# X-RAY CRYSTALLOGRAPHY OF DAVIDITE

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## Abstract

Partly or wholly metamict davidite from Pima County, Arizona and from Iveland, Norway, has been reconstituted to single crystals or twins by heating in air. The cell dimensions are $a_0$ 10.37 ±0.02, $c_0$ 20.87 ±0.02 Å. The space group is $R\bar{3}$ or $R3$. The suggested ideal content for the rhombohedral cell is $Y_6Z_{15}O_{36}$ or $3(Y_2Z_5O_{12})$, Y representing the larger cations, mostly Fe″ with some Ce, U, etc. and Z the smaller cations, mostly Ti with some Fe‴, V, Cr, etc. Davidites from seven localities yield the same powder diffraction pattern which can be fully indexed on this cell. Small amounts of contaminants, mostly rutile, can be identified in some reconstituted davidites. The reported morphology of davidite from Mozambique can be reconciled with the structure cell. Rough crystals of davidite from Billeroo, South Australia, also appear rhombohedral.

## Introduction

The name davidite was applied by Mawson (1906) to a "bright black mineral" from Radium Hill, South Australia, shown "to contain over 50 per cent titania, a large quantity of iron, and a notable amount of rare earths, uranium, vanadium and chromium." An analysis was not published until ten years later (Cooke, 1916). The mineral at the type locality occurs in an intimate intergrowth with ilmenite and rutile from which it is difficult to separate a pure concentrate. Probably because of this the status of the species had been questioned even before the publication of Cooke's analysis (Crook and Blake, 1910) and long remained in doubt (Palache, Berman and Frondel, 1944, p. 542) though Mawson (1916) had reasserted its validity when the analysis was published. This may have been the reason for the caution exercised by Bannister and Horne (1950) when they referred to material they described as "A radioactive mineral from Mozambique related to davidite."

Studies by Kerr and Holland (1951) showed that davidite yields a characteristic DTA curve as well as x-ray powder diffraction pattern though analyses indicate wide variation in composition and in recent years davidite has been reported from many other localities in Australia (Whittle, 1954 and 1955, Lawrence, *et al.* 1957, Ramdohr and Lawrence, 1958). In spite of this its status continues to be questioned and Whittle (1959, p. 80) has recently stated "that davidite is perhaps not a finite mineral species, but that it could consist of a mechanical mixture of two or even more minerals, which are intimately associated at submicroscopic sizes."

The finding of davidite in Arizona which could be made to yield single crystal diffraction patterns (Pabst and Thomssen, 1959) has led to a unit cell and probable space group for davidite on the basis of which

powder patterns of davidite from many localities can be indexed. These results have been further supported by single crystal x-ray examination of davidite from Norway and by the reconciliation of the reported morphology of davidite from Mozambique and meager observations on the morphology of davidite from Billeroo, South Australia, with the lattice found by x-ray diffraction.

## MATERIAL

Davidite specimens available for study included material from:

1. Pandora prospect, Quijotoa Mountains, Pima County, Arizona. (Several pieces collected by R. W. Thomssen, showing the association described by Thomssen (1961).)
2. Radium Hill, South Australia, the type locality. (Mawson 1906, 1944)
    a. ($3 \times 4''$ specimen, mostly davidite intimately intergrown with ilmenite and rutile and much black mica, with which are mixed minor amounts of chalcopyrite and carbonates.)
    b. (A smaller specimen, similar to 2a, some parts nearly pure davidite.)
    Presumably equivalent to type material.
3. Crocker's Well, South Australia. Locality described by Whittle (1954).
    a. (Black, pitchy mass, $1\frac{1}{2} \times 1\frac{1}{2}''$, with albite, mostly pale brownish in color, presumably due to many minute, high index, colored inclusions.)
    b. (A specimen similar to 3a, kindly lent for study by Mr. Joseph Urban.)
4. Billeroo, South Australia. Mentioned by Whittle (1959).
    a. (A small cluster of crystals, ca. $1 \times 1''$.)
    b. (3 larger, rough, single crystals, $22\frac{1}{2}$, 17 and $8\frac{1}{2}$ grams.)
5. Thackeringa, New South Wales, Australia.
    ($1\frac{1}{2}'' \times 2''$. Small amount of davidite with a bit of anatase coating and large rutile crystals, some coarse gray quartz in fine granular yellowish matrix of quartz with a bit of mica.)
6. Portuguese East Africa (Mozambique). Geological setting described by Davidson and Bennett (1950), and by Roso de Luna and Freitas (1952), referred to as mavudzite by Pinto Coelho (1954). ("Rich mass," a $1 \times 2''$ rough fragment of pure davidite.)
7. Iveland, Setesdal, Norway.
    ($1\frac{1}{2} \times 1\frac{1}{2}''$ crystal fragment with a bit of adhering quartz and mica.)
    Specimens 2a, 4a, 5, 6, and 7 were purchased from the Scott Williams Mineral Co., specimens 2b, 3a and 4b from Specimen Minerals (Australia) Ltd.
    (See supplementary note (2) on page 718 of this paper)
    Other specimens examined (no davidite found):
8. Heavy mineral concentrates from east side of the Sierra Nevada, California. Said to contain "uranium-bearing ilmenite" (Shawe, 1953). Kindly supplied by Professor C. O. Hutton.
9. Coarse, heavy mineral concentrates. Red River placer gravels. Idaho County, Idaho. Reported to contain davidite (Armstrong and Weis, 1957, table 1, p. 28). Kindly supplied by L. L. Brown, U. S. Bureau of Mines, Albany, Oregon.

## X-RAY PROCEDURE

X-ray examination of davidites was carried out mostly on fragments. Untreated fragments were first mounted in Norelco powder cameras at

the tips of glass fibers and the x-ray diffraction recorded. Thereupon the fragments were dismounted, heat treated, remounted and again examined by x-ray diffraction. In some cases fragments were repeatedly treated and remounted for further examination to follow the course of changes. If single crystal diffraction was detected in either untreated or treated material the fragments were remounted on x-ray goniometer heads and fully examined by the Weissenberg or Buerger precession methods. X-ray photographs were also made from powdered material for the sake of obtaining more favorable conditions for recording powder patterns but only after the same material had been checked by the examination of fragments.

## General Survey of Results

Davidites from all seven localities are initially metamict or show only faint x-ray indications of a remnant of structure. Upon heating all yielded the same x-ray powder diffraction pattern which can be indexed on the basis of a rhombohedral cell. The temperature at which reconstitution is effected varies in different davidites but once the reconstitution is complete no further changes are produced in the powder patterns by heating fragments to temperatures as high as 1375° C. Lima de Faria (1956, p. 8) noted that "it makes no difference whether davidite samples are heated at 1000° C. for 1 hour or for 24 hours."

