OPTICAL AND X-RAY DATA FOR IRON-RICH ORTHOPYROXENES FROM NORTHERN QUEBEC

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Kranck (1961), studying mineral phase relations in metamorphic iron formation of the Mount Reed area, Quebec, analysed a number of iron-rich orthopyroxenes. Moore later determined optical properties of some of the original concentrates. Recently, Chao measured cell dimensions of samples separated from impure concentrates of the original hand specimens. Several of the indices were also checked by Kranck, using the same material. Because physical data on orthopyroxenes of the compositions studied are not abundant, it was deemed advisable to publish our data.

Refractive indices were measured in white light at room temperature, using the oblique illumination-colour fringe method and oils calibrated with an Abbe refractometer. Alpha and gamma indices were measured on grains showing an optic normal figure. Precision of measurement is estimated at ±.003. Optic angles were measured on crushed grains, mounted on gelatin-coated slides, in ordinary light, with a Leitz 5-axis Universal stage. Four to eight grains from each concentrate were measured, yielding standard deviations not exceeding 1.4° (total variations were 3°–6°). Appropriate refractive index corrections were applied. Of three specimens studied by Chao, two exhibited refractive indices identical to those of the analysed concentrates (within the estimated error of analysis, ±0.001), but the third deviated appreciably and its *x*-ray data are not reproduced here. In addition to the iron-rich specimens, two metamorphic bronzites were studied optically and these data are also included (Table 1).

Except for a few magnetite inclusions in A-12 and H-1, the grains are free of inclusions and exsolution lamellae. Some grains show wavy or patchy extinction. A-12 and H-1 are pleochroic, with $Y \simeq Z$ = pale green; X = pale brown; H-4 has the pleochroic scheme $Y \simeq Z$ = pale greenish-grey, X = pale pinkish brown. The others are uniformly pale greyish-brown. Modal and chemical analyses may be consulted in Kranck (1961). TiO_2 was not determined, but the lack of pleochroism in all but one of the iron-rich specimens may be explained by their low (<0.03 weight percent) Al_2O_3 content (see Burns, 1966). By contrast,

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TABLE 1. OPTICAL PROPERTIES AND COMPOSITION OF ORTHOPYROXENES

	Specimen Number							
Property[1]	H-4	H-7	H-9	Bl-6	Bl-21	Bl-3	A-12	H-1
$\gamma(\pm.003)$	1.757	1.760	1.756	1.754	1.750	1.745	1.692	1.682
$\alpha(\pm.003)$	1.741	1.746	1.742	1.734	1.729	1.725	1.678	1.670
$2V_\alpha(\pm1°)$	74	67	65	64	61	53	70	80
mg[2]	.218	.229	.235	.288	.310	.405	.760	.827

[1] ± values in parentheses are estimated error of the values given.

[2] mg = molar $Mg/(Mg + Fe^{2+} + Fe^{3+} + Mn)$.

TABLE 2. X-RAY POWDER DATA FOR EULITES

H-4				H-7			
hkl	d_{obs}	I/I_0	d_{calc}	hkl	d_{obs}	I/I_0	d_{calc}
—	8.340[1]	<5		—	8.327[1]	10	
210	6.444	25	6.4409	210	6.441	20	6.4384
400	4.612	50	4.6012	400	4.599	45	4.5992
—	4.250[2]	5	—	—	—	—	—
211	4.061	10	4.0603	211	4.058	5	—
121	3.345[3]	40	—	121	3.347	5	—
420	3.214	100	—	420	3.216	100	—
221			—	221			—
321	2.9828	35	2.9840	321	2.9851	30	2.9871
610	2.8997	90	2.9041	610	2.9032	95	2.9028
511	2.8547	6	2.8553	511	2.8554	5	2.8579
421	2.7397	25	2.7423	421	2.7429	20	2.7446
131	2.5802	50	2.5805	131	2.5813	50	2.5823
521	2.5038	55B	2.5036	521	2.5074	55	2.5051
231	2.4065	5	2.5076	231	2.4103	5	2.5092
302			2.4057	302			2.4137
431	2.2725	<5	2.2677	—	weak		—
711			2.2738				
				531	2.1303	40B	2.1278
				322			2.1279
				721	2.0817	5	2.0839
				512			2.0796
				811			2.0512
				820	2.0505	10	2.0484
				241	2.0209	10	2.0205
				631	1.9850	25	1.9866
a	18.401 ± 0.012[4]				18.397 ± 0.010[4]		
b	9.006 ± 0.007[4]				9.015 ± 0.006[4]		
c	5.233 ± 0.004[4]				5.251 ± 0.004[4]		
R[5]	0.113				0.159		
N[6]	11				18		

[1] Ascribed to amphibole.

