

TABLE IV. Interatomic distances and standard deviations.

Atom pair (No.)			Distance, A	σ , A	Atom pair (No.)			Distance, A	σ , A	
Ga _I O ₄ tetrahedron	Ga—O _I	1.80	0.03	Ga _{II} O ₆ octahedron	Ga—O _I (2)	1.95	0.03	Averages	Ga _I —O	1.83
	Ga—O _{II} (2)	1.83	0.01		Ga—O _{II}	1.95	0.03		Ga _{II} —O	2.00
	Ga—O _{III}	1.85	0.03		Ga—O _{III}	2.02	0.03		O—O, octa-	2.84
	O _I —O _{II} (2)	2.93	0.04		Ga—O _{III} (2)	2.08	0.02		hedron	3.02
	O _I —O _{III}	3.13	0.04		O _I —O _I	3.04	0.01		O—O, tetra-	
	O _{II} —O _{II}	3.04	0.01		O _I —O _{II} (2)	2.90	0.04		hedron	
	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							
	Ga _{II} —Ga _{II} (2)	3.04	0.01							
	Ga _{II} —Ga _{II} (2)	3.11	0.01							
	Ga _I —Ga _{II}	3.28	0.01							
	Ga _I —Ga _{II} (2)	3.30	0.01							
	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		Ga _I —O—Ga _I (tetrahedral-tetrahedral) angles	
2 Ga—O _I —Ga	123.3° (2 different Ga _I 's)	2 Ga—O _{II} —Ga	112.0° (2 different O _{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 _{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 observation¹⁸ 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_I²⁻ 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

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

being occupied by an O_I²⁻ and an O_{III}²⁻ ion each lying in the mirror plane containing the Ga_I³⁺ ion within the tetrahedron.

Thus each O_I²⁻ 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_I²⁻, 1½, at O_{II}²⁻, 2; and at O_{III}²⁻, 2½. 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