497 0.680013 1
O O75 1 0.146809 0.848400 0.176342 1
O O76 1 0.847834 0.144389 0.823827 1
O O77 1 0.145864 0.847598 0.32389( )]TJETQ0.000008871 0 595.32 841.92 reW*nBT/F1 12 Tf1 0 0 1 59.52 7

NbO_2

```
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  Nb  Nb2  1  0.720519  0.487464  0.243637  1
  Nb  Nb3  1  0.970489  0.740168  0.513078  1
  Nb  Nb4  1  0.970526  0.256885  0.490994  1
  Nb  Nb5  1  0.220589  0.009600  0.260422  1
  Nb  Nb6  1  0.220551  0.987414  0.743636  1
  Nb  Nb7  1  0.470541  0.240130  0.013076  1
  Nb  Nb8  1  0.470561  0.756929  0.990968  1
  Nb  Nb9  1  0.272387  0.487437  0.743672  1
  Nb  Nb10  1  0.272456  0.509582  0.260428  1
  Nb  Nb11  1  0.522316  0.756880  0.490915  1
  Nb  Nb12  1  0.522391  0.240125  0.513125  1
  Nb  Nb13  1  0.772464  0.987470  0.243659  1
  Nb  Nb14  1  0.772463  0.009579  0.760395  1
  Nb  Nb15  1  0.022443  0.256933  0.990972  1
  Nb  Nb16  1  0.022475  0.740096  0.013068  1
  O  O17  1  0.741175  0.150235  0.900689  1
  O  O18  1  0.741180  0.846734  0.103422  1
  O  O19  1  0.991149  0.599667  0.153544  1
  O  O20  1  0.991054  0.397369  0.850494  1
  O  O21  1  0.240954  0.650282  0.400679  1
  O  O22  1  0.241072  0.346716  0.603442  1
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O	O23	1	0.491071	0.099715	0.653686	1
O	O24	1	0.491115	0.897280	0.350364	1
O	O25	1	0.756096	0.362104	0.611880	1
O	O26	1	0.756078	0.635087	0.392008	1
O	O27	1	0.006150	0.888958	0.365898	1
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_gamma   89.97714155
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_chemical_formula_structural   NbO
_chemical_formula_sum   'Nb3 O3'
_cell_volume   78.57824324
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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
```

Nb_2O_5

```
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_cell_angle_alpha   64.37219889
_cell_angle_beta   90.00103500
_cell_angle_gamma   90.00214144
_symmetry_Int_Tables_number   1
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_chemical_formula_sum   'Nb28 O70'
_cell_volume   1446.69434171
_cell_formula_units_Z   14
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 _atom_site_fract_x
 _atom_site_fract_y
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 _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
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  Nb  Nb22  1  0.984298  0.844413  0.432737  1
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O O71 1 0.996472 0.086485 0.804171 1
O O72 1 0.498953 0.501014 0.272165 1

O	O23	1	0.002169	0.749996	0.755711	1
O	O24	1	0.248539	0.253625	0.005544	1
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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
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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	Ba23	1	0.999850	0.333520	0.670661	1
Ba	Ba24	1	0.999809	0.668282	0.003186	1
Ba	Ba25	1	0.999880	0.668330	0.335765	1
Ba	Ba26	1	0.999880	0.668363	0.670635	1
Nb	Nb27	1	0.167677	0.165627	0.167949	1
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
Nb	Nb31	1	0.165949	0.500925	0.503229	1
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
Nb	Nb35	1	0.167709	0.836220	0.838470	1
Nb	Nb36	1	0.497141	0.165603	0.167886	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
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O O125 1 0.499038 0.667688 0.836537 1
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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

$Ba_9Nb_{10}O_{30}$

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
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$Ba_2Nb_5O_9$

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 _atom_site_occupancy
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  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
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$BaNb_7O_9$

```
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_cell_angle_gamma   90.00029533
_symmetry_Int_Tables_number   1
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_cell_volume   229.93753073
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 _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.[illegible]  0.[illegible]  0.[illegible]  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
```

$BaNb_5O_8$

```
_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_
 _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
```

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
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$BaNb_8O$

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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
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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
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Nb Nb66 1 0.124232 0.923952 0.317082 1
Nb Nb67 1 0.375768 0.423952 0.682918 1
Nb Nb68 1 0.875768 0.576048 0.817082 1
Nb Nb69 1 0.375768 0.923952 0.817082 1

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Nb Nb71 1 0.624232 0.576048 0.317082 1
Nb Nb72 1 0.124232 0.423952 0.182918 1
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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
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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
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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 O164 1 0.228666 0.318930 0.000347 1
O O165 1 0.241464 0.083710 0.061080 1
O O166 1 0.741464 0.916290 0.438920 1
O O167 1 0.758536 0.416290 0.561080 1
O O168 1 0.258536 0.583710 0.938920 1
O O169 1 0.758536 0.916290 0.938920 1
O O170 1 0.258536 0.083710 0.561080 1
O O171 1 0.241464 0.583710 0.438920 1
O O172 1 0.741464 0.416290 0.061080 1
O O173 1 0.258178 0.095366 0.188295 1
O O174 1 0.758178 0.904634 0.311705 1
O O175 1 0.741822 0.404634 0.688295 1
O O176 1 0.241822 0.595366 0.811705 1
O O177 1 0.741822 0.904634 0.811705 1
O O178 1 0.241822 0.095366 0.688295 1
O O179 1 0.258178 0.595366 0.311705 1
O O180 1 0.758178 0.404634 0.188295 1
O O181 1 0.000000 0.000000 0.000000 1
O O182 1 0.500000 0.000000 0.500000 1
O O183 1 0.000000 0.500000 0.500000 1
O O184 1 0.500000 0.500000 0.000000 1

$Ba_4Nb_{14}O_{23}$