Twelve fragments from Arizona and 9 from Norway were heated and examined by x-rays. All were reconstituted to single crystals, twins or coarse aggregates. No fragments from the other five localities were reconstituted in this way by heating, though 27 such fragments were examined, at least 4 from each locality. In most cases smooth arcs were observed in the powder patterns but the best patterns of reconstituted davidite from Radium Hill, the type locality, show some degree of orientation, suggesting that there might be a possibility of finding fragments of this material that could be reconstituted to single crystals.

## Space Group and Cell Dimensions

Indexing of all patterns indicates a rhombohedral lattice and the Laue group is $\bar{3}$ so that the possible space groups are $R\bar{3}$ or $R3$, the latter if the $c$ axis is polar as concluded from the morphology by Horne (Bannister & Horne, 1950, p. 102). The cell dimensions as determined from shrinkage-corrected Weissenberg or precession patterns of davidite from Arizona and Norway are $a_0$ 10.37 ± 0.02 Å, $c_0$ 20.87 ± 0.02 Å, averages of 11 and 6 determinations respectively, corresponding to $a_r$ 9.178 Å, $\alpha$ 68° 48′, for the rhombohedral cell. The large indicated ranges of uncertainty span all values obtained. A greater precision was not

attained because of the diffuseness of high angle spots on most films and the high background on films with Cu or Co radiation due to high Ti content of the mineral. Powder patterns show no measurable back reflection lines but multiple correlation using 14 and 16 selected lines free of coincidence in the interval 3.0 to 1.4 Å on Co powder patterns of Arizona and Norway davidite respectively, made from powder rods 0.1 mm. thick and perfectly centered, yielded good checks of the values obtained from single crystals. Powder patterns of davidite from the five other localities gave no indication of differences in cell dimensions that would exceed the stated limits.

## INDEXED POWDER PATTERN

In Table 1 is given an indexed powder pattern of davidite from Arizona heated for one hour at 970° C. in air. The indexing has been completely checked by comparison with single crystal patterns giving proper consideration to intensities. All expected lines are observed and there are no surplus lines. Most of the indices listed in the table represent superposition of 2 and some of 4 sets of reflections. For instance, $41\bar{5}6$ represents $\{41\bar{5}6\}$, $\{41\bar{5}6\}$, $\{51\bar{4}6\}$ and $\{51\bar{4}6\}$. The relative intensities of spots representing these four sets, as observed on a single precession pattern, are 6, 5, 3 and 1. This statement can be taken to define the orientation adopted for indexing davidite single crystal patterns. In Table 1 the indices listed do not in all cases correspond to the set of reflections with highest intensity as in the example just given.

The indexed powder pattern agrees fairly well with patterns of davidite from Mozambique, specimen 1, published by Kerr and Holland (1951, table 2) and of "the Tete mineral after heating in air at 1000° C." published by Bannister and Horne (1950, Fig. 6, pattern A) as well as with patterns of davidite from Australian localities published by Lawrence *et al.* (1957) and by Whittle (1959), but includes a number of weaker lines not recorded by those observers. Similar patterns were obtained from all the davidites examined though some also showed extraneous lines to be discussed later. No change was observed in patterns obtained from fragments heated for longer periods or to higher temperatures. The highest temperatures employed were: specimen 1, 2 hours at 1375° C.; specimen 3$b$, 1$\frac{1}{2}$ hours at 1150° C; specimen 4$a$, 1$\frac{1}{4}$ hours at 1180° C. and specimen 6, 1 hour at 1220° C.

## DENSITY, COMPOSITION AND CELL CONTENT

In Table 2 are shown the chemical analyses of three of the davidites examined, two quoted from earlier publications. A somewhat different analysis of davidite with density 4.60 from the Tete district, Mozam-

TABLE 1. X-RAY POWDER DIFFRACTION PATTERN OF DAVIDITE FROM ARIZONA, RECONSTITUTED BY HEATING FOR ONE HOUR AT 970° C.

