SYNTHESIS OF CONDENSED 1,2,4-TRIAZINE SYSTEMS FROM 2(8)-METHYLMERCAPTOIMIDAZOLES

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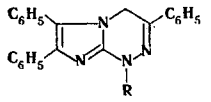
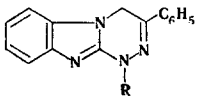
UDC 547.785.5.07

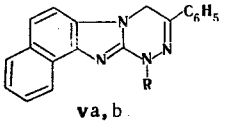
The corresponding 2-substituted N-acylmethylimidazoles (benzimidazoles) (I-II) were obtained by reaction of 4,5-diphenyl-2-imidazolyl methyl sulfone and 2-methylmercaptobenzimidazole with α-halo ketones. Compounds III-VI were obtained by heating I and II and 3-phenacyl-2-methylmercaptonaphtho-[1,2-d]imidazole and 7-phenacyl-8-methylmercaptotheophylline with hydrazine hydrate or phenylhydrazine.



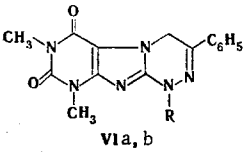
III a, b



IV a, b



Va, b



VIa, b

EXPERIMENTAL

1-Phenacyl-4,5-diphenyl-2-imidazolyl Methyl Sulfone (I). This compound was obtained as colorless needles with mp 199-200° (from methanol). IR spectrum (KBr): 1705 cm^{-1} (CO).

1-Phenacyl-2-methylmercaptobenzimidazole (II). This compound was obtained as colorless prisms with mp 185-186° (from aqueous alcohol). IR spectrum (KBr): 1690 cm^{-1} (CO).

The structures of the compounds obtained were confirmed by the results of elementary analysis, the UV spectra, and alternative synthesis of some of the compounds from the appropriate N-acylmethyl-2-haloimidazoles and hydrazines.

TABLE 1. Characteristics of Derivatives III-VI

Compound	R	mp, °C (dec.)	Crystallization solvent	IR spectrum, cm^{-1}, NH (KBr)	PMR spectrum, $-CH_2-$, δ, ppm (in CF_3COOH)	Yield, %
IIIa	H	269—270	Acetic acid—water	3230, 3280	4,75	80
IIIb	C_6H_5	249—250	Dioxane—water	—	4,85	75
IVa	H	305—308	DMFA	3210, 3280	5,33	92
IVb	C_6H_5	228—230	Dioxane	—	5,15	68
Va	H	312—313	DMFA	3200, 3250	4,78	60
Vb	C_6H_5	245—246	Dioxane—water	—	4,65	68
VIa	H	319—320	DMFA—water	3230, 3280	5,34	85
VIb	C_6H_5	228—230	Isopropyl alcohol	—	5,10	

Kherson Branch, M. V. Lomonosov Odessa Technologic Institute of the Food Industry. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 12, pp. 1696-1697, December, 1974. Original article submitted June 3, 1974.