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Structural Investigation of K^+ and Tl^+ β-Aluminas

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Structures of K^+ and Tl^+ aluminas were investigated by single-crystal X-ray diffraction. In the final refinements, corresponding to R values of 0.034 and 0.058, respectively, the distribution of conducting ions was found to be similar to that of Na β-alumina. In K^+ β-alumina clear evidence of additional electronic density in the spinel-like blocks is obtained and is interpreted as due to a Frenkel defect.

Introduction

β-Alumina compounds are double oxides with the general formula nA_2O_3–B_2O where

$$A = Al^{3+}, Ga^{3+}, Fe^{3+},$$
$$B = Na^+, Ag^+, K^+, Rb^+, Tl^+.$$

The structure has hexagonal symmetry (space group $P6_3/mmc$). The outstanding feature is the stacking of close-packed spinel blocks separated by mirror planes perpendicular to the c axis and containing B^+ ions (*1*, *2*).

The great interest in these compounds arises from their very high ionic conductivity in the solid state, which allows them to be put among superionic conductors (*3*). This conductivity is due to the diffusion of B^+ ions in the intermediate conduction planes; major questions to be answered concern the origin of the temperature dependance of their electrical properties and their variation with regard to temperature. An X-ray diffuse scattering investigation of the distribution conducting ions (*4–6*) revealed the existence of two-dimensional ordered microdomains, the size of which varies with temperature and cation type

For silver β-alumina, the average distribution of electron density in the mirror planes, obtained by X-ray diffraction study (*7*), allowed a semiquantitative analysis of diffuse intensities and gave a description of cation distribution within the microdomains (*8*).

To account for the variations in the scattered intensity distribution (related to local order changes) which are observed for different types of B^+ ions and preparation conditions (*5*, *6*), it is necessary to have a good knowledge of the mean structures of those different compounds.

This paper reports an X-ray diffraction investigation of the nature and mean occupancy factors of the sites occupied by conducting ions in potassium and thallium β-aluminas.

Experimental

Sodium β-alumina crystals are obtained by the slow cooling of a melt heated by direct induction at high frequency through the oxide (Kyropoulos self-crucible method). Their composition, deduced from neutron activation analysis, is about 11 Al_2O_3–1.3 ± 0.03 Na_2O. Replacement of Na^+ by K^+ or Tl^+ is obtained by an exchange reaction in molten salts (*9*).

β-alumina single crystals grow in the shape of easily cleavable thin platelets. The choice of

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crystals for structural determination was made according to the quality of diffraction spots observed. In both studies, intensities were measured on a $P2_1$ Syntex four-circle diffractometer, between $2\theta = 0$ to 65°, using Mo$K\alpha$ radiation with a graphite monochromator. A standard reflection was measured every 30 reflections. For each crystal, data was collected in a section of reciprocal space where h, k, and l were all >0, and equivalent reflections were averaged.

Absorption corrections were needed for crystals in platelet form (especially for Tl^+). They were performed with the ψ scan technique using 15 reflections.

Refinement was done according to the ORXFLS III routine (*10*) with all the measured intensities (even zero values) by using Na β-alumina as starting positional parameters (*11*).

Refinement of K β-Alumina Structure

The single crystal of K β-alumina had a triangular shape (350 μm for the side and 150 μm for thickness). The lattice constants of the hexagonal cell have the following values: $a = 5.602$ Å, $c = 22.734$ Å. Four hundred and ninety-four independent reflections were collected on the four-circle diffractometer. The first cycles of refinement using all the variable parameters—scale factor, positional parameters, occupancy, and individual temperature factors in the intermediate planes—revealed very high terms in the correlation matrix. Therefore we employed the least number of variable parameters in the refinements.

In the first step, the scale factor, general temperature factor, and occupancy coefficient of potassium atoms located in the Beevers–Ross (BR) and mid-oxygen (mO) positions were refined (Fig. 1).

The successive cycles indicated that:

1. some K^+ ions were located on the anti-Beevers–Ross (aBR) site,
2. some interstitial aluminum was found on the position previously mentioned by Reidinger *et al.* for Na β-alumina (*12*) (Fig. 2),
3. all atoms were, more or less, shifted out of the theoretical positions BR, mO, and

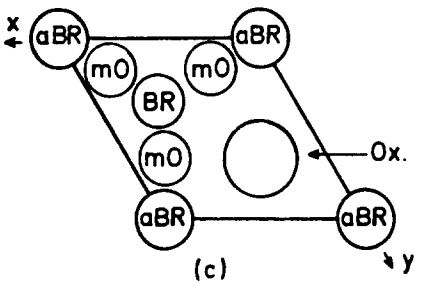
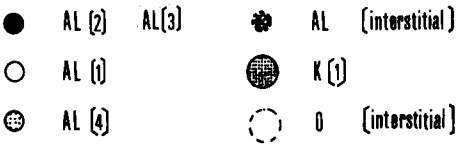


FIG. 1. Simplified site model with the conventional site denomination. BR = Beevers–Ross, aBR = anti-Beevers–Ross, mO = mid-oxygen.

aBR, and the same thing occurred for O (5) in the plane.

We then froze the scale factor and refined the occupancy coefficients of aluminum atoms in the spinel blocks together with the occupancy factors of potassium atoms, interstitial Al, and the general temperature factor. This showed that the Al_1 position was partly vacant and on the other positions the variations were within the error limits.

In the next step, refinements were attempted alternatively either on individual isotropic temperature factors or on occupancy factors,



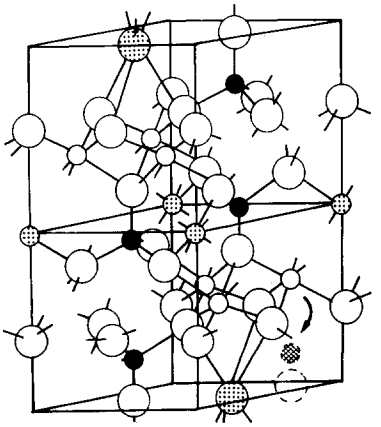


FIG. 2. Frenkel defect on K^+ β-alumina.

TABLE I

POTASSIUM β-ALUMINA: POSITION AND THERMAL PARAMETERS

	Position	Number per unit cells	$x \times 10^4$	$z \times 10^4$	$\beta_{11} \times 10^5$	$\beta_{22} \times 10^5$	$\beta_{33} \times 10^5$	$\beta_{13} \times 10^5$	B
Al (1)	12(*k*)	11.50 (3)	8322 (1)	1052 (1)	819 (23)	743 (31)	38 (1)	3 (3)	
Al (2)	4(*f*)	4	3333	245 (1)	676 (32)	β_{11}	34 (1)	0	
Al (3)	4(*f*)	4	3333	1749 (1)	1034 (36)	β_{11}	31 (2)	0	
Al (4)	2(*a*)	2	0	0	773 (46)	β_{11}	30 (3)	0	
Al interstitial	12(*k*)	0.36 (2)	8380 (28)	1750 (10)					0.2 (2)
O (1)	12(*k*)	12	1571 (2)	496 (1)	880 (52)	718 (74)	38 (3)	−6 (7)	
O (2)	12(*k*)	12	5027 (2)	1454 (1)	721 (48)	792 (70)	46 (3)	−8 (7)	
O (3)	4(*f*)	4	6666	552 (2)	758 (79)	β_{11}	37 (5)	0	
O (4)	4(*e*)	4	0	1411 (2)	670 (74)	β_{11}	41 (5)	0	
O (5)	6(*h*)	2	3151 (10)	2500	1400 (220)	1060 (454)	32 (8)	0	
K (3)	6(*h*)	0.28 (1)	9707 (22)	2500					0.8 (2)
K (2)	6(*h*)	0.75 (1)	8824 (9)	2500	1995 (186)	3218 (365)	29 (8)	0	
K (1)	6(*h*)	1.56 (1)	6887 (3)	2500	1347 (72)	1352 (68)	48 (3)	0	