| hkil | I | $d_{obs.}$ | $d_{calc.}$ | hkil | I | $d_{obs.}$ | $d_{calc.}$ | hkil | I | $d_{obs.}$ | $d_{calc.}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 10$\bar{1}$1 | | | 8.25 Å | 30$\bar{3}$6 | | | 2.267 | 50$\bar{5}$2 | | | 1.770 |
| 0003 | 18 | 6.86 | 6.96 | 20$\bar{2}$8 | | | 2.256 | 20$\bar{2}$·11 | | | 1.748 |
| 01$\bar{1}$2 | | | 6.81 | 13$\bar{4}$4 | 50 | 2.248 | 2.248 | 000·12 | <5 | 1.741 | 1.739 |
| 11$\bar{2}$0 | 15 | 5.21 | 5.18 | 21$\bar{3}$7 | | | 2.240 | 22$\bar{4}$9 | | | 1.728 |
| 10$\bar{1}$4 | | | 4.51 | 40$\bar{4}$1 | | | 2.232 | 33$\bar{6}$0 | | | 1.728 |
| 02$\bar{2}$1 | | | 4.39 | 04$\bar{4}$2 | ‡ | | 2.195 | 41$\bar{5}$6 | 22 | 1.708 | 1.707 |
| 11$\bar{2}$3 | 24 | 4.18 | 4.16 | 31$\bar{4}$5 | 40 | 2.139 | 2.139 | 04$\bar{4}$8 | | | 1.702 |
| 20$\bar{2}$2 | | | 4.12 | 11$\bar{2}$9 | | | 2.117 | 05$\bar{5}$4 | | | 1.698 |
| 01$\bar{1}$5 | 7 | 3.81 | 3.79 | 22$\bar{4}$6 | | | 2.079 | 32$\bar{5}$7 | | | 1.695 |
| 0006 | | | 3.48 | 12$\bar{3}$8 | 5 | 2.072 | 2.068 | 24$\bar{6}$1 | ‡ | | 1.692 |
| 02$\bar{2}$4 | 72 | 3.42 | 3.40 | 40$\bar{4}$4 | | | 2.062 | 33$\bar{6}$3 | | | 1.677 |
| 21$\bar{3}$1 | 8 | 3.36 | 3.35 | 32$\bar{5}$1 | | | 2.048 | 42$\bar{6}$2 | | | 1.675 |
| 12$\bar{3}$2 | 20* | 3.21 | 3.228 | 10$\bar{1}$·10 | 5 | 2.029 | 2.033 | 12$\bar{3}$·11 | | | 1.656 |
| 20$\bar{2}$5 | 50 | 3.065 | 3.057 | 23$\bar{5}$2 | | | 2.021 | 50$\bar{5}$5 | | | 1.650 |
| 30$\bar{3}$0 | 40 | 3.000 | 2.994 | 04$\bar{4}$5 | 12 | 1.982 | 1.977 | 11$\bar{2}$·12 | 12 | 1.652 | 1.649 |
| 11$\bar{2}$6 | 100 | 2.895 | 2.889 | 41$\bar{5}$0 | | | 1.960 | 13$\bar{4}$·10 | 40 | 1.601 | 1.600 |
| 21$\bar{3}$4 | 60 | 2.850 | 2.845 | 32$\bar{5}$4 | 25 | 1.919 | 1.916 | 42$\bar{6}$5 | <5 | 1.572 | 1.572 |
| 10$\bar{1}$7 | | | 2.829 | 13$\bar{4}$7 | | | 1.911 | 33$\bar{6}$6 | 10 | 1.548 | 1.548 |
| 30$\bar{3}$3 | 22 | 2.755 | 2.748 | 02$\bar{2}$·10 | 5 | 1.897 | 1.893 | 31$\bar{4}$·11 | 15 | 1.509 | 1.509 |
| 12$\bar{3}$5 | 33 | 2.640 | 2.633 | 41$\bar{5}$3 | | | 1.886 | 32$\bar{5}$·10 | 5 | 1.467 | 1.466 |
| 22$\bar{4}$0 | 18 | 2.595 | 2.593 | 01$\bar{1}$·11 | | | 1.856 | 52$\bar{7}$0 | 40 | 1.439 | 1.438 |
| 01$\bar{1}$8 | | | 2.505 | 23$\bar{5}$5 | 10 | 1.849 | 1.847 | | 8 | 1.419 | |
| | | | | 30$\bar{3}$9 | | | 1.833 | | 10 | 1.376 | |
| 02$\bar{2}$7 | | | 2.484 | | | | | | 5 | 1.360 | |
| | | | | 31$\bar{4}$8 | 38 | 1.803 | 1.801 | | 8 | 1.346 | |
| 13$\bar{4}$1 | 38† | 2.480 | 2.473 | 40$\bar{4}$7 | | | 1.793 | | 6 | 1.302 | |
| | | | | 05$\bar{5}$1 | | | 1.789 | | <5 | 1.275 | |
| 22$\bar{4}$3 | 25 | 2.429 | 2.429 | 21$\bar{3}$·10 | 12 | 1.780 | 1.778 | | 5 | 1.246 | |
| 31$\bar{4}$2 | | | 2.423 | | | | | plus ca. a dozen more weak, diffuse lines. | | | |
| 0009 | | | 2.319 | | | | | | | | |

Co radiation, Fe filter, Norelco 114.59 camera. Intensities estimated by comparison with standard intensity scale.

\* Intensity reported for 12$\bar{3}$2 is on hydrothermally reconstituted davidite. Ordinarily traces of the strongest rutile line at 3.245 obscure this.

† May be enhanced and slightly displaced towards lower angles by rutile line at 2.489 or by "subsidiary reflections" discussed in text.

‡ Lines in these positions reported in most published davidite patterns are probably attributable to (111) and (211) of rutile, spacings 2.188 and 1.687, intensities 22 and 50, NBS Circ. 539, vol. I, p. 45.

bique, has been published by Colin (1950). So far as known neither the davidites of Billeroo, Thackeringa and Crocker's Well, Australia, nor that from Iveland, Norway,* have been analyzed. Published analyses of davidites not examined during this study include one of material from Houghton, South Australia (Whittle, 1954) and three from the Mt. Isa-Cloncurry district, Queensland (Lawrence et al. 1957). Among the latter is an analysis of "davidite type 3" having a much higher density, 4.89,

\* See supplementary note (2), page 718, this issue.

TABLE 2. CHEMICAL ANALYSES OF DAVIDITE

|  | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| $Al_2O_3$ | — | — | 0.37 | 0.39 |
| $SiO_2$ | — | 0.06 | 1.69 | 0.34 |
| $TiO_2$ | 54.3 | 54.5 | 54.37 | 55.20 |
| $V_2O_5$ | * | 1.4 | 0.31 | 0.33 |
| $Cr_2O_3$ | * | 0.17 | 0.87 | 0.91 |
| $Fe_2O_3$ | 13.0 | 10.2 | 18.84 | 19.80 |
| MgO | 0.6 | nil | 0.73 | 0.77 |
| CaO | 1.5 | 0.3 | 1.28 | |
| MnO | — | — | 0.21 | 0.22 |
| FeO | 16.0 | 16.5 | 7.14 | 7.50 |
| SrO | — | — | 0.26 | 0.27 |
| PbO | 1.5 | 0.72 | — | |
| $ZrO_2$ | — | 0.4 | 0.52 | 0.55 |
| R.E. | 8.3 | 5.6 | 8.96§ | 9.42 |
| $ThO_2$ | 1.1 | 0.07 | 0.43 | 0.45 |
| $UO_2$ | 4.6* | 9.8† | 3.56 | 3.74 |
| $Na_2O$ | — | 0.15‡ | 0.03 | 0.03 |
| $K_2O$ | — | — | 0.08 | 0.08 |
| $H_2O^+$ | — | 0.05 | 0.17 | |
| $H_2O^-$ | — | — | 0.00 | |
| Total | 100.9 | 99.92 | 99.82 | 100.00 |
| Sp. Gr. | — | 4.46 | 4.42 | |

* Represents $U_3O_8$, $Cr_2O_3$ and $V_2O_5$.

† Uranium reported as $UO_3$

‡ Alkali metals as $Na_2O$.

§ Includes $Ce_2O_3$ (1.5–2%), $Sc_2O_3$, $Y_2O_3$, etc.

1. Radium Hill, South Australia. W. T. Cooke (1916).

2. Tete district, Mozambique. Bannister and Horne (1950, Analysis 1, Table I).

3. Pandora prospect, Quijotoa Mountains, Pima County, Arizona. C. A. Ingamells, analyst.

4. Analysis of column 3 adjusted to a total of 100% after deducting sphene equivalent to 1.28% CaO and omitting water.

and higher uranium content, 20.16% $U_3O_8$, than any other recorded davidite.

