

General Disclaimer

One or more of the Following Statements may affect this Document

- This document has been reproduced from the best copy furnished by the organizational source. It is being released in the interest of making available as much information as possible.
- This document may contain data, which exceeds the sheet parameters. It was furnished in this condition by the organizational source and is the best copy available.
- This document may contain tone-on-tone or color graphs, charts and/or pictures, which have been reproduced in black and white.
- This document is paginated as submitted by the original source.
- Portions of this document are not fully legible due to the historical nature of some of the material. However, it is the best reproduction available from the original submission.

THE LATTICE PARAMETERS OF NOHSO_4 AND NOHS_2O_7

Carl-Friedrich Linström and Joachim Löscher

(NASA-TT-F-16880) THE LATTICE PARAMETERS OF
 NOHSO_4 AND NOH_2O_7 (Agnew Techn.-Tran, Inc.,
Woodland Hills, Calif.) 7 p HC \$3.50

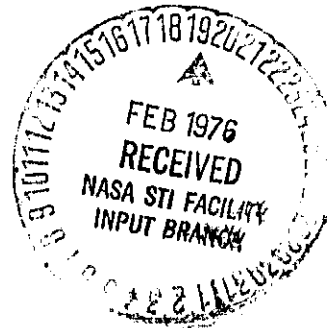
N76-19976

CSCS 20L

Unclass

G3/76 13641

Translation of "Die Gitterparameter von NOHSO_4 und NOHS_2O_7 ",
Zeitschrift für Chemie, Vol. 9, 1969, pp. 353-354



| | | | |
|---|--|--|---------------------------------|
| 1. Report No. NASA TT F-16880 | 2. Government Accession No. | 3. Recipient's Catalog No. | |
| 4. Title and Subtitle THE LATTICE PARAMETERS OF NOHSO_4 AND NOHS_2O_7 | | 5. Report Date February 1976 | 6. Performing Organization Code |
| | | 8. Performing Organization Report No. NASW-2789 | 10. Work Unit No. |
| 7. Author(s) Carl-Friedrich Linström and Joachim Löscher. | | 11. Contract or Grant No. | |
| | | 13. Type of Report and Period Covered Translation | |
| 9. Performing Organization Name and Address Agrew Tech-Tran Inc. Woodland Hills CA 91364 | | 14. Sponsoring Agency Code | |
| 12. Sponsoring Agency Name and Address National Aeronautics and Space Adminis- tration, Washington, D.C. 20546 | | 15. Supplementary Notes Translation of "Die Gitterparameter von NOHSO_4 und NOHS_2O_7 ", <u>Zeitschrift für Chemie</u> , Vol. 9, 1969, pp. 353-354. | |
| 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. | | | |
| 17. Key Words (Selected by Author(s)) | | 18. Distribution Statement Unclassified-Unlimited | |
| 19. Security Classif. (of this report) Unclassified | 20. Security Classif. (of this page) Unclassified | 21. No. of Pages 5 | 22. Price |

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 ($\lambda=1.5418 \text{ \AA}$) 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 diagram.

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.

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

Both compounds crystallize in an orthorhombic lattice.

NOHSO₄ $a = 10,682 \pm 4 \cdot 10^{-3} \text{ \AA}$
 $b = 11,658 \pm 8 \cdot 10^{-3} \text{ \AA}$
 $c = 10,367 \pm 7 \cdot 10^{-3} \text{ \AA}$

NOHS₂O₇ $a = 11,663 \pm 5 \cdot 10^{-3} \text{ \AA}$
 $b = 12,806 \pm 4 \cdot 10^{-3} \text{ \AA}$
 $c = 10,773 \pm 3 \cdot 10^{-3} \text{ \AA}$

The measured angles of incidence θ_0 , the relative intensities, I_0 , the lattice plane separations d_0 , the Q_0 -values ($Q_0 = 1/d_0^2$), the differences between the measured and calculated Q -values ($Q_0 - Q_c$) and the Miller indices (hkl) are given in Tables 1 and 2.

