than + 7%) increase the microhardness by increasing the dislocation density due to lattice strains. Multivalent dopants creat ion vacancies which provide obstacles to the dislocation motion thereby raising the microhardness of the crystals.

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THE CRYSTAL STRUCTURE OF SULPHAMOXOLE

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SULPHAMOXOLE (2-*p*-aminobenzene sulphonamido-4,5-dimethyloxazole, $C_{11}H_{13}N_3O_3S$) is a well known antibacterial drug. The crystal structure of sulphamoxole is reported in this paper as part of our programme on the crystal and molecular structure studies of sulphonamides[1-3].

Large yellow coloured crystals of sulphamoxole were obtained by slow evaporation at room temperature from its solution in methanol. The crystals belong to monoclinic space group $P2_1/c$ with $a = 7.93(2)$, $b = 12.88(1)$, $c = 13.38(3)$ A, $\beta = 106.1°(5)$, $d_m = 1.378(5)$, $d_c = 1.373\,g\,cm^{-3}$ with $Z = 4$.

Three-dimensional x-ray intensity data were recorded on multiple films by Weissenberg technique. The structure was solved by the direct method and successive difference Fourier technique; 250 reflexions with $E \geq 1.30$ were used for sign determination. The co-ordinates of the atoms as read from the *E*-map and individual isotropic temperature factors were refined by structure factor least squares refinement. The present *R* value is 0.175. The intramolecular bond distances and angles are listed in table 1. The packing of the molecules in the unit cell is shown in figure 1.

The bond lengths and angles are in good agreement with the values observed in other sulphonamides *e.g.* sulphisoxazole[4], sulphisomidine[1], sulphadiazine[3], sulphadimethoxine[2], etc. The planes of both the rings are inclined at an angle of approx. 55° The dihedral angle 30° along S—N bond seems to be very small as compared to other sulphonamides. The tetrahedral geometry around sulphur is also distorted, as angles

TABLE 1

Intramolecular bond distances (a) and angles (b)

(a)	C1—C2	1.43 Å
	C1—S8	1.76
	C1—C6	1.40
	C2—C3	1.39
	C3—C4	1.39
	C4—C5	1.40
	C4—N7	1.40
	C5—C6	1.39
	S8—O9	1.49
	S8—O10	1.46
	S8—N11	1.56
	N11—C12	1.30
	C12—O13	1.37
	O13—C14	1.42
	C14—C15	1.35
	C14—C18	1.52
	C15—N16	1.40
	C15—C17	1 49
	N16—C12	1 33
(b)	C2—C1—C6	121.1°
	C2—C1—S8	121.4
	C6—C1—S8	117.5
	C1—C2—C3	120.0
	C2—C3—C4	119.3
	C3—C4—C5	119.8
	C3—C4—N7	118.7
	C5—C4—N7	121.6
	C4—C5—C6	122.8
	C5—C6—C1	116.7
	C1—S8—O9	105.7
	C1—S8—O10	109.8
	C1—S8—N11	102.6
	N11—S8—O9	110.9°
	N11—S8—O10	107.9
	O9—S8—O10	118.8
	S8—N11—C12	119.8
	N11—C12—O13	132.3
	N11—C12—N16	117.5
	N16—C12—O13	110.0
	C12—O13—C14	107.7
	O13—C14—C15	105.0
	O13—C14—C18	120.9
	C15—C14—C18	134.1
	C14—C15—N16	110.9
	C14—C15—C17	133.7
	N16—C15—C17	115.0
	C15—N16—C12	106.3

vary from 102° to 119°. Hydrogen bonds are not yet clear. At this stage, the molecule looks very much twisted along the centre of symmetry. Molecular packing is mainly due to van der Waals forces. Further refinement of the structure is in progress and the details will appear elsewhere.

