TABLE I. Trial parameters.

Atom	Coordinates		B, A²
	x	z	
Ga_I	0.087	−0.204	0.2
Ga_{II}	0.341	−0.312	0.2
O_I	0.153	0.092	0.8
O_{II}	0.492	0.248	0.8
O_{III}	0.829	0.443	0.8

REFINEMENT OF THE STRUCTURE

Refinement of the structure was carried out with the Busing-Levy[15] least-squares program for the IBM 704 computer. Only *h0l* and *h1l* amplitudes were used. In the first refinement cycles 824 data were included. All observed amplitudes were weighted unity; all unobserved amplitudes included at one-half threshold value were weighted 0.01. Two scale factors corresponding to the two k values (zero and first layers about b) of the data were refined. Both of these were started at 1.000 and are the scale factors mentioned earlier. Atomic scattering factors used for the structure amplitude calculations were those of Thomas and Umeda[16] for Ga^{3+} and for O^{2-} those given by Berghuis *et al.*[17] for O arbitrarily modified such that $f_{O^{2-}}=10$ at $\sin\theta/\lambda=0$ and $f_{O^{2-}}=f_O$ at $\sin\theta/\lambda\geq 0.20$.

Convergence was attained within three cycles: in the final cycle, the largest change in any coordinate was 0.003 A by O_{II} in the a direction. The weighted R factor was 0.171 for the data calculated on the basis of the parameters of the second cycle. The final scale factors were 0.988 and 0.997 with σ's of 0.010, meaning that these are not significantly different from 1.000.

Examination of the calculated and observed data indicated some large discrepancies in the high-angle data taken with the Mo$K\alpha$ radiation. These data had been taken with Kodak type *KK* film, which unfortunately has rather large grain size. Small weak spots are difficult to see in this case; the difficulty is more pronounced when the α_1, α_2 doublet is resolved. Because the data were plentiful, it was decided to omit a large portion of the high-angle reflections. The total data were therefore reduced from 824 to 522. Two least-squares cycles were run. The largest difference in coordinates between the results so obtained and those obtained previously was 0.005 A for atom O_{III} in the a direction. The final parameters with their standard deviations are given in Table II.

The weighted R factor calculated by the Busing-Levy program was 0.166. However, if unobserved reflections are excluded; the R factor

$$\sum | F_{obs}-F_{calc} | / \sum | F_{obs} |$$

for the *hOl* reflections is 0.143 and for the *h1l*, 0.130. The comparison of calculated and observed structure amplitudes is given in Table III.

INTERATOMIC DISTANCES AND ANGLES

The estimated standard deviations of the positions of the atoms are 0.004, 0.004, 0.033, 0.028, and 0.028 A for Ga(I), Ga(II), O(I), O(II), and O(III), respectively. These standard deviations of position should be considered as radii of circles in the mirror planes. Standard deviations in bond lengths were computed taking into consideration the angle made between the bond direction and the symmetry planes. The interatomic distances and their standard deviations are given in Table IV.

The important angles are given in Table V. Individual standard deviations were not calculated for these, but an estimate of the standard deviation of an O—Ga—O angle is 1.3° and of a Ga—O—Ga angle, 0.9°.

DESCRIPTION OF THE STRUCTURE

The arrangement of the ions in the β-Ga_2O_3 structure is shown in Figs. 1 and 2. The oxygen ions are arranged in a "distorted cubic" close-packed array. There are two crystallographically nonequivalent gallium and three nonequivalent oxygen ions in the unit cell. Each Ga_I^{3+} ion is surrounded by a distorted tetrahedron of oxygen ions: one O_I^{2-} at 1.80 A, two O_{II}^{2-} ions at 1.83 A, and one O_{III}^{2-} ion at 1.85 A (average 1.83 A). Each Ga_{II}^{3+} ion is surrounded by a highly distorted octahedron of oxygen ions: two O_I^{2-} at 1.95 A, one O_{II}^{2-} ion at 1.95 A, one O_{III}^{2-} ion at 2.02 A, and two O_{III}^{2-} ions at 2.08 A (average 2.00 A). A tetrahedron shares *only* corners with other tetrahedra in the b-axis direction and with octahedra in other directions. An octahedron shares edges with adjacent octahedra in the b axis direction and in roughly the [102] direction: the shared edges are, respectively, O_I–O_{III} and O_{III}–O_{III}, each of length 2.67 (Table IV). The distance 2.67 A is the shortest O–O distance in the structure. This is

TABLE II. Final parameters.

	Scale factors	Standard deviations
1	0.984	0.013
2	0.988	0.014

Atom	Coordinates		B, A²	$\sigma(x)$	$\sigma(z)$	$\sigma(B)$
	x	z				
Ga_I	0.0904	−0.2052	0.33	0.0002	0.0005	0.05
Ga_{II}	0.3414	−0.3143	0.28	0.0002	0.0005	0.05
O_I	0.1674	0.1011	0.76	0.0019	0.0041	0.32
O_{II}	0.4957	0.2553	0.43	0.0016	0.0034	0.25
O_{III}	0.8279	0.4365	0.46	0.0015	0.0034	0.25

[15] W. R. Busing and H. A. Levy, ORNL Central Files Memorandum 59-4-37 (April, 1959).
[16] L. H. Thomas and K. Umeda, J. Chem. Phys. 26, 293 (1957).
[17] J. Berghuis, I. J. M. Haanappel, M. Potters, B. O. Loopstra: C. H. MacGillavry, and A. L. Veenendaal, Acta Cryst. 8, 478 (1955).