Additional information on the composition of the Arizona davidite was obtained from an $x$-ray fluorescence spectrogram and counts on selected peaks kindly run by Mr. Kenneth Johnson of the Kearney Foundation of Soil Science. The spectrogram showed lines for Y, Ce, La and Gd and no others among the elements included under rare earths in the analysis.

Spectrographic examinations of the Arizona and Norwegian davidites by Mr. George Gordon of the Division of Mineral Technology showed them to have similar compositions but with these differences: less Mg. Si, Ca, Th and U but more V, Mn and Sc in the Norwegian than in the Arizona material.

The specific gravity recorded in Table 2 for the Arizona davidite was determined by pycnometer on the concentrate used for analysis. Similar values were obtained on individual fragments by Berman balance. No reliable specific gravity has been reported for the Radium Hill davidite and the available samples of this provide no material suitable for a determination. A selection of new specific gravity determinations of davidite follows:

| Specimen | Locality | Method | Sp. Gr. |
|---|---|---|---|
| 3a | Crocker's Well | Jolly balance | 4.49 |
| 4 | Billeroo | Jolly balance | 4.38 |
| 7 | Norway | Berman balance | 4.37 |

The weight loss after heating was determined for fragments of the Arizona, Crocker's Well and Norwegian material to be about 0.3%. The Arizona davidite increased in sp. gr. to about 4.55 on heating, whereas changes in the others were within the limits of uncertainty.

In Table 3 are shown the results of cell content calculations for the three davidites for which analyses are given in Table 2. For the Arizona davidite the figures of the adjusted analysis, column 4, Table 2, were used. The same cell volume, 1,943.6 $Å^3$, was assumed for all. Since it seems probable that davidite in its reconstituted state contains no hydroxyl, water was excluded from consideration. In the absence of a specific gravity determination for the Radium Hill davidite the calculation for this shown in column 1 was adjusted to an oxygen content of 35 atoms for the rhombohedral cell, close to the average for the other two davidites as given in columns 2 and 3. Following Bannister and Horne (1950, p. 107), "$V_2O_5$ and $U_3O_8$, reported together in the analysis, have been arbitrarily assigned the values 1.4 and 3.2% respectively" for the Radium Hill davidite.

Bannister and Horne (1950) derived the provisional formula $AB_3(O, OH)_7$, where A represents smaller and B larger cations, for davidite. Five such formula units in the rhombohedral cell are indicated. The ratios of $A+B/O$ for the Mozambique and Arizona davidites agree with this fairly well. If $Fe'''$ is counted with the B cations, as was done by Bannister and Horne, their number is too large, 16.71 instead of 15.00, in the Arizona davidite. This is connected with the fact that $Fe^3$ exceeds $Fe^2$ in this davidite. An adjustment to the formula can be obtained by counting a part of the ferric iron with the B cations.

TABLE 3. CELL CONTENTS OF DAVIDITE

|  | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| Al | — | — | 0.13 | — | — | 0.13 |
| Si | — | 0.02 | 0.09 | — | 0.02 | 0.09 |
| Ti | 11.87 | 11.87 | 11.95 | 12.21 | 12.28 | 12.14 |
| V | 0.38 | 0.27 | 0.06 | 0.39 | 0.28 | 0.06 |
| Cr | — | 0.04 | 0.21 | — | 0.04 | 0.21 |
| Fe''' | 2.85 | 2.21 | 4.27 | 2.93 | 2.29 | 4.34 |
| $\Sigma'$ | 15.10 | 14.41 | 16.71 | 15.53 | 14.91 | 16.97 |
| Mg | 0.26 | — | 0.33 | 0.27 | — | 0.34 |
| Ca | 0.46 | 0.09 | — | 0.47 | 0.09 | — |
| Mn | — | — | 0.05 | — | — | 0.05 |
| Fe'' | 3.87 | 3.99 | 1.80 | 3.98 | 4.13 | 1.83 |
| Sr | — | — | 0.05 | — | — | 0.05 |
| Pb | 0.09 | 0.06 | — | 0.09 | 0.06 | — |
| Zr | — | 0.06 | 0.08 | — | 0.06 | 0.08 |
| Ce* | 0.89 | 0.59 | 0.99 | 0.92 | 0.61 | 1.01 |
| Th | — | 0.01 | 0.03 | — | 0.01 | 0.03 |
| U | 0.20 | 0.61 | 0.24 | 0.21 | 0.63 | 0.24 |
| Na | — | 0.08 | 0.01 | — | 0.08 | 0.01 |
| K | — | — | 0.03 | — | — | 0.03 |
| $\Sigma''$ | 5.77 | 5.49 | 3.61 | 5.94 | 5.67 | 3.67 |
| $\Sigma(\Sigma'+\Sigma'')$ | 20.87 | 19.90 | 20.32 | 21.47 | 20.58 | 20.64 |
| O | 35.00 | 34.70 | 35.44 | 36.00 | 36.00 | 36.00 |
| Sp. Gr. | 4.45 (calc.) | 4.46 (meas.) | 4.42 (meas.) | 4.58 (calc.) | 4.61 (calc.) | 4.49 (calc.) |

Columns 1 and 4, Radium Hill, South Australia.
Columns 2 and 5, Tete district, Mozambique.
Columns 3 and 6, Pima County, Arizona.
* R. E. treated as $Ce_2O_3$. See text for other details.

The specific gravities used in the cell content calculations were determined on metamict material. It seems probable that somewhat higher values, as indicated by the increase in specific gravity on heating the Arizona davidite, would be appropriate for the crystalline material. This could lead to a cell content of 36 oxygens (see columns 4 to 6, Table 3) and possibly to a formula $Y_6Z_{15}O_{36}$, or $3(Y_2Z_5O_{12})$, for the rhombohedral cell, perhaps corresponding to no atoms on the 3-fold axes, a not unlikely situation. Probably only a determination of the structure, not contemplated at present, could firmly establish the ideal cell content and formula.

