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X-ray data correlation through common reflexions. By A. D. RAE, *Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England* and A. B. BLAKE, *Department of Chemistry, The University, Hull, England*

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It should be pointed out that there exists a more general solution of the equations generated in the method of data correlation described by Rae (1965).

The equations, $\sum_{j=1}^N a_{ij}l_j = b_i$, $i=1$ to N , generated by the least-squares minimization of $\sum_{\text{all pairs } h,i,j} w_{hij} \Delta_{hij}^2$, where w_{hij} is the weight of the residual $\Delta_{hij} = \log k_i F_{hi} - \log k_j F_{hj}$, have the property that $\sum_{j=1}^N a_{ij} = \sum_{j=1}^N a_{ji} = 0 = \sum_{j=1}^N b_i$. The equations are redundant but may be solved with the use of some extra condition upon the l_i . The condition used by Rae (1965), viz. $\sum_{i=1}^N a_{ii}l_i = 0$, is only one of many possible extra conditions.

The equations may be rewritten as $\sum_{j=1}^N a_{ij}(l_j - l_K) = b_i - l_K \sum_{j=1}^N a_{ij} = b_i$, since $\sum_{j=1}^N a_{ij} = 0$. This gives $N-1$ non-redundant equations in $N-1$ unknowns ($l_j - l_K$) which may be solved. The solutions, $l_i - l_K = \log(k_j/k_K)$ are the logarithms of the ratios of the scale constants, which may be put on an absolute scale by the use of an extra condition, the simplest being $l_K = 0$, i.e. $k_K = 1$.

References

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Variation of the Debye parameter B with temperature. By K. LONSDALE AND K. EL SAYED, *University College, London W.C. 1, England*

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In the first line of the caption to Fig. 1 in a recent Short Communication under the above title (Lonsdale & El Sayed, 1965) for *metals* read *crystals*.

Reference

LONSDALE, K. & EL SAYED, K. (1965). *Acta Cryst.* **19**, 487.

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The structure of the intermetallic compound Ce_3In . By M. DARIEL, *Nuclear Research Center, Negev, Israel*.

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The equilibrium diagram of the cerium-indium system was investigated by Vogel & Klose (1954). The experimental methods used were thermal-analysis, metallography and X-ray diffraction. Five intermetallic compounds were found in the system, namely: Ce_3In , Ce_2In , $CeIn$, Ce_2In_3 and $CeIn_3$. Only the structure of $CeIn_3$ was identified; it is of the $L1_2$ ($AuCu_3$) type with a lattice parameter of 4.689 ± 0.008 Å. It was not possible to identify the structures of the other compounds, as they decomposed and were oxidized at an extremely fast rate. For the present investigation a chain of dry boxes under inert atmosphere (Erez, 1965) was used in an attempt to identify the structures of the cerium-rich compounds of the cerium-indium system.

The cerium metal used in preparing the alloys was supplied by Johnson & Matthey; it is stated to contain 200 ppm of metallic impurities and 100 ppm of other rare earths. The indium was of 99.99% nominal purity. Weighed and cleaned lumps of the two metals were melted in an induction furnace, in degassed magnesia crucibles, under a purified argon atmosphere and were then bottom poured into split copper moulds. The alloys thus obtained were sealed in evacuated silica tubes and heat-treated for homogenization. After the heat treatment, they were introduced into the dry box chain. Filings taken from the alloys were

then passed through 200-mesh sieves, wrapped in tantalum foils and stress relieved in evacuated Pyrex tubes. Glass capillaries of 0.5 mm diameter were filled and sealed inside the dry box. The capillaries were taken out of the dry box chain, mounted on 11.9 mm Debye-Scherrer cameras and exposed to filtered copper radiation.

The structure of the alloys containing 25 at. % indium (that is, corresponding to the compound of formula Ce_3In) was found to be $L1_2$ ($AuCu_3$ type) with a lattice parameter (after extrapolation with the Nelson & Riley (1945) function) of 4.9610 ± 0.0005 Å.

It was found, upon examination of the diffraction patterns of alloys having a higher indium content (up to 70 at. % In), that the compounds decomposed rapidly even in an inert atmosphere, giving a diffraction pattern which contained all the diffraction lines of pure metallic indium, besides some additional faint lines which we were not able to index.

References

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