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X-ray powder data for villamaninite

In a recent review of the literature, the Joint Committee of Powder Diffraction Standards has been unable to find powder X-ray diffraction data for villamaninite. This mineral has been described by Ympa *et al.* (1968) from the type-locality of the Providencia Mine, near Cármenes, Villamanín, León, Spain, with a chemical composition determined by electron-probe of $Cu_{0.60}Fe_{0.23}Ni_{0.14}Co_{0.03}S_2$. They determined the space group as $Pa3$ with $a = 5.6927(5)$ Å. A villamaninite sample from this locality was obtained from Dr. Ympa. A diffractometer trace was obtained with Cu-$K\alpha$ radiation (1·5405 Å) and a 002 graphite monochromator from 10° to 90° 2θ at a scanning speed of 0·125°/min. A least-squares refinement in space group $Pa3$ with the program of Appleman *et al.* (1972) gave $a = 5.6944(3)$ Å. The *hkl*, *d* calculated, *d* observed, and relative intensities (I/I_1) are presented in Table I.

TABLE I. *X-ray powder data for villamaninite*

hkl	d_{calc} Å	d_{obs} Å	I/I_1	*hkl*	d_{calc} Å	d_{obs} Å	I/I_1	*hkl*	d_{calc} Å	d_{obs} Å	I/I_1
111	3·288	3·289	15	222	1·6438	1·6434	5	420	1·2733	1·2732	3
200	2·847	2·852	100	230	1·5793	1·5786	10	421	1·2426	1·2431	1
210	2·547	2·548	30	321	1·5219	1·5220	10	332	1·2140		
211	2·325	2·325	25	400	1·4236			422	1·1624	1·1623	3
220	2·013	2·014	25	410	1·3811	1·3813	2	430	1·1389	1·1389	1
221	1·898			411	1·3422	1·3419	1	431	1·1168		
311	1·7169	1·7174	40	331	1·3064	1·3060	5	511	1·0959	1·0959	15

Villamaninite is a pyrite-type mineral with Cu as the dominant metal atom. This corresponds to the 'idiomorphic villamaninite' with *a* 5·69–5·71 Å unit cell of Ympa *et al.* (1968). However, their 'nodular villamaninite' with *a* 5·65–5·67 Å unit cell is a misnomer, since it has Ni as the dominant metal atom and hence is a ferroan cuprian vaesite.

Disordered gersdorffite–NiAsS (Bayliss, 1968) has space group $Pa3$ with a unit cell of 5·693 Å and a pyrite-type structure. Therefore villamaninite and disordered gersdorffite have the same space group, the same unit cell, and the same structure-type. Generally, the intensity of the 200 is greater than the 210 for AX_2 minerals (e.g. vaesite) whereas the intensity of the 200 is less than the 210 for AXY minerals (e.g. ullmannite). However, the data of Bayliss (1969) indicates that the intensity ratio of 200:210 for gersdorffite is variable. Therefore villamaninite may be misidentified as gersdorffite if only X-ray powder data is used.

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