

oxygens enclosing a layer of iodine, parallel to the (010) plane. The H_5IO_6 structure is found by displacement of the atoms and a slight deformation of the ideal unit cell as shown in Figs. 1 and 2.

In the ideal structure half of the oxygens are in the position $y=1/16$ and the other half in the position $y=3/16$. The iodine atoms lie in the plane $y=1/8$. In the actual structure these values are:

$$\begin{aligned} \text{I: } & y = 1/8 - 0.004; & \text{O}_1: & y = 1/16 - 0.012; \\ \text{O}_2: & y = 1/16 + 0.019; & \text{O}_3: & y = 1/16 + 0.001; \\ \text{O}_4: & y = 3/16 + 0.008; & \text{O}_5: & y = 3/16 - 0.020; \\ \text{O}_6: & y = 3/16 - 0.006. \end{aligned}$$

The unit cell contains four of these double layers of oxygen perpendicular to the b -axis, connected by the

Table 2

$$\begin{aligned} \text{O}_1(x, y, z) - \text{O}'_3(x, y, z) &= 2.76 \text{ \AA} \\ \text{O}_6(x, y, z) - \text{O}'_4(x, y, z) &= 2.79 \\ \text{O}_2(x, y, z) - \text{O}''_5(x, y, z) &= 2.69 \\ \text{O}_1(x, y, z) - \text{O}_2(\bar{x}, \bar{y}, \bar{z}) &= 2.64 \\ \text{O}_6(x, y, z) - \text{O}_4(\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z) &= 2.81 \text{ \AA} \end{aligned}$$

Note: The parameters in brackets give the symmetry relation between the oxygen atoms and the primes refer to an oxygen atom in neighbouring unit cells (see Fig. 2).

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Lattice constants and space group of sodium tungstate dihydrate.* By CARL W. F. T. PISTORIUS† and W. E. SHARP, *Institute of Geophysics, University of California, Los Angeles 24, California, U.S.A.*

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The crystallographic properties of $Na_2WO_4 \cdot 2H_2O$ have only been superficially investigated. Marignac (1863) found that the crystalline substance is orthorhombic bipyramidal. His goniometric measurements indicate that

$$a:b:c = 0.8002:1:0.6470.$$

Baker's Analyzed Reagent grade $Na_2WO_4 \cdot 2H_2O$ was used in the present investigation. The company's analysis is as follows: insoluble matter 0.002%; alkalinity (as Na_2CO_3) 0.08%; chloride (as Cl) 0.001%; nitrogen compounds (as N) 0.0003%; sulfate (as SO_4) 0.003%; arsenic (as As) 0.0001%; heavy metals (as Pb) 0.0002%; iron (as Fe) 0.0001% and molybdenum (as Mo) 0.0001%. The substance was used without further purification.

Under the microscope the crystals have the appearance of basal tablets, elongated parallel to a or b , with a perfect {001}, and less perfect {110} and {120} cleavages. The optic plane is (010); $r < v$ strong. The refractive indices for NaD light are

$$\begin{aligned} n_x &= 1.5530 \pm 0.001, & n_y &= 1.5535 \pm 0.001, \\ n_z &= 1.5650 \pm 0.001; & n_z - n_x &= 0.012; \\ (+)2V &= 26^\circ; & X &= a, Y = b, Z = c. \end{aligned}$$

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symmetry elements. As the structure of $Al(OH)_3$ is also derived from the same ideal model, the crystal structure of H_5IO_6 is closely related to that of $Al(OH)_3$ (Megaw, 1934). In $Al(OH)_3$ two of the three oxygen octahedra are filled by aluminium. In H_5IO_6 only one of the three octahedra contains an iodine atom. The shortest distances between oxygen in neighbouring octahedra are shown in Table 2. These distances give the impression that an oxygen octahedron in a double layer is linked by three hydrogen bonds to octahedra in the same layer and by two hydrogen bonds to octahedra of adjacent layers. An attempt will be made to determine the positions of the hydrogen atoms from neutron diffraction data.

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The X-ray powder diffraction pattern of finely ground $Na_2WO_4 \cdot 2H_2O$ at 25 °C. was obtained in a Norelco high angle recording diffractometer, using $Cu K\alpha$ radiation ($\lambda = 1.5418 \text{ \AA}$) and a Ni filter. The scanning speed was $1/8^\circ (2\theta)$ per min. High-purity sodium chloride was used as an internal standard.

The assignment of the peaks was made with the aid of some runs emphasizing preferred orientation, and by using the goniometric value for $a:b:c$. All of the observed diffraction peaks could be satisfactorily assigned as being due to an orthorhombic lattice with the following unit-cell dimensions, obtained by a least-squares treatment:

$$\begin{aligned} a_0 &= 8.456 \pm 0.005, & b_0 &= 10.601 \pm 0.005, \\ c_0 &= 13.842 \pm 0.005 \text{ \AA}. \end{aligned}$$

The present axial ratio,

$$a_0:b_0:c_0 = 0.7978:1:2(0.6530),$$

agrees reasonably well with the goniometric value (Marignac, 1863).

The calculated density of $Na_2WO_4 \cdot 2H_2O$ at 25 °C., assuming 8 molecules per unit cell, is 3.532 g.cm.^{-3} . Clarke & Davis (1877) found that the pycnometric density at 19 °C. is $3.2314 \text{ g.cm.}^{-3}$. However, according to Zamboni (1923) this value is too low. His pycnometric measurements on carefully selected material gave a density at 15 °C. of 3.50 g.cm.^{-3} , which is in fair agreement with X-ray density.

