

LETTERS TO THE EDITOR

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THE USE OF ANOMALOUS SCATTERING WITHOUT PHASE CHANGE IN CRYSTAL STRUCTURE ANALYSIS

MANY novel methods have recently been suggested for the determination of the phases in non-centro-symmetric structures. These can in general be classified into two categories: (i) those in which isomorphous crystals are used, and (ii) those in which one set of atoms in the crystal scatters the incident radiation anomalously with a change of phase. By the use of two isomorphous crystals, the determination is ambiguous to the extent that two values can be assigned for the phase of each reflexion (Bijvoet¹). This ambiguity can however be resolved by the use of the double-isomorphous replacement method (Harker²). In method (ii) also (where the intensities of the hkl and $\bar{h}\bar{k}\bar{l}$ reflexions are used to determine the phases) a similar ambiguity exists. Here again it can be overcome by the use of two isomorphous crystals along with the anomalous scattering technique (Ramachandran and Raman³ and Okaya and Pepinsky⁴).

Recently, the present writers⁵ had occasion to solve a centro-symmetric structure ($KMnO_4$)

using two radiations, one on either side of the absorption edge of one of the atoms (Mn). From a knowledge of the differences in the scattering factors for the two wavelengths and the position of the anomalously scattering atom, it was possible to determine the signs of more than half the total number of reflexions. This method practically amounts to the isomorphous replacement technique. In this note the writers wish to draw attention to the fact that wherever one uses the isomorphous replacement method for the determination of non-centro-symmetric structures, one could substitute the method of anomalous scattering without change of phase.

Thus it should be possible to determine the phases in an acentric case by an analogue of Harker's method by using three radiations, two of which have wavelengths that are respectively scattered anomalously (without change of phase) by two kinds of atoms that occupy different sites in the structure. In practice only relatively simple structures with favourable scatterers in them will prove amenable to solution by this method.

If two incident wavelengths on each side of and close to the absorption edge of one of

the atoms be used, since for one of the wavelengths there is only an amplitude change, while for the other there exist changes both in phase and amplitude, the method suggested by Ramachandran and Raman for isomorphous crystals (*loc. cit.*) could be directly applied for the unequivocal determination of the phases of non-centro-symmetric crystals.

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Bangalore-3, September 24, 1957.

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AN INTERPRETATION OF THE VERTICAL MAGNETIC ANOMALIES OVER THE KODUR MANGANESE BELT

THE high magnetic character of the Indian manganese ores was first brought to light by Fermor,¹ who further indicated the possibility of finding new deposits by magnetic prospecting.

Very recently we have carried out extensive investigations with the vertical magnetometer over the Kodur manganese belt in the Srikulam District (Andhra State). These were followed by laboratory investigations of the magnetic properties of these manganese ores. The results of the susceptibility measurements showed that the manganese samples exhibited susceptibilities over a wide range. Further the variation of susceptibility with field strength in the region of 0-1,000 oersteds was different in most cases. Most of the ore samples exhibited strong ferromagnetic characteristics and all of them showed only one susceptibility maximum, which may indicate the presence of a single ferromagnetic mineral responsible for the magnetism of the ores. The high values of the remanence and coercivity of the ore samples indicated that the ores were susceptible to high remanent magnetism.

Chemical analysis of the ore samples showed that most of the samples collected contain moderate to high percentages of manganese and fair amounts of iron. The susceptibility values appeared to bear no relation with the individual amounts of iron or manganese. It was

generally observed from the susceptibility measurements that high susceptibilities were associated with samples containing mangan-magnetite and Vredenburgite, whereas samples rich in the hydrated oxides like psilomelane possessed low susceptibilities.

The normative values of mangan-magnetite and Vredenburgite were also calculated from the chemical analysis of the ore samples. The relation between the normative percentages of $(\text{MnFe})_3\text{O}_4$ and susceptibility was found to be almost linear. Extrapolation of the statistically best fitted line gave rise to a value of $150,000 \times 10^{-6}$ (C.G.S. units) for cent. per cent. normative $(\text{MnFe})_3\text{O}_4$, which was found to be in the range of susceptibilities quoted by Mason² for hausmannite, jacobsite series.

It was finally concluded, therefore, that the presence of minerals like mangan-magnetite and Vredenburgite (which are almost identical with one another) resulted in the high magnetic character of some ore samples. The variation in percentage of these metamorphosed minerals was the cause of the wide range of magnetic properties exhibited by these ores. This could hence explain the wide variation in the vertical magnetic anomalies over this area.

Further details of the above investigations will be published elsewhere.

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Waltair, September 9, 1957.

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USE OF COMMERCIAL ELECTRO- LYTIC COPPER ELECTRODES IN SPECTROGRAPHIC ANALYSIS

IMPORTED copper electrodes of spectrographic purity have been in use at this Institute, for the determination of boron and manganese in soils and plants, with bismuth as the internal standard. In view of recent import difficulties, the possibility of using commercial electrolytic copper known for its high purity was explored.

Spectrographic comparison of commercial electrolytic and pure copper rods made by means of a Hilger Large Quartz Spectrograph, using a direct current arc, showed absence of boron and