## Relation to Ilmenite

It has been suggested by Shawe (1953, p. 38) that davidite is but a "uranium-bearing ilmenite." The cell dimensions of ilmenite, $a_0$ 5.082, $c_0$ 14.027 Å (Crystal Data, p. 453), if multiplied by 4/2 and 3/2 respectively, give a multiple cell with $a_0$ 10.164 and $c_0$ 21.041, very close to the dimensions, 10.37 and 20.37, for davidite. The content of the rhombohedral cell corresponding to this multiple of the ilmenite cell would be $Fe_{12}Ti_{12}O_{36}$. The cells can be compared on the basis of the volumes per oxygen atom. This is 17.34 Å$^3$ for ilmenite and either 18.51 or 18.00 for davidite, depending on whether there are 35 or 36 oxygens
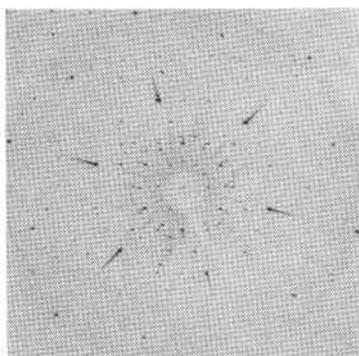


Fig. 1. Davidite, Norway, heated to 960° C. 30° $hki0$ precession photograph of twin on (52$\overline{7}$0). Mo-Zr, 28 hours.

per rhombohedral cell. The volume per oxygen in close packing is 13.01 or 15.09 corresponding to the radii 1.32 or 1.40 Å. One may speculate that the structure of a davidite cell is related to the structure of a multiple of the ilmenite cell by the omission of one eighth of the cations and the partial subsitution of others by cations of higher charge. Such a possibility is not excluded by the marked difference in the diffraction patterns whose aspect is largely determined by the heavier atoms.

## Twinning as Revealed by X-Rays

The third crystal of Arizona davidite examined by x-rays showed a repetition of spots in $hki0$ to $hki3$ precession patterns indicating twinning on a plane parallel to $c$. No indications of such twinning were found in other crystals of Arizona davidite but the same kind of twinning was observed in all of the reconstituted fragments of Norwegian davidite of which single crystal patterns were taken.

Manifestation of the twinning in an x-ray diffraction pattern is shown in Fig. 1. The interpretation is shown in the reciprocal lattice diagram in Fig. 2 which is reproduced to the same scale. Within the range of a 30°

Mo $hki0$ precession pattern only the reciprocal lattice points $52\overline{7}0$, $39.\overline{12}.0$ and $10.4\cdot\overline{14}.0$ and their symmetrical equivalents are in common for the two lattices. The $hki0$ section of the combined lattices shows the symmetry $6mm$, intensity differences of equivalent spots arising from the two parts of the twin being disregarded. Upper level sections parallel to $hki0$ show only the symmetry $3m$. In $hki1$ and $hki2$, only the points plotted in Fig. 3 are in common for the two lattices. $(52\overline{7}0)$ or equivalents, which are symmetry planes for the rhombohedrons $\{13\overline{4}1\}$ and $\{4\overline{1}32\}$, may be taken as the twin planes.
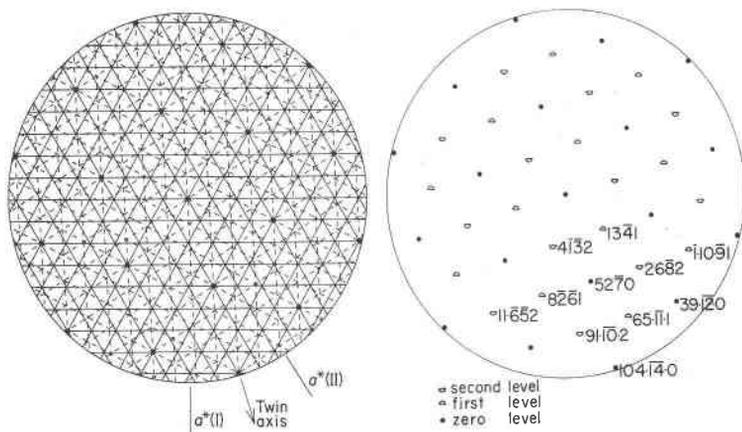


Fig. 2 (left). The $hki0$ plane of the reciprocal lattice of davidite, twinned on $(52\overline{7}0)$. Same scale as Fig. 1. Small black circles are lattice points common to both parts of twin. Intersections of lattice lines correspond to points for which $h-k-l=3n$ only. Same scale as Fig. 1.

Fig. 3 (right). Common reciprocal lattice points on the zero, first and second levels of a davidite twin on $(52\overline{7}0)$. Same scale as Fig. 2.

The common sets of reciprocal lattice points, $\{52\overline{7}0\}$, $\{13\overline{4}1\}$ and $\{4\overline{1}32\}$, correspond to the strongest reflections of their levels. The simplest indices that can be assigned to these sets of points are $\{11\overline{2}0\}$, $\{10\overline{1}1\}$ and $\{01\overline{1}2\}$, corresponding to an hexagonal cell with $a_0=2.878$ and $c_0=20.87$ Å.

<center>SUBSIDIARY X-RAY REFLECTIONS</center>

On Fig. 1 there may be noted weak arcs or short tangential streaks, regularly distributed in a trigonal or hexagonal pattern. The most prominent of these are close to the position of $13\overline{4}0$, a "forbidden" reflection for a rhombohedral lattice. On the zero layer of a $c$-axis rotation pattern these streaks are reduced to spots which are slightly diffuse. Three such spots, the innermost one corresponding to the streaks near

13$\bar{4}$0, the others on either side of 52$\bar{7}$0, are indicated by arrows on the zero line of the c-axis rotation pattern of which one quadrant is shown in Fig. 4. On this pattern another arrow indicates a line of slightly diffuse spots between the 4th and 5th layer lines. Weissenberg resolution of this level shows only streaks similar to the subsidiary streaks on the zero level, whereas resolution of the 4th and 5th levels shows only sharp reflections. In accordance with expectation both sharp spots and diffuse streaks are present on the 9th level. No streaks were seen on other levels nor were any observed on $h0\bar{h}l$ or $hh\bar{2}\bar{h}l$ patterns.

The diffuse subsidiary streaks are present in the indicated regions on all well exposed patterns of twins as well as single crystals. A single crystal of the Arizona davidite and a twin of the Norwegian davidite, first reconstituted at 980 and 960° C. respectively and used for a survey of the subsidiary streaks, were further heated to 1170° C. Reexamination by c-axis rotation and $hki0$ Weissenberg patterns showed no change in the subsidiary streaks. In powder patterns corresponding lines are not recorded with the possible exception of the strong streaks near 13$\bar{4}$0 which may account for the diffuse shoulder usually seen on the low angle side of the 13$\bar{4}$1 line.

The subsidiary layer level, close to a "4$\frac{1}{2}$ level", corresponds to a c axis spacing of 4.64. This is very close to the spacing of the third level of ilmenite, 4.68. Likewise the spacing of 13$\bar{4}$0, 2.488, is close to that of 11$\bar{2}$0, 2.541, of ilmenite.

