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# Davanite, $K_2TiSi_6O_{15}$, in the Smoky Butte (Montana) lamproites: Discussion of X-ray powder data

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Davanite, the Ti analogue of dalyite ($K_2ZrSi_6O_{15}$), was described as a new mineral from Murunski, USSR, by Lazebnik et al. (1984). Wagner and Velde (1986) have reported the second find of davanite, from Smoky Butte, Montana. X-ray powder data for the Montana davanite are listed by Wagner and Velde (1986) together with data for the Russian mineral taken from the original description.

TABLE 1. X-ray powder-diffraction data for davanite

| Synthetic $K_2TiSi_6O_{15}$* | | | Murunski† | | Smoky Butte‡ | | Synthetic $K_2TiSi_6O_{15}$* | | | Murunski† | | Smoky Butte‡ | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| *hkl* | $d_{calc}$ | $I_{calc}$ | $d_{obs}$ | $I_{obs}$ | $d_{obs}$ | $I_{obs}$ | *hkl* | $d_{calc}$ | $I_{calc}$ | $d_{obs}$ | $I_{obs}$ | $d_{obs}$ | $I_{obs}$ |
| 100 | 6.377 | 12 | | | 6.375 | w | 220 | 2.051 | 10 | 2.057 | 1 | 2.053 | w |
| 001 | 5.931 | 6 | | | | | 2$\bar{3}$1 | 2.036 | 3 | | | | |
| 10$\bar{1}$ | 5.868 | 34 | 5.88 | 5 | 5.878 | m | 130 | 1.976 | 3 | | | | |
| 1$\bar{1}$1 | 4.285 | 32 | 4.31 | 1 | 4.290 | w | 112 | 1.973 | 5 | | | 1.974 | w |
| 110 | 4.102 | 53 | 4.09 | 5 | 4.104 | ms | 022 | 1.925 | 4 | 1.929 | <1 | | |
| 1$\bar{1}$1 | 3.873 | 5 | | | 3.878 | vw | 310 | 1.878 | 11 | 1.886§ | 1 | 1.880 | w |
| 011 | 3.849 | 4 | | | | | 3$\bar{3}$0 | 1.860 | 3 | | | 1.866 | vw |
| 101 | 3.604 | 47 | | | 3.605 | w | 1$\bar{4}$1 | 1.857 | 5 | | | | |
| 02$\bar{1}$ | 3.594 | 5 | | | | | 23$\bar{1}$ | 1.833 | 4 | | | 1.833 | w |
| 1$\bar{2}$0 | 3.491 | 96 | 3.51 | 10 | 3.490 | s | 1$\bar{1}$3 | 1.807 | 4 | | | | |
| 020 | 3.435 | 26 | | | 3.423§ | w | 202 | 1.802 | 10 | 1.799 | 1 | 1.802 | w |
| 11$\bar{2}$ | 3.344 | 47 | 3.34 | 5 | 3.349 | s | 32$\bar{1}$ | 1.800 | 4 | | | | |
| 2$\bar{1}$0 | 3.293 | 18 | | | 3.305 | w | 32$\bar{3}$ | 1.766 | 9 | | | 1.766 | w |
| 1$\bar{2}$1 | 3.183 | 29 | | | | | 23$\bar{3}$ | 1.762 | 9 | 1.762§ | 1 | | |
| 01$\bar{2}$ | 3.176 | 32 | 3.19 | 5 | 3.179 | ms | 1$\bar{4}$2 | 1.747 | 4 | | | | |
| 21$\bar{1}$ | 3.023 | 100 | 3.022 | 10 b | 3.022 | vs | 2$\bar{3}$2 | 1.735 | 3 | | | | |
| 002 | 2.966 | 34 | | | 2.970 | w | 21$\bar{4}$ | 1.719 | 3 | | | | |
| 02$\bar{2}$ | 2.807 | 26 | | | | | 1$\bar{3}$3 | 1.712 | 5 | | | | |
| 2$\bar{2}$0 | 2.790 | 13 | | | | | 12$\bar{4}$ | 1.684 | 4 | | | 1.684 | w |
| 21$\bar{2}$ | 2.785 | 20 | 2.789§ | 7 | 2.790 | m b | 4$\bar{1}$0 | 1.667 | 3 | | | | |
| 111 | 2.777 | 10 | | | | | 20$\bar{4}$ | 1.664 | 5 | | | | |
| 120 | 2.705 | 3 | | | 2.706 | vw | 40$\bar{3}$ | 1.663 | 15 | 1.667 | 3 b | 1.668 | w |
| 2$\bar{1}$2 | 2.619 | 60 | 2.615 | 9 b | 2.623 | m b | 3$\bar{3}$2 | 1.652 | 8 | | | | |
| 210 | 2.610 | 9 | | | | | 122 | 1.645 | 4 | | | | |
| 021 | 2.591 | 19 | | | 2.588 | m b | 3$\bar{2}$3 | 1.641 | 3 | | | | |
| 2$\bar{1}$1 | 2.576 | 18 | | | | | 24$\bar{1}$ | 1.622 | 3 | | | | |
| 1$\bar{1}$2 | 2.516 | 5 | | | 2.514 | vw | 1$\bar{4}$1 | 1.612 | 6 | | | 1.613 | w |
| 03$\bar{1}$ | 2.458 | 10 | | | | | 14$\bar{3}$ | 1.606 | 4 | | | | |
| 2$\bar{2}$1 | 2.432 | 3 | | | | | 320 | 1.606 | 9 | 1.604 | 3 | 1.607 | w |
| 1$\bar{2}$2 | 2.410 | 4 | | | | | 30$\bar{4}$ | 1.605 | 5 | | | | |
| 1$\bar{3}$1 | 2.403 | 8 | | | | | 3$\bar{4}$0 | 1.588 | 3 | | | | |
| 201 | 2.392 | 7 | | | | | 43$\bar{1}$ | 1.569 | 5 | | | | |
| 31$\bar{1}$ | 2.384 | 15 | 2.391 | 3 | 2.391 | w | 24$\bar{2}$ | 1.541 | 2 | | | | |
| 22$\bar{1}$ | 2.341 | 3 | | | 2.340 | vw | 14$\bar{3}$ | 1.539 | 2 | 1.542§ | <1 | | |
| 13$\bar{1}$ | 2.198 | 5 | | | | | 42$\bar{2}$ | 1.511 | 4 | | | | |
| 31$\bar{2}$ | 2.197 | 6 | 2.215§ | 2 | 2.201§ | w | 21$\bar{3}$ | 1.511 | 3 | | | 1.510§ | w |
| 2$\bar{3}$0 | 2.197 | 6 | | | | | 3$\bar{3}$2 | 1.509 | 3 | | | | |
| 22$\bar{2}$ | 2.143 | 13 | | | 2.144 | w | 2$\bar{3}$3 | 1.497 | 12 | 1.498 | 4 | 1.500 | w |
| 01$\bar{3}$ | 2.116 | 14 | 2.119 | 2 b | 2.115 | w | 023 | 1.494 | 2 | | | | |
| 121 | 2.109 | 4 | | | | | 42$\bar{3}$ | 1.494 | 3 | | | | |
| 1$\bar{3}$2 | 2.091 | 18 | | | | | 15$\bar{1}$ | 1.492 | 3 | | | 1.496§ | w |
| 2$\bar{3}$1 | 2.086 | 3 | | | | | 43$\bar{2}$ | 1.492 | 5 | | | | |
| 02$\bar{3}$ | 2.070 | 4 | | | 2.076§ | vw | | | | +16 lines to $d$ = 1.011 Å | | | |

