

Ag formation in $\text{Ag}_3\text{Al}_{22}\text{O}_{34+x}$ under reduced atmosphere. (a) The powder X-ray diffraction of $\text{Ag}_3\text{Al}_{22}\text{O}_{34.5}$ can be indexed to the JCPDS reference pattern #01-084-0514, corresponding with the phase " $\text{Ag}_3\text{Al}_{22}\text{O}_{34}$ " identified by Tofield³. (b) Any attempts to reduce $\text{Ag}_3\text{Al}_{22}\text{O}_{34.5}$ and introduce carriers results in the precipitation of free metallic silver and the possible formation of $\text{Ag}_{2.5}\text{Al}_{22}\text{O}_{34.25}$.

Ba

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_cell_length_b 4.35636704
_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

BaO₂

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1 'x, y, z'
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_atom_site_fract_x
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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

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Nb₈O

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_atom_site_occupancy
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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

Nb₁₂O₂₉

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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 070 1 0.638284 0.351434 0.679804 1
O 071 1 0.742572 0.252292 0.179970 1
O 072 1 0.252602 0.740888 0.820121 1
O 073 1 0.741039 0.250981 0.320149 1
O 074 1 0.249942 0.738497 0.680013 1
O 075 1 0.146809 0.848400 0.176342 1
O 076 1 0.847834 0.144389 0.823827 1
O 077 1 0.145864 0.847598 0.32389()JTJET@0.000008871 0 595.32 841.92 reW*BT/F1 12 Tf1 0 0 1 59.52 7

NbO₂

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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
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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

O 023 1 0.491071 0.099715 0.653686 1
O 024 1 0.491115 0.897280 0.350364 1
O 025 1 0.756096 0.362104 0.611880 1
O 026 1 0.756078 0.635087 0.392008 1
O 027 1 0.006150 0.888958 0.365898 1
O 028 1 0.006125 0.108100 0.638169 1
O 029 1 0.256071 0.862216 0.111769 1
O 030 1 0.255937 0.134902 0.892191 1
O 031 1 0.506085 0.388753 0.865734 1
O 032 1 0.505954 0.608185 0.138238 1
O 033 1 0.236968 0.362047 0.111990 1
O 034 1 0.236980 0.634862 0.892207 1
O 035 1 0.487004 0.388982 0.365957 1
O 036 1 0.486886 0.608057 0.638125 1
O 037 1 0.736760 0.862152 0.611815 1
O 038 1 0.736735 0.134877 0.392233 1
O 039 1 0.986987 0.888783 0.865719 1
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O 041 1 0.501930 0.099700 0.153588 1
O 042 1 0.501896 0.897331 0.850414 1
O 043 1 0.751882 0.346835 0.103318 1
O 044 1 0.751779 0.650199 0.900709 1
O 045 1 0.001783 0.599713 0.653569 1
O 046 1 0.001784 0.397365 0.350534 1
O 047 1 0.251897 0.846721 0.603355 1
O 048 1 0.251917 0.150367 0.400629 1

NbO

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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

Nb₂O₅

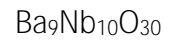
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Nb Nb3 1 0.005453 0.004647 0.763546 1
Nb Nb4 1 0.984459 0.156122 0.566579 1
Nb Nb5 1 0.001231 0.693061 0.628814 1
Nb Nb6 1 0.004717 0.995881 0.235761 1
Nb Nb7 1 0.998223 0.152055 0.302579 1
Nb Nb8 1 0.498459 0.734115 0.839873 1
Nb Nb9 1 0.999145 0.316040 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

O 070 1 0.995534 0.914039 0.195169 1
O 071 1 0.996472 0.086485 0.804171 1
O 072 1 0.498953 0.501014 0.272165 1

O 023 1 0.002169 0.749996 0.755711 1
O 024 1 0.248539 0.253625 0.005544 1
O 025 1 0.252281 0.249588 0.505538 1
O 026 1 0.248412 0.746074 0.005525 1
O 027 1 0.252495 0.750109 0.505533 1
O 028 1 0.755781 0.253719 0.005523 1
O 029 1 0.752092 0.249495 0.505519 1
O 030 1 0.755963 0.745978 0.005511 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

