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Letter

Discreditation of paraspurrite

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Abstract

Paraspurrite is discredited as a mineral species. No type material was available necessitating collecting new material from the original locality. A crystallographic study shows paraspurrite to be polysynthetically twinned spurrite, twin law by reflection on {001}. The spurrite cell calculated from XRPD unit-cell refinement is a = 10.478(3), b = 6.700(2), c = 14.127(3) Å, β = 101.02(2)°, V = 972.8(3) Å^3. The cell refined on two "twinned" crystals yielded: a = 10.494(1), b = 6.7116(6), c = 28.216(3) Å, α = 90.059(6), β = 100.132(5), γ = 90.023(6)°. This monoclinic primitive cell transforms to monoclinic B (Fig. 2): a = 10.494, b = 6.7116, c = 55.56 Å, α = 90, β = 90.6, γ = 90°, which corresponds to a sub-cell described as "paraspurrite" by Colville and Colville (1977); space group $P2_1/a$ with cell parameters: a = 10.473, b = 6.706, c = 27.78 Å, α = 90, β = 90.58, γ = 90°. The discreditation has been approved by the IMA Commission on New Minerals, Nomenclature and Classification.

Keywords: Paraspurrite, discreditation, twin, crystallography

Introduction

Paraspurrite, from Inyo County, California, was first described as a new mineral by Colville and Colville (1977). It was determined to be a polymorph of spurrite "having a doubled unit cell in the c* direction." "Precession photographs provided crystal geometry, systematic extinctions, and preliminary cell parameters. Accurate cell parameters were calculated using a least-squares analysis of 15 reflections measured with an automated four-circle single-crystal diffractometer." There was no mention of using this crystal to collect an intensity data set to solve the crystal structure. A "proposed" crystal structure was given and briefly discussed.

Here, paraspurrite is shown to be twinned spurrite. As there is no type specimen, voucher specimens used in the discreditation will be stored at the Canadian Museum of Nature (Ottawa), Smithsonian Institution (Washington, D.C.), and the Los Angeles County Natural History Museum. The discreditation was unanimously approved by the IMA Commission on New Minerals, Nomenclature and Classification.

Type material

The new mineral proposal of paraspurrite was presented to the IMA CNMNC in 1977 (number 77-16). This proposal stated the "Type material will be deposited at the U.S. National Museum, Washington, D.C., U.S.A." This was never done. Type material was also sought at the Los Angeles County Natural History Museum and the California State University, where the original research was conducted; only to discover no type material exists. In the Smithsonian collection, there are two "paraspurrite" samples from "California" (NMNH 157372 and NMNH 153997). Both samples were donated by David Wilson. Chips from these samples were generously provided by the Smithsonian Institution and both were identified as spurrite by X-ray single-crystal and X-ray powder-diffraction methods. As it was impossible to verify the structure of "paraspurrite," it was omitted in the study of crystal structure relationships in silicate-carbonate minerals (Grice 2005). This was duly noted by Editor Bob Martin and this study brings resolution to this problem. Discreditation of a mineral species that has no type material is problematic (Dunn 1990) and requires extra care to make sure a valid species is not inadvertently discarded.

Both authors, Alan Colville and Patricia Colville, were contacted and neither had any material left from their research. P.M.A. located the "type" locality, which was confirmed by Alan Colville. The locality, which consists of three spurrite bodies in a small roof pendant, was mapped and systematically sampled.

Occurrence

Colville and Colville (1977) describe "paraspurrite" occurring with gehlenite, vesuvianite, and apatite with sparse larnite in a small roof pendant with an outer zone of massive grossular. The locality, as described in this paper, is "Inyo County, California, north of the small mining town of Darwin." Our detailed mapping and sampling showed that the spurrite occurs in three small close, but separate, skarn bodies in a roof pendant. X-ray powder diffraction (XRPD) showed that in many areas melilite is the predominant second phase, however, tilleyite is also relatively common. In even more localized areas, spurrite + melilite ± tilleyite can be found with merwinite, rankinite, kilchoanite, monticellite, and an (SiO_4)-(SO_4) apatite mineral, in various combinations. Larnite was not identified in our study.