```
_symmetry_space_group_name_H-M   'P 1'
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_cell_length_b   12.66576800
_cell_length_c   21.13886408
_cell_angle_alpha   89.65959083
_cell_angle_beta   90.00121860
_cell_angle_gamma   90.00008583
_symmetry_Int_Tables_number   1
_chemical_formula_structural   Ba4Nb14O23
_chemical_formula_sum   'Ba8 Nb28 O46'
_cell_volume   1129.57945662
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
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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
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

$Ba_3Nb_{16}O_{23}$

```
_symmetry_space_group_name_H-M   'P 1'
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_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
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 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
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  0.996455  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
```

Nb Nb23 1 0.496437 0.168853 0.101008 1
Nb Nb24 1 0.496710 0.831285 0.898868 1
Nb Nb25 1 0.496358 0.831349 0.100976 1
Nb Nb26 1 0.496754 0.168813 0.898884 1
Nb Nb27 1 0.498231 0.669383 0.600995 1
Nb Nb28 1 0.497885 0.331937 0.398895 1
Nb Nb29 1 0.498239 0.331871 0.601020 1
Nb Nb30 1 0.497859 0.669433 0.398892 1
Nb Nb31 1 0.496523 0.333144 0.195068 1
Nb Nb32 1 0.496950 0.667309 0.804871 1
Nb Nb33 1 0.496462 0.667417 0.195000 1
Nb Nb34 1 0.496925 0.333058 0.804840 1
Nb Nb35 1 0.498105 0.833343 0.695003 1
Nb Nb36 1 0.497702 0.167694 0.304832 1
Nb Nb37 1 0.498172 0.167602 0.695061 1
Nb Nb38 1 0.497642 0.833421 0.304867 1
O O39 1 0.496433 0.499956 0.999942 1
O O40 1 0.498196 0.000749 0.499950 1
O O41 1 0.996507 0.333567 0.999954 1
O O42 1 0.996446 0.666368 0.999930 1
O O43 1 0.998130 0.834333 0.499944 1
O O44 1 0.998141 0.167154 0.499951 1
O O45 1 0.996358 0.500087 0.096401 1
O O46 1 0.996677 0.500027 0.903489 1
O O47 1 0.998288 0.000644 0.596403 1
O O48 1 0.997926 0.000701 0.403492 1
O O49 1 0.496567 0.159192 0.999953 1
O O50 1 0.496442 0.840765 0.999920 1
O O51 1 0.498169 0.659947 0.499941 1
O O52 1 0.498161 0.341515 0.499959 1
O O53 1 0.996449 0.161059 0.099220 1
O O54 1 0.996720 0.839060 0.900733 1
O O55 1 0.996365 0.839123 0.099095 1
O O56 1 0.996770 0.161009 0.900711 1
O O57 1 0.998246 0.661604 0.599125 1
O O58 1 0.997907 0.339730 0.400707 1
O O59 1 0.998251 0.339663 0.599212 1
O O60 1 0.997879 0.661663 0.400743 1
O O61 1 0.496739 0.165962 0.199695 1
O O62 1 0.497209 0.834420 0.800171 1
O O63 1 0.496673 0.834538 0.199679 1
O O64 1 0.497274 0.165880 0.800204 1
O O65 1 0.497952 0.666216 0.699692 1
O O66 1 0.497599 0.334881 0.300211 1
O O67 1 0.497942 0.334778 0.699700 1
O O68 1 0.497480 0.666300 0.300186 1
O O69 1 0.997713 0.160509 0.300507 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'
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_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
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 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
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 _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
```

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

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_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
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  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

Al

Al

```
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_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
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 _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
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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
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 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
```

$CaAl_2$

```
_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
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loop_
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CaO

$CaAl_4O_7$

```
_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_
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 _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 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
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_cell_angle_alpha   109.47122063
_cell_angle_beta   109.47122063
```

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_length_b   12.08491300
_cell_length_c   12.15689086
_cell_angle_alpha   90.00000000
_cell_angle_beta   89.95748726
_cell_angle_gamma   90.00000000
_symmetry_Int_Tables_number   1
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_chemical_formula_sum   'Ca22 Al28 O64'
_cell_volume   1769.50007290
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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

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

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  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
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  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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1. Zhang, X., Zhang, L., Perkins, J. D., and Zunger, A., (2015), Intrinsic transparent conductors without doping. Phys. Rev. Lett., 115, 176602.
2. Kummer, J. T., (1972), β-Alumina electrolytes. Prog. Solid State Chem., 7, 141-175.2 7
3. England, W. A., Jacobson, A. J., and Tofield, B. C., (1982), Structural studies of highly non-stoichiometric polycrystalline sodium and silver beta-aluminas. Solid State Ion., 6, 21-27.
4. Iyi, N., Inoue, Z., and Kimura, S., (1986), The crystal structure of highly nonstoichiometric potassium β-alumina, $K_{1.50}Al_{11.0}O_{17.25}$. J. Solid State Chem., 61, 81-89.
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