### DIFFERENCES IN LOCALITIES

*Extraneous phases in untreated material*

X-ray examination of untreated fragments revealed no impurities in the davidites from Arizona, Norway or Mozambique and only a trace of anatase in one fragment from Thackeringa. Some fragments from the Crocker's Well specimens are completely x-ray amorphous but one fragment of specimen 3a showed streaky spots near 3.3, 2.7 and 1.7 Å and two fragments of specimen 3b showed weak diffuse lines near 3.5. Faint rutile lines are detectable in the patterns of some untreated fragments from both of the Billeroo specimens even though detached from what seem to be single crystals.

The Radium Hill davidite is intimately intergrown with rutile, partly in coarse crystals, ilmenite and possibly other black, opaque minerals as has been noted by others. The complexity of the intergrowth is indicated by the autoradiograph of specimen 2a shown in Fig. 5. Many untreated fragments were examined by x-rays. Those which could be converted to davidite or to mixtures including davidite all showed faint rutile lines and some also diffuse ilmenite spots in the untreated state. It seems not improbable that the cryptocrystalline rutile in untreated
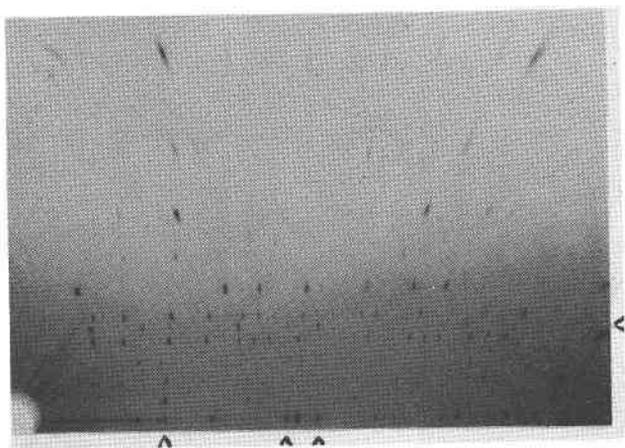
FIG. 4. One quadrant of *c*-axis rotation pattern of davidite, Arizona. Co-Fe, 16 hours. Arrows indicate features discussed in text.

Radium Hill davidite and in some fragments of the Billeroo davidite corresponds to the extremely fine-grained rutile isolated from davidite by Whittle (1959).

*X-ray evidence of other phases in reconstituted davidite*

Traces of cryptocrystalline rutile can be found by *x*-rays in most davidites reconstituted by simple heating in air. The four strongest rutile lines, with *d* and *I* 3.245–100; 2.489–41; 2.188–22 and 1.687–50, are close to possible davidite lines. The presence of rutile is suggested by the variation in intensity of this set of lines relative to the intensities of all other lines which remain nearly constant in the patterns. Examples of this variability can be found in several sets of published patterns, for
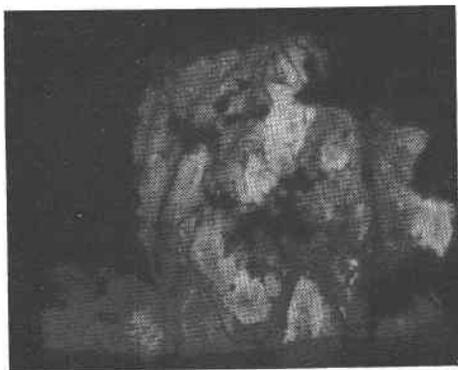


FIG. 5. Autoradiograph of polished surface of specimen 2a, Radium Hill, South Australia. Natural size. Compare Plate XXI, Mawson (1944).

instance those of Lawrence *et al.* (1957, table III), who report *d* and *I* 1.71–4, 1.69–4 for their specimen 1 and 1.70–10, 1.69–1 for their specimen 2, the second line of this pair being due to rutile which is present in much smaller amount in specimen 2. Reconstitution of davidite under hydrothermal conditions, to be reported in detail at some future date, yields material giving no trace of rutile lines.

Pseudobrookite lines were found in several patterns obtained from heated fragments of Radium Hill davidite. In two cases these fragments
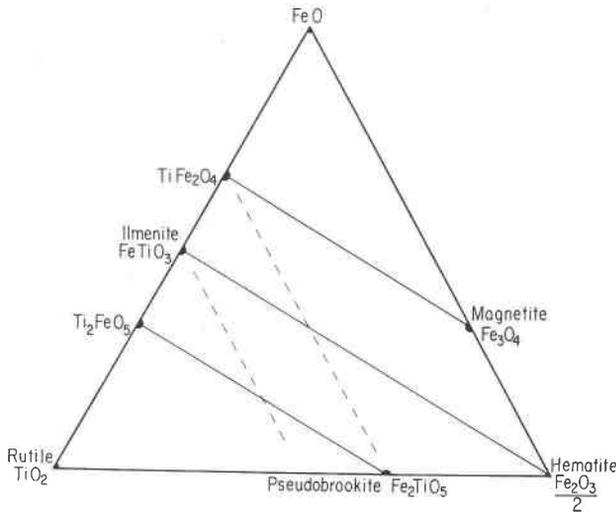


Fig. 6. Concentration triangle for the system $FeO$-$Fe_2O_3$-$TiO_2$. Following Gorter (1957), components are formulated so that each has the same number of metal atoms in order that the several mix-crystal series may be represented by parallel lines. Dashed lines show the trends of composition changes with oxidation or reduction.

showed diffuse ilmenite spots before treatment but not after heating. The Radium Hill fragment yielding the best pseudobrookite pattern showed only rutile spots before heating and some of these remained, though weakened, in the pattern of the heated fragment. Bannister (Bannister and Horne, 1950, footnote p. 110) reported that heated ilmenite yields a pseudobrookite pattern and wrote the equation $2FeTiO_3 + O \rightarrow Fe_2TiO_5 + TiO_2$ to represent the change though no $TiO_2$ lines were observed. It is now known that a complete series of pseudobrookite structure exists with the composition range $Fe_2TiO_5$ to $FeTi_2O_5$ as shown on Fig. 6. Such phases may arise by oxidation of phases in the Ti-rich portion of the series $FeTiO_3$-$Fe_2O_3$ or by reaction between phases or combinations of phases in any part of this series and $TiO_2$. No pseudo-

brookite lines were observed in patterns from untreated Radium Hill fragments. Oxidation would be most effective if powder is heated in air. It may be presumed to be less effective when fragments are heated.