TABLE II

THALLIUM β-ALUMINA: POSITION AND THERMAL PARAMETERS

	Position	Number per unit cell	$x \times 10^4$	$z \times 10^4$	$\beta_{11} \times 10^5$	$\beta_{22} \times 10^5$	$\beta_{33} \times 10^6$	$\beta_{13} \times 10^6$
Al (1)	12(*k*)	12	8324 (3)	1042 (2)	795 (72)	715 (94)	440 (40)	10 (80)
Al (2)	4(*f*)	4	3333	246 (2)	610 (98)	β_{11}	350(60)	0
Al (3)	4(*f*)	4	3333	1748 (2)	845 (103)	β_{11}	250 (60)	0
Al (4)	2(*a*)	2	0	0	691 (132)	β_{11}	270 (80)	0
O (1)	12(*k*)	12	1577 (6)	488 (2)	594 (138)	582 (201)	310 (70)	260 (180)
O (2)	12(*k*)	12	5021 (6)	1437 (2)	649 (137)	437 (184)	440 (80)	50 (180)
O (3)	4(*f*)	4	6666	548 (4)	628 (216)	β_{11}	250 (140)	0
O (4)	4(*e*)	4	0	1397 (4)	483 (201)	β_{11}	300 (140)	0
O (5)	6(*h*)	2	3333	2500	2613 (536)	β_{11}	90 (210)	
Tl (1)	6(*h*)	1.75 (2)	6807 (32)	2500	2246 (308)	2649 (765)	630 (20)	0
Tl (2)	6(*h*)	0.51 (2)	9099 (15)	2500	2630 (283)	5367 (746)	300 (90)	0
Tl (3)	2(*b*)	0.21 (2)	0	2500	3397 (585)	β_{11}	250 (140)	0

the general scale factor being fixed; then complete convergence was reached ($R = 0.040$). The very last attempt was to refine anisotropic temperature factors; a final R value of 0.034 was obtained, corresponding to the values gathered in Table I.

The last refinement cycle dealing with all the variable parameters brought no meaningful difference in the values of structural parameters and confirmed the reliability of the results.

Description of the Structure

(*a*) *Spinel blocks.* As pointed out by Reidinger, a partial occupation of the interstitial tetrahedral Al site is noticed. For this atom only a very weak thermal coefficient is obtained; thus if the partial occupation of this position is firmly established, the absolute value of the occupancy factor is not known with precision. But we observed that this occupancy factor is nearly identical to the lack of

TABLE III

COMPONENTS OF PRINCIPAL AMPLITUDES OF THERMAL VIBRATION OF ATOMS IN POTASSIUM β-ALUMINA, AND IN THALLIUM β-ALUMINA[a]

Atoms in the mirrorplane	$(\bar{U}_{11}^2)^{1/2}$ (Å)	(Å)	$(\bar{U}_{22}^2)^{1/2}$ (Å)
K(1)	0.127	0.127	0.112
K(2)	0.154	0.196	0.087
Tl(1)	0.163	0.177	0.129
Tl(2)	0.177	0.253	0.089
Tl(3)	0.201	0.201	0.082

[a] $\bar{U}_{11}$, $\bar{U}_{22}$, $\bar{U}_{33}$ are the root mean square deplacements of the vibration parallel to a*, b*, and c*.

aluminum in the Al (1) site, and this is consistent with the hypothesis of a Frenkel-type defect within the spinel blocks (Fig. 2).

(*b*) *Mirror planes.* All three possible cationic sites (BR, mO, aBR) are simultaneously occupied (but partly), and the refinement did not reveal a lack of oxygen in the O (5) position.

No pronounced anisotropy is detected for the atoms in the conducting plane (Table III).

The final formula may be written as follows:

$$Al_{21.86(5)}K_{2.59(3)}O_{34},$$

i.e., 68.17 positive charges for 68 negative ones. This formula is not accurate enough to confirm the charge compensation model, by in-

TABLE IV

INTERATOMIC DISTANCES

	Number of bonds	K β-Al_2O_3 (Å)	Tl β-Al_2O_3 (Å)
Octahedra			
Al(1)–O(1)	2	2.023	2.025
–O(2)	2	1.841	1.840
–O(3)	1	1.968	1.965
–O(4)	1	1.823	1.817
Al(4)–O(1)	6	1.896	1.895
Tetrahedra			
Al(2)–O(1)	3	1.802	1.791
–O(3)	1	1.811	1.819
Al(3)–O(2)	3	1.775	1.784
–O(5)	1	1.716	1.723
Al(interstitial)–O(1)	2	1.762	
–O(4)	1	1.751	
–O[a]	1	1.758	
Polyhedron 9-coordinated			
K(1) or Tl(1)–O(2)	2	2.810	2.876
–O(2)	2	2.810	2.876
–O(2)	2	2.986	2.988
–O(5)	3(average of three)	3.192	3.232
Polyhedron 8-coordinated			
K(2) or Tl(2)–O(5)	2(average of three)	2.841	2.895
–O(4)	2	2.727	2.673
–O(2)	4	3.040	3.205
Polyhedron 9-coordinated			
K(3) or Tl(3)–O(4)	2	2.493	2.527
–O(5)	3	3.243	3.231
–O(2)	4	3.492	

[a] Interstitial oxygen located in the mid-oxygen position.

terstitial oxygen on mid-oxygen positions, that would be suggested by a Frenkel defect in the blocks.

Three outstanding differences are to be noticed in regard to Dernier and Remeika's (D.R.) paper (*13*):

1. the presence, in our crystal, of interstitial aluminium,

2. the occupation of the aBR position, as in previously described alumina structures (7, 8, 12, 14),

3. and a noticeable difference in the occupancy rate of K atoms.

	D.R.	This work
BR	1.42 (2)	1.56 (1)
mO	1.22 (2)	0.75 (1)
aBR	0.0	0.28 (1)
	2.64 (4)	2.59 (3)

The total amount of potassium in both cases is very similar; there is in fact a different distribution between the positions.

The divergence between Remeika's and our results is presumably due to different preparation conditions: our crystals were obtained at higher temperatures than those of Dernier and Remeika, which were prepared by flux method; in our method, the occupation of aBR sites is favored, in which the environment of the potassium ion is less favorable (K (3)–O (4) distances are short), (Table IV).

