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A NOTE ON THE UNIT CELL CONSTANTS, AND *X*-RAY DIFFRACTION POWDER PATTERN, OF PYROBELONITE

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Pyrobelonite, $PbMn(VO_4)(OH)$, is one of several vanadates the structures of which have been determined in this laboratory but for which powder identification data have not yet appeared in the *ASTM Index* (1968). The specimen at our disposal, kindly supplied by Professor C. Frondel, was Harvard 94831 from the type locality, Långban, Sweden. It consists largely of massive to well-crystallized hausmannite in contact with, and cut by, calcite. The pyrobelonite occurs as very fine grains with a few small crystals (commonly $<100\,\mu$ in largest dimension) primarily in the hausmannite but at least one was found at an interface with the calcite. The isolation of a reasonable number of crystals, free from hausmannite and calcite, and their authentication by precession photographs, for the purpose of preparing a suitable powder specimen was in progress when Moore (1967) published *x*-ray diffraction powder data for Långban pyrobelonite. It is a relief, therefore, not to have to sacrifice the very few satisfactory crystals isolated from the Harvard specimen. It is particularly gratifying that Moore not only had access to an adequate supply of good material, but located one sample large enough for a reliable density measurement (see a discussion of the density of pyrobelonite in Donaldson & Barnes, 1955, pp. 594, 595).

There has been some speculation (Strunz, 1939) about the possible replacement of some of the Pb in pyrobelonite by Mn, based on the original analysis by Mauzelius (Flink, 1919) and on the relatively low value of the measured density reported by Flink (1919). The accuracy of the analysis, however, has been seriously questioned (Richmond, 1940; Dana, 1951). Powder photographs of the hausmannite from Harvard 94831 commonly show pyrobelonite lines. It is possible, therefore, that the high manganese content found by Mauzelius may be indicative of the presence of some hausmannite, or other manganese minerals, although it would require about 10.3% of the former to raise the Mn:Pb ratio from 1:1 to 35:22 as calculated by Strunz (1939). The water content (3%) given by Mauzelius is certainly too high, and the SiO_2, FeO, MgO, CaO, and P_2O_5 (total $>2\%$) presumably represent impurities, including calcite. The *x*-ray diffractometer study described in the present note has shown that even the smaller crystals of pyrobelonite are not necessarily free from internal flaws which could entrap air; this may have contributed to the low values of earlier density measurements (Flink, 1919; Donaldson & Barnes, 1955). Finally, the structure analysis (Donaldson & Barnes, 1955) and the recent density determination of Moore (1967) demonstrate that very strong evidence would now be required to prove that there is any significant replacement of Pb by Mn in Långban pyrobelonite.

Pyrobelonite is listed three times in *Crystal Data* (Donnay, 1963). The unit cell dimensions of Moore (1967), which differ slightly from those of Barnes & Qurashi (1952), now make a fourth entry possible. It seemed desirable, therefore, to remeasure the unit cell constants with greater accuracy than heretofore and, in view of the discussion in the preceding paragraph, to make a single entry feasible. The crystal system is orthorhombic and the space group is *Pnma* so that the odd orders of all three sets of axial reflections are extinguished. To conform with the *Crystal Data* convention, $c < a < b$, the axes b and c have been interchanged in the present note so that the space group designation becomes *Pnam*, but this should cause no confusion in any comparison of the present data with those reported previously (Barnes & Qurashi, 1952; Donaldson & Barnes, 1955; Moore, 1967).