TABLE 1. NOHSO₄ INTERFERENCES
 STANDARD DEVIATION OF THE Q_0 -VALUES: $9.79 \cdot 10^{-4}$

| Nr. | J_0 | θ_0 | d_0 | Q_0 | $Q_0 - Q_c$ $\cdot 10^{-4}$ | (hkl) |
|-----|-------|------------|---------|----------|--------------------------------|-------------|
| 1 | 2 | 8,20 | 5,3650 | 0,03473 | -2,3 | (200) |
| 2 | 3 | 8,54 | 5,1913 | 0,03711 | -1,4 | (020) |
| 3 | 2 | 8,79 | 5,0618 | 0,03903 | 2,4 | (020) |
| 4 | 3 | 10,37 | 4,2820 | 0,05453 | 27,8 | (311) |
| 5 | 0 | 10,50 | 4,2302 | 0,05388 | 25,3 | (112) |
| 6 | 3 | 11,40 | 3,9001 | 0,06374 | -5,9 | (030) |
| 7 | 1 | 12,08 | 3,6836 | 0,07370 | -1,4 | (231) |
| 8 | 0 | 12,82 | 3,4742 | 0,08285 | -8,0 | (003) |
| 9 | 7 | 13,41 | 3,3340 | 0,09050 | -8,0 | (013) |
| 10 | 10 | 13,70 | 3,2540 | 0,09439 | -11,6 | (311) |
| 11 | 3 | 14,17 | 3,1401 | 0,10084 | -5,5 | (230) |
| 12 | 3 | 14,27 | 3,1274 | 0,10224 | 4,8 | (232) |
| 13 | 0 | 14,47 | 3,0851 | 0,10506 | 16,1 | (032) |
| 14 | 0 | 15,33 | 2,9159 | 0,11761 | -0,4 | (321) |
| 15 | 0 | 16,76 | 2,6733 | 0,13802 | -3,0 | (100) |
| 16 | 0 | 17,31 | 2,6000 | 0,14887 | 1,1 | (004) |
| 17 | 1 | 17,95 | 2,5014 | 0,15982 | 0,0 | (133) |
| 18 | 1 | 18,41 | 2,4410 | 0,16783 | -18,7 | (420) |
| 19 | 1 | 18,70 | 2,4044 | 0,17267 | 20,0 | (313) |
| 20 | 4 | 19,52 | 2,3071 | 0,18787 | 7,6 | (124) |
| 21 | 1 | 20,32 | 2,2190 | 0,20253 | 8,0 | (151) |
| 22 | 1 | 21,20 | 2,1531 | 0,22183 | 3,6 | (032) |
| 23 | 1 | 22,00 | 2,0958 | 0,24850 | -0,8 | (520) |
| 24 | 3 | 22,37 | 1,94332 | 0,26470 | -5,7 | (030) |
| 25 | 3 | 22,65 | 1,92171 | 0,27078 | -0,6 | (125) |
| 26 | 1 | 24,71 | 1,84412 | 0,29404 | -0,3 | (334) |
| 27 | 1 | 25,14 | 1,81458 | 0,30360 | 2,0 | (233) |
| 28 | 1 | 25,58 | 1,78541 | 0,31370 | -18,0 | (600) |
| 29 | 1 | 26,10 | 1,75220 | 0,32568 | 8,7 | (601) |
| 30 | 1 | 26,31 | 1,73926 | 0,33057 | -16,1 | (011) |
| 31 | 1 | 26,50 | 1,72769 | 0,33501 | 0,7 | (006) |
| 32 | 1 | 27,02 | 1,69687 | 0,34720 | 4,2 | (353) |
| 33 | 3 | 27,30 | 1,67078 | 0,35397 | -3,2 | (621) |
| 34 | 1 | 27,56 | 1,64671 | 0,35997 | -1,1 | (012) |
| 35 | 1 | 27,91 | 1,61601 | 0,36808 | -4,8 | (533) |
| 36 | 1 | 28,00 | 1,58700 | 0,39700 | -4,5 | (524) |
| 37 | 1 | 30,00 | 1,54178 | 0,42007 | -0,0 | (543) |
| 38 | 1 | 31,21 | 1,48770 | 0,45181 | 1,2 | (305) (253) |
| 39 | 1 | 32,33 | 1,41885 | 0,49726 | -0,7 | (065) |
| 40 | 1 | 33,52 | 1,33990 | 0,54913 | -0,2 | (703) |
| 41 | 1 | 34,02 | 1,32144 | 0,56200 | 2,4 | (373) |
| 42 | 1 | 34,07 | 1,32218 | 0,56150 | -0,6 | (274) |
| 43 | 1 | 34,07 | 1,32501 | 0,55870 | 5,4 | (554) |
| 44 | 1 | 35,20 | 1,23438 | 0,66161 | 2,0 | (510) |
| 45 | 1 | 36,43 | 1,20814 | 0,58334 | -3,3 | (075) |
| 46 | 1 | 37,08 | 1,20117 | 0,62020 | -0,4 | (164) |
| 47 | 1 | 38,25 | 1,24510 | 0,64404 | 3,1 | (734) (603) |
| 48 | 1 | 39,35 | 1,21581 | 0,67735 | 7,0 | (670) |
| 49 | 1 | 41,81 | 1,15634 | 0,74785 | 7,6 | (092) |
| 50 | 1 | 43,68 | 1,11826 | 0,79060 | -2,2 | (771) |
| 51 | 1 | 46,72 | 1,05830 | 0,89183 | -8,8 | (717) |
| 52 | 1 | 54,32 | 0,94004 | -1,11020 | 0,0 | (703) |