Refinement of the Tl β-Alumina Structure

The lattice constants are: $a = 5.596$ Å, $c = 22.912$ Å. Four hundred ninety-nine independent reflections were collected. (Tables V and VI). The refinement was performed in the same way as in K^+ β-alumina.

No interstitial aluminum was detected in the spinel blocks, probably because the corresponding electron density was too low in relation to that of Tl atoms.

The final value of the R parameter was 0.058 corresponding to the parameters of Table II.

Discussion

Here again we find simultaneous partial occupation of the three possible cationic sites in the conducting planes; these positions are all slightly shifted off the theoretical ones.

The main differences with a recent paper of Kodama and Muto (K.M.) (*14*) are:

1. First, no negative thermal coefficient was noticed when the necessary absorption corrections were correctly made,

2. Also, the strong correlation between the theoretical BR position ($\frac{2}{3}\ \frac{1}{3}\ \frac{1}{4}$) and the actual BR position ($\frac{2}{3}+\varepsilon,\ \frac{1}{3}-\varepsilon,\ \frac{1}{4}$) does not allow their simultaneous occupations as in the K.M. paper,

3. Finally occupancy factors for cationic sites are different from those of K.M.:

	K.M.[1]	This work
BR	1.86	1.76 (2)
mO	0.73	0.51 (2)
aBR	0.07	0.21 (2)
	2.66	2.48 (6)

The divergence between these results may again be related to:

1. the difference in preparation methods as for K β-alumina,

2. the lack of absorption corrections in K.M.'s work; this led to imprecise values of occupancy and thermal coefficients (especially anisotropic factors).

Conclusion

For crystals obtained in the same way, the occupancy factor of the BR position increases when Tl^+ takes the place of K^+, and simultaneously the mO site occupancy factor decreases. The aBR site is always weakly occupied. Also the total amount of M^+ in the conducting planes decreases when Tl^+ substitutes for K^+.

On the other hand, if our results are compared with the parameters of Na β-alumina the shift from the theoretical positions is related to the nature of the conducting ion.

	Theoretical position	Na[11]	K	Tl
BR	0.666	0.706	0.689	0.681
mO	0.833	0.873	0.882	0.910
aBR	1.0	—	0.971	1.00

[1] K.M. do not reveal the error for occupancy factors.

TABLE V

Observed and Calculated Structure Factors (K^+ β-Alumina)

