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THE LATTICE PARAMETERS OF $NOHSO_4$ AND $NOHS_2O_7$

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16. Abstract

Data are lacking on the crystal system, the magnitude of the lattice parameters and the Miller indices of individual X-ray interferences. The positions and intensities of X-ray reflections were measured by using Ni-filtered copper radiation. Peak heights were used to determine the relative intensities and the peak height of the strongest line was set equal to 10. Graphically determined Miller indices were used for refining the lattice parameters by means of a compensation calculation. Lattice parameter errors may result in the line indices being incorrect at the greater interference angles.

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THE LATTICE PARAMETERS OF $NOHSO_4$ and $NOHS_2O_7$

Carl-Friedrich Linström and Joachim Löscher

Many X-ray bar graphs of $NOHSO_4$ [1] and $NOHS_2O_7$ [2], [3] have /353 already been published. However, data are lacking on the crystal system, the magnitude of the lattice parameters and the Miller indices of individual X-ray interferences.

The positions and intensities of X-ray reflections have been measured, using Ni-filtered copper radiation (λ=1.5418 Å) with a HZG 1 horizontal counter tube goniometer of the VEB (Volks Eigener Betrieb = People's Owned Enterprise) Freiberg Precision Mechanics. Since the compounds are very hygroscopic, the samples had to be masked with polystyrene foil and had to be replaced several times during the exposure of the X-ray film diagrsm.

We used peak heights to determine the relative intensities and set the peak height of the strongest line equal to 10.

The indexing of the uncorrected interference positions as per the Gattow and Plotter procedure [4] resulted first in only inexact lattice parameters and--as a result--(hkl) values, which still contained certain errors. Assuming nevertheless, that the major part of the interferences had been correctly indexed, the Miller indices, graphically determined as per [4], were used for refining the lattice parameters by means of a compensation calculation. /354
The calculation of the theoretical line sequence from these corrected parameters using a program written in FORTRAN 63--which can be used upon request--and the comparison with the measured values resulted in more exact indices. The final lattice parameters and (hkl)--values were obtained from numerous repetitions of these steps.

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* Numbers in the margin indicate pagination in the foreign test.

Both compounds crystallize in an orthorhombic lattice.

NOHSO$_4$	$a = 10{,}682 \pm 4 \cdot 10^{-3}$ Å $b = 11{,}648 \pm 8 \cdot 10^{-3}$ Å $c = 10{,}367 \pm 7 \cdot 10^{-3}$ Å	NOHS$_2$O$_7$	$a = 11{,}663 \pm 5 \cdot 10^{-3}$ Å $b = 12{,}806 \pm 4 \cdot 10^{-3}$ Å $c = 10{,}773 \pm 3 \cdot 10^{-3}$ Å

The measured angles of incidence ϑ_o, the relative intensities, I_o, the lattice plane separations d_o, the Q_o-values ($Q_o = 1/d_o^2$), the differences between the measured and calculated Q-values ($Q_o - Q_c$) and the Miller indices (hkl) are given in Tables 1 and 2.