Weak, diffuse, unidentified lines appeared in x-ray diffraction patterns of several heated fragments of davidite from Mozambique near 5.9 or 3.7, from Crocker's Well near 4.7, or near 4.7 and 2.70 or near 6.0 and 3.18, and in one pattern of powdered Arizona davidite near 6.1 and 4.7. These cannot be matched with lines of any expected phases. Though some of these lines appeared in several patterns their occurrence seems to be accidental. At least a few of them, e.g. the 4.7 line from a Crocker's Well davidite fragment, persist after heating at higher temperature, $1\frac{1}{4}$ hours at 1150° C. It may be that these lines arise from unknown phases formed during the reconstitution of the davidite, possibly in part by reaction with original impurities. No systematic study of these extraneous lines, present on only a few photographs, was carried out.

*Differential thermal analysis*

Kerr and Holland (1951) published differential thermal analysis curves of davidite from Mozambique and reported that "samples after heating to 710° C. give no distinct lines even after extended exposure, but patterns of samples heated to 830° C. and 1020° C. give groups of lines that are identical." Mr. Larry Godwin kindly ran differential thermal curves to 920°C. on powdered davidite from Crocker's Well (specimen 3a) and from Arizona, using a constant heating rate of 12 degrees per minute. The curve obtained from the Crocker's Well davidite is somewhat similar to those for the Mozambique davidite published by Kerr and Holland, with a principal exothermic peak at 660° C. and a lower, broader, exothermic peak at 820° C. The differential thermal curve for Arizona davidite, on the other hand, shows no peaks. Powder diffraction photographs of the two samples after the DTA runs are nearly identical, showing the full davidite pattern plus a weak line near 2.70 from the Crocker's Well material only.

*Degree of metamictness*

The degree of metamictness differs markedly in the several davidites. All but the Arizona davidite are x-ray amorphous in the untreated state. Untreated fragments of this yielded x-ray photographs showing a few faint, diffuse, single-crystal spots. These are so weak that any x-ray pattern prepared from powdered material might be interpreted as indicating an x-ray amorphous substance.

Sharp single crystal patterns were obtained from a fragment of Arizona davidite heated to 775° C. for 2 hours. Fragments heated to 915° C.

or higher yielded the same patterns. The powder pattern of material used for a DTA run to 920° at 12° per minute, which had been above the presumed temperature of reconstitution only about 25 minutes, showed sharp lines that could be fully indexed on the lattice derived from the single crystal patterns.

No lower limit can be set for the temperature at which reconstitution occurs. After the lattice had been established it was possible to orient untreated fragments showing a few faint spots and to interpret the rather weak precession and Weissenberg pattern obtained from them on the basis of this lattice. On these patterns, obtained from 3 untreated fragments, spots corresponding to spacings greater than 3.5 Å are absent and spots corresponding to spacings less than about 1.5 are most diffuse and usually not observable. The absence of the low angle spots is attributable to absorption and that of the high angle spots to the smallness of the volumes within which a degree of order sufficient for $x$-ray diffraction persists. However, the remnants of order in this davidite are enough to determine the reconstitution of the fragments to single crystals upon heating. It may be recalled that Mügge's (1922) studies on the optical properties of partly metamict crystals indicated that intermediate stages may consist of a web- or sponge-like crystal whose meshes are filled with amorphous substance.

Fragments of the davidite from Norway are $x$-ray amorphous. A fragment heated for 44 hours at 510° C. acquired about the same degree of crystallinity found in untreated fragments of Arizona davidite. Fragments heated to various temperatures in the range 680 to 960° C. all yielded sharp patterns of similar character. Though no remnant of crystallinity can be detected by $x$-rays in untreated Norway davidite, the fact that reconstitution invariably leads to single crystals or twins suggests that metamictization of this davidite was not complete. According to Pellas (1954, p. 454) radiation damaged material will appear $x$-ray amorphous when 20 per cent of its atoms have been displaced.

Several fragments of Crocker's Well davidite, which may show faint lines even before heating, were heated at relatively low temperatures for long periods. Several weak diffuse lines that might be correlated with the principal groups of davidite lines appeared in a fragment heated for 44 hours at 510° C. Continued heating of this and other fragments below 600° C. for up to five days failed to produce sharp patterns, but all such fragments yielded sharp patterns on further heating at higher temperatures. Similar observations were made on davidite from Mozambique but in this case a fragment heated to 510° for 44 hours yielded no lines and only three weak lines were produced by the same fragment after further heating at the same temperature for a total of 106 hours.

TABLE 4. COORDINATE ANGLES FOR DAVIDITE FROM MOZAMBIQUE

| As recorded by Horne (Bannister and Horne, 1950, p. 102) | | | | Calculated for axial ratio 2.013 | | |
|---|---|---|---|---|---|---|
| Lower | Upper | $\phi$ | $\rho$ | $hkil$ | $\phi$ | $\rho$ |
| $\bar{c}$ | $\bar{c}(0001)$ | — | $0°$ | $(0001)$ | — | $0°$ |
| | $h(21\bar{3}0)$ | $11°$ | 90 | $(21\bar{3}0)$ | $10°54'$ | 90 |
| | $-h(1\bar{2}\bar{3}0)$ | $-11$ | 90 | $(1\bar{2}\bar{3}0)$ | $-10\ 54$ | 90 |
| | $-l(2\bar{5}\bar{7}0)$ | $-14$ | 90 | $(2\bar{5}\bar{7}0)$ | $-13\ 54$ | 90 |
| $-\bar{n}$ | $(0\bar{3}\bar{3}4)$ | $-30$ | 50 | $(01\bar{1}2)$ | $-30$ | 49 16 |
| | $o(11\bar{2}1)$ | 0 | 70 | $(22\bar{4}3)$ | 0 | 69 34 |
| $\bar{p}$ | $(22\bar{4}1)$ | 0 | 80 | $(44\bar{8}3)$ | 0 | 79 27 |
| | $s(52\bar{7}8)$ | 14 | 51 | $(527\cdot12)$ | 13 54 | 50 25 |
| | $t(41\bar{5}6)$ | 19 | 50 | $(41\bar{5}9)$ | 19 06 | 49 48 |
| | $-u(34\bar{7}3)$ | $-5$ | 73 | $(68\overline{14}\cdot9)$ | $-4\ 43$ | 72 20 |
| $-\bar{v}$ | $(34\bar{7}2)$ | $-5$ | 78 | $(34\bar{7}3$ | $-4\ 43$ | 78 18 |
| $-\bar{w}$ | $(12\bar{3}3)$ | $-11$ | 54 | $(24\bar{6}9)$ | $-10\ 54$ | 53 48 |
| $-\bar{x}$ | $(26\bar{8}9)$ | $-16$ | 52 | $(4\cdot12\cdot\overline{16}\cdot27)^*$ | $-16\ 06$ | 51 19 |
| $-\bar{y}$ | $(13\bar{4}4)$ | $-16$ | 55 | $(13\bar{4}6)$ | $-16\ 06$ | 54 24 |
| $-\bar{z}$ | $(16\bar{7}8)$ | $-22$ | 52 | $(16\bar{7}\cdot12)$ | $-22\ 24$ | 51 47 |

* See text for comment and alternative interpretation.

