

ELECTRIC DIPOLE MOMENTS OF SUBSTITUTED-3-AMINOMETHYLBENZOXAZOLIN-2-THIONES

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A series of substituted-3-aminomethylbenzoxazolin-2-thiones have been synthesised and their electric dipole moments in benzene have been determined.

Recently a series of substituted-3-aminomethylbenzoxazolin-2-thiones have been synthesised^{1,2}. These compounds have been found to possess antimicrobial activity³. It has been reported⁴⁻¹⁸ that dipole moment measurements of various organic compounds have been found to reveal valuable structural information. From this point of view the electric dipole moments of compounds I and II have been determined.

E X P E R I M E N T A L

The dielectric constant measurements were carried out with the help of a Toshniwal Dipolemeter and the refractive indices of the solvent and solution were determined with the help of a ASCO Abbe-Refractometer at 35° as described earlier¹⁹. The dipole moments are recorded in Table 1.

TABLE 1

DIPOLE MOMENTS OF BENZOXAZOLIN-2-THIONE(I) AND SUBSTITUTED-3-AMINOMETHYLBENZOXAZOLIN-2-THIONES(II) IN BENZENE AT 35°.

Compound No.	—NR ₁ R ₂	M.P. °C	μ × 10 ¹⁸	(e.s.u.)
I		188-190	5.68 5.70	
IIa	piperidino	130-131	5.34 5.24	
IIb	2m-ethylpiperidino	97-100	insoluble	
IIc	3-methylpiperidino	136-138	6.66 6.64	
IId	4-methylpiperidino	106-108	6.85 6.89	
IIe	morpholino	157-158	4.94 4.90	
IIf	3-azabicyclo (3.2.2) nonano	173-175	5.59 5.65	
IIg	dimethylamino	105-106	6.09 6.01	
IIh	anilino	167-169	7.35 7.37	7.36

Substituted-3-aminomethylbenzoxazolin-2-thiones (II)

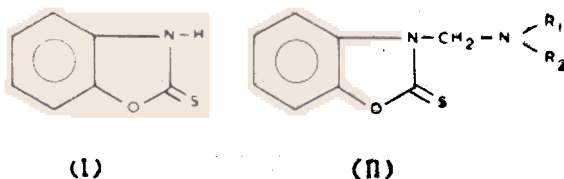
Benzoxazolin-2-thione (0.01 mole) was suspended in 20 ml of boiling ethanol. To this suspension 2 ml of 37% formalin and 0.01 mole of an amine were added and the reaction mixture warmed on a waterbath with stirring for 10 min. The contents were then cooled, filtered, washed with petroleum-ether (b.p. 60-80°) and crystallised from ethanol.

DISCUSSION

It has been observed that the dipole moments (Table I) of substituted-3-aminomethylbenzoxazolin-2-thiones (II) are either higher or lower as compared with the parent compound, benzoxazolin-2-thione (I) thereby indicating that the moments of substituent groups are directed towards the same or in opposite direction resulting in an increase or decrease in the net moments of II. The comparatively larger or smaller values of μ for IIh and IIe appear to suggest the higher moments for anilino and lower for morpholino groups.

The dipole moments of *N*-methylpiperidine²⁰ (0.80 D), trimethylamine²¹ (0.86D), *N*-methylaniline²² (1.65D) and benzoxazolin-2-thione (I) have been used to determine μ values of IIa, IIg and IIh, which differ widely from the experimental results for IIa and IIg, leading to the conclusion that in general these compounds are non-planar except IIh. This suggests that the resultant moments of the substituents- NR_1 , R_2 are definitely directed towards different planes with respect to the plane of the parent compound (I). The inclination angles have been calculated²¹ from the reported²⁰⁻²² and experimental data which have been found to be 131.5° , 69.1° and 0° for IIa, IIg and IIh respectively. The zero degree angle of inclination indicates that IIh is planar.

Thus it may be concluded from the reported results that II are non-planar in general and the moments of the substituents are directed towards different planes either reinforcing or opposing the moment of I, thereby resulting in an increase or decrease in the net moments of II.



Benzoxazolin-2-thione (I) and substituted-3-Aminomethylbenzoxazolin-2-thiones(II)

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