

Table 3. Magnetic data for some rare earth oxide carbonates.

Compound	$\theta_{P(K)}$	Molar Curie constant C_M		Magnetic moments (in μ_B)	
		Exptl.	Calc.	Exptl.	Calc.
Dy ₂ O ₂ CO ₃	- 3	10.74	14.17	9.3	10.6
Ho ₂ O ₂ CO ₃	0	14.28	14.08	10.7	10.6
Er ₂ O ₂ CO ₃	- 6	9.08	11.50	8.5	9.6
Yb ₂ O ₂ CO ₃	- 47	2.36	2.58	4.3	4.5

mixtures of solid carbon dioxide and methyl alcohol. The magnetic parameters obtained from the measurements on the four components are listed in Table 3. The inverse molar susceptibilities of Dy₂O₂CO₃, Ho₂O₂CO₃, and Er₂O₂CO₃ are shown in Fig. 1, and that of Yb₂O₂CO₃ in Fig. 2. The compounds have no magnetically ordered state at 77 K and $1/\chi_{mol}$ vs. temperature follows the Curie-Weiss law from 77 K to room temperature. In this paramagnetic temperature range all four oxide carbonates have molar Curie constants close to the values expected for the free ions. Further investigation of the magnetic properties of the compounds over the temperature range 4.2 K to 77 K is planned.

Acknowledgement. I am indebted to Dr. S. J. Jensen, Department of Technology, the Royal Dental College, Aarhus, C, for use of the recording microdensitometer.

1. Christensen, A. N. *Acta Chem. Scand.* **20** (1966) 896.
2. Christensen, A. N. *Les Éléments des Terres Rares*, Colloques Internationaux du Centre National de la Recherche Scientifique No. 180. Edited by: Centre National de la Recherche Scientifique, Paris 1970, Vol. I, p. 279.
3. Christensen, A. N. *J. Solid State Chem.* **4** (1972) 46.

Received June 13, 1973.

Crystallographic Computer Programs for CYBER-74

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The series of crystallographic CDC-3300 programs at the University of Oslo¹ has been modified for CYBER-74.

Among the few changes made in the file structures may be mentioned the addition of the raw intensity of each reflection, and an extra record containing estimated standard deviations of atomic parameters.

The file concept of the 6000-computers is somewhat different from that of the 3000-series, and a number of file handling routines have been added to the program system.

Data reduction programs were not adapted to the CYBER-computer since these calculations more conveniently are carried out at CDC-3300.

A new feature in the structure determination programs based upon direct methods is the possibility of changing sign or phase for all reflections of one specified parity group. Peaks from scanned Fourier synthesis may be plotted on line printer.

The program for translation of all (or a part of) the atoms through desired areas of the cell, calculating the R -value for each step, has been rewritten. In the new version, which is more than 10 times faster than the old one, trigonometric calculations are carried out only for the first step.

The maximum number of parameters that can be refined simultaneously by the modified full-matrix least squares refinement program is 300.

The system contains some new routines preparing tables suitable for publication of atomic parameters, observed and calculated structure factors, bond distances and angles *etc.*

1. Dahl, T., Gram, F., Groth, P., Klewe, B. and Rømming, Chr. *Acta Chem. Scand.* **24** (1970) 2232.

Received June 27, 1973.