

SYNTHESIS OF DERIVATIVES OF A NEW
HETEROCYCLIC SYSTEM -
DIBENZIMIDAZO[1,2,2',1'-b,f]-1,3,6-
THIADIAZEPIN

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We have established that 1,2-di(2'-chloro-1'-benzimidazolyl)ethanes (III, IV) are formed when 2-chlorobenzimidazole (I) or its 5,6-dimethyl homolog (II) is refluxed with 1,2-dibromoethane in alcoholic sodium ethoxide solution; III and IV are converted to dibenzimidazo[1,2,2',1'-b,f]-1,3,6-thiadiazepin derivatives (V, VI) in high yields when they are refluxed with 2 moles of thiourea in dimethylformamide (DMF) for 2 h. The structure of V was confirmed by alternative synthesis by reaction of dibenzimidazolyl sulfide (VII) with 1,2-dibromoethane in the presence of sodium ethoxide.

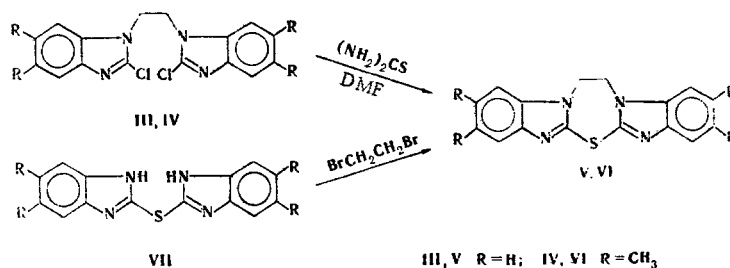


TABLE 1. Characteristics of the Compounds Obtained

Compound	R	mp, °C	Empirical formula	Found, %					Calculated, %					Yield, %
				C	H	Cl	N	S	C	H	Cl	N	S	
III	H	227-228 ^a	C ₁₆ H ₁₂ Cl ₂ N ₄	57.9	3.4	21.2	16.6	—	58.0	3.6	21.4	16.9	—	93
IV	CH ₃	315-316 ^b	C ₂₀ H ₂₀ Cl ₂ N ₄	62.2	5.2	18.4	14.4	—	62.0	5.2	18.3	14.5	—	83
V	H	330-333 ^b	C ₁₆ H ₁₂ N ₄ S	65.7	4.1	—	19.4	10.8	65.7	4.1	—	19.2	10.9	90
VI	CH ₃	360 ^b	C ₂₀ H ₂₀ N ₄ S	69.2	6.0	—	15.7	9.1	68.9	5.8	—	16.1	9.2	69

^aFrom ethanol-water (2:1).

^bFrom dimethylformamide.

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