ORIGINAL PAGE IS
 OF POOR QUALITY

TABLE 2. NOHS_2O INTERFERENCES:
STANDARD DEVIATION OF THE Q_0 -values: $5.73 \cdot 10^{-4}$

| Nr. | l_0 | θ_0 | r_0 | Q_0 | $Q_0 - Q_c$ $\cdot 10^4$ | (hkl) |
|-----|-------|------------|---------|---------|-----------------------------|-------------|
| 1 | | 6,95 | 6,871 | 0,02401 | 2,1 | (020) |
| 2 | | 7,56 | 6,8504 | 0,02913 | -2,8 | (200) |
| 3 | | 7,91 | 6,8807 | 0,03211 | 3,0 | (120) |
| 4 | | 8,16 | 6,8312 | 0,03300 | 8,0 | (021) |
| 5 | | 8,23 | 6,8854 | 0,03448 | 0,1 | (002) |
| 6 | | 8,44 | 6,8522 | 0,03625 | 7,5 | (210) |
| 7 | | 10,17 | 4,9659 | 0,05246 | -13,4 | (220) |
| 8 | | 10,43 | 4,2583 | 0,05515 | 2,6 | (030) |
| 9 | | 11,04 | 4,0257 | 0,06170 | -5,3 | (130) |
| 10 | | 11,25 | 3,9515 | 0,06401 | 1,7 | (202) |
| 11 | | 11,43 | 3,8960 | 0,06608 | -0,8 | (300) (122) |
| 12 | | 11,85 | 3,7540 | 0,07096 | 1,1 | (131) |
| 13 | | 12,84 | 3,4769 | 0,08272 | -0,3 | (013) |
| 14 | | 13,30 | 3,4436 | 0,08915 | 1,0 | (002) |
| 15 | | 13,59 | 3,2898 | 0,09200 | 0,0 | (231) |
| 16 | | 13,84 | 3,2220 | 0,09629 | -4,1 | (132) |
| 17 | | 13,97 | 3,1932 | 0,09807 | 5,0 | (040) |
| 18 | | 14,15 | 3,1534 | 0,10050 | -0,7 | (302) |
| 19 | | 14,48 | 3,0810 | 0,10520 | 2,8 | (140) |
| 20 | | 14,70 | 3,0194 | 0,10905 | 3,6 | (320) |
| 21 | | 14,80 | 3,0059 | 0,11007 | -23,8 | (213) |
| 22 | | 15,07 | 2,9009 | 0,11375 | 2,1 | (141) |
| 23 | | 15,33 | 2,8150 | 0,11761 | 0,0 | (400) |
| 24 | | 15,30 | 2,8048 | 0,11851 | -2,4 | (232) |
| 25 | | 15,75 | 2,8469 | 0,12398 | 2,6 | (410) |
| 26 | | 16,52 | 2,7111 | 0,13605 | 4,6 | (241) |
| 27 | | 16,63 | 2,6936 | 0,13782 | -0,4 | (004) |
| 28 | | 16,70 | 2,6827 | 0,13805 | -4,4 | (142) |
| 29 | | 17,02 | 2,6317 | 0,14417 | 2,1 | (014) |
| 30 | | 17,09 | 2,6292 | 0,14592 | 1,1 | (104) |
| 31 | | 18,36 | 2,4474 | 0,16005 | -3,2 | (204) |
| 32 | | 18,68 | 2,4009 | 0,17201 | 1,1 | (400) (341) |
| 33 | | 19,10 | 2,3453 | 0,18181 | -0,5 | (250) |
| 34 | | 19,87 | 2,2681 | 0,19499 | 1,2 | (152) |
| 35 | | 20,50 | 2,2012 | 0,20637 | -5,9 | (432) |
| 36 | | 20,98 | 2,1550 | 0,21532 | -0,0 | (005) |
| 37 | | 21,37 | 2,1156 | 0,22343 | -3,8 | (441) |
| 38 | | 21,70 | 2,0849 | 0,23004 | 0,5 | (053) |
| 39 | | 22,11 | 2,04811 | 0,23838 | -2,8 | (530) |