No observations were made on Billeroo, Thackeringa or Radium Hill davidite heated at temperatures below 950° C. At this temperature all of the davidites are fully reconstituted in less than an hour, possibly within minutes.

Among the davidite specimens examined the least metamict are those from Arizona, followed by the specimen from Norway. It may not be a coincidence that the Arizona davidite is youngest, probably being late Cretaceous-early tertiary (Thomssen, 1961), and that the Norwegian davidite has a lower uranium content than analyzed davidites.

## MORPHOLOGY

The morphology of davidite from Mozambique was described by Horne (Bannister and Horne, 1950) on the basis of contact goniometer measurements on large rough crystals. He stated that "the mineral appears to belong to the ditrigonal pyramidal class" and, adopting the axial ratio 1.37, recorded coordinate angles to one degree for 15 forms. His angle table is reproduced in the first four columns of table 4, form names being omitted. The axial ratio of the structure cell, $c_0/a_0 = 2.013$, being close to three halves the axial ratio adopted by Horne, the indices given in column 5 have been obtained from Horne's indices by the transformation $100/010/00\frac{3}{2}$. The calculated coordinate angles all agree with

Horne's reported measurements within the limits to be expected from rough goniometer measurements but this must not be taken as confirming the indices either as originally given or as transformed. $-\bar{x}$ may be considered to be $(26\bar{8}\cdot13)$, with $\rho = 52°$ 12′, and simpler indices might also be found for some of the other forms.

Unfortunately no traces of morphology can be found on the Arizona or Norway davidites which have been reconstituted to single crystals but some crude observations on forms are possible on the crystals from Billeroo, South Australia. On the smallest of these a pinacoid (or pair of pedions), a rhombohedron with $\rho$ close to 63° and some smaller steeper faces can be recognized. The larger crystals show fewer faces and are rougher but on the largest a 63° angle can also be found. For $c/a = 2.013$, $\rho_{11\bar{2}2}$ is 63° 35′ and $\rho_{44\bar{8}9}$ is 60° 48′. The commonest rhombohedral form on ilmenite is $\{22\bar{4}3\}$ referred to the axial ratio 1.3846. Transformed as indicated above this would be $\{44\bar{8}9\}$.

Though it has not been possible to connect the morphology with the structure lattice by single crystal $x$-ray diffraction from faceted crystals the observations suggest that the structure lattice found in the reconstituted davidites does correspond to the lattice of original single crystals from Mozambique and Billeroo and that this is indeed the original lattice of davidites generally.

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<center>SUPPLEMENTARY NOTES</center>

(1) A few days after the completion of this paper an article by J. D. Jayton, entitled "The Constitution of Davidite," appeared in Economic Geology, 55, 1030–1038, August, 1960. Hayton records ten new analyses of davidite. With 5 of the new analyses densities from 4.41 to 4.50 are given. Using the cell dimensions given in the preliminary report by Pabst and Thomssen (1959) Hayton calculated the cell contents for all of the newly ana-

lyzed davidites and also for the Mozambique davidite, using Bannister and Horne's analysis 3, the same one used in this paper, Table 2 and 3.

In his table 7 Hayton has tabulated the calculated contents of the hexagonal cell in three different ways, varying in the grouping of cations. The oxygen count is of particular interest. His figures for this, divided by 3 to correspond to the rhombohedral cell content given in Table 3 of this paper, are:

|  | Anal. 8 (Maximum) | Anal. 5 (Minimum) | arithmetic mean | standard deviation |
|---|---|---|---|---|
| oxygen atoms per rh. cell | 34.15 | 32.20 | 33.22 | 0.63 |

All of these figures are substantially below those reported in Table 3 of this paper.

Many factors contribute to the difference. Minor factors are:

1. Difference in the preliminary (10.36, 20.85) and revised (10.37, 20.87) cell dimensions.
2. Difference in the value taken for the weight of the unit of atomic weight. Hayton used $1.649 \times 10^{-24}$ grs., which is the value, now obsolete, that would have been appropriate had dimensions been stated in kX units. I used $1.6604 \times 10^{-24}$ grs., consistent with dimensions given in Ångstrom units.
3. Differences in atomic weight values used in calculation.
4. Differences in rounding of figures.

Factors 1 and 2 would tend respectively to raise and to lower the calculated oxygen content and hence tend to cancel each other. Factors 3 and 4 are negligible.

Major factors contributing to differences in the oxygen count are:

5. State of oxidation assumed for Fe. Hayton has taken all the Fe to be ferrous in every case. This reduces the oxygen count.
6. Departure of summation of analysis from 100%.

As seen from Hayton's sample calculation the atom counts obtained are only a proportion of the full cell content corresponding to the summation of the analysis used. There may be some doubt as to the propriety of adjusting an analysis to sum to 100% before starting the calculation but, in any case, using an analysis with a low total in the manner shown in Hayton's sample calculation necessarily leads to a low cell content. If the number of oxygens per hexagonal cell, 102.46, shown in Hayton's table 6, calculated from an analysis totalling 97.5%, is adjusted for a total of 100% it becomes 105.09, or 35.03 for the rhombohedral cell. If some of the iron were ferric the figure would be still higher.

Hayton considers three formulas, $A_8B_{12}O_{33}$, $A_2B_{19}O_{33}$ and $A_2B_6C_{12}O_{33}$, corresponding to cation/oxygen ratios 0.606, 0.636 and 0.606. The ratio of his mean values is 61.54/99.65 or 0.618. The lower ratios suggested in Table 3 of this paper arise in part from the higher proportion of oxygen connected with the higher valence state of part of the iron as reported in the analyses used.

(2) Four months after this paper was submitted, an article "Contributions to the Mineralogy of Norway. No. 8. Davidite from Tuftan, Iveland," by Henrich Neumann and Thor L. Sverdrup, appeared in *Norsk Geologisk Tidsskrift*, **40**, 277–288, Dec. 1960. A chemical analysis, and density of 4.29 are reported for davidite. It seems highly probable that it corresponds to specimen No. 7 of this paper.