TABLE 1. NOHSO$_4$ INTERFERENCES
STANDARD DEVIATION OF THE Q_o-VALUES: $9.79 \cdot 10^{-4}$

Nr.	I_0	ϑ_0	d_0	Q_0	$Q_0 - Q_c \cdot 10^{-4}$	(hkl)
1	2	8,26	5,3650	0,03473	−3,3	(200)
2	3	8,54	5,1913	0,03711	−1,1	(002)
3	2	8,70	5,0918	0,03863	2,4	(021)
4	3	10,37	4,2820	0,05453	27,8	(211)
5	6	10,50	4,2302	0,05588	25,3	(112)
6	3	11,40	3,9001	0,06574	−5,0	(030)
7	1	12,08	3,6836	0,07370	−1,4	(221)
8	6	12,82	3,4743	0,08285	−6,0	(003)
9	7	13,41	3,3240	0,09050	−6,0	(013)
10	10	13,70	3,2540	0,09439	−11,6	(311)
11	3	14,17	3,1491	0,10084	−5,5	(230)
12	3	14,27	3,1274	0,10224	4,8	(222)
13	6	14,47	3,0851	0,10506	15,1	(032)
14	4	15,33	2,9159	0,11761	−0,4	(321)
15	4	16,76	2,6733	0,13992	−3,0	(400)
16	2	17,31	2,5900	0,14907	1,1	(004)
17	<1	17,95	2,5014	0,15982	9,9	(133)
18	1	18,41	2,4410	0,16783	−18,7	(420)
19	1	18,70	2,4044	0,17297	20,9	(313)
20	4	19,53	2,3071	0,18787	7,6	(124)
21	<1	20,32	2,2199	0,20293	5,9	(151)
22	1	21,20	2,1231	0,22183	3,6	(052)
23	1	22,60	2,00598	0,24850	−0,8	(520)
24	3	23,37	1,94342	0,26476	−5,7	(060)
25	3	23,65	1,92171	0,27078	−0,6	(125)
26	1	24,71	1,84412	0,29404	−0,3	(334)
27	2	25 14	1,81458	0,30369	2.0	(253)
28	<1	25,58	1,78541	0,31370	−18,0	(600)
29	<1	26,10	1,75226	0,32568	8,7	(601)
30	<1	26,31	1,73926	0,33057	−16,1	(611)
31	<1	26,50	1,72769	0,33501	0,7	(006)
32	<1	27,02	1,69687	0,34729	4,2	(353)
33	2	27,30	1,68078	0,35397	−3,2	(621)
34	<1	27,56	1,66671	0,35997	−1,1	(612)
35	1	27,91	1,64601	0,36908	−4,8	(533)
36	<1	29,06	1,58709	0,39700	−4,5	(624)
37	1	30,00	1,54178	0,42067	−0,9	(643)
38	1	31,21	1,48770	0,45181	1,2	(505) (253)
39	<1	32,93	1,41885	0,49726	−6,7	(065)
40	<1	33,52	1,39599	0,51315	−0,2	(703)
41	1	33,92	1,38144	0,52399	2,4	(373)
42	<1	34,67	1,35518	0,54450	−5,6	(274)
43	<1	34,97	1,34501	0,55276	5,4	(554)
44	1	35,20	1,33438	0,56161	2,0	(610)
45	<1	36,43	1,29814	0,59334	−3,5	(075)
46	<1	37,68	1,26117	0,62926	−0,6	(184)
47	<1	38,25	1,24519	0,64494	3,1	(734) (803)
48	<1	39,35	1,21581	0,67735	7,0	(670)
49	<1	41,81	1,15634	0,74785	7,0	(092)
50	<1	43,58	1,11826	0,79968	−2,2	(771)
51	<1	46,72	1,05830	0,89183	−8,8	(717)
52	<1	54,32	0,94904	1,11026	0,9	(703)

TABLE 2. $NOHS_2O$ INTERFERENCES:

STANDARD DEVIATION OF THE Q_o-values: $5.73 \cdot 10^{-4}$

Nr.	I_0	θ_0	d_0	Q_0	$Q_0 - Q_c \cdot 10^4$	(hkl)
1	<1	6,95	6,371	0,02461	2,4	(020)
2	<1	7,56	5,8594	0,02913	−2,8	(200)
3	1	7,94	5,5807	0,03211	3,6	(120)
4	1	8,16	5,4312	0,03390	8,0	(021)
5	2	8,23	5,3854	0,03448	0,1	(002)
6	5	8,44	5,2522	0,03625	7,5	(210)
7	4	10,17	4,3650	0,05246	−13,4	(220)
8	2	10,43	4,2583	0,05515	2,6	(030)
9	<1	11,01	4,0257	0,06170	−5,3	(130)
10	<1	11,25	3,9515	0,06401	1,7	(202)
11	1	11,43	3,8900	0,06608	−0,8	(300) (122)
12	<1	11,85	3,7540	0,07096	1,1	(131)
13	2	12,81	3,4769	0,08272	−0,3	(013)
14	<1	13,33	3,3436	0,08945	−1,0	(032)
15	<1	13,59	3,2808	0,09290	0,0	(231)
16	2	13,84	3,2220	0,09629	−4,1	(132)
17	2	13,97	3,1932	0,09807	5,0	(040)
18	10	14,15	3,1534	0,10056	−0,7	(302)
19	<1	14,48	3,0830	0,10520	2,8	(140)
20	<1	14,70	3,0108	0,10965	3,6	(123)
21	<1	14,86	3,0059	0,11067	−23,8	(213)
22	1	15,07	2,9609	0,11375	2,1	(141)
	<1	15,33	2,9150	0,11761	0,0	(400)
	<1	15,39	2,9048	0,11851	−2,4	(232)
25	<1	15,75	2,8460	0,12308	2,6	(410)
26	3	16,52	2,7111	0,13605	4,6	(241)
27	2	16,63	2,6936	0,13782	−0,4	(004)
28	1	16,70	2,6827	0,13895	−4,4	(142)
29	3	17,02	2,6337	0,14417	2,1	(014)
30	3	17,09	2,6232	0,14532	1,1	(104)
[illegible]	1	18,36	2,4474	0,16695	−3,2	(204)
	<1	18,68	2,4069	0,17261	1,1	(430) (341)
[illegible]	2	19,19	2,3453	0,18181	−0,5	(250)
34	<1	19,67	2,2681	0,19439	1,2	(152)
35	<1	20,50	2,2012	0,20637	−5,9	(432)
36	<1	20,96	2,1550	0,21532	−0,9	(005)
37	<1	21,37	2,1156	0,22343	−3,8	(441)
38	<1	21,70	2,0840	0,23004	0,4	(053)
39	<1	22,11	2,04814	0,23838	−2,8	(530)
40	<1	22,18	2,04200	0,23982	0,1	(025)
41	<1	22,42	2,02125	0,24477	−0,5	(205)
42	<1	23,18	1,95846	0,26071	−6,3	(162)
43	<1	23,40	1,93638	0,26669	−7,3	(513)
44	<1	23,75	1,91408	0,27294	−1,8	(532) (001)
45	<1	24,23	1,87838	0,28341	0,1	(262)
46	<1	25,12	1,81503	0,30324	−11,9	(163)
47	<1	25,35	1,80053	0,30845	10,3	(071)
48	<1	25,61	1,78146	0,31438	−3,0	(171)
49	<1	26,13	1,75039	0,32638	−1,1	(263)
50	<1	26,23	1,74419	0,32870	5,6	(631) (270)
51	<1	26,79	1,71035	0,34184	−0,9	(126)
52	<1	26,80	1,70622	0,34349	11,1	(245) (603)
53	<1	27,24	1,68420	0,35253	−5,1	(414)
54	1	27,94	1,64528	0,36941	6,0	(701)
55	<1	28,02	1,64096	0,37136	−2,6	(462)
56	<1	29,31	1,57474	0,40325	−0,6	(560)
57	1	30,56	1,51619	0,43499	0,5	(065)
58	<1	32,41	1,43830	0,48338	6,9	(436) (660)
59	<1	32,74	1,42539	0,492	1,3	(256) (742)
60	<1	33,02	1,41465	0,49968	−3,9	(510)
61	<1	35,40	1,33077	0,56465	4,4	(118)
62	<1	35,75	1,31945	0,57438	3,2	(580) (057)

One should note, however, that as a result of the lattice parameter errors, the line indices may be incorrect at the greater interference angles. If no unambiguous correlation could be made by comparing the observed values with the calculated values, all indices in question were included in Tables 1 and 2.

Some crystal-optical data are given in Table 3.

TABLE 3

Substance	$NOHSO_4$	$NOHS_2C_7$
Optical axis angle 2 v	$\approx 65^{\circ}$, r < v	$\approx 30^{\circ}$, r < v (very strong)
Optical characteristic	+	+
Color	colorless, transparent	color, transparent

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