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SHORT COMMUNICATIONS

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Crystal data for iodostrychninesulphonic acid.

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Crystal data for iodostrychninesulphonic acid ($IC_{21}H_{22}N_2O_2SO_3$) are: orthorhombic, $P2_12_12$, $Z=4$, $F(000)=1140$; $a=12{\cdot}53$ (2), $b=15{\cdot}67$ (1), $c=10{\cdot}81$ (1) Å, $D_m=1{\cdot}72$, $D_c=1{\cdot}69$ g cm^{-3}.

The structure of strychninesulphonic acid tetrahydrate has been solved by direct methods (Sake Gowda, Cartz & Natarajan, 1973). If this structure had not been solved by this method, an alternative approach was to have been by the use of a heavy-atom derivative of strychninesulphonic acid. For this purpose, iodostrychninesulphonic acid in powder form was kindly supplied by Professor John T. Edward, McGill University, Canada. Crystals were grown from a solution of dilute ammonium hydroxide and were very tiny, needle-like, and yellow-white in colour. The space group was determined on a single-crystal diffractometer with the crystal mounted about the needle axis (*c* axis) and Cu $K\alpha$ radiation. The extinction conditions were $h00$ ($h=2n$), $0k0$ ($k=2n$) with no other systematic absence, so that the space group is $P2_12_12$. The cell dimensions were determined from a least-squares analysis of 10 high-angle reflections. The crystal data are given in Table 1.

The density was measured by the flotation technique in bromobenzene and bromoform. The agreement between the measured and the calculated density indicates the absence of water of crystallization in iodostrychninesulphonic acid whereas four water molecules of crystallization were found to be present in crystals of strychninesulphonic acid. The molecular packing is likely to be different for the iodo derivative, because of the different crystal symmetry, with the sulphur oxygen atoms involved in the intermolecular bonding. The detailed crystal structure of the iodo derivative is not being determined.

Table 1. *Crystal data for iodostrychninesulphonic acid*

Chemical formula: $IC_{21}H_{22}N_2O_2SO_3$
Crystal system and space group: orthorhombic, $P2_12_12$
$Z=4$
$F(000)=1140$
$a=12{\cdot}53$ (2) Å
$b=15{\cdot}67$ (1)
$c=10{\cdot}81$ (1)
$D_m=1{\cdot}72$ g cm^{-3}
$D_c=1{\cdot}69$

Reference

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