syringe. The Nessler results after 8 h hydrolyses were the same as the 20 h micro-Kieldahl.

As Kendrew has mentioned in Structure and function in myoglobins and other proteins, "myoglobins from different species have amino acid compositions which are broadly similar, but differ in detail". We may only confirm his statement by comparing the compositions of the purified myoglobins which are presently available, namely sperm whale had and horse myoglobin. The results show that these myoglobins differ only in details.

The amino acid analysis of Mb II, Mb III, Mb IV and Mb V are in progress using the procedure of Moore and Stein.

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- Rumen, N. M. Acta Chem. Scand. 13 (1959) 1542.
- Moore, S., Spackman, D. H. and Stein, W. H. Anal. Chem. 30 (1958) 1185.
- Moore, S. and Stein, W. H. J. Biol. Chem. 211 (1954) 907.
- Laki, K., Kominz, D. R., Symonds, P., Lorand, L. and Seegers, W. H. Arch. Biochem. Biophys. 49 (1954) 276.
- Kendrew, J. C. Federation Proc. 18 (1959) 740.
- Edmundson, A. B. Personal communication to Benson, E. E. and Linderstrøm-Lang, K. Biochim. et Biophys. Acta 32 (1959) 579.
- 7. Theorell, H. and Åkeson, A. In press.

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Structure of Rhodan Hydrate

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So far X-ray structure determinations of two unsaturated five-membered cyclic disulphides have been reported 1,2. Observed bond lengths in the thiuret ion 1 and in 4 - methyl - 1,2 - dithia - 4 - cyclopentene -3 - thione 2 indicate that the five-membered ring has some aromatic character. This seems to explain the relatively high stability of unsaturated five-membered cyclic

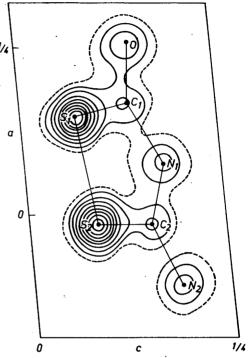


Fig. 1. Electron density projection of rhodan hydrate along the b-axis showing one asymmetric unit. Plane group p2 and origin in center of symmetry in the projection. Contours at arbitrary but equal intervals.

disulphides as contrasted with saturated ones. It is hoped that a determination of the molecular structure of rhodan hydrate will give further information that can be used to test this idea. The rhodan hydrate molecule has, according to Söderbäck³, the following structure:

The preparation of rhodan hydrate has been described by Söderbäck 3,4 , and the unit cell and space group have been reported by Foss 5 . The crystals are monoclinic, a=12.50 Å, b=5.24 Å, c=14.67 Å,

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Table 1. Atomic coordinates, in fractions of corresponding cell edges.

	$oldsymbol{x}$	z
S_1	0.1470	0.0695
$S_1 \\ S_2$	-0.0150	0.0865
C_1	0.1635	0.1365
C_2	-0.0135	0.1550
N,	0.0760	0.1750
N,	-0.1060	0.1885
oʻ	0.2585	0.1450

 $\beta = 95 \text{ 1/2}^{\circ}$. Preliminary results of a complete crystal structure determination of rhodan hydrate are given here.

rhodan hydrate are given here.

The space group of rhodan hydrate was found to be either $C2/\rho$ or C/c. The morphology of the crystals indicates ⁵ the presence of a twofold axis and thus the correctness of the centrosymmetric space group. The "average test" and "zero moment test" ⁶ also indicated centrosymmetry.

Attempts to solve the structure from Patterson projections did not succeed, and the solution was then sought by means of Harker Kasper inequalities and the "multiplication rule". This led to three possible sets of signs for the 35 strongest reflections in the b-axis projection. The molecule was recognised in one of the corresponding Fourier maps, and after three Fourier-refinements the reliability factor R was 0.115. The electron density map is reproduced in Fig. 1. The map shows that the cyclic form of rhodan hydrate, anticipated by Söderbäck 3, is correct. Further refinement will be carried out by means of $(F_0 - F_c)$ -technique.

- Foss, O. and Tjomsland, O. Acta Chem. Scand. 12 (1958) 1799.
- Kehl, W. L. and Jeffrey, G. A. Acta Cryst. 11 (1958) 813.
- 3. Söderbäck, E. Ann. 419 (1919) 217.
- 4. Söderbäck, E. Ann. 465 (1928) 184.
- Foss, O. Acta Chem. Scand. 10 (1956) 868.
 International Tables for X-Ray Crystallography. The Kynoch Press, Birmingham,
- England, 1959, Vol. II, p. 356. 7. Zachariasen, W. H. Acta Cryst. 5 (1952) 68.

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The σ-Phase Ta₂Al

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In the course of a study of the tantalumaluminium system recently started at this Institute, the existens of a σ -type phase has been observed in samples of the approximate composition Ta₂Al prepared by arc-melting in an argon atmosphere.

The dimensions of the tetragonal unit cell obtained from a Guinier powder pat-

tern were found to be:

$$a = 9.828 \text{ Å}$$
 $c = 5.232 \text{ Å}$

The axial ratio c/a=0.532 is similar to that found for other σ -phases such as the one occurring in the nickel-vanadium system studied by Kasper and Waterstrat using neutron diffraction techniques. Since the ratios of the atomic radii $r_{\rm Ta}/r_{\rm Al}$ and $r_{\rm V}/r_{\rm Nl}$ are comparable, the atomic distribution reported for the nickel-vanadinium phase was tentatively adopted for Ta₂Al:

Space-group: $D_{4h}^{14} - P4/mnm$. Unit cell content: 10 Ta₂Al.

Table 1. The Guinier powder pattern of Ta_2Al (Cu Ka_1 radiation).

hkl	$\sin^2\!\Theta_{ m obs}$	$\sin^2\!\Theta_{ m calc}$	$I_{ m obs}$	$I_{ m calc}$
110	0.01228	0.01228	vw	0.5
200	_	0.02457		0.0
101	0.02782	0.02781	\mathbf{st}	5.5
210	0.03068	0.03071	st *	2.5
111	0.03396	0.03396	w	2.0
220	0.04911	0.04914	vw	0.8
211	0.05238	0.05238	vw	0.8
310	0.06142	0.06142	$\mathbf{v}\mathbf{w}$	1.0
221		0.07081		0.0
301	0.07696	0.07695	W	2.2
320	0.07982	0.07985	$\mathbf{v}\mathbf{w}$	1.1
311	0.08311	0.08310	\mathbf{m}	4.5
002	0.08670	0.08668	vw	0.7
400	0.09831	0.09828	$\mathbf{v}\mathbf{w}$	1.5
112	0.09898	0.09897	$\mathbf{v}\mathbf{w}$	1.3
321	0.10153	0.10152	vvw	0.6
410	0.10443	0.10442	\mathbf{vst}	10.7
330	0.11059	0.11057	\mathbf{st}	5.8
202	0.11130	0.11125	\mathbf{st}	6.8
212	0.11739	0.11739	\mathbf{vst}	10.0
420	0.12285	0.12285	vvw	0.5
411	0.12603	0.12609	\mathbf{vst}	9.5
331	0.13224	0.13224	\mathbf{m}	4.0
				_

^{*} Line overlaps line of neighbouring phase.