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The unit cell and space group of $\text{Na}_2\text{HPO}_4 \cdot 2\text{H}_2\text{O}$. By EVA ZSOLDOS, *Research Institute for Technical Physics of the Hungarian Academy of Sciences, Budapest, Hungary*

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The inorganic compound Na_2HPO_4 (sodium hydrogen orthophosphate) occurs in four hydrated modifications:

Na_2HPO_4	
$\text{Na}_2\text{HPO}_4 \cdot 2\text{H}_2\text{O}$	orthorhombic
$\text{Na}_2\text{HPO}_4 \cdot 7\text{H}_2\text{O}$	monoclinic
$\text{Na}_2\text{HPO}_4 \cdot 12\text{H}_2\text{O}$	monoclinic or orthorhombic.

The white powder $\text{Na}_2\text{HPO}_4 \cdot 2\text{H}_2\text{O}$ was studied in our laboratory. X-ray powder photographs were taken in a de Wolff type fourfold Guinier camera with copper $K\alpha$ radiation monochromatized by a curved-quartz-crystal monochromator. The film contained 87 lines, of which only the first 73 were measurable by a coincidence measuring rule. The indexing was carried out according to the Lipson (1949) and Hesse (1948) difference method completed by Zsoldos (1962).

The compound was unambiguously indexed in the orthorhombic system. The lattice parameters were

$$a = 10.34 \pm 0.03, \quad b = 13.64 \pm 0.03, \quad c = 16.98 \pm 0.04 \text{ \AA}.$$

Table 1. *X-ray data*

No.	<i>hkl</i>	$\sin^2 \theta_{\text{calc.}}$	$\sin^2 \theta_{\text{meas.}}$	$\Delta \sin^2 \theta \cdot 10^5$
1.	002	0.00824	0.00834	14
2.	112	0.01628	0.01626	2
3.	003	0.01854	0.01862	8
4.	121	0.02037	0.01957	80
5.	022	0.02100	0.02132	30
	013	0.02173		41
6.	200	0.02222	0.02222	0
7.	201	0.02428	0.02488	60
8.	211	0.02747	0.02765	18
9.	031	0.03077	0.03063	14
	202	0.03046		17
10.	212	0.03365	0.03321	44
11.	104	0.03851	0.03796	55
12.	203	0.04076	0.04045	31
13.	132	0.04250	0.04257	7
14.	024	0.04472	0.04453	19
15.	040	0.05104	0.05101	3
16.	041	0.05310	0.05302	8
17.	204	0.05518	0.05510	8
18.	140	0.05659	0.05601	58
19.	105	0.05705	0.05706	1
20.	042	0.05928	0.05906	22
21.	115	0.06024	0.06030	6
22.	320	0.06275	0.06258	17
23.	134	0.06732	0.06730	2
24.	303	0.06853	0.06907	54
25.	043	0.06958	0.06947	11
	233	0.06947		0
26.	313	0.07172	0.07227	55
27.	241	0.07532	0.07605	73
28.	016	0.07735	0.07723	12
29.	050	0.07975	0.07960	15
	106	0.07971		11
30.	331	0.08076	0.08066	10

Table 1 (cont.)

No.	<i>hkl</i>	$\sin^2 \theta_{\text{calc.}}$	$\sin^2 \theta_{\text{meas.}}$	$\Delta \sin^2 \theta \cdot 10^5$
31.	304	0.08295	0.08301	6
32.	150	0.08530	0.08509	21
	135	0.08576		67
33.	400	0.08888	0.08893	5
34.	152	0.09354	0.09302	52
	126	0.09247		45
35.	206	0.09638	0.09634	4
36.	333	0.09724	0.09789	65
37.	216	0.09957	0.09963	6
38.	244	0.10622	0.10599	23
39.	145	0.10809	0.10775	34
	403	0.10742		33
40.	334	0.11166	0.11156	10
41.	054	0.11271	0.11308	37
	027	0.11370		62
42.	061	0.11690	0.11639	1
43.	161	0.12245	0.12265	20
	062	0.12380		43
44.	460	0.12372	0.12351	21
	207	0.12316		35
45.	351	0.13180	0.13166	14
	008	0.13184		18
46.	108	0.13739	0.13731	8
47.	118	0.14058	0.14015	43
	405	0.14038		17
48.	510	0.14206	0.14258	52
49.	064	0.14780	0.14799	19
50.	307	0.15093	0.15095	2

Only the following systematic absences were found:

$$\text{in } h00 \quad h = 2n$$

and

$$\text{in } 0k0 \quad k = 2n,$$

the space group thus being $P2_12_12(D_2^3)$.

The result of the indexing process is presented in Table 1. The inaccuracy of measurement in $\sin^2 \theta$ for the first lines was 10^{-4} and for the final lines $5 \cdot 10^{-4}$. The measured and calculated $\sin^2 \theta$ are in good agreement.

The density of $\text{Na}_2\text{HPO}_4 \cdot 2\text{H}_2\text{O}$ at 15 °C.—according to Koglin (1954) is 2.066 g.cm.^{-3} and the density calculated from the X-ray data with 16 molecules in the unit cell is 2.079 g.cm.^{-3} .

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References

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