H	K	L	Y(OBS)	Y(CALC)	H	K	L	Y(OBS)	Y(CALC)	H	K	L	Y(OBS)	Y(CALC)	H	K	L	Y(OBS)	Y(CALC)	H	K	L	Y(OBS)	Y(CALC)
0	0	2	155.3284	145.4021	0	2	0	78.1669	81.2364	0	3	21	2.8530	1.6350	0	5	15	16.2551	14.8224	1	1	26	69.6190	68.5825
0	0	4	162.3029	149.0669	0	2	1	129.8728	126.5582	0	3	22	2.8142	4.4338	0	5	16	2.8404	4.1410	1	1	28	20.8947	20.2563
0	0	6	25.1425	24.8320	0	2	2	87.1052	77.5675	0	3	23	11.7124	12.5750	0	5	17	12.6723	13.5903	1	1	30	10.5585	10.4237
0	0	8	169.3707	154.8050	0	2	3	52.3339	65.0152	0	3	24	34.0810	34.4065	0	5	18	25.9768	26.3632	1	1	32	32.6111	33.5216
0	0	12	17.9181	18.8587	0	2	4	97.7980	80.9851	0	3	25	1.6939	1.2838	0	5	19	17.3124	16.4010	1	2	0	35.3933	33.6726
0	0	14	215.5700	216.6901	0	2	5	168.6682	162.6714	0	3	26	53.2491	54.1755	0	5	20	27.7221	26.1591	1	2	1	7.4813	7.3348
0	0	16	4.9302	3.3749	0	2	6	197.0785	187.7158	0	3	27	10.8606	11.3846	0	5	21	42.1397	41.7493	1	2	2	40.5196	41.0440
0	0	18	71.3583	74.2975	0	2	7	140.1839	137.9408	0	3	28	12.7541	12.5483	0	5	22	18.6582	19.0486	1	2	3	1.6516	3.2738
0	0	20	202.0519	206.2721	0	2	8	110.6716	102.9191	0	3	29	4.4341	4.8116	0	5	23	1.6067	2.0358	1	2	4	39.5860	38.9130
0	0	22	13.7985	10.6546	0	2	9	86.7848	84.0904	0	3	30	8.6211	3.4481	0	5	24	3.2030	.2757	1	2	5	7.3512	7.6101
0	0	24	101.0877	102.6729	0	2	10	81.9941	81.5497	0	3	31	5.3373	4.2691	0	5	25	11.4892	11.3727	1	2	6	12.9545	13.5999
0	0	26	103.6865	104.3846	0	2	11	179.8632	184.2990	0	4	0	65.0665	64.2751	0	6	0	251.1590	246.9376	1	2	7	163.7301	167.8631
0	0	28	140.6247	140.9862	0	2	12	26.7231	25.1268	0	4	1	87.9342	85.9463	0	6	1	5.2191	5.1703	1	2	8	54.4172	54.1627
0	0	30	34.4856	33.7589	0	2	13	254.8654	258.8965	0	4	2	39.3032	38.8770	0	6	2	60.9356	59.5800	1	2	9	35.2444	35.7013
0	0	32	65.4027	64.6823	0	2	14	260.9411	258.1257	0	4	3	76.1788	76.4188	0	6	3	6.0659	5.0307	1	2	10	79.6525	83.9590
0	0	34	11.3840	11.9458	0	2	15	14.9014	16.0557	0	4	4	23.4333	23.0826	0	6	4	64.1500	63.1057	1	2	11	12.4838	11.2693
0	1	0	8.9594	7.9067	0	2	16	3.5660	3.4293	0	4	5	94.0222	95.7956	0	6	5	5.8227	4.8681	1	2	12	8.5485	8.6520
0	1	1	2.8024	.4302	0	2	17	53.4350	53.9884	0	4	6	104.0967	105.9939	0	6	6	13.6681	13.8014	1	2	13	30.8027	32.9555
0	1	2	66.6927	63.6882	0	2	18	88.2756	93.3769	0	4	7	71.2719	72.1181	0	6	7	5.9177	5.0079	1	2	14	45.9971	48.7279
0	1	3	29.9329	27.5212	0	2	19	56.9032	57.8708	0	4	8	54.4745	56.3739	0	6	8	41.7763	40.3712	1	2	15	31.6166	31.7854
0	1	4	24.9702	23.9375	0	2	20	21.7292	20.9502	0	4	9	40.9826	40.4611	0	6	9	6.3176	4.8939	1	2	16	10.8671	10.7153
0	1	5	13.1039	12.5689	0	2	21	30.5617	31.8316	0	4	10	56.2154	56.1351	0	6	10	.0000	.6876	1	2	17	22.4059	22.6392
0	1	6	32.8718	31.0807	0	2	22	58.8469	61.4894	0	4	11	131.5142	133.5118	0	6	11	3.5166	4.6216	1	2	18	44.5508	46.0659
0	1	7	198.9477	194.5752	0	2	23	3.8630	1.6062	0	4	12	19.6234	17.4816	0	6	12	.0000	5.3923	1	2	19	37.4916	37.7195
0	1	8	57.9834	58.3473	0	2	24	14.8420	10.4145	0	4	13	169.2683	169.0402	0	6	13	6.6616	4.5637	1	2	20	49.7521	49.5026
0	1	9	40.6787	39.5299	0	2	25	92.0351	91.6444	0	4	14	168.7605	174.3846	0	6	14	66.5375	63.5058	1	2	21	73.2722	74.2077
0	1	10	66.7152	67.4596	0	2	26	65.4970	63.2647	0	4	15	12.1851	12.7214	0	6	15	1.7171	4.2571	1	2	22	33.9805	34.1782
0	1	11	16.6631	15.5348	0	2	27	125.9623	125.8667	0	4	16	6.4214	6.9913	0	6	16	19.7965	18.9795	1	2	23	8.4880	6.6529
0	1	12	18.0770	16.1130	0	2	28	14.6938	17.3505	0	4	17	48.2596	48.1958	0	6	17	3.1820	4.1317	1	2	24	5.1682	4.2985
0	1	13	50.4229	52.2041	0	2	29	3.5858	2.2461	0	4	18	65.9084	65.9558	0	6	18	43.1333	41.6988	1	2	25	14.0746	11.5496
0	1	14	45.0077	46.1298	0	2	30	2.3618	3.2463	0	4	19	47.3997	47.4911	0	6	19	4.9594	3.9895	1	2	26	42.1816	41.2285
0	1	15	39.8577	39.0437	0	2	31	59.0809	58.2030	0	4	20	17.9750	16.9938	0	7	0	10.6207	10.6694	1	2	27	4.9179	5.6656
0	1	16	29.0212	28.7856	0	2	32	18.6246	18.5997	0	4	21	19.2019	18.3117	0	7	1	2.6376	1.1854	1	2	28	17.5201	16.6359
0	1	17	32.3411	35.4048	0	2	33	5.3194	5.1534	0	4	22	44.9280	46.1726	0	7	2	17.8714	15.9486	1	2	29	16.4475	18.1315
0	1	18	50.8459	52.6712	0	3	0	122.4819	122.7993	0	4	23	3.9564	3.6102	0	7	3	18.4996	17.4188	1	2	30	33.6758	34.1690
0	1	19	47.4756	47.9967	0	3	1	6.9158	7.4284	0	4	24	7.2783	6.4425	0	7	4	2.6646	3.9884	1	2	31	12.5935	12.1165
0	1	20	74.6963	74.8219	0	3	2	9.4988	6.3976	0	4	25	77.0973	75.1329	0	7	5	2.7880	1.6829	1	2	32	1.2187	2.0517
0	1	21	90.5421	88.9507	0	3	3	30.4784	29.0889	0	4	26	50.0481	47.7312	0	7	6	11.8130	12.9684	1	3	0	11.3597	10.6982
0	1	22	40.3788	40.0573	0	3	4	136.1986	135.6564	0	4	27	94.3357	91.4503	0	7	7	45.4896	45.1932	1	3	1	12.0580	11.0146
0	1	23	17.3486	17.3177	0	3	5	13.4669	12.6601	0	4	28	16.1991	16.6772	0	7	8	8.0787	9.6118	1	3	2	39.3836	39.2496
0	1	24	16.3111	17.9821	0	3	6	108.7794	110.1801	0	5	0	23.2677	22.3559	0	7	9	13.1088	12.1064	1	3	3	29.6136	28.9975
0	1	25	13.0253	14.1353	0	3	7	20.1492	19.4183	0	5	1	11.9864	12.6991	0	7	10	4.9031	2.8179	1	3	4	21.9182	21.6419
0	1	26	38.7701	38.3958	0	3	8	6.5988	6.6380	0	5	2	16.4267	16.8809	1	1	0	191.4793	176.9480	1	3	5	3.1510	2.6354
0	1	27	9.1022	9.8213	0	3	9	10.9926	10.7071	0	5	3	.0000	.7005	1	1	2	19.5102	17.1623	1	3	6	15.4932	15.7857
0	1	28	17.6473	18.5390	0	3	10	41.0049	42.9146	0	5	4	25.6742	25.6093	1	1	4	194.5754	185.1751	1	3	7	119.1472	121.1135
0	1	29	20.0720	19.7439	0	3	11	10.9910	10.3522	0	5	5	4.1029	3.8327	1	1	6	106.5638	111.0085	1	3	8	35.5665	36.3993
0	1	30	24.8289	24.7423	0	3	12	79.3989	77.9435	0	5	6	9.1201	8.6652	1	1	8	27.1736	26.0177	1	3	9	34.4105	36.3040
0	1	31	14.9330	15.7383	0	3	13	13.9115	14.7931	0	5	7	95.3225	96.2667	1	1	10	70.3342	70.1788	1	3	10	50.4917	52.5386
0	1	32	.8000	.1941	0	3	14	14.7158	15.6329	0	5	8	39.8820	38.7617	1	1	12	103.2618	107.9993	1	3	11	.0000	.7817
0	1	33	41.3474	41.5328	0	3	15	7.7323	8.0314	0	5	9	28.8216	29.5760	1	1	14	30.9201	30.2457	1	3	12	9.7955	12.0067
0	1	34	18.5847	19.7504	0	3	16	51.3147	53.0989	0	5	10	58.0507	59.2074	1	1	16	74.2416	76.2294	1	3	13	42.4618	44.8968
					0	3	17	41.8171	41.3800	0	5	11	5.7167	2.9347	1	1	18	60.4911	60.9893	1	3	14	38.0593	38.1113
					0	3	18	43.0672	43.7745	0	5	12	3.7265	1.2305	1	1	20	71.0937	70.6793	1	3	15	21.5678	22.2261
					0	3	19	5.9604	6.1245	0	5	13	18.3503	18.6906	1	1	22	12.3630	11.5372	1	3	16	15.0342	15.2329
					0	3	20	67.6772	67.4056	0	5	14	31.4756	30.2994	1	1	24	46.9691	47.7999	1	3	17	34.3157	34.7378

