

an IBM 7090 digital computer using programs written by Charles W. Burnham. His program for calculating unit-cell parameters by least squares is described elsewhere in this report. His program for calculating  $d$  values permitted by the space group from the parameters of the unit cell was used in indexing powder patterns.

TABLE 1. Miller Indices and  $d$  Values of Reflections Used in Calculating Unit-Cell Parameters of Diopsidic Pyroxenes

$hkl$	$d$ Value	
	Diopside	Lime Tschermak's Molecule
221	2.9897	2.9412
310	2.9492	2.8997
311	2.8924	2.8613
311	2.3009	2.2739
330	2.1546	2.1062
331	2.1322	2.0902
421	2.1067	2.0752
132	1.9679	1.9468
150	1.7535	1.7026

The starting point in our investigation was a carefully indexed powder pattern of pure diopside. This pattern was compared with patterns obtained on material prepared by completely crystallizing glasses on the join diopside-lime Tschermak's molecule at 20 kb. The positions of the peaks were found to shift smoothly as a function of composition from one end of the join to the other. No peaks appeared that could not be traced into their counterparts in the diopside pattern;

this plus optical examination provides evidence that only one phase, a pyroxene, was present in these runs. As a check, the complete pattern for the composition 50 per cent diopside, 50 per cent lime Tschermak's molecule, was calculated. No unexpected interferences between peaks were found. The reflections used and their  $d$  values for diopside and lime Tschermak's molecule are given in table 1. These reflections were chosen because they can be indexed unambiguously and are sharp and strong—an important feature if they are to be used for determinative purposes in mixtures of phases that do not contain very much pyroxene.

The first three reflections listed in table 1 fall at  $2\theta$  angles less than  $31^\circ$  for copper radiation. Hence the  $d$  values cannot be determined with high accuracy. The parameters of the unit cells were calculated by least-squares adjustment both with and without these peaks. The resulting parameters do not differ significantly, but the standard errors are usually smaller if the low-angle peaks are rejected.

The unit-cell parameters of lime Tschermak's molecule and diopside are given in table 2, along with parameters for diopside from other observers. The agreement is good. The change of parameters along the joins diopside-lime Tschermak's molecule and diopside-enstatite is shown in figures 4 and 5. The data in figure 5 were obtained by applying the procedures described above to a series of glasses that had previously been crystallized at 1 atmosphere. Compositions containing more than 40 per cent

TABLE 2. Unit-Cell Parameters of Lime Tschermak's Molecule and Diopside

	Lime Tschermak's Molecule (present)	Diopside (present)	Diopside (Sakata, 1957)	Diopside (H. H. Hess, unpublished)
$a$ , Å	$9.615 \pm 0.003$	$9.745 \pm 0.001$	9.743	9.741
$b$ , Å	$8.661 \pm 0.002$	$8.925 \pm 0.001$	8.923	8.924
$c$ , Å	$5.272 \pm 0.003$	$5.248 \pm 0.001$	5.251	5.247
$\beta$ , deg	$73.88 \pm 0.03$	$74.13 \pm 0.01$	74.07	74.15
$V$ , Å <sup>3</sup>	$421.79 \pm 0.28$	$439.08 \pm 0.07$	438.98	438.77