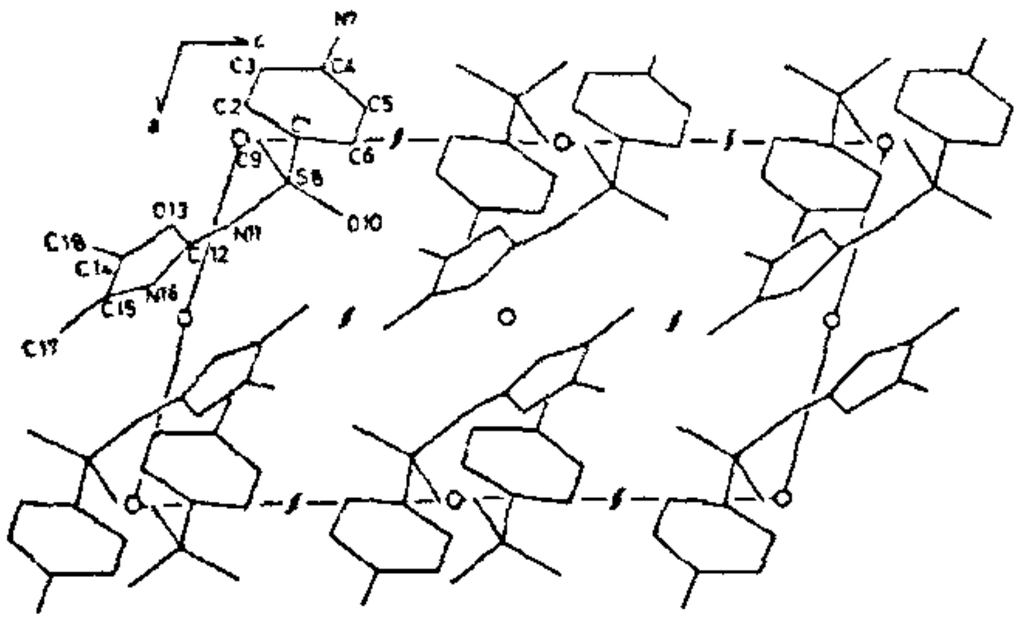

Figure 1. The structure viewed along the *b*-axis.

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ACTIVATED NITRILES IN HETEROCYCLIC SYNTHESIS: A NOVEL SYNTHESIS OF PYRIDINONES, QUINOLINES AND THIAZOLINONES