Ideally, the unit cell dimensions should have been remeasured with the G.E. manual XRD-5 diffractometer (practical upper limit of $2\theta \approx 160°$) and with both Mo and Cu radiation as was done in the case of vanadinite (Barnes, 1962). Unfortunately, however, this equipment was in use on a long-term project, and a Picker automatic diffractometer (practical upper limit of $2\theta \approx 135°$) and Cu radiation, therefore, were employed, thus reducing the number of even-order axial reflections available for examination by more than one-half and greatly increasing the effect of absorption (μ = 480 cm^{-1} for Mo, 1154 cm^{-1} for Cu). The present investigation, therefore, was carried out with Cu $K\alpha_1$ (λ = 1.54050 Å) and $K\alpha_2$ (λ = 1.54434 Å) radiations, and was restricted to the following reflections: $h00$ with h = 4, 6, 8; $0k0$ with k = 6, 8, 10; $00l$ with l = 2, 4, 6. The $K\alpha_2$ reflection from 002 was not resolved sufficiently for an accurate measurement of 2θ and was omitted. A small prismatic crystal of approximate dimensions 0.04 × 0.07 × 0.13 mm., elongated along c, with c^* coincident with the φ-axis, and a^* and b^* in the equatorial plane of the goniostat at $\chi = 0°$, was employed with a take-off angle of 1° and a narrow slit. Two values of 2θ (180° apart around φ) for each of 400, 600, and 800, were measured at $\chi = 0°$ with both $K\alpha_1$ and $K\alpha_2$ radiations, and the complete set of values for 800 was repeated as a check on the satisfactory reproducibility of measurement (estimated standard deviation (e.s.d.) $\approx$ 0.0001); these data yielded 16 values for $d(100) = a$, over a range $\approx 23.8° < \theta < 54.0°$. Similarly, 12 values for $d(010) = b$, over a range $\approx 29.0° < \theta < 54.4°$, were obtained, also at $\chi = 0°$. At $\chi = 90°$, four values of 2θ (90° apart around φ) for each of 004 and 006 with both $K\alpha_1$ and $K\alpha_2$ radiations, and for 002 with $K\alpha_1$ only, were measured to give 20 values for $d(001) = c$ over a range $\approx 14.4° < \theta < 48.6°$.

All values for each of the axial lengths were plotted against $\frac{1}{2}[(\cos^2\theta/\sin\theta) + (\cos^2\theta/\theta)]$ (Azároff & Buerger, 1958, pp. 236–239, 321–323). For each axis a straight line was drawn through a point representing the arithmetic mean of the axial lengths derived from the data from the highest order and passing midway between the means of those from the two lower orders (±0.0004 Å for a, ±0.0005 Å for b, ±0.0007 Å for c). Extrapolation to $\frac{1}{2}[(\cos^2\theta/\sin\theta) + (\cos^2\theta/\theta)] = 0$ gave a = 7.6435 Å, b = 9.5085 Å, c = 6.1816 Å (last digits uncertain). The maximum deviation of any point from the straight line was 0.0009 Å for a, 0.0016 Å for b, and 0.0017 Å for c. The e.s.d. values are as follows: a (from 400, 600, 800), 0.0001, 0.0002, 0.0001 Å, respectively; b (from 060, 080, 0.10.0), 0.0007, 0.0007, 0.0004 Å, respectively; c (from 002, 004, 006), 0.0006, 0.0003, 0.0003 Å, respectively; root mean square deviation = 0.0004 Å. Therefore, although only three orders from each set of axial planes were employed to derive values for a, b, and c, and the absorption coefficient for Cu is very high, an e.s.d. of 0.001 Å for the final value of each axial length seems reasonable.

Revised crystal data, and discussion

The unit cell data for pyrobelonite, therefore, are as follows: orthorhombic, *Pnam*, a = 7.644, b = 9.508, c = 6.182 Å ($\sigma \approx$ 0.001 Å in each case), $U = 449.3025$ Å^3, F.W. = 1576.30, $D_x = 5.824$ g.ml^{-1}, $Z = 4$, $D_m = 5.82$ g.ml^{-1} (Moore, 1967; temperature not stated).

Dimensions previously reported are compared with the remeasured values in Table 1, where their sources are identified as S. (Strunz, 1939), R. (Richmond, 1940), B. & Q. (Barnes & Qurashi, 1952), M. (Moore, 1967), B. & A. (Barnes & Ahmed, this note). Those of Strunz differ from the new ones by 0.6 to 1.3%, those of Richmond by 0.6 to 2.6%, those of Barnes & Qurashi by 0.14 to 0.24%, and those of Moore by 0.19 to 0.40%. There is nothing surprising about these differences; Strunz relied on rotation and oscillation photographs, Richmond measured Weissenberg films, Barnes & Qurashi employed precession films corrected for film shrinkage (Barnes, Przybylska & Shore, 1951), and Moore derived his values from a powder pattern (114.6 mm camera diameter; Fe/Mn radiation, with which absorption effects could be highly significant). In fact, taking into account the various techniques and possible errors involved, the data in Table 1 are consistent with the argument that Långban pyrobelonite has a constant composition with Mn:Pb = 1:1.