H	K	L	Y(OBS)	Y(CALC)
1	3	18	41.8958	42.4713
1	3	19	27.4619	27.7751
1	3	20	49.3894	48.9971
1	3	21	58.9021	58.3419
1	3	22	33.7570	34.3128
1	3	23	20.3010	20.1747
1	3	24	7.0056	8.9462
1	3	25	15.8973	14.9505
1	3	26	33.9065	32.7980
1	3	27	12.9577	12.6112
1	3	28	10.9272	11.1772
1	3	29	9.7982	10.1716
1	3	30	24.4268	23.6225
1	4	0	82.6779	82.5301
1	4	1	1.0601	1.2825
1	4	2	13.0940	11.8961
1	4	3	13.1401	12.2885
1	4	4	90.8457	92.5588
1	4	5	12.6754	12.9724
1	4	6	81.2131	81.7001
1	4	7	6.9101	6.1614
1	4	8	1.3590	.9519
1	4	9	1.3130	1.7606
1	4	10	29.9322	29.9674
1	4	11	1.8009	2.0359
1	4	12	50.1007	51.1785
1	4	13	4.9018	4.7691
1	4	14	7.6769	8.4331
1	4	15	11.1616	10.4626
1	4	16	35.1953	36.8159
1	4	17	11.3963	10.6789
1	4	18	31.3346	31.3000
1	4	19	3.1296	.0555
1	4	20	41.1356	40.7433
1	4	21	4.1381	3.2078
1	4	22	5.4818	2.0724
1	4	23	4.9946	5.4258
1	4	24	24.5360	24.6386
1	4	25	6.8715	5.3269
1	4	26	42.1286	41.5915
1	5	0	6.8372	8.2903
1	5	1	8.7736	8.7712
1	5	2	13.0072	13.1486
1	5	3	12.6602	12.0890
1	5	4	14.3414	14.9138
1	5	5	1.9652	2.9013
1	5	6	12.0607	11.8743
1	5	7	75.2686	75.5037
1	5	8	32.6170	33.0217
1	5	9	26.1203	25.6941
1	5	10	38.5307	38.8686
1	5	11	2.3899	.7512
1	5	12	1.2509	1.5179
1	5	13	24.9808	24.5867
1	5	14	21.6564	22.1254
1	5	15	13.6767	14.6872
1	5	16	9.1183	9.6042
1	5	17	20.9224	20.3114
1	5	18	21.5344	21.2096
1	5	19	14.6627	14.4263
1	5	20	29.9899	29.6993
1	5	21	37.4887	37.2380
1	5	22	17.2957	17.4354
1	6	0	1.5985	.2709
1	6	1	5.3672	.8308
1	6	2	20.5884	19.7471
1	6	3	16.4003	18.1532
1	6	4	6.3578	7.1683
1	6	5	.5893	.7142
1	6	6	7.9264	7.0738
1	6	7	53.2680	52.5084
1	6	8	11.8560	11.9562
1	6	9	15.1736	15.7626
1	6	10	18.1886	17.9038
1	6	11	2.3450	2.8789
1	6	12	8.8585	8.7845
1	6	13	23.9845	25.5457
1	6	14	18.3360	17.6771
1	6	15	16.1730	14.3590
2	2	0	505.5654	516.8460
2	2	2	99.2119	98.6856
2	2	4	104.8147	103.3297
2	2	6	8.9644	6.4435
2	2	8	82.2659	87.0907
2	2	10	25.7648	27.0883
2	2	12	8.9509	6.0606
2	2	14	133.5284	137.7538
2	2	16	18.4946	17.1242
2	2	18	66.9990	65.8100
2	2	20	126.9791	126.3610
2	2	22	6.6679	2.5340
2	2	24	90.0677	89.2535
2	2	26	69.2068	67.9618
2	2	28	99.1425	98.0330
2	2	30	19.3092	19.0310
2	3	0	9.7028	8.5253
2	3	1	1.0428	.8976
2	3	2	31.0464	31.3100
2	3	3	24.4546	24.8478
2	3	4	1.9566	2.3723
2	3	5	3.4200	3.3929
2	3	6	22.6208	22.8186
2	3	7	104.2532	104.0892
2	3	8	28.4594	28.1446
2	3	9	21.8621	22.0563
2	3	10	23.4248	23.7132
2	3	11	8.9214	7.3421
2	3	12	9.1868	9.1078
2	3	13	37.1942	38.0373
2	3	14	23.6459	24.1909
2	3	15	25.1072	25.0226
2	3	16	23.7618	24.2623
2	3	17	28.5843	28.4388
2	3	18	34.1825	34.9304
2	3	19	31.6322	30.8379
2	3	20	52.9530	52.9875
2	3	21	56.9067	55.6905
2	3	22	31.1485	30.5878
2	3	23	19.0985	18.7102
2	3	24	16.3608	17.7446
2	3	25	9.1657	8.4867
2	3	26	21.8359	21.8101
2	3	27	9.4348	8.3379
2	4	0	42.3167	41.3234
2	4	1	69.9295	68.1027
2	4	2	30.1097	30.7996
2	4	3	54.5402	53.9896
2	4	4	6.6938	7.6660
2	4	5	59.7929	59.1046
2	4	6	67.7092	69.0370
2	4	7	54.9463	54.9736
2	4	8	43.2553	43.8988
2	4	9	23.0975	23.1852
2	4	10	47.9184	46.5966
2	4	11	93.4014	92.7787
2	4	12	17.1401	17.3009
2	4	13	128.6614	128.4413
2	4	14	124.3294	125.2907
2	4	15	4.9838	5.4430
2	4	16	7.6245	8.9960
2	4	17	32.2935	31.1755
2	4	18	54.5135	55.2449
2	4	19	30.9989	30.9856
2	4	20	19.1904	18.1706
2	4	21	17.6583	17.6270
2	4	22	32.2575	32.5878
2	4	23	4.3667	2.1825
2	5	0	47.6371	46.1175
2	5	1	1.1633	2.5194
2	5	2	12.5716	13.0409
2	5	3	14.2844	14.3880
2	5	4	54.3125	54.0345
2	5	5	17.6988	17.8699
2	5	6	54.2473	55.2307
2	5	7	6.0730	7.0376
2	5	8	1.4316	1.5662
2	5	9	4.3805	1.3739
2	5	10	14.0485	12.8200
2	5	11	3.3227	1.7172
2	5	12	29.7770	28.6424
2	5	13	6.1849	5.6796
2	5	14	1.1439	1.2441
2	5	15	17.2186	15.5811
2	5	16	20.6641	20.4298
2	5	17	14.0587	14.3589
2	5	18	19.3042	18.2691
2	6	0	20.6984	18.6100
2	6	1	34.1654	36.0691
2	6	2	19.4696	20.8873
2	6	3	32.4171	31.9747
2	6	4	8.5202	7.5633
2	6	5	38.7415	38.1841
2	6	6	44.8793	41.9556
3	3	0	74.3488	76.0292
3	3	2	6.8379	7.8435
3	3	4	84.5584	84.1751
3	3	6	65.4113	65.7184
3	3	8	4.2904	3.7492
3	3	10	32.6784	32.5610
3	3	12	47.2689	46.0270
3	3	14	9.5842	10.1631
3	3	16	36.3373	36.3492
3	3	18	32.2430	30.7627
3	3	20	38.5956	38.3502
3	3	22	2.9493	4.3672
3	3	24	24.7333	24.8336
3	4	0	7.8087	9.1705
3	4	1	8.9562	9.3262
3	4	2	5.7493	4.2209
3	4	3	2.2522	1.3307
3	4	4	12.6228	12.5898
3	4	5	4.5066	3.6214
3	4	6	12.7687	12.9908
3	4	7	70.0541	69.5532
3	4	8	35.7732	36.5328
3	4	9	22.9759	23.7912
3	4	10	37.6186	38.1782
3	4	11	1.1948	1.9119
3	4	12	8.7885	8.1778
3	4	13	14.2339	15.1874
3	4	14	17.0154	16.6773
3	4	15	12.5415	11.6139
3	4	16	10.2127	9.1963
3	4	17	11.9933	12.0074
3	4	18	14.3572	13.5475
3	4	19	11.6097	10.8114
3	5	0	3.4638	2.0237
3	5	1	2.7708	5.5476
3	5	2	12.6919	11.3273
3	5	3	16.2866	16.9557
3	5	4	9.4041	8.6962
3	5	5	4.3267	3.6953
3	5	6	7.8136	6.9208
3	5	7	44.8821	43.8397
3	5	8	17.8987	18.0058
3	5	9	18.5700	19.2039
3	5	10	21.5533	21.0893
4	4	0	189.7543	190.8160
4	4	2	44.7082	46.0097
4	4	4	48.3613	49.7418
4	4	6	10.6529	11.8461
4	4	8	33.4856	31.7772
4	4	10	3.7619	4.0938