| 40 | | 22,18 | 2,04200 | 0,23982 | 0,1 | (025) |
| 41 | | 22,42 | 2,02125 | 0,24477 | -0,5 | (205) |
| 42 | | 23,18 | 1,95816 | 0,25671 | -6,3 | (162) |
| 43 | | 23,46 | 1,93638 | 0,26069 | -7,4 | (513) |
| 44 | | 23,75 | 1,91408 | 0,27204 | -1,8 | (532) (001) |
| 45 | | 24,29 | 1,87838 | 0,28311 | 0,1 | (262) |
| 46 | | 25,12 | 1,81509 | 0,30324 | -11,0 | (163) |
| 47 | | 25,35 | 1,80053 | 0,30815 | 10,3 | (071) |
| 48 | | 25,61 | 1,78416 | 0,31438 | -3,0 | (171) |
| 49 | | 26,13 | 1,75039 | 0,32638 | -1,1 | (263) |
| 50 | | 26,23 | 1,74419 | 0,32870 | 5,0 | (601) (270) |
| 51 | | 26,79 | 1,71035 | 0,34184 | -0,9 | (126) |
| 52 | | 26,80 | 1,70822 | 0,34310 | 11,1 | (245) (003) |
| 53 | | 27,24 | 1,68420 | 0,35253 | -5,1 | (414) |
| 54 | | 27,04 | 1,64528 | 0,36041 | 5,0 | (701) |
| 55 | | 28,02 | 1,61096 | 0,37130 | -2,6 | (462) |
| 56 | | 28,31 | 1,57474 | 0,40325 | -0,6 | (560) |
| 57 | | 30,56 | 1,51619 | 0,43499 | 0,5 | (065) |
| 58 | | 32,41 | 1,43830 | 0,48398 | 0,9 | (436) (060) |
| 59 | | 32,74 | 1,42539 | 0,492 | 1,3 | (256) (742) |
| 60 | | 33,02 | 1,41465 | 0,49968 | -3,9 | (510) |
| 61 | | 35,40 | 1,33077 | 0,56405 | 4,4 | (118) |
| 62 | | 35,75 | 1,31045 | 0,57436 | 3,2 | (580) (057) |

ORIGINAL PAGE IS
OF POOR QUALITY

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 | 1 NOHSO_4 | NOHS_2C_7 |
|-------------------------|---------------------------|---|
| Optical axis angle $2v$ | $\approx 65^\circ, r < v$ | $\approx 30^\circ, r < v$ (very strong) |
| Optical characteristic | + | + |
| Color | colorless, transparent | color, transparent |

We wish to thank G. Malyska (Dipl. Chem.), Dept. of Chemistry, for providing the substances, Dr. H. H. Seyfarth, Chemical Engineering, for the crystal-optical investigations and the colleagues of the Computer Center of the VEB Leuna-Werke "Walter Ulbricht" for performing the calculations.

RE NCES

1. Stopperka, K., and Kilz, F., Zeitschrift für anorganische allgemeine Chemie, 348, 1, 1966.
2. Linström, C. F., and Malyska, G., Zeitschrift für Chemie, 8, 345, 1968.
3. Stopperka, K., and Kilz F., Zeitschrift für Chemie, 8, 437, 1968.
4. Gattow, G., and Plotter, H., Zeitschrift für anorganische allgemeine Chemie, 336, 1, 1965.