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Common accessory/trace phases in these assemblages are, but not limited to, perovskite, Ti-containing andradite, and sulfides. Sparse outcrops and the ubiquitous chalky white appearance of weathered specimens prevented discrimination of detailed metamorphic/metasomatic zones. An outer zone of grossular, vesuvianite, wollastonite, microcline, albite, and calcite, in various proportions, separates the spurrite assemblages from quartz monzonite. A retrograde zone occurs between the spurrite and grossular/vesuvianite zones. Spurrite/tilleyite first appears to be altered to wollastonite + calcite and ultimately to foshagite + calcite. Melilite is altered to a hydrogarnet + vesuvianite ± a clinochlore-like mineral.

Analysis

Transmitted light microscopy

Thin sections were made from 16 samples that contained spurrite as a significant phase. Spurrite displays high birefringence and a xenoblastic texture with individual grains ranging from 0.15 to 25 mm. Cleavage is indistinct. Melilite is commonly associated, and spurrite- and melilite-rich bands are common. Melilite commonly forms small (0.10–0.20 mm) inclusions in spurrite. Most spurrite is not twinned. In the two northernmost spurrite-melilite bodies, simple twins and polysynthetic twinning in spurrite is uncommon. Only two specimens from the southernmost spurrite-melilite bodies contained large spurrite grains displaying polysynthetic twinning. In other specimens from that body, twinning in spurrite is uncommon. An example of polysynthetic twinning of spurrite in thin section is shown in Figure 1.

X-ray diffraction

Data presented by Colville and Colville (1977) appear to have reflections that are unique to the larger cell they propose (Table 1). These are reflections that have odd indices for *l*. They list 22 such reflections; 12 of these reflections Colville and Colville (1977) mark as "overlapping peaks" and 9 reflections are not indicated as overlapping (shaded in Table 2). If the indexing were correct, the *c* cell parameter would in fact need to be doubled as they proposed. Colville and Colville (1977) indicated that the (00*l*) reflections of paraspurrite show some enhancement but that it was not extreme.

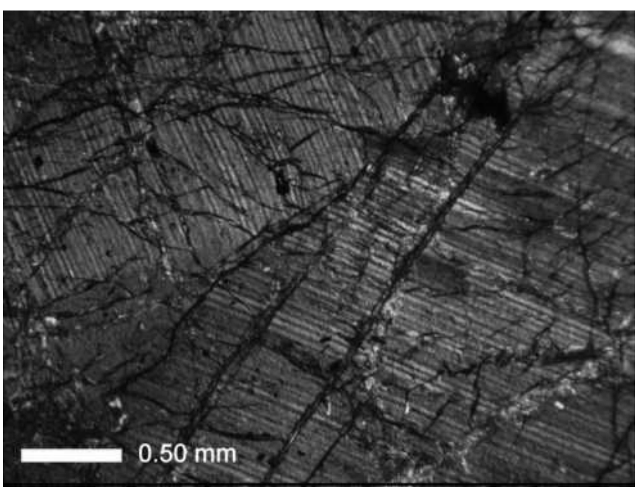

Figure 1. Polysynthetic twinning in spurrite (crossed polarized light). Sample from near Darwin, Inyo County, California.

Table 1. Spurrite and "paraspurrite:" Comparison of crystallographic data

Parameter	Spurrite*	"Paraspurrite"†
a, Å	10.478	10.473
b, Å	6.700	6.706
c, Å	14.127	27.78
β, °	101.02	90.58
V, Å^3	492.8	1951.0
Cell contents	$4[Ca_5(SiO_4)_2(CO_3)]$	$8[Ca_5(SiO_4)_2(CO_3)]$
Space group	$P2_1/a$	$P2_1/a$
D_{calc}, g/cm^3	3.01	3.01

* This study.
† Colville and Colville (1977).

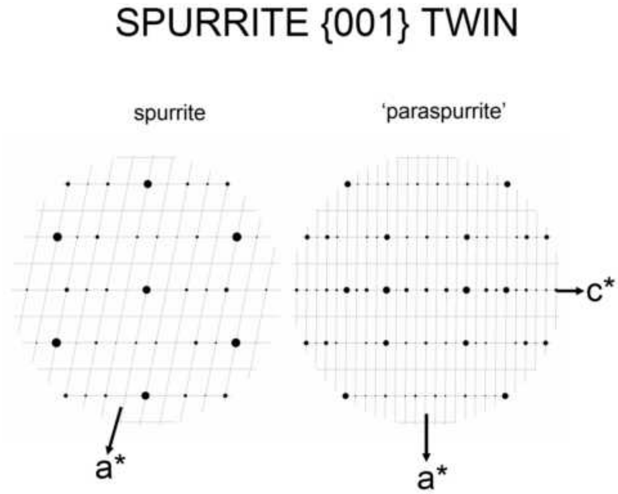

Figure 2. The reciprocal lattice of untwinned (**left**) and twinned (**right**) spurrite. β* changes from 79 to 90°. *c** is halved on the 20*l* row and on 001 plane *c** would be quartered.

