The Crystal Structure of Ethylzinc Iodide

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THE structure of ethylzinc iodide is of interest, not only on account of the antiquity[1] of the compound, but also in connection with the controversy[2] concerning the nature of the organometal halides of the Group II elements, other than those of mercury. Since then, convincing evidence for the existence of monomeric solvated alkylmagnesium halides has been obtained by molecular-weight[3] and crystallographic[4] studies. Though there is now evidence for the existence of solvated monomeric alkylzinc halides[5] also, and the tetrameric unsolvated ethylzinc chloride and bromide are believed[6] to have cubane-type structures similar to that of tetrameric methylzinc methoxide,[7] there have been hitherto no structural studies of any of the unsolvated Group II organometal halides, except those of mercury.

We now report that crystalline ethylzinc iodide is a co-ordination polymer, the iodine–zinc linkages giving rise to a layer structure, as shown in the Figure.

Crystals were prepared by the method of Jander, Fischer, and Winkler[8] from a solution in ethyl iodide. An *X*-ray examination has shown that ethylzinc iodide crystallises in an orthorhombic cell with $a = 21{\cdot}17$, $b = 4{\cdot}33$, $c = 5{\cdot}38$ Å, space group *Pnma*. The unit cell contains four units of C_2H_5ZnI which are situated on the mirror planes at $y = 0{\cdot}25$ and $0{\cdot}75$.

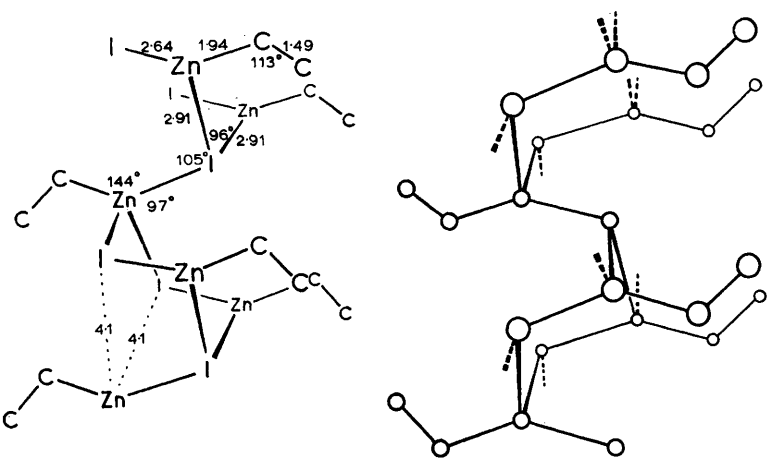

FIGURE. *Part of the ethylzinc iodide polymer.*

Each iodine atom is at a distance of 2·64 Å from a zinc atom lying on the same mirror plane, the I–Zn–C angle in the plane (143·9°) being considerably removed from 180°. In addition, each iodine is 2·91 Å from two other zinc atoms, which lie on adjacent mirror planes half a unit-cell length above and below it respectively. There are no other zinc atoms at a distance of less than 4 Å. Thus each iodine forms two long and one more normal bond to

zinc and has a nearly pyramidal environment, whereas the arrangement at zinc departs considerably from the tetrahedral. The structure can be compared with that of mercury(II) cyanide[9] where almost linear $Hg(CN)_2$ molecules are linked together by long Hg–N bonds.

The structure was solved by the heavy-atom method and is being refined by the method of least squares. At the present time, the reliability index, R, for the 335 independent reflections is 0·11.

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