The observed and calculated d -spacings, assigned indices and observed relative intensities are listed in Table 1. The selection rules appear to be:

$h00$: $h = 2n$ $h0l$: $l = 2n$
 $0k0$: $k = 2n$ $hk0$: $h = 2n$ (?)
 $00l$: $l = 2n$ hkl : no restriction
 $0kl$: $k = 2n$

Table 1. Powder data

d_o (Å)	d_c (Å)	hkl	$(I/I_0) \times 100$
6.902	6.921	002	100
5.959	5.965	111	20
5.288	5.301	020	25
4.773	4.780	112	22
4.238	4.228	200	67
4.209	4.208	022	68
3.936	3.927	210	2
3.782	3.784, 3.778	113, 211	16
3.613	3.608	202	69
3.463	3.460	004	20
3.418	3.416	212	11
3.308	3.305	220	48
3.218	3.218	123	14
3.170	3.174	131	75
3.066	3.066	114	50
2.985	2.991, 2.983	213, 222	71
2.950	2.950	132	2
2.897	2.898	024	22
2.745	2.741	124	10
2.680	2.678, 2.673	204, 311	54
2.664	2.663, 2.661	133, 231	34
2.598	2.603, 2.596	041, 214	6
2.551	2.554	115	2
2.468	2.475	042	3
2.451	2.450, 2.454	321, 025	6
2.392	2.390	224	13
2.355	2.357	125	5
2.343	2.346	313	17
2.338	2.338	233	9
2.306	2.307	006	6
2.296	2.298	043	6
2.178	2.176, 2.178	331, 116	39
2.144	2.141	314	7
2.138	2.134, 2.136	234, 242	4
2.120	2.114	400	5
2.114	2.110	135	17
2.104	2.104	044	5
2.030	2.034, 2.025	151, 206	29
1.990	1.986, 1.989, 1.989	412, 333, 216	24
1.967	1.964, 1.971	420, 152	7
1.912	1.912, 1.914	341, 045	4
1.892	1.889, 1.891, 1.895	422, 413, 250	21
1.883	1.884, 1.883	244, 136	4
1.878	1.878	251	32
1.861	1.860, 1.859	342, 334	2
1.854	1.851, 1.853	325, 027	6
1.808	1.807, 1.804, 1.810	423, 404, 127	8
1.789	1.785	306	4
1.783	1.781, 1.779	343, 414	6
1.764	1.761, 1.767	316, 060	15
1.745	1.744	245	11
1.724	1.724	335	14
1.710	1.708, 1.712	424, 062	12
1.697	1.695, 1.697	108, 227	5
1.692	1.691, 1.692	137, 326	3
1.682	1.682	351	19
1.675	1.678, 1.674	162, 118	21

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Table 1 (cont.)

d_o (Å)	d_c (Å)	hkl	$(I/I_0) \times 100$
1.650	1.653, 1.651, 1.650	440, 155, 063	9
1.616	1.615, 1.619	128, 261	2
1.609	1.609, 1.607, 1.608	246, 434, 442	3
1.603	1.601, 1.600, 1.602, 1.600	208, 317, 425, 521	5
1.590	1.591	353	12
1.586	1.585, 1.583, 1.587, 1.584	047, 218, 262, 345	10
1.560	1.559, 1.558	406, 147	5
1.539	1.535, 1.537	156, 263	2
1.531	1.528, 1.533	138, 228	3
1.519	1.521, 1.520	523, 504	6
1.508	1.504	514	3
1.485	1.484	247	12
1.480	1.481	346	12
1.473	1.475, 1.475, 1.472	264, 308, 337	5
1.463	1.463, 1.461, 1.461, 1.463	452, 524, 318, 362	8
1.451	1.449	048	4
1.445	1.445	355	8
1.417	1.418, 1.418	271, 541	7
1.404	1.405, 1.403	265, 066	4
1.395	1.394, 1.396, 1.396, 1.396	229, 272, 534, 542	6
1.383	1.384, 1.384	166, 0, 0, 10	5
1.356	1.356, 1.356, 1.355	460, 621, 1, 1, 10	12
1.338	1.339, 1.339, 1.337, 1.337, 1.338, 1.339	319, 408, 437, 613; 239; 0, 2, 10	5
1.330	1.330, 1.331, 1.330	049, 266, 462	4
1.317	1.317, 1.317, 1.318, 1.316, 1.318, 1.318	365, 455, 544, 551, 274, 067	6
1.308	1.308, 1.308	329, 630	3
1.299	1.298, 1.299	428, 552	4
1.281	1.282	373	3
1.275	1.274, 1.274, 1.276	083, 1, 3, 10, 517	4
1.269	1.268, 1.269	447, 249	11
1.258	1.258	267	3
1.244	1.244, 1.244	640, 282	3
1.235	1.235, 1.235, 1.236, 1.236	419, 554, 068, 1, 1, 11	6
1.226	1.226	471	2
1.218	1.218	465	5
1.203	1.203, 1.203, 1.203	349, 562, 606	4
1.1943	1.1936, 1.1947, 1.1951, 1.1936, 1.1951, 1.1943	367, 381, 448, 457, 616, 259	3
1.1870	1.1865	268	3
1.1751	1.1740, 1.1760	1, 3, 11; 2, 2, 11	4
1.1727	1.1721, 1.1732, 1.1729	3, 3, 10; 439, 626	5
1.1558	1.1549	376	3
1.1373	1.1367, 1.1375	0, 4, 11; 653	6
1.1272	1.1278, 1.1266	732; 1, 4, 11	5

The space group is probably either $Pbcn-D_{2h}^1$ or $Pbca-D_{2h}^5$. If the very weak (210) peak is real, the space group must be $Pbca-D_{2h}^5$, but the possibility that this reflection is spurious cannot yet be ruled out with certainty. All of the other observed peaks are allowed in both of the above space groups.

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