TABLE 1. UNIT CELL DIMENSIONS (Å) OF PYROBELONITE IN *Pnam*; S. AND R. PROBABLY *kX* UNITS

	a	*b*	*c*
S.	7.74	9.57	6.22
R.	7.84	9.45	6.09
B. & Q.	7.66_8	9.52_2	6.19_1
M.	7.62	9.47	6.17
B. & A.	7.644	9.508	6.182

Indexed powder data, with *d* values calculated on an IBM/360 computer with a program which uses 16 decimal digits of precision (Ahmed, Hall, Pippy & Huber, 1966), are listed in Table 2 for $d >$ 1.900 Å (the limit adopted by Moore, 1967, whose list of *observed d* values extends for a further 50 lines and for which his paper should be consulted). The print-out of the NRC spacings routine shows the unit cell data used by the computer, lists all permissible values of *d* (with corresponding indices) in decreasing magnitude to any desired minimum limit within the sphere of reflection, and, as a further check, lists separately the *d* values (with corresponding indices) of all reflections prohibited by the space group. All values of *d* are rounded off and printed to four decimal digits which may then be further rounded off by hand to three or two as desired. In Table 2, the first column shows I/I_1 (values of I/I_0 (*sic*) from Moore's Table 2 multiplied by 10), the second column, M(calc.) lists the values of *d* calculated by Moore, the third column, M(recalc.), lists all possible values of *d* (not prohibited by the space

TABLE 2. X-RAY DIFFRACTION POWDER DATA FOR PYROBELONITE, PbMn(VO$_4$)(OH); TABLE HEADINGS EXPLAINED IN THE TEXT

	d(Å)					hkl	
I/I_1	M(calc.)	M(recalc.)	M(obs.)	M(obs.;c.)	BA(calc.)	*Pnma*	*Pnam*
—	—	5.937	—	—	5.957	101	110
70	5.16	5.170	5.14	5.172	5.183	011	011
30	4.73	4.735	4.75	4.777	4.754	002	020
40	4.27	4.278	4.27	4.292	4.290	111	111
20	4.01	4.022	4.00	4.019	4.037	102	120
—	—	3.810	—	—	3.822	200	200
30	3.53	3.535	3.54	3.555	3.546	201	210
20	3.36	3.369	3.36	3.373	3.380	112	121
100	3.24	3.242	3.24	3.252	3.251	210	201
30	3.084	3.085	3.085	3.096	3.091	020	002
—	—	3.067	—	—	3.076	211	211
—	—	2.968	—	—	2.979	202	220
50	2.909	2.916	2.914	2.924	2.928	103	130
—	—	2.810	—	—	2.820	013	031
30	2.735	2.737	2.734	2.742	2.744	121	112
65	2.673	2.675	2.672	2.680	2.683	212	221
70	2.631	2.637	2.635	2.643	2.646	113	131
25	2.582	2.585	2.583	2.590	2.591	022	022
20	—	2.453	2.452	2.458	2.461	301	310
	2.445	2.448			2.454	122	122
—	—	2.431	—	—	2.440	203	230
—	—	2.398	—	—	2.403	220	202
—	—	2.367	—	—	2.377	004	040
70	2.324	2.324	2.323	2.329	2.330	221	212
—	—	2.280	—	—	2.287	311	311
20	2.254	2.261	2.262	2.267	2.270	104	140
	—	2.262			2.269	213	231
—	—	2.238	—	—	2.246	302	320
—	—	2.139	—	—	2.145	222	222
50	—	2.123	2.121	2.125	2.131	114	141
	2.117	2.119			2.126	123	132
20	2.103	2.104	2.108	2.112	2.111	312	321
—	—	2.011	—	—	2.018	204	240
10	2.009	2.010	2.012	2.016	2.014	031	013
20	1.978	1.979	1.983	1.987	1.986	303	330
10	1.943	1.943	1.943	1.947	1.947	131	113
—	—	1.920	—	—	1.925	321	312
—	—	1.912	—	—	1.919	214	241
—	—	1.909	—	—	1.915	223	232
20	1.906	1.905	1.908	1.911	1.911	400	400
			+ 50 lines not indexed				