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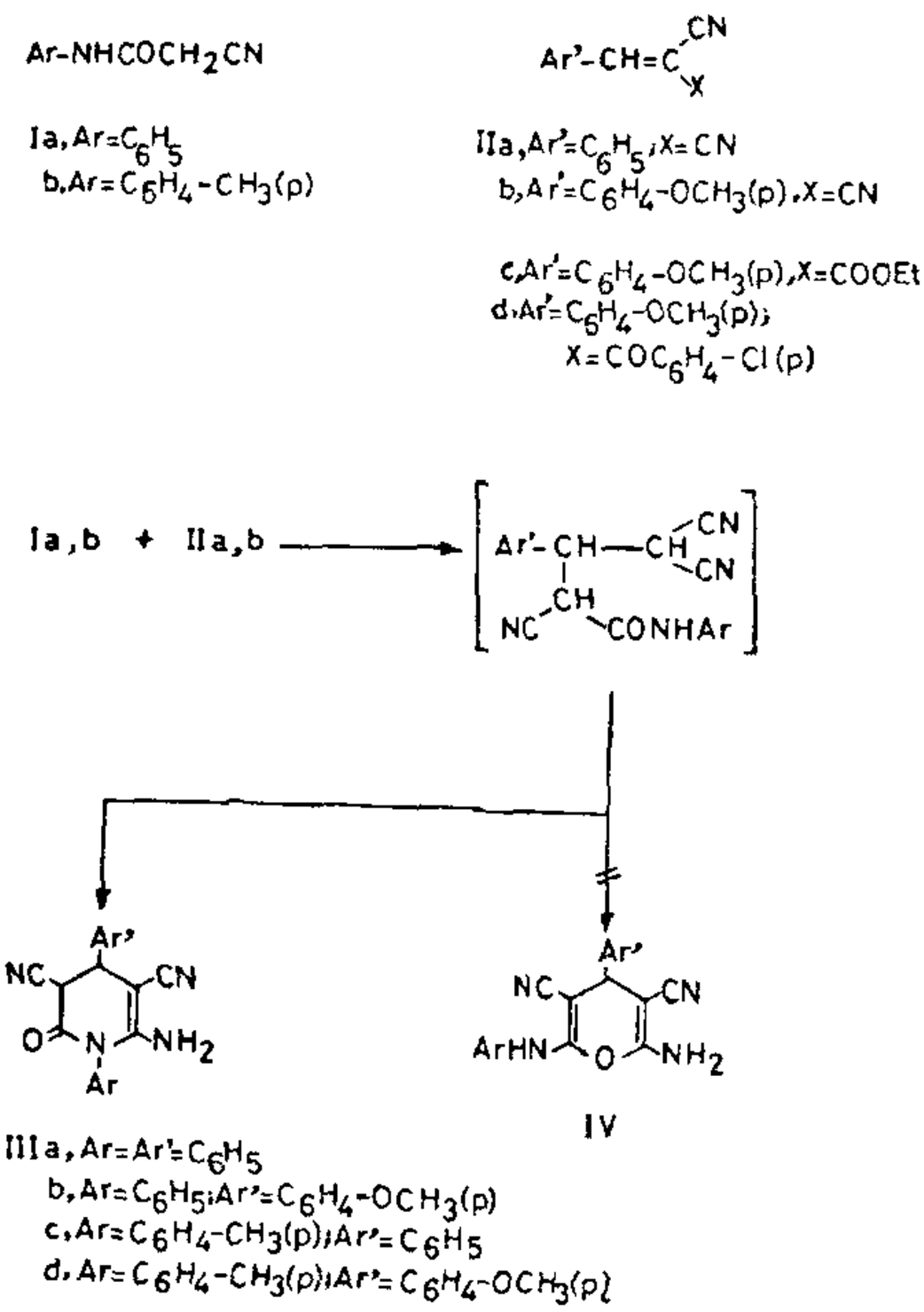
POLYFUNCTIONAL nitriles are versatile reagents extensively utilized in heterocyclic syntheses[1-3]. In continuation of our programme of developing new procedures to synthesise azoles and azines utilizing readily accessible polyfunctional nitriles as starting materials, we report here the utility of cyanoacetanilide (I) for the synthesis of pyridinones, thiazolines and quinolines. It has been found that Ia,b reacted with the cinnamonitrile derivatives IIa,b to yield 1:1 adducts IIIa-d. The IR spectra of the products revealed absorption band characteristic for carbonyl group and another band for amino group. Two theoretically possible isomeric structures were considered (cf. III and IV). However, structure III could be established for the reaction products based on their stability *towards acetic-ammonium acetate mixture. The for*mation of III from the reaction of I and IIa,b is assumed to proceed *via* addition to the activated double bond followed by cyclization of the Michael adduct intermediates.



Similarly, Ia,b reacted with IIc,d under the same conditions to yield the pyridinones derivatives Va,b and Va,b (or alternate tautomers) respectively. A novel synthesis of thiazole was earlier reported *via* reaction of malononitrile, benzalacetonitrile and ethyl cyanoacetate with thioglycollic acid[4-6]. It has now been found that Ia,b reacts with thioglycollic acid to yield 2-carboxamidomethyl-4-hydroxythiazole derivatives VIIa,b.

Compound Ia,b could also be converted into quinolines *via* treatment of their arylazo derivatives with hydrazines or dimethylformamide. This constitutes an interesting direct synthesis of arylazoquinolines IXa,b.