Some 40 specimens were identified as containing a significant amount of spurrite, not paraspurrite, based on XRPD patterns. In the screening process, the side drifting method was used to mount samples for XRPD and to minimize preferred orientation (Bish and Reynolds 1989). Significant care is needed to prevent preferred orientation of the (00*l*) reflections as this is the plane of parting due to the polysynthetic twinning. Table 2 displays the X-ray powder diffraction data of spurrite, obtained with a Bruker AXS Discover 8 micro-diffractometer using Hi-Star 2-D area detector and Cu*K*α radiation and refined by the method of Rowe (2009). By comparison the powder X-ray data given for paraspurrite can be indexed on the spurrite cell (Table 1) calculated from XRPD unit-cell refinement with a = 10.478(3), b = 6.700(2), c = 14.127(3) Å, β = 101.02(2)°, V = 972.8(3) Å^3.

Eight samples of spurrite from the "type locality," which included samples from each roof pendant, were used for single-crystal X-ray diffraction studies. Care was taken to include samples that exhibited polysynthetic twinning in thin section. All samples X-rayed showed only spurrite.

Colville and Colville (1977) report polysynthetic twinning on {001}, but failed to realize that the cell they derived using 15 reflections with an automated four-circle single-crystal diffractometer was derived on a twinned crystal. The unit cell

TABLE 2. Comparison of "paraspurrite" and spurrite X-ray powder data

Spurrite X-ray powder diffraction data (Cu*K*α) (this study)					Paraspurrite original X-ray powder diffraction data (Cu$K\alpha_1$) (Colville and Colville 1977)			
I_{obs}	I_{calc}*	d_{obs}	d_{calc}†	*hkl*	I_{obs}	d_{obs}‡	d_{calc}	*hkl*
35	80	6.920	6.929	002	**78**	**6.92**	**6.95**	**004**
21	49	6.030	6.032	011	34	6.03	6.04	012
21	27	5.143	5.156	−201	14	5.15	5.15	−201
	23		5.139	200	27	5.12	5.13	201
6	13	5.020	5.020	111				
13	23	4.625	4.619	003	**37**	**4.62**	**4.63**	**006**
					2	4.54	4.54	203
2	2	4.089	4.086	−211	2	4.09	4.087	−211
	2		4.078	−210	2	4.08	4.078	211
33	37	3.798	3.825	−203	11	3.83	3.829	−205
	32		3.803	013	12	3.82	3.81	016
	21		3.790	202	12	3.80	3.78	205
	18		3.778	−212	8	3.78	3.78	−213
	13		3.758	211	5	3.76	3.758	213
19	44	3.465	3.464	004	**100**	**3.47**	**3.47**	**008**
9	9	3.344	3.394	113	16	3.35	3.355	020
	17		3.350	020	4	3.30	3.301	215
3	4	3.292	3.322	−213				
	6		3.299	212				
19	45	3.184	3.185	120	12	3.18	3.18	−207
11	26	3.097	3.099	−114	4	3.08	3.08	018
17	29	3.032	3.050	−310	20	3.017	3.02	024
	33		3.016	022				
	15		2.989	−312				
4	5	2.817	2.817	114				
	3		2.809	−221				
	4		2.806	220				
5	15	2.774	2.776	−313				
100	92	2.702	2.712	023	42	2.716	2.717	026
	97		2.703	−222	34	2.707	2.706	−223
	100		2.695	221	48	2.698	2.698	223
44	92	2.668	2.665	−205	25	2.671	2.671	−209
44	89	2.645	2.644	204	39	2.647	2.647	209
	18		2.629	312				
37	72	2.619	2.619	−401	8	2.617	2.617	400
2	5	2.515	2.515	−314				
7	5	2.458	2.460	214	8	2.443	2.442	404
	11		2.458	−403				
	9		2.443	401				
11	27	2.416	2.416	−321				
	4		2.310	006	**28**	**2.313**	**2.315**	**0.0.12**
9	13	2.309	2.308	321	12	2.307	2.307	−227
						2.292	2.295	227
					4	2.288	2.288	−406
					2	2.282	2.284	−2.0.11
20	43	2.258	2.255	−323	4	2.268	2.268	406

