

Tschernichite, the Mineral Analogue of Zeolite Beta

Joseph V. Smith,*^a Joseph J. Pluth,^{a,b} Russell C. Boggs^c and Donald G. Howard^d

^a Consortium for Theoretical Frameworks, Department of the Geophysical Sciences, The University of Chicago, Chicago, IL 60637, USA

^b Materials Research Laboratory, The University of Chicago, Chicago, IL 60637, USA

^c Department of Geology, Eastern Washington University, Cheney, WA 99004, USA

^d Physics Department, Portland State University, P.O. Box 751, Portland, OR 97207, USA

Tschernichite, a new mineral that occurs with boggsite near Goble, Oregon, has a disordered structure of the Beta type.

Tschernichite,¹ is a new mineral that is associated with several other zeolites including boggsite^{2,3} in hydrothermally altered basalt near Goble, Columbia County, Oregon. Its chemical composition ranges from *ca.* $\text{CaSi}_6\text{Al}_2\text{O}_{16}\cdot 8\text{H}_2\text{O}$ to *ca.* $\text{Ca}_{0.7}\text{Na}_{0.1}\text{Si}_{6.3}\text{Al}_{1.7}\text{O}_{16}\cdot 4\text{H}_2\text{O}$. Diffractometer X-ray diffraction patterns were indexed on a tetragonal unit cell with $a = 12.88$ and $c = 25.02$ Å, but the fit was not fully satisfactory. Although tschernichite occurs as well-shaped crystals bounded by tetragonal dipyramids, especially $\{302\}$, all single-crystal X-ray photographs showed complex sharp and diffuse spots unsuitable for structure analysis. Even a tiny fragment from the apex of a crystal showed a complex pattern. To test whether the diffractometer powder pattern was consistent with the single-crystal photographs, Gandolfi powder patterns were taken of a single fragment 0.5 mm across. To reduce the background from air scattering, the camera was evacuated.

Table 1 compares the d -values for the diffractometer and Gandolfi patterns of tschernichite with ones calculated for the

ordered arrangements A and B of the Beta structure.^{4,5} There is a satisfactory match between the overall features of the patterns, but the details do not fit. The tschernichite patterns match best with the computed X-ray pattern for an approximately equal amount of the A and B arrangements in a random sequence (Fig. 17 of ref. 4). It is concluded that tschernichite is the natural analogue of synthetic zeolite Beta, and has a similar degree of disorder.

Some details need discussion. The observed powder diffractions patterns of different preparations of zeolite Beta differ slightly (*e.g.* see refs. 4–6), and it is not clear what are the relative contributions from changes of bulk composition, possible variations in stacking disorder, and possible presence of minor impurities. The calculated powder diffraction patterns vary slightly because of minor differences in the predictions of the atomic coordinates.⁷ None of these details compromise the conclusion that tschernichite has a disordered Beta type of structure.

Table 1 Comparison of X-ray powder diffractometer and Gandolfi diffraction data of tschernichite with calculated data for Beta-A and Beta-B

I ^a	d _X (Tsch) ^a	d _G (Tsch) ^b	d(Beta-A) ^c	d(Beta-B) ^c
2	25.98			
10	12.52		12.66	
32	11.63	11.97	11.4,9.14	12.03,10.63
7	6.24	6.31	7.22,6.60,6.16	7.72-6.25
2	5.63		5.70	
2	4.97		4.88	5.10
2	4.74			
2	4.45		4.56	4.56
14	4.22	4.21	4.30,4.24	4.36,4.28,4.23
1	4.12		4.16	4.19
100	4.03	4.02	4.06,4.02	4.06
4	3.971		3.96	3.98,3.86
6	3.708			3.73,3.70
2	3.651		3.64,3.61	
13	3.569	3.564	3.56	3.58
7	3.500	3.482	3.48	3.46-3.50
5	3.333	3.322	3.30,3.24	3.25
16	3.156	3.155	3.17	3.15-3.10
15	3.062	3.064	3.05	3.03
7	2.990	2.991	2.93	2.99
1	2.950			2.94
2	2.818		2.86	2.85
10	2.730	2.724	2.72,2.75	2.79,2.72
2	2.617		2.66	2.66
5	2.527	2.527	2.53	2.53,2.51
3	2.439		2.44	2.46,2.41
1	2.300		2.29	2.37
2	2.220		2.22	2.25
2	2.191			2.21
2	2.164		2.16,2.15	
16	2.114	2.111	2.11	2.11

^a Intensities and d-spacings from Table 1 of ref. 1. ^b d-Spacings from Gandolfi pattern. ^c d-Spacings calculated from Tables 1 and 2 of ref. 4.

The occurrence of the Beta structure type as a natural mineral in basaltic rock is important because it implies that an organic structure-directing agent, such as methylammonium ion,⁸ may not be necessary for synthesis. Furthermore, tschernichite has a lower Si:Al ratio (3.0-3.6) than synthetic Beta (5-100; typically 10) described in the primary patent.⁸ Hence a systematic search for inorganic syntheses of the Beta structure type is indicated. Valuable applications in molecular sieve technology might ensue.

Further studies on tschernichite are in progress to determine (a) how the X-ray patterns change in response to chemical treatment, and (b) whether different natural samples vary in the stacking ratio.

We thank the Exxon Education Foundation and UOP for support of the Consortium for Theoretical Frameworks, and NSF DMR for support of the Materials Research Laboratory.

Received, 23rd November 1990; Com. 0/05283C

References

- 1 R. C. Boggs, D. G. Howard and J. V. Smith, *Am. Mineral.*, in the press.
- 2 J. J. Pluth and J. V. Smith, *Am. Mineral.*, 1990, **75**, 501.
- 3 D. G. Howard, R. W. Tschernich, J. V. Smith and G. L. Kline, *Am. Mineral.*, in the press.
- 4 J. M. Newsam, M. M. J. Treacy, W. T. Koetsier and C. B. de Gruyter, *Proc. R. Soc. London, Ser. A*, 1988, **420**, 375.
- 5 J. B. Higgins, R. B. LaPierre, J. L. Schlenker, A. C. Rohrman, J. D. Wood, G. T. Kerr and W. J. Rohrbaugh, *Zeolites*, 1988, **8**, 446.
- 6 J. Perez-Pariante, J. A. Martens and P. A. Jacobs, *Appl. Catal.*, 1987, **31**, 35.
- 7 S. M. Tomlinson, R. A. Jackson and C. R. A. Catlow, *J. Chem. Soc., Chem. Commun.*, 1990, 813.
- 8 R. L. Wadlinger, G. T. Kerr and E. J. Rosinski, 1967, U.S. Pat. No. 3 308 069.