*Note:* vs = very strong, s = strong, ms = medium strong, w = weak, vw = very weak, b = broad.

* Pattern calculated with the program LAZY PULVERIX (Yvon et al., 1977) from structural data of Gebert et al. (1983). Cell dimensions: $a$ = 7.250(2), $b$ = 7.474(2), $c$ = 6.909(3) Å, $\alpha$ = 105.59(5), $\beta$ = 112.81(5), $\gamma$ = 99.28(5)°. All reflections with $I_{calc} \geq 3$ and $d > 1.490$ Å are listed. Diffraction geometry: Debye-Scherrer. $\lambda_{CuK\alpha}$ = 1.5418 Å.

† Lazebnik et al. (1984).

‡ Wagner and Velde (1986).

§ Not used for calculation of cell parameters.

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Wagner and Velde (1986) remarked as an "interesting fact" that the strongest reflection in the two patterns could not be indexed satisfactorily. Again, there are unexplained differences in the indexing of the two patterns. Wagner and Velde claimed that the cell dimensions of the two davanites are not identical, the $a$ parameter differing by 0.11 Å. However, no explanation is offered for this discrepancy. The chemical analyses reported for the two davanites are virtually identical (Table 2 in Wagner and Velde, 1986), and no such difference in the cell dimensions would actually be expected.

These apparent inconsistencies are quite simply explained by incorrect indexing of the powder patterns. The crystal structure of synthetic $K_2TiSi_6O_{15}$ was published by Gebert et al. (1983). They have also tabulated observed and calculated X-ray powder data, but have neglected to include the intensities. Again, some of the stronger reflections have somehow been omitted. Based on the structural data of Gebert et al. (1983), a calculated pattern for $K_2TiSi_6O_{15}$ is presented here (Table 1). It was computed with the program LAZY PULVERIX (Yvon et al., 1977). With this information, the patterns of the Murunski and Smoky Butte davanites can be easily indexed (Table 1). Least-squares refinements of the cell parameters of the Murunski mineral based on 16 reflections gave $a$ = 7.26(1), $b$ = 7.51(2), $c$ = 6.92(1) Å, $\alpha$ = 105.6(2)°, $\beta$ = 112.9(1)°, $\gamma$ = 99.4(2)°, $V$ = 319.0(7) Å$^3$. The Smoky Butte mineral has nearly identical cell parameters, based on 33 reflections: $a$ = 7.272(3), $b$ = 7.480(4), $c$ = 6.910(2) Å, $\alpha$ = 105.55(3)°, $\beta$ = 112.82(3)°, $\gamma$ = 99.42(3)°, $V$ = 318.2(1) Å$^3$.

## References

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