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O 0120 1 0.499018 0.334114 0.169756 1
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O 0122 1 0.499014 0.334154 0.836580 1
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O 034 1 0.449866 0.399685 0.249370 1
O 035 1 0.549318 0.600288 0.750191 1
O 036 1 0.304851 0.101130 0.999421 1
O 037 1 0.399448 0.299779 0.499587 1
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O 041 1 0.349983 0.199847 0.749609 1
O 042 1 0.100611 0.694219 0.999745 1
O 043 1 0.199869 0.899685 0.499649 1
O 044 1 0.050663 0.101495 0.745160 1
O 045 1 0.349615 0.699505 0.249469 1
O 046 1 0.049753 0.600130 0.250316 1
O 047 1 0.152045 0.796380 0.745679 1
O 048 1 0.999696 0.499919 0.499805 1
O 049 1 0.152319 0.304752 0.253419 1

Ba₂Nb₅O₉

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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

Ba₆Nb₂O₁₁

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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

BaNb₅O₈

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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

Ba₄Nb₂O₉

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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
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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

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Ba₇Nb₆O₂₁

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Ba₂Nb₁₅O₃₂

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Nb	Nb26	1	0.877054	0.072918	0.317622	1
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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
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Nb	Nb35	1	0.618191	0.338615	0.620165	1
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Nb	Nb37	1	0.618191	0.838615	0.879835	1
Nb	Nb38	1	0.118191	0.161385	0.620165	1
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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
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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
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Ba₄Nb₁₄O₂₃

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O 072 1 0.498238 0.333700 0.802139 1
O 073 1 0.498468 0.997286 0.595980 1
O 074 1 0.498475 0.001069 0.404219 1
O 075 1 0.498016 0.497162 0.095988 1
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O 079 1 0.498341 0.837641 0.499571 1
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Ba₃Nb₁₆O₂₃

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Ba Ba3 1 0.997041 0.000301 0.201349 1
Ba Ba4 1 0.997601 0.000231 0.798534 1
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Ba Ba6 1 0.997053 0.500554 0.298517 1
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Nb Nb11 1 0.996413 0.329049 0.101486 1
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Nb Nb13 1 0.996320 0.671150 0.101449 1
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Nb Nb15 1 0.998249 0.829577 0.601462 1
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O O41 1 0.996507 0.333567 0.999954 1
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O 082 1 0.496696 0.000053 0.896717 1
O 083 1 0.498494 0.500621 0.603133 1
O 084 1 0.497931 0.500669 0.396786 1

BaNb₂O₆

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O 025 1 0.654909 0.464715 0.213837 1
O 026 1 0.154757 0.532969 0.285507 1
O 027 1 0.352448 0.533061 0.785473 1
O 028 1 0.852428 0.464696 0.713819 1
O 029 1 0.494506 0.249297 0.647454 1
O 030 1 0.994630 0.748378 0.851843 1
O 031 1 0.512485 0.748482 0.351825 1
O 032 1 0.012747 0.249300 0.147375 1
O 033 1 0.613995 0.749793 0.637868 1
O 034 1 0.113981 0.247912 0.861271 1
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Ba₃Nb₅O₁₅

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1 'x, y, z'

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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

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O 041 1 0.496963 0.858115 0.067794 1
O 042 1 0.497166 0.139711 0.930815 1
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Ca₈Al₃

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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  
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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  
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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
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CaAl₄

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CaAl₂

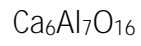
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CaO

CaAl₄O₇

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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  
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O O12 1 0.637289 0.748638 0.920266 1  
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AI AI26 1 0.965857 0.965857 0.965857 1
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O O28 1 0.867850 0.500000 0.000000 1
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Ca₁₁Al₁₄O₃₂

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O	O58	1	0.066420	0.068541	0.064401	1
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O	O61	1	0.650831	0.034504	0.055681	1
O	O62	1	0.349081	0.534514	0.444171	1
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O	O66	1	0.194720	0.286557	0.100521	1
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Ca₂₃Al₂₈O₆₄

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O 073 1 0.605362 0.302827 0.713907 1
O 074 1 0.894638 0.302827 0.286093 1 Tf1 0 0 1 59.52 597.34 Tm0 g0 G(O On./F1 12 582.65 0 0 1 59.52 6
O 075 1 0.097627 0.195947 0.282170 1
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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), γ -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.
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- 5.3 Van Berkel, F. P. F., Zandbergen, H. W., Verschoor, G. C., and Jdo., D. J. W., (1984), The structure of barium aluminate $Ba_{0.95}Al_{11}O_{17.25}$. *Acta r, ecr198*