TABLE VI

Observed and Calculated Structure Factors (Tl^+ β-Alumina)

H	K	L	Y(OBS)	Y(CALC)	H	K	L	Y(OBS)	Y(CALC)	H	K	L	Y(OBS)	Y(CALC)	H	K	L	Y(OBS)	Y(CALC)	H	K	L	Y(OBS)	Y(CALC)
0	0	2	109.1612	138.5034	0	3	20	23.5453	13.4399	0	1	34	19.8071	21.8755	0	5	13	18.9618	14.0918	1	1	20	51.2052	54.7375
0	0	4	186.1857	139.2710	0	3	21	16.0792	21.0702	0	2	0	134.2749	140.9092	0	5	14	61.0165	64.5918	1	1	22	126.9931	135.0143
0	0	6	339.0108	329.4066	0	3	22	87.0909	86.7255	0	2	1	24.6274	14.6129	0	5	15	43.8982	44.7561	1	1	24	153.9907	159.4895
0	0	8	483.3685	439.9105	0	3	23	24.8486	25.0722	0	2	2	40.4720	21.7673	0	5	16	20.6192	22.7105	1	1	26	161.3318	166.4500
0	0	10	433.6477	404.1596	0	3	24	104.6103	107.2960	0	2	3	196.1607	212.4437	0	5	17	17.0629	19.4483	1	1	28	105.9134	111.0919
0	0	12	248.8939	264.6723	0	3	25	11.9961	12.4186	0	2	4	184.8735	181.0272	0	5	18	51.4370	52.9616	1	1	30	94.0830	92.4496
0	0	14	437.0671	438.9772	0	3	26	112.7979	119.1953	0	2	5	308.2335	290.2754	0	5	19	47.7701	48.0164	1	1	32	105.2913	102.1322
0	0	16	196.6636	197.8665	0	3	27	20.7457	25.1771	0	2	6	252.9905	243.2867	0	5	20	3.1313	4.3453	1	2	0	96.2915	93.4841
0	0	18	133.4965	133.9357	0	3	28	68.5926	72.9812	0	2	7	40.4130	23.6983	0	5	21	70.1395	73.1859	1	2	1	134.7937	132.4506
0	0	20	372.7165	381.9824	0	3	29	13.7786	13.3669	0	2	8	81.8505	64.5721	0	5	22	44.0489	41.8287	1	2	2	102.6281	103.7353
0	0	22	139.0972	136.6719	0	3	30	58.7565	57.7739	0	2	9	186.9098	187.9819	0	5	23	16.7616	16.6353	1	2	3	132.5210	131.5976
0	0	24	51.8334	46.4850	0	3	31	10.1818	18.3701	0	2	10	39.8163	33.3122	0	5	24	20.0396	22.2598	1	2	4	101.0525	98.5212
0	0	26	266.5711	255.9753	0	4	0	112.8827	112.9509	0	2	11	270.3045	295.1936	0	5	25	10.9823	10.4372	1	2	5	144.7291	145.4880
0	0	28	261.9791	254.9098	0	4	1	28.8478	22.4404	0	2	12	32.7433	34.3819	0	6	0	300.8660	298.2485	1	2	6	41.9855	41.0427
0	0	30	123.7409	120.1286	0	4	2	11.2406	5.5913	0	2	13	162.9016	160.1457	0	6	1	5.7668	9.4458	1	2	7	308.1497	304.1826
0	0	32	35.4403	29.6387	0	4	3	182.9039	188.5602	0	2	14	300.9284	305.1337	0	6	2	29.3371	26.5371	1	2	8	15.2823	2.1479
0	0	34	114.9109	118.0639	0	4	4	68.8124	72.8831	0	2	15	118.8564	128.0670	0	6	3	6.8356	9.9925	1	2	9	88.6559	86.9094
0	1	0	49.3584	49.4524	0	4	5	192.4121	198.1589	0	2	16	18.9778	12.5436	0	6	4	31.5744	26.7151	1	2	10	144.5553	137.7007
0	1	1	184.9796	182.1912	0	4	6	148.9266	155.1086	0	2	17	142.4949	144.7111	0	6	5	12.4504	9.1686	1	2	11	136.8984	130.5336
0	1	2	113.4472	106.0752	0	4	7	31.9225	20.5330	0	2	18	63.4297	61.6672	0	6	6	30.3392	31.3865	1	2	12	59.9139	55.9501
0	1	3	155.4338	149.8646	0	4	8	24.7849	19.5906	0	2	19	137.1612	126.8012	0	6	7	8.8486	9.6942	1	2	13	82.8979	76.4229
0	1	4	67.9867	63.2914	0	4	9	146.0672	147.3829	0	2	20	23.2995	25.2963	0	6	8	81.4473	80.3076	1	2	14	98.5021	96.7937
0	1	5	201.1792	190.0666	0	4	10	19.8326	14.5802	0	2	21	44.9926	39.6767	0	6	9	9.1989	8.6151	1	2	15	139.7379	130.9856
0	1	6	18.0621	8.9296	0	4	11	224.2399	226.9703	0	2	22	85.8325	92.8390	0	6	10	37.1778	37.2653	1	2	16	32.2019	32.2502
0	1	7	358.8207	366.9813	0	4	12	26.8497	31.5570	0	2	23	76.0618	75.4714	0	6	11	9.5046	8.6161	1	2	17	71.5734	73.7935
0	1	8	30.5824	20.9506	0	4	13	97.1218	87.4553	0	2	24	13.9691	13.0509	0	6	12	29.1254	25.7803	1	2	18	82.9565	85.1299
