

ured with a Joyce-Loebl microdensitometer. The results are listed in Table 1.

Comparison with other results

In comparison with the ionic conductor $N(CH_3)_4GeCl_3$ (Möller & Felsche, 1979), in $NH(CH_3)_3GeCl_3$ the deviations from an ideal cubic perovskite-like structure are more obvious. There is a larger difference between the short axes a and b [1.302 \AA for $NH(CH_3)_3GeCl_3$; 0.217 \AA for $N(CH_3)_4GeCl_3$], indicating a stronger distortion along

$[110]_{\text{cubic}}$. Furthermore, in $NH(CH_3)_3GeCl_3$ a transition to a cubic high-temperature form has not been observed. The compound decomposes above 393 K.

References

- MÖLLER, A. & FELSCHE, J. (1979). *J. Appl. Cryst.* **12**, 617-618.
 MÖLLER, A., HUTTNER, G. & FELSCHE, J. (1982). In preparation.
 POSKOZIM, P. S. & STONE, A. L. (1970). *J. Inorg. Nucl. Chem.* **32**, 1391-1393.

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Crystal powder data of $MoGa_5(CuS_2)_{0.0556}$. By R. HORYŃ and R. ANDRUSZKIEWICZ, *Institute for Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland*

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Abstract

The X-ray powder data have been obtained for a new phase $MoGa_5(CuS_2)_{0.0556}$. The powder patterns were indexed on the basis of a tetragonal body-centred unit cell with the lattice constants $a = 12.872$, $c = 5.284 \text{ \AA}$, $c/a = 0.410$, $d_m = 6.825(8)$, $d_x = 6.869 \text{ Mg m}^{-3}$, $Z = 8$.

The new phase was obtained in the shape of single crystals as a result of a reaction of the Chevrel-type phase $Cu_{1.2}Mo_6S_8$ with metallic gallium. The reaction was performed at 1073 K both under vacuum and in an argon atmosphere.

The X-ray microprobe analysis has revealed the chemical composition of the phase corresponding to $MoGa_5(CuS_2)_{0.0556}$.

The powder diffraction data of the phase were obtained with a Guinier-type camera with Cu $K\alpha$ radiation. The single crystal and X-ray powder diffraction patterns show tetragonal symmetry and the lattice constants $a = 12.872$, $c = 5.284 \text{ \AA}$, $c/a = 0.410$. The first 14 lines are listed in Table 1. The standard deviation for 2θ is 0.019.

The density of the phase $MoGa_5(CuS_2)_{0.0556}$, $d_m = 6.825(8) \text{ Mg m}^{-3}$, was measured pycnometrically in CCl_4 ; $Z = 8$. The calculated density corresponds to $d_x = 6.869 \text{ Mg m}^{-3}$.

Table 1. Powder diffraction data of $MoGa_5(CuS_2)_{0.0556}$

<i>hkl</i>	d_{exp}	d_{calc}	<i>I</i>
110	9.092	9.094	rw
200	6.421	6.431	rw
101	4.879	4.884	m
220	4.542	4.547	rw
310	4.063	4.067	m
211	3.886	3.889	m
321	2.955	2.956	rw
420	2.875	2.876	m
411	2.686	2.686	w
002	2.640	2.640	rrw
112	2.535	2.535	m
510	2.524	2.522	w
202	2.443	2.442	rrw
431	2.312	2.312	s

The compounds $MoGa_5S_{0.1667}$, $MoGa_5Se_{0.1667}$ and $MoGa_5Te_{0.1667}$, synthesized at 973 K, are isostructural with the $MoGa_5(CuS_2)_{0.0556}$ phase. Their unit-cell constants are $a = 12.874$, $c = 5.286 \text{ \AA}$, $a = 12.904$, $c = 5.286 \text{ \AA}$ and $a = 12.938$, $c = 5.309 \text{ \AA}$, respectively.

The new phases show superconducting properties.

Crystallographers

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This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England).

John Walter Gruner died in 1981, at the age of 91. Immigrating from his native Silesia (now Poland) to America in 1912, John Gruner received his BA degree from the University of New Mexico

(1917), and MS (1919) and PhD (1922) degrees from the University of Minnesota. He became a member of the geology faculty at Minnesota in 1920 and held that position until retiring in 1959. He was an exceptionally successful teacher at both undergraduate and graduate levels. He was among the first in an American geology department to introduce X-ray diffraction (1927). He served as an advisor to 12 MS and 28 PhD students. He discovered several new minerals, pioneered in mineral synthesis, and solved the crystal structures of some difficult clay minerals. He published

nearly 100 papers. He was the second President (1947) of the Crystallographic Society of America, the predecessor of the American Crystallographic Association. He served as President of the Mineralogical Society of America (1948) and as Vice-President of the Geological Society of America (1949). His contributions to the advancement of science were recognized by such honors as the Distinguished Service Award of Sigma Xi (1960), the Roebling Medal of MSA (1962), and the honorary degree of Doctor of Science from the University of New Mexico (1963).

In February 1982 Professor **E. F. Bertaut** retired as Director of the Laboratoire de Cristallographie, CNRS, Grenoble. Professor Bertaut was a member of the IUCr Executive Committee between 1975 and 1981. He was also involved in the establishment of the Commission on Charge, Spin and Momentum Densities, being its first Chairman between 1975 and 1978, and has worked for many years with other members of the Commission on *International Tables* in the preparation of a new volume of this publication on direct space.

