

Experimental) and the fact that repeated susceptibility measurements have always given the same result (Oostra, 1984) make it reasonable to assume that the measured $\chi(T)$ curve belongs to the most accessible modification ($I\alpha$).

It is noteworthy that the phase transition of (I) to ($I\alpha$) leads to octameric rather than to tetrameric stacks, as is expected for isolated stacks in which the exchange interaction between the conduction electrons is modified (Huizinga, Kommandeur, Jonkman & Haas, 1982). In the above discussion of the ($I\alpha$) structure the changes in the stack have been attributed to the ordering of the DMM groups, indicating that the phase transition is most probably driven by this ordering. However, it is not clear to what extent the modification of the exchange interactions at T_c also contributes to the stability of the low-temperature structure.

The current interest and many helpful suggestions of Professor Dr A. Vos are gratefully acknowledged. Part of this work was supported by the Netherlands Foundation for Chemical Research (SON) with financial aid from the Netherlands Organization for the Advancement of Pure Research (ZWO). The computations were carried out at the Computing Centre of the University of Groningen.

References

- BODEGOM, L. VAN (1979). PhD thesis, Groningen.
 BODEGOM, L. VAN (1981). *Acta Cryst.* B37, 857-863.
 BODEGOM, L. VAN & DE BOER, J. L. (1981). *Acta Cryst.* B37, 119-125.
 BOER, J. L. DE (1970) PhD thesis, Groningen.

- BOLHUIS, F. VAN (1971). *J. Appl. Cryst.* 4, 263-264.
 BOSCH, A. & VAN BODEGOM, L. (1977). *Acta Cryst.* B33, 3013-3021.
 BRUCE, M. R. & MURPHY, L. C. (1984). *Nature (London)*, 309, 119-126.
 CROMER, D. T. & MANN, J. B. (1968). *Acta Cryst.* A24, 321-324.
 CRUICKSHANK, D. W. J. (1949). *Acta Cryst.* 2, 65-82.
 FLANDROIS, S. & CHASSEAU, D. (1977). *Acta Cryst.* B33, 2744-2750.
 HAMILTON, W. C., ROLLETT, J. S. & SPARKS, C. A. (1965). *Acta Cryst.* 18, 129-130.
 HELMHOLDT, R. B. & VOS, A. (1977). *Acta Cryst.* A 33, 456-465.
 HUIZINGA, S. (1980). PhD thesis, Groningen.
 HUIZINGA, S., KOMMANDEUR, J., JONKMAN, H. T. & HAAS, C. (1982). *Phys. Rev. B*, 25, 1717-1725.
 HUIZINGA, S., KOMMANDEUR, J., SAWATZKY, G. A., THOLE, B. T., KOPINGA, K., DE JONGE, W. J. M. & ROOS, J. (1979). *Phys. Rev. B*, 19, 4723-4732.
 KAMMINGA, P. & VAN BODEGOM, L. (1981). *Acta Cryst.* B37, 114-119.
 KORVING, W. H., HYMAN, T. W., BROM, H. B., OOSTRA, S., SAWATZKY, G. A. & KOMMANDEUR, J. (1983). *J. Phys. (France), Colloq.* C3, 1425-1428.
 MORSINK, H. J. & VAN BODEGOM, L. (1981). *Acta Cryst.* B37, 107-114.
 OOSTRA, S. (1984). Private communication.
 OOSTRA, S. & VISSER, R. J. J. (1985). In preparation.
 SCHWERDTFEGER, C. F., OOSTRA, S., VISSER, R. J. J. & SAWATZKY, G. A. (1981). *Solid State Commun.* 39, 1133-1135.
 SMAALEN, S. VAN, DE BOER, J. L., HAAS, C. & KOMMANDEUR, J. (1985). *Phys. Rev. B*, 31, 3496-3503.
 SMAALEN, S. VAN & KOMMANDEUR, J. (1985). Accepted by *Phys. Rev. B*.
 STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* 42, 3175-3187.
 VISSER, R. J. J. & DE BOER, J. L. (1985). In preparation.
 VISSER, R. J. J., OOSTRA, S., VETTIER, C. & VOIRON, J. (1983). *Phys. Rev. B*, 28, 2074-2077.
 XRAY system (1976). Dutch version of the XRAY system. Tech. Rep. TR-192. Computer Science Centre, Univ. of Maryland, College Park, Maryland.

International Union of Crystallography

Acta Cryst. (1985). B41, 374

Compilation of Temperature Factors for Elements and Binary Compounds

The Commission on Neutron Diffraction has initiated a new project for compiling *accurate* temperature factors. The compilation will be restricted to elements and binary compounds. Later, it may be extended to other compounds, replacing the compilation published in Volume III of *International Tables for X-ray Crystallography*.

Interested crystallographers are requested to contact any one of the following:

Dr N. M. Butt, Nuclear Physics Division, PINSTECH, Post Office Nilore, Rawalpindi, Pakistan.

Dr G. Heger, Kernforschungszentrum, Karlsruhe IAK 1, Postfach 3640, D-7500 Karlsruhe, West Germany.

Dr B. T. M. Willis, Chemical Crystallography Laboratory, 9 Parks Road, Oxford, England.

A copy of a preliminary compilation can be obtained from Dr N. M. Butt.

Acta Cryst. (1985). B41, 374

Commission on Journals Reporting an Absolute-Configuration Determination

A structural paper reporting an absolute-configuration determination should, if practicable, also report a chiral property of the source material which can be linked uniquely to the structural handedness. If such a linkage is not made, the result should be reported only as a determination of structural handedness or chirality. Should the source material be a product of reactions with condition-dependent stereospecificity, the experimental conditions of the preparation should be given or referenced and a linkage made between the claimed stereospecificity and the structure. In the event that a linkage cannot be made, a disclaimer is necessary stating that the structural handedness may not be representative of the bulk material.