[2] Ascribed to quartz.

[3] Not used in refinement because of possible quartz interference.

[4] The ± values are the computed standard deviations after cell refinement.

[5] $[(\Sigma|d_{obs} - d_{calc}|)/\Sigma d_{obs}] \times 100$.

[6] Number of reflections used in refinement.

A-12 and H-1 contain, respectively, 4.0 and 5.8 percent Al_2O_3. The concentration of CaO does not exceed 2.2 weight percent in any sample.

Cell dimensions were determined by least-squares computer refinement (using a program based on the discussion given by Burnham, 1962) of 11–18 reflections, measured from photographs taken with a Siemens 114.6 mm powder camera and FeKα radiation using silicon as internal standard. Reflections were indexed with the aid of single-crystal precession and Weissenberg photographs. Those parts of the patterns measured and indexed are given in Table 2, together with the cell dimensions and their calculated standard errors.

Comparison of optical data with recent compilations (Deer, *et al.*, 1963; Leake, 1968) reveal no significant discord. Cell parameters are close to those predicted by the variation curves of Hess (1952) for orthopyroxenes of the Bushveld type. The *c*-dimension is, inexplicably, significantly different for the two specimens, despite their similar composition. The regression values of Winchell and Leake (1965) for orthopyroxenes poor in Al and Ca provide a slightly better fit for *a*, but their value for *b* of the orthoferrosilite end member in this group is clearly in error. The cell dimensions of H-4 were also determined by Howie (1963, p. 219) as *a* 18.384 Å; *b* 9.006 Å; *c* 5.228 Å. Our values for *a* and *c* are slightly larger. The contraction of the *a* and *b* dimensions observed by Howie in most metamorphic orthopyroxenes is not seen, evidently a result of the low Al content of our specimens, a function of the alumina-poor character of the host rock.

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CELL CONSTANTS OF BIRCH PORTAGE BERYL, SASKATCHEWAN

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In an earlier paper (Radcliffe and Campbell, 1966) the cell edges of three beryl crystals were reported and correlated with chemical composition. At that time the cell constants were determined by a step-wise procedure involving *h*00 with *h* odd and 112. This was done because most diffraction peaks of beryl can be indexed on more than one possible *hkl* value, *e.g.*, 002 ≈ 110, 200 ≈ 102 etc., due to the similarity of the *a* and *c* dimensions.

To improve the precision and accuracy of these measurements it is necessary to calculate cell edge simultaneously by least squares analysis on at least 15 uniquely indexed reflections. Since most peaks may be non-unique a discrimination of tolerance 0.01–0.05° (2θ) has been utilized. The smaller value (0.01) represents the maximum measuring error and the range 0.01–0.05° represents the variation of spacings acceptable in the least squares analysis. Thus any two *hkl* values with calculated 2θ with a difference less than 0.01° are excluded from the computations. These were done automatically with an IBM 7094 using the program of Evans, Appleman and Hardwerker (1963), which assigns Miller indices, computes cell edges and iterates through 10 progressive cycles of least squares refinement.

The results of this procedure are given in Table 1. While the cell edges are somewhat less variable than those reported previously, similar correlation trends of cell constants with chemistry exist. This correlation involves the total of elements other than those required by the beryl formula $Be_3Al_2Si_6O_{18}$. These are for the most part R_2O and R_2O_3 group members, and the values used in the least squares approximation are the average of 5 analytical measurements on each crystal. The inverse linear regressions of $\Sigma(R_2O + R_2O_3)$ with lattice constants, measured density and two refractive indices as independent variables are given in Table 2. This gives four methods of estimating the total of non-