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CRYSTAL AND MOLECULAR STRUCTURE OF 1-NITRO-9(3--DIMETHYLAMINOPROPYLAMINO)-ACRIDINE (C-283) MONOIODIDE

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From among several hundreds of 9-aminoacridine derivatives, compound C-283 exhibits the highest antitumour activity in vitro, in vivo and in the clinical tests [1–5]. In order to explain the high specific activity of this compound many physicochemical, biochemical, pharmacological and other studies have been done [5].

In the present communication the results of X-ray investigations on compound C-283 as monoiodide have been presented. This is the first nitroacridine derivative the whole structure of which has been solved by X-ray analysis.

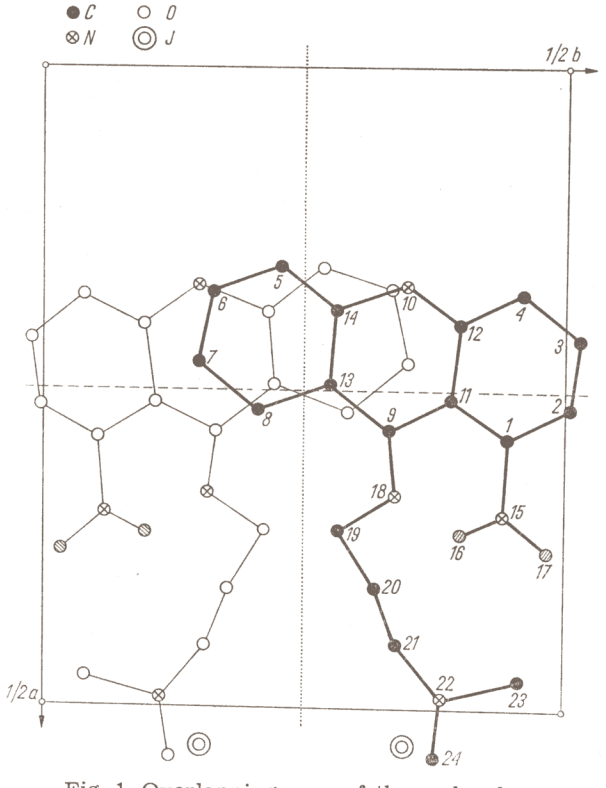

Fig. 1. Overlapping area of the molecules

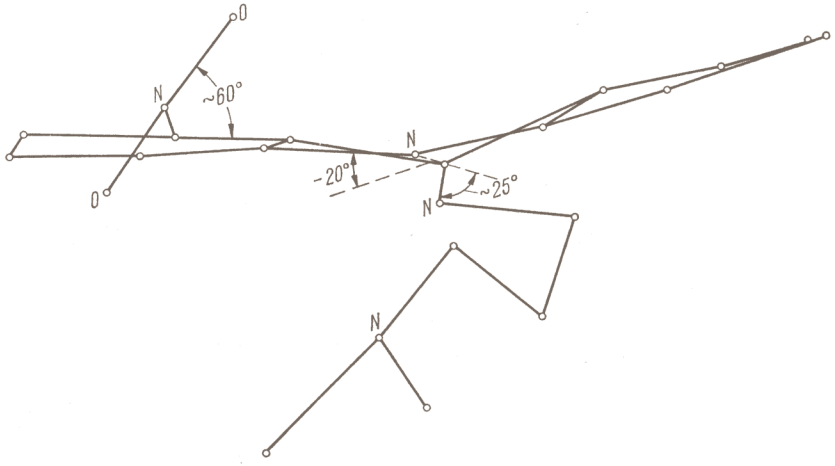

Fig. 2. The structure viewed along the *a* axis

Crystals of monoiodide C-283, $C_{18}H_{21}N_4O_2I$, have the space group *Pbca* with unit-cell dimensions: $a = 24.53$ Å, $b = 19.94$ Å, $c = 7.83$ Å and with eight molecules per unit-cell. $V = 3832$ Å^3, $D_{obs.} = 1.57$ g cm^{-3}, $D_x = 1.59$ g cm^{-3}. Intensity data were collected with an automated diffractometer using Cu K_α radiation. The structure was solved by the methods of Patterson and Fourier and refined by the method of least squares to $R = 0.06$ for the 1500 observed reflexions.

The acridine ring system is folded along C(9)—N(10) (Fig. 1) line by 20° (Fig. 2). The nitro group is distorted from plane of the benzene ring, dihedral angle along C(1)—N(15) is about 60° (Fig. 2). The bond C(9)—N(18) has a partially double character (1.312 Å). The distances between the ni-

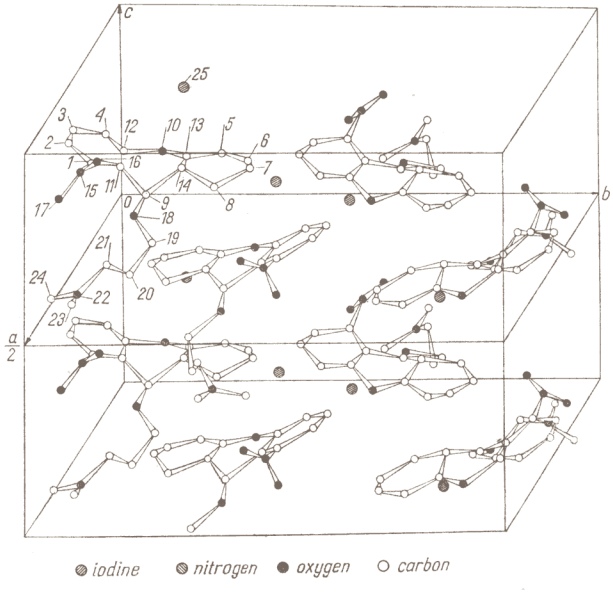

Fig. 3. Arrangement of the molecules in the unit cell

trogen atom N(18) of aliphatic side chain and two oxygen atoms of nitro group are the same and are of about 3 Å, due to the deviation from C(9)—N(10) line. It makes possible the bifurcated hydrogen bond to appear between atoms mentioned.

From the difference Fourier synthesis protonization of atom N(10) was stated.

The distances of iodine atom from nitrogen atoms N(10) and $N_{\omega}(22)$ are nearly 4 Å (Fig. 1).

The packing of the molecules in the crystal is illustrated in Fig. 3 and is atypical as compared with other acridine derivative structures[6–12]. In this structure "head to head" arrangement occurs with the distance between molecules of about 3.9 Å.

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STRESZCZENIE

Metodą rentgenograficznej analizy strukturalnej określono strukturę cząsteczkową i krystaliczną monojodowodorku 1-nitro-9(3-dwumetyloaminopropyloamino)-akrydyny, preparatu C-283, wykazującego wysoce specyficzne działanie przeciwnowotworowe. Jest to pierwsza pochodna nitroakrydyny, której budowę wyjaśniono metodą rentgenograficzną.

Przestrzenny model cząsteczki i sposób ułożenia cząsteczek w krysztale różnią się od wszystkich zbadanych dotychczas rentgenograficznie pochodnych akrydyny.

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