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Hartree-Fock-Slater coherent scattering factors for ions*. By H. P. HANSON and R. F. POHLER, *Department of Physics, The University of Texas, Austin 12, Texas, U.S.A.*

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Coherent scattering factors for 70 different ionic configurations have been calculated from HFS wave functions. The compilation of these results represents an extension of the work reported previously by Hanson, Herman, Lea & Skillman (1964). Form factors have been calculated for the more common ionic configurations of elements in the first three rows of the periodic table, for the 3d transition elements, and for Ga³⁺, Ga⁺, Ge⁴⁺, Ge²⁺, Br⁻, Rb⁺, Mo⁺, Ag⁺, Au⁺, Hg⁺, Tl³⁺, Tl⁺, and U⁶⁺. The list of these configurations includes essentially all of those ions which are stable within the framework of the HFS model. Thus Cl⁻, O⁻, and S⁻ were calculable but not O²⁻ or S²⁻.

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However, in view of the recent publication of Dirac-Slater scattering factors for many of these same ions (Cromer & Waber, 1965), the use of journal space for detailed HFS results does not seem justified. Nevertheless, the HFS values have a certain merit and utility; in order that they be generally accessible, they have been placed on file with the American Documentation Institute. Moreover an abridged set of these results may be obtained by writing to the authors.

References

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The anti-Th₃P₄ structure type for rare earth germanides, antimonides and bismuthides. By D. HOHNKE and E. PARTHÉ, *School of Metallurgical Engineering and Laboratory for Research on the Structure of Matter, University of Pennsylvania, Philadelphia, Pennsylvania, U.S.A.*

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The Th₃P₄ structure type was first described by Meisel (1939) and has been found since for numerous lanthanide and actinide compounds. Kripyakevich (1963) has shown that the structure can be represented as an arrangement of polyhedra such as [ThP₈] or [PTh₆] where each Th atom is surrounded with 8 P atoms and, conversely, each P atom has 6 nearly octahedral Th neighbors. Most of the early known compounds with the Th₃P₄ structure are the homologues of Th and P. During the last few years, however, a number of isostructural rare earth sulfides, selenides and tellurides were reported (in certain cases with deviations from the ideal composition R₃X₄, where R denotes rare earth element and X the metalloid). (Flahaut, 1965; Holtzberg, Okaya & Stemple, 1965).

The fourteen new rare earth germanides, antimonides and bismuthides which are reported here have the composition R₄X₃ and crystallize with the anti-Th₃P₄ structure type. Here the rare earth elements occupy the centers of the distorted octahedra.

The rare earth elements with a stated purity of 99.9% were obtained from the Research Chemicals Division of Nuclear Corporation of America, Phoenix. All compounds were prepared by fusing the components in an arc melting furnace. Appropriate control of the operating conditions assured negligible weight losses. A homogenization annealing was performed on La₄Ge₃, but it was subsequently found that this procedure was unnecessary as the arc melted samples were already homogeneous and well crystallized.

All investigated germanides are stable in air, while the antimonides and bismuthides react with the moisture of

the air in varying degrees. To avoid decomposition during the diffraction experiments, those materials were enclosed in quartz capillaries filled with dried ligroin. The experiments were performed with Cu K α or Cr K α radiation.

La₄Ge₃ gave a cubic diffraction pattern with $a=9.3563 \pm 0.0004$ Å. The conditions for possible reflections were found to be $hkl: h+k+l=2n$ only and $hhl: 2h+l=4n$ only, which lead to the unique space group I43d (T_d^2). Only a limited number of equipoints are available in this space group, the lowest multiplicity being twelve. Assuming the smallest possible number of formula units per unit cell, $M=4$, a theoretical density of 6.17 g.cm⁻³ is obtained. The next higher number of formula units which can be accommodated in the space group, $M=12$, leads to an unreasonably high density of 18.8 g.cm⁻³. Thus only the 12-fold and one 16-fold equipoint position are available for the positioning of the atoms. A simple geometrical consideration showed that the only reasonable arrangement is:

16 La in 16 (c) with $x \sim \frac{1}{6}$

12 Ge in 12 (a)

Such an arrangement can be called the anti-Th₃P₄ structure type.

The line intensities of the La₄Ge₃ diffractometer pattern, obtained from a flat specimen, were measured with a planimeter. Owing to the many coincidences of the 44 measured diffraction lines only 30 could be used for a least-squares analysis of the adjustable parameter x of the La atoms in 16 (c). The least-squares refinement program of Gantzel, Sparks & Trueblood (1961) was used. $\sum w(F_o - |F_c|)^2$ was