0	1	9	106.1460	114.8460	0	4	14	202.0324	217.3910	0	2	25	143.8030	146.1815	0	6	13	11.6711	8.6826	1	2	19	127.4854	130.8441
0	1	10	100.5003	102.9550	0	4	15	96.6438	107.7597	0	2	26	82.1932	78.8093	0	6	14	98.3410	95.9307	1	2	20	21.1241	16.8482
0	1	11	159.4321	162.5077	0	4	16	16.4751	13.5291	0	2	27	89.2300	81.9672	0	6	15	13.2935	7.7711	1	2	21	187.8342	158.7292
0	1	12	46.4853	43.8027	0	4	17	122.7433	127.9280	0	2	28	5.1699	5.6934	0	6	16	13.1720	10.3098	1	2	22	63.0722	67.0494
0	1	13	84.2238	85.9338	0	4	18	37.4676	36.6021	0	2	29	61.9803	60.2228	0	6	17	6.2643	7.8555	1	2	23	56.9051	60.4759
0	1	14	72.0433	71.2847	0	4	19	110.3772	112.2374	0	2	30	27.2602	25.8179	0	6	18	11.3078	5.7346	1	2	24	23.2071	24.7228
0	1	15	155.7371	160.8880	0	4	20	21.4117	24.2047	0	2	31	105.8542	95.9735	0	6	19	.0000	6.7495	1	2	25	53.3388	46.0399
0	1	16	12.5909	.9298	0	4	21	50.2240	48.3985	0	2	32	4.2770	5.2396	0	6	20	91.3051	104.1889	1	2	26	64.0207	65.4449
0	1	17	74.0978	78.9312	0	4	22	76.2353	77.1543	0	2	33	39.0315	38.6816	0	7	0	.0000	.2787	1	2	27	54.2213	54.7453
0	1	18	68.3675	60.8899	0	4	23	72.3968	72.1311	0	3	0	257.7654	265.1793	0	7	1	13.4047	17.4918	1	2	28	4.7971	9.1029
0	1	19	149.3174	150.1869	0	4	24	16.8762	18.4586	0	3	1	28.6368	28.9956	0	7	2	30.8653	31.5464	1	2	29	66.1653	62.9823
0	1	20	58.7117	61.1378	0	4	25	133.8058	128.6861	0	3	2	131.9791	137.3917	0	7	3	.0000	1.4683	1	2	30	58.0406	56.1385
0	1	21	177.5629	186.9441	0	4	26	69.9868	69.9124	0	3	3	58.7589	49.5393	0	7	4	6.9604	9.4977	1	2	31	38.3423	39.1089
0	1	22	57.2334	56.8416	0	4	27	57.5095	47.6568	0	3	4	288.4764	273.1453	0	7	5	13.0366	17.8296	1	2	32	15.0428	15.2354
0	1	23	63.8561	63.8418	0	4	28	7.4643	2.7963	0	3	5	7.4899	11.0930	0	7	6	.0000	.4799	1	3	0	64.4514	66.4384
0	1	24	12.6727	8.1487	0	4	29	57.2582	61.3785	0	3	6	31.0104	17.5060	0	7	7	64.3153	66.1023	1	3	1	64.1002	64.3407
0	1	25	67.6934	64.9269	0	5	0	99.1177	97.8748	0	3	7	43.5396	42.1126	0	7	8	.0000	.0410	1	3	2	94.3309	95.2873
0	1	26	58.9704	49.7392	0	5	1	33.3297	30.4416	0	3	8	136.0153	134.8794	0	7	9	5.1378	4.0468	1	3	3	43.8326	45.0154
0	1	27	63.7602	53.1827	0	5	2	58.3643	54.5372	0	3	9	28.8173	28.5822	0	7	10	13.8427	13.9019	1	3	4	78.4618	73.9739
0	1	28	10.8118	18.0989	0	5	3	42.7598	42.5193	0	3	10	164.1476	169.1634	1	1	0	406.0867	402.5059	1	3	5	73.7965	74.1624
0	1	29	61.2871	73.1809	0	5	4	61.8068	63.4782	0	3	11	27.3126	32.0906	1	1	2	284.7216	285.4280	1	3	6	35.6004	33.1144
0	1	30	39.4171	33.1942	0	5	5	35.8472	40.3851	0	3	12	180.8202	194.1264	1	1	4	417.7171	408.0113	1	3	7	198.6593	196.9929
0	1	31	43.8125	41.2672	0	5	6	28.0886	29.7989	0	3	13	29.8381	34.5459	1	1	6	187.3760	96.2875	1	3	8	17.9395	12.9159
0	1	32	2.8434	.1831	0	5	7	136.9680	144.4353	0	3	14	114.0397	125.3768	1	1	8	244.3063	226.5101	1	3	9	31.7476	30.0024
0	1	33	100.9532	92.9772	0	5	8	9.2785	4.2898	0	3	15	12.8714	10.7369	1	1	10	269.7310	266.5783	1	3	10	104.6045	103.6385
					0	5	9	18.1254	8.1183	0	3	16	151.4876	169.7105	1	1	12	291.6919	287.2567	1	3	11	65.7993	64.9464
					0	5	13	93.8898	91.8340	0	3	17	37.3134	39.0683	1	1	14	289.8977	289.4435	1	3	12	96.8461	96.3677
					0	5	11	48.8478	48.2786	0	3	18	131.8219	131.9276	1	1	16	238.0862	238.6062	1	3	13	24.3088	16.4039
					0	5	12	90.7776	89.1878	0	3	19	21.2831	29.0850	1	1	18	178.2890	197.3438	1	3	14	83.8817	80.5114