Spurrite X-ray powder diffraction data (Cu*K*α) (this study)					Paraspurrite original X-ray powder diffraction data (Cu$K\alpha_1$) (Colville and Colville 1977)			
I_{obs}	I_{calc}*	d_{obs}	d_{calc}†	*hkl*	I_{obs}	d_{obs}‡	d_{calc}	*hkl*
					6	2.262	2.265	2.0.11
7	16	2.203	2.205	031	6	2.208	2.208	032
28	20	2.170	2.183	016	8	2.186	2.188	0.1.12
	9		2.182	130				
	12		2.174	322				
	41		2.170	−131				
	20		2.165	−414	7	2.165	2.165	−416
7	15	2.149	2.150	412	8	2.149	2.149	416
7	11	2.115	2.126	032	2	2.140	2.139	0.2.10
	21		2.115	314				
	12		2.099	−405				
2	11	2.079	2.080	403	17	2.080	2.080	408
4	7	2.050	2.060	116	5	2.065	2.064	420
	4		2.049	−231	4	2.050	2.050	231, −231
	7		2.048	−230				
11	29	2.017	2.017	−316	8	2.015	2.014	036
18	11	1.9870	1.9981	−511	5	2.008	2.009	−233
	24		1.9903	−512	**63**	**1.983**	**1.983**	**0.0.14; −424**
	9		1.9868	413				
	9		1.9796	007				
7	8	1.9358	1.9425	133				
	12		1.9323	−117				
29	50	1.9013	1.9015	026	4	1.905	1.905	0.2.12
	11		1.8985	017				
	16		1.8946	315				
	26		1.8891	−424	10	1.890	1.891	−426
					5	1.887	1.888	−2.2.11
21	33	1.8799	1.8791	422	7	1.880	1.880	038
5	9	1.8580	1.8556	324	7	1.879	1.879	426
4	6	1.8030	1.8047	512				
	4		1.8019	−333				
7	8	1.7751	1.7784	−425				
	11		1.7753	−521				
9	14	1.7679	1.7653	−515	11	1.767	1.768	428
2	5	1.7377	1.7322	008				
13	11	1.7050	1.7051	−227				
	10		1.7043	027				
	7		1.7035	521				
7	5	1.6765	1.6812	135				
	9		1.6750	040				
	5		1.6734	333				
2	4	1.6498	1.6476	−141				
5	5	1.6367	1.6355	141				
	5		1.6331	−335				
4	5	1.5941	1.5930	−241				
10	5	1.5443	1.5454	−621				
	6		1.5424	227				

* Calculated based on results from crystal-structure data.
† Calculated from XRPD unit-cell refinement with a = 10.478(3), b = 6.700(2), c = 14.127(3) Å, β = 101.02(2)°, V = 972.8(3) Å^3.
‡ Peaks as identified in Colville and Colville (1977). Those in boxes have severe overlap and were evidently measured by Colville and Colville in the fine structure of the spectrum at the top (an unconventional method). Bold peaks show 00*l* reflections that were thought to show the effect of preferred orientation by Colville and Colville (1977). Shaded peaks are those with *l* indices odd.

and space group derived for paraspurrite can be generated by twinning of the spurrite unit cell. Two polysynthetically twinned crystals (Fig. 1) were mounted for single-crystal experimental work. Both crystals gave identical results within one standard deviation using some 230 reflections for each cell refinement: a = 10.494(1), b = 6.7116(6), c = 28.216(3) Å, α = 90.059(6), β = 100.132(5), γ = 90.023(6)°.

Figure 2 shows the relationship, in reciprocal space, of spurrite to "paraspurrite." Reflections of the **a*-c***-plane show *h*0*l* reflections with h = 2n (*c*-glide extinctions). This extinction condition exists in both the single and twinned crystals. In the calculated, twinned "paraspurrite" diffraction pattern γ approaches 90° and the c^* reciprocal spacing is divided into 4 parts (i.e., the c cell parameter is 4× larger).

This monoclinic primitive cell transforms to monoclinic *B* centered cell (Fig. 2): a = 10.494, b = 6.7116, c = 55.56 Å, α = 90, β = 90.6, γ = 90°. This corresponds to the monoclinic *P* cell of Colville and Colville (1977). They refined the cell on 15 strong reflections and obtained a c cell parameter of one-half the actual twin cell dimension. They give space group $P2_1/a$ with cell parameters: a = 10.473, b = 6.706, c = 27.78 Å, α = 90, β = 90.58, γ = 90°. The twin transformation matrix is 100/010/104.

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