Sir **Charles Frank**, formerly Henry Overton Wills Professor of Physics at the University of Bristol, has been awarded the Guthrie Medal and Prize of the British Institute of Physics for his extensive contributions to the physics of solids.

The Charles Vernon Boys Prize of the British Institute of Physics for 1982 has been awarded to Dr **B. J. Isherwood** of GEC's Hirst Research Centre for his development and use of X-ray topography and multiple diffraction in the diagnosis of surface behaviour and crystalline quality.

International Union of Crystallography

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Commission on Journals Chemical Formulae and Nomenclature

Authors are reminded that chemical formulae and nomenclature in papers submitted to *Acta Crystallographica* and *Journal of Applied Crystallography* should conform to the rules of nomenclature established by the International Union of Pure and Applied Chemistry (IUPAC), the International Union of Biochemistry (IUB) and other appropriate bodies. As far as possible the crystallographic nomenclature should correspond to the systematic name. A structural formula should generally be given for all organic and organometallic compounds.

All papers in *Acta Crystallographica*, Section B, reporting crystal structure determinations and all Crystal Data in *Journal of Applied Crystallography* should include the approved name(s) of the compound(s) in the title of the paper or in a footnote to the title. Any paper in *Acta Crystallographica*, Section A, or in *Journal of Applied Crystallography* dealing with the crystal physics or the properties of a particular material should also include the approved name of the compound concerned. It is desirable that any accepted trivial name, trade mark,

recommended International Non-proprietary Name (INN), United States Adopted Name (USAN) or British Pharmacopoeia Approved Name be retained, but the corresponding systematic (IUPAC) name should be provided. For a list of available nomenclature sources see *J. Appl. Cryst.* (1979). **12**, 640. [Approved Names 1977 – a list of approved names for pharmaceutical compounds with their corresponding systematic (IUPAC) names, published for the British Pharmacopoeia Commission – is available from Her Majesty's Stationery Office.]

Assistance in the naming of compounds in accordance with IUPAC and IUPAC-IUB rules may be obtained from Dr K. L. Loening, Director of Nomenclature, Chemical Abstracts Service, PO Box 3012, Columbus, Ohio 43210, USA; from Mr E. W. Godly, Chemical Nomenclature Advisory Service (CNAS), Laboratory of the Government Chemist, Department of Industry, Room A-510, Cornwall House, Stamford Street, London SE1 9NQ, England; and in the particular naming of inorganic compounds from Professor Y. Jeannin, Laboratoire de Chimie des Métaux de Transition, Université Pierre et Marie Curie, 4 place Jussieu, 75230 Paris CEDEX 05, France. Enquiries may also be addressed to Dr J. E. Derry, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. If advice on chemical nomenclature is sought from any of the above advisory sources authors are requested, when submitting a manuscript to the Union's journals, to indicate the source consulted.

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Commission on Journals Decisions taken at meeting in Ottawa, August 1981

The attention of authors planning to submit papers to *Acta Crystallographica* or *Journal of Applied Crystallography* is drawn to the following decisions taken by the Commission on Journals at meetings held in Warsaw, 14–16 August 1981. These and other revisions in editorial policy since 1978 will be published in a new version of *Notes for Authors*, which is presently in preparation.

International Symbols for Units

The Commission has recognized that, although multiples of 10^3 are the preferred prefixes in the SI System of Units, the centimetre is not prohibited by the SI system and therefore density and absorption coefficients may be given in units of g cm^{-3} and cm^{-1} respectively, if authors so wish. In all other cases, however,

authors are asked to use the recommended prefixes of decimal multiples and submultiples of the SI units rather than using " $\times 10^n$ ".

Structural papers

Estimated standard deviations for B_{eq} : The requirement of estimated standard deviations on equivalent values of the Debye-Waller factor was reviewed. The Commission agreed that the significance of such estimated standard deviations is ambiguous. In the case of high anisotropy, the estimated standard deviation is necessarily large although the individual anisotropic parameters may be well determined. In future, the presence of unusual anisotropy should be referred to in the text (including the maximum and minimum amplitudes and any nonpositive-definite coefficients found), or in the table of B_{eq} (by use of an asterisk), or illustrated by a plot of the atomic vibrational ellipsoids.

Calculated hydrogen-atom coordinates: Calculated hydrogen-atom coordinates will be published in future only at the Co-editor's discretion and if they are necessary to the understanding of the paper. They will otherwise be deposited.

Graphical chemical formulae: A graphical structural formula should always be given in the report of a structure determination of an organic or organometallic compound. The figure showing the atomic positions is not adequate for this purpose. However, a plot of the atomic vibrational ellipsoids can be used to illustrate atomic positions. Authors should ensure that such plots are of good contrast and quality. The numbering of atoms should be consistent throughout a paper and, as far as possible, correspond to the systematic name [*J. Appl. Cryst.* (1982). **15**, 250].

Least-squares planes: Least-squares planes and the deviations from them will only be published if they are referred to in the text of the paper and are significant in the consideration of the structure. They will otherwise be deposited.

Absorption correction: In a structural paper the absorption correction, if any, should always be described and the maximum and minimum corrections stated.

Melting point: In a structural paper the melting point of a compound should always be given if it is known.

Stereofigures: The requirement on stereofigures is one per structure unless the Co-editor and referees feel that more are necessary for the understanding of the structure described in the paper. These stereoviews must fit into a single