group) recalculated from the unit cell dimensions of Moore, the fourth column, M(obs.), repeats the observed values from Moore's Table 2, the fifth column, M(obs.;c.), shows the effect of an empirical correction for absorption (see next paragraph) on M(obs.), the sixth column, BA(calc.), lists the values calculated with the new cell dimensions, and the last two columns give the corresponding indices, *hkl*, for space groups *Pnma* and *Pnam*, respectively. Because the resolution of lines in the original powder photographs is not indicated by Moore, possible lines separated by $S \leq 0.10$ mm ($2\theta \leq 0.10°$) for Fe $K\alpha$ radiation are shown in parentheses.

In Table 2, corresponding values of d for M(obs.) tend to be consistently lower than those for BA(calc.). Therefore, the observed values of 2θ for Fe $K\alpha$ radiation in the indexed range $21° < 2\theta < 61°$ are higher than the calculated values by 0.05° to 0.30° (mean, 0.13°). This effect is precisely that found in the case of undiluted vanadinite (Barnes, 1962) where an increase of about 0.1° in the range $20° < 2\theta < 75°$ was observed for undiluted vanadinite in 0.2 mm capillaries and the use of Cu $K\alpha$ radiation, with the same camera diameter as that of Moore, and was shown to arise from absorption. With pyrobelonite, the effect of absorption for Fe radiation would be expected to be high, $\mu(\text{Fe}) = 1710\ \text{cm}^{-1}$, and better agreement between M(obs.) and BA(calc.) undoubtedly could be achieved by heavy dilution of the pyrobelonite powder with powdered gum tragacanth as has been demonstrated in the case of vanadinite and Cu $K\alpha$ radiation (Barnes, 1962). This expectation is supported by the application of an empirical absorption correction to the values of M(obs.) based on the assumption that the differences between BA(calc.) and M(obs.) arise entirely from absorption. The correction factor to be applied to each value of M(obs.) was obtained from the best straight line drawn through a plot of d[BA(calc.)]/d[M(obs.)] against $\frac{1}{2}[(\cos^2\theta/\sin\theta) + (\cos^2\theta/\theta)]$, and decreased from 1.0063 for the 011 reflection to 1.0018 for the 400 reflection. The values of M(obs.) corrected for absorption in this manner are shown in column five of Table 2 under the heading M(obs.;c.).

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A NOTE FROM THE ACTING EDITOR

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We undertook the duties of acting editor after the tragically sudden death of W. W. Moorhouse and consequently the current issue of the journal was delayed a few months. However, the delay was not entirely due to the sudden shift of editorial responsibility: it was partly due to the difficulty of arriving at a compromise between the profound lack of knowledge of scientific logic, semantics and mathematics on the part of the authors and a conceptual ideal for this journal.

Currently, we are involved in a research project consisting of computer storage and retrieval of scientific information required in modern research in the field of physical geochemistry. Less than one percent of the items (paper, books, and reports) are from mineralogical and geological sources, and nearly half of the total number of relevant items originated in the USSR. The purpose in mentioning these facts is that we have read approximately 6,800 scientific communications in the immediate past and thus are in a position to compare what is currently practiced in sciences closely related to mineralogy. In every respect (except possibly the paper on which the journal is printed) the quality of our efforts is poor by comparison. The principal defects appear to be 1) inordinate length of the papers and 2) unusable numerical data.

In regard to the length of scientific papers, the criterion is not, of course, the number of pages, but the number of concepts and/or data transmitted to the reader per word or number in the published item. As a rough estimate, the papers currently published in this journal could be condensed about 90% without losing their critical information. That is, the facts which the readers are looking for could be presented without being imbedded in essay-style reports which were acceptable a century ago. We assume, of course, that this is a scientific journal addressing itself to scientists and if so the papers contained in it should be written as if the readers were well acquainted with the necessary theory to understand the problem attacked, the methods and apparatus used, and