

x-ray diffraction investigations, they are very small. PRANDL's work includes the determination of anisotropic thermal parameters. However, while there are *apparent* differences in results between the neutron and x-ray investigations, the limits of error in each preclude any conclusion as to their reality. PRANDL also made 77°K measurements of the neutron-diffraction intensities of reflections in the [111] zone. Positional and isotropic thermal parameters were deter-

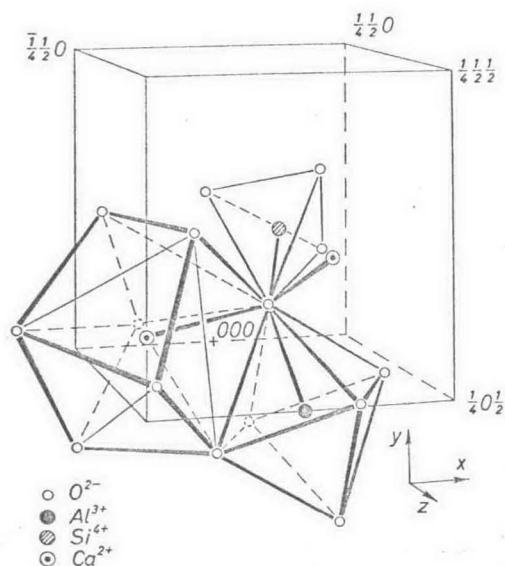


Fig. 1. Coordination about an oxygen ion in grossularite (after ABRAHAMS and GELLER¹⁷)

mined from these and showed no significant difference from those determined from the [111] zone data taken at room temperature.

The x-ray data with which PRANDL's refinement was made were obtained with a Buerger precession camera; intensities were measured with a photodensitometer. The neutron data were also obtained from a single crystal. Our data¹⁷ were obtained from Weissenberg photographs and the intensities were estimated visually. Further, the origins and compositions of the specimens are different. Yet the differences in positional parameters of the oxygen ions are not large. If the averages of the four values for each parameter given in PRANDL's Table 10 are compared with the final set of parameters of the Abrahams-Geller paper, we obtain:

	<i>x</i>	<i>y</i>	<i>z</i>
ABRAHAMS-GELLER	-0.0389	0.0456	0.1524
PRANDL	-0.0382	0.0456	0.1513

The standard errors for the Abrahams-Geller parameters were calculated to be 0.0005 and for the Prandl set 0.0001.

The interionic distances and angles in grossularite are given in the Abrahams-Geller¹⁷ and Prandl¹⁶ papers. The actual values are not strictly those for single cation-oxygen distances because the minerals do not have ideal formulas. In fact, if the chemical analysis given for the grossularite we investigated may be taken as that for the particular spherical specimen from which the x-ray data were collected, the formula may be written:



(The formula does not quite balance, there being an excess of 0.05 cations, but this is probably within the error of the chemical analysis.) If the $\text{Fe}^{3+}-\text{O}^{2-}$ and $\text{Ti}^{4+}-\text{O}^{2-}$ distances are assumed to be 2.01 Å and the $\text{Mg}^{2+}-\text{O}^{2-}$ distances 2.10 Å, the octahedral $\text{Al}^{3+}-\text{O}^{2-}$ distance in this grossularite would be 1.92 Å. The composition of the garnet investigated by PRANDL is much closer to that of pure $\text{Ca}_3\text{Al}_2\text{Si}_3\text{O}_{12}$ and therefore the octahedral cation-oxygen distance in his specimen should be closer to 1.92 Å than to 1.95 Å found¹⁷ in the Chihuahua garnet. Thus there *should* actually be some difference between the two sets of oxygen coordinates. The distance found by PRANDL is 1.927 ± 0.004 Å. Of course, the error limits on our value are not as good, but these results appear to make sense anyway. However, the Si-O distances do not: PRANDL's value, 1.65 Å, is higher than ours, 1.64 Å, and probably the situation should be reversed; thus, perhaps we cannot draw any firm conclusions regarding the small differences, especially since our error limits are about four times as large as PRANDL's.

ZEMANN and ZEMANN¹⁸ found a value of 1.89 Å for the $\text{Al}^{3+}-\text{O}^{2-}$ distance in the synthetic pyrope. Some years ago, I used the Busing-Levy least-squares program on their data and found the standard errors in the oxygen positional parameters to be 0.0005, 0.0004, and 0.0005, respectively. Thus the limits of error on the distances are the same as those in our grossularite investigation. The difference of the $\text{Al}^{3+}-\text{O}^{2-}$ distances in the two garnets (PRANDL's grossularite and ZEMANN's pyrope) therefore appears to be significant. The $\text{Si}^{4+}-\text{O}^{2-}$