TABLE IV. Interatomic distances and standard deviations.

	Atom pair (No.)	Distance, A	σ, A		Atom pair (No.)	Distance, A	σ, A
Ga_IO_4 tetrahedron	$Ga—O_I$	1.80	0.03	$Ga_{II}O_6$ octahedron	$Ga—O_I(2)$	1.95	0.03
	$Ga—O_{II}(2)$	1.83	0.01		$Ga—O_{II}$	1.95	0.03
	$Ga—O_{III}$	1.85	0.03		$Ga—O_{III}$	2.02	0.03
	$O_I—O_{II}(2)$	2.93	0.04		$Ga—O_{III}(2)$	2.08	0.02
	$O_I—O_{III}$	3.13	0.04		$O_I—O_I$	3.04	0.01
	$O_{II}—O_{II}$	3.04	0.01		$O_I—O_{II}(2)$	2.90	0.04
	$O_{II}—O_{III}(2)$	3.02	0.03		$O_I—O_{III}(2)$	2.85	0.04
					$O_I—O_{III}(2)$	2.67	0.04
					$O_{II}—O_{III}(2)$	2.89	0.03
					$O_{III}—O_{III}(2)$	2.67	0.04
					$O_{III}—O_{III}$	3.04	0.01
Shortest Ga–Ga distances	$Ga_I—Ga_I(2)$	3.04	0.01	Averages	$Ga_I—O$	1.83	
	$Ga_{II}—Ga_{II}(2)$	3.04	0.01		$Ga_{II}—O$	2.00	
	$Ga_{II}—Ga_{II}(2)$	3.11	0.01		O—O, octahedron	2.84	
	$Ga_I—Ga_{II}$	3.28	0.01				
	$Ga_I—Ga_{II}(2)$	3.30	0.01		0—0, tetrahedron	3.02	
	$Ga_I—Ga_{II}(2)$	3.33	0.01				
	$Ga_I—Ga_{II}(2)$	3.45	0.01				

TABLE V. Bond angles.

Within a tetrahedron (involve only Ga_I)		Within an octahedron (involve only Ga_{II})	
2 $O_I—Ga—O_I$	107.6°	$O_I—Ga—O_I$	102.7°
$O_I—Ga—O_I$	117.8	2 $O_I—Ga—O_{II}$	96.1
$O_{II}—Ga—O_{II}$	112.0	2 $O_I—Ga—O_{III}$	91.9
2 $O_{II}—Ga—O_{III}$	110.2	2 $O_I—Ga—O_{III}$	83.1
		2 $O_{II}—Ga—O_{III}$	91.5
		$O_{III}—Ga—O_{III}$	94.1
		2 $O_{III}—Ga—O_{III}$	81.4

$Ga_I—O—Ga_{II}$ (tetrahedral-octahedral) angles		
2 $Ga—O_I—Ga$	123.3°	(2 different Ga_{II}'s)
2 $Ga—O_{II}—Ga$	123.0	(2 different O_{II}'s)
2 $Ga—O_{III}—Ga$	122.3	(2 different Ga_{II}'s)
$Ga—O_{III}—Ga$[a]	115.4	

$Ga_I—O—Ga_I$ (tetrahedral-tetrahedral) angles		
2 $Ga—O_{II}—Ga$	112.0°	(2 different O_{II}'s)

$Ga_{II}—O—Ga$ (octahedral-octahedral) angles		
2 $Ga—O_{III}—Ga$	98.4°	(2 different Ga_I's)
2 $Ga—O_{III}—Ga$	98.4	(2 different O_{III}'s)
$Ga—O_I—Ga$	102.7	
$Ga—O_{III}—Ga$	94.1	

[a] Ga_I and Ga_{II} in same plane.

in agreement with the observation[18] that in ionic structures, the mutual repulsion of the positive ions tends to reduce the length of shared edges of anion polyhedra.

Because of the short *b* axis, there are two O_I^{2-} and two O_{III}^{2-} ions (along the *b* axis) at corners of an octahedron. The structure cannot possibly then have two O_{II}^{2-} ions at the remaining corners of the octahedron, since these must lie in the mirror plane containing the Ga_{II}^{3+} ion within the octahedron. Thus there is only one O_{II}^{2-} ion at a corner of the octahedron, the remaining corner being occupied by a third O_{III}^{2-} ion.

At the corners of the tetrahedron, there are two O_{II}^{2-} ions which are along the *b* axis, the other corners being occupied by an O_I^{2-} and an O_{III}^{2-} ion each lying in the mirror plane containing the Ga_I^{3+} ion within the tetrahedron.

Thus each O_I^{2-} ion is at the corner of two octahedra and one tetrahedron; each O_{II}^{2-} ion is at the corner of one octahedron and two tetrahedra; and each O_{III}^{2-} ion is at the corner of three octahedra and one tetrahedron. *If* the octahedra and tetrahedra were regular, it would be doubtful that such a structure could exist, because the sums of the bond numbers of the bonds at all oxygen ions would not be 2 (see footnote reference 18). They would be: at O_I^{2-}, $1\frac{3}{4}$, at O_{II}^{2-}, 2; and at O_{III}^{2-}, $2\frac{1}{4}$. However, the polyhedra are probably not regular. In fact, the four bonds to O_{III}^{2-} are the longest ones: $Ga_I–O_{III}=1.85$ A, $Ga_{II}–O_{III}=2.08(2)$ and 2.02

[18] L. Pauling, *Nature of the Chemical Bond* (Cornell University Press, Ithaca, New York, 1960), 3rd ed., Chap. 13, Sec. 6.