H	K	L	Y(OBS)	Y(CALC)	H	K	L	Y(OBS)	Y(CALC)	H	K	L	Y(OBS)	Y(CALC)	H	K	L	Y(OBS)	Y(CALC)	H	K	L	Y(OBS)	Y(CALC)
1	3	15	80.7343	75.2542	1	5	11	46.1126	44.2465	2	3	11	81.8851	76.5014	2	5	13	2.0993	3.3457	3	5	9	5.9299	.6507
1	3	16	29.6829	27.0861	1	5	12	11.9452	15.7495	2	3	12	39.1559	38.1944	2	5	14	39.3492	38.8196	3	5	10	28.8338	29.2545
1	3	17	19.3159	16.3410	1	5	13	21.6070	16.1914	2	3	13	37.4796	29.3231	2	5	15	17.1107	17.5962	4	4	0	239.3222	240.6544
1	3	18	77.2787	78.2674	1	5	14	40.7406	40.9192	2	3	14	53.9936	50.1104	2	5	16	63.6315	59.6530	4	4	2	17.4159	13.9428
1	3	19	78.3221	81.1354	1	5	15	54.6416	51.4749	2	3	16	52.2763	5.4197	2	5	17	15.2781	14.0753	4	4	4	21.0899	14.9898
1	3	20	19.7080	17.9185	1	5	16	3.3250	6.2575	2	3	15	44.8931	84.3431	2	5	18	52.2592	49.7821	4	4	6	29.4758	29.9755
1	3	21	102.9884	103.5464	1	5	17	16.8577	16.3360	2	3	17	31.1489	28.9300	2	6	0	29.4295	26.2507	4	4	8	73.6366	69.7785
1	3	22	65.4855	66.4265	1	5	18	35.2025	37.6439	2	3	18	61.3833	54.4165	2	6	1	23.6246	15.3338	4	4	10	43.3828	41.2900
1	3	23	14.3229	15.2965	1	5	19	52.3513	53.2410	2	3	19	92.2784	89.5370	2	6	2	17.6257	16.2096					
1	3	24	17.4194	17.2783	1	5	20	16.2129	17.0158	2	3	20	35.3583	36.0448	2	6	3	53.8342	53.9171					
1	3	25	22.6429	21.9190	1	5	21	69.9385	71.6201	2	3	21	110.3805	106.8800	2	6	4	19.1846	18.5024					
1	3	26	54.9613	59.5000	1	5	22	33.0379	30.5372	2	3	22	55.5556	52.7604	2	6	5	59.0761	57.5890					
1	3	27	21.0356	17.1178	1	6	0	19.6953	19.8081	2	3	23	25.7773	24.9942	2	6	6	53.9444	52.5614					
1	3	28	10.3912	13.1441	1	6	1	29.2520	26.2447	2	3	24	2.7921	3.5366	3	3	0	149.1611	152.3765					
1	3	29	37.8663	33.4266	1	6	2	41.6809	40.9031	2	3	25	33.9703	33.6155	3	3	2	65.6526	68.7934					
1	3	30	47.6974	46.5091	1	6	3	11.2711	9.9485	2	3	26	35.2060	41.2296	3	3	4	164.5161	161.2307					
1	4	0	164.0419	164.2772	1	6	4	26.9713	25.2315	2	3	27	29.4324	27.4652	3	3	6	17.8520	2.4830					
1	4	1	17.0432	13.9515	1	6	5	30.3380	28.9300	2	4	0	63.7546	62.1691	3	3	8	78.2518	72.8260					
1	4	2	66.6328	70.3859	1	6	6	8.9398	9.4196	2	4	1	34.0142	23.5034	3	3	10	105.4579	101.6155					
1	4	3	7.2931	.0626	1	6	7	85.1384	83.1414	2	4	2	11.5690	13.0386	3	3	12	114.5967	111.6728					
1	4	4	173.1091	172.4389	1	6	8	.0000	4.5955	2	4	3	102.2549	101.1227	3	3	14	75.1386	76.3377					
1	4	5	24.1152	23.1627	1	6	9	8.6358	10.1941	2	4	4	30.4774	30.5910	3	3	16	101.1153	98.9615					
1	4	6	26.0979	10.1919	1	6	10	38.0497	37.1417	2	4	5	106.8036	102.1064	3	3	18	85.8401	81.5785					
1	4	7	4.5234	3.6917	1	6	11	29.0604	27.6204	2	4	6	91.5537	92.1469	3	3	20	17.2042	7.5612					
1	4	8	75.6455	74.4192	1	6	12	28.4470	26.2573	2	4	7	22.2433	20.1209	3	3	22	57.9213	53.7143					
1	4	9	5.8903	10.7990	1	6	13	11.1381	1.2405	2	4	8	35.1418	31.7385	3	3	24	65.2383	72.7073					
1	4	10	103.8415	103.4241	1	6	14	33.7839	33.3306	2	4	9	72.7721	70.0869	3	4	0	15.6302	14.3929					
1	4	11	10.6806	7.3541	1	6	15	42.0339	35.4660	2	4	10	32.1509	29.6108	3	4	1	30.1849	25.4207					
1	4	12	117.5691	120.2124	2	2	0	620.2534	647.7234	2	4	11	136.2749	131.9813	3	4	2	10.2583	10.4608					
1	4	13	3.2226	6.2150	2	2	2	27.1212	12.2757	2	4	12	7.1428	6.4201	3	4	3	33.4899	33.4133					
1	4	14	74.6786	75.3767	2	2	4	26.9932	12.5037	2	4	13	107.1031	98.8315	3	4	4	17.4965	18.6377					
1	4	15	24.1063	20.1543	2	2	6	116.6205	123.9513	2	4	14	154.5907	146.4022	3	4	5	31.0299	33.0223					
1	4	16	103.0048	102.9228	2	2	8	200.7018	205.3662	2	4	15	46.7237	49.4964	3	4	6	10.7495	9.2559					
1	4	17	9.7924	1.5643	2	2	10	134.0654	128.8648	2	4	16	5.7747	5.0660	3	4	7	110.1466	109.7864					
1	4	18	83.6866	83.4963	2	2	12	111.0275	102.8431	2	4	17	67.2210	63.4117	3	4	8	34.9969	31.7874					
1	4	19	10.9480	10.7771	2	2	14	250.5198	234.1243	2	4	18	48.4096	45.8652	3	4	9	10.5606	7.8870					
1	4	20	14.0502	2.6112	2	2	16	78.0710	66.1194	2	4	19	61.3784	55.3577	3	4	10	48.5846	43.0511					
1	4	21	13.4344	8.9194	2	2	18	36.3875	30.4594	2	4	20	6.1043	2.5800	3	4	11	37.3223	34.4929					
1	4	22	52.8341	52.7096	2	2	20	213.0757	211.3791	2	4	21	14.2569	10.2304	3	4	12	9.9333	5.1090					
1	4	23	3.6194	4.1902	2	2	22	44.2545	43.5603	2	4	22	48.2727	47.3041	3	4	13	14.9565	13.4469					
1	4	24	72.0019	70.8850	2	2	24	29.9416	21.4729	2	4	23	31.5022	27.1993	3	4	14	23.6489	23.9468					
1	4	25	12.6810	13.1103	2	2	26	134.1487	144.7253	2	4	24	5.7603	3.4246	3	4	15	39.6766	37.3841					
1	4	26	79.0973	81.9591	2	2	28	145.7829	148.0626	2	5	0	95.7198	94.5522	3	4	16	9.1509	7.2946					
1	4	27	1.9489	1.0006	2	2	30	50.3983	52.1394	2	5	1	1.6465	5.0261	3	4	17	15.9968	16.4113					
1	5	0	28.7440	31.3652	2	3	0	25.1208	24.7277	2	5	2	33.1414	34.5125	3	4	18	19.5605	17.0126					
1	5	1	42.2980	39.7345	2	3	1	80.3687	79.3786	2	5	3	14.6011	12.9105	3	4	19	40.8839	38.7407					
1	5	2	36.2706	36.0075	2	3	2	69.2747	67.0114	2	5	4	101.4991	97.4087	3	5	0	9.8678	10.3965					
1	5	3	36.8033	35.6290	2	3	3	56.6097	54.7856	2	5	5	18.6343	19.0786	3	5	1	14.7852	13.4612					
1	5	4	35.4906	35.1629	2	3	4	33.9011	35.4996	2	5	6	21.0839	17.1716	3	5	2	12.5199	18.8100					
1	5	5	46.2867	47.7252	2	3	5	87.4845	84.0123	2	5	7	3.9250	7.3785	3	5	3	3.7522	2.2400					
1	5	6	7.7972	5.9649	2	3	6	9.7878	8.0576	2	5	8	43.0314	41.0922	3	5	4	8.5895	12.9759					
1	5	7	127.1058	127.2766	2	3	7	191.0072	184.2604	2	5	9	7.4579	2.8737	3	5	5	18.3765	18.0163					
1	5	8	17.8623	12.6792	2	3	8	9.1892	.1330	2	5	10	55.5191	55.5017	3	5	6	10.1173	4.1604					
1	5	9	20.6362	18.7975	2	3	9	50.2315	49.2359	2	5	11	7.0195	1.4493	3	5	7	69.1473	66.3448					
1	5	10	60.6483	60.5249	2	3	10	58.4497	55.0222	2	5	12	69.5121	69.9314	3	5	8	10.8857	12.7860					

Both Tl and K β-alumina compounds are similar in nature to Na β-alumina, rather than to Ag β-alumina, in which aBR positions have significant occupation factors.

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