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Author	与田, 玲子(Yoda, Reiko)
	山本, 有一(Yamamoto, Yuichi)
	岡田, 智子(Okada, Tomoko)
	松島, 美一(Matsushima, Yoshikazu)
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Pyrolytic Products of N-Alkyl-N'-(4-methyl-2-thiazolyl)-S-methylisothioureas*

Reiko Yoda, Yuichi Yamamoto, Tomoko Okada and Yoshikazu Matsushima

与田玲子, 山本有一, 岡田智子, 松島美一

We reported previously that pyrolysis of N,N-dimethyl-N'-(4-methyl-2-thiazolyl)-S-methylisothiourea at 155°C for 14 h gave N,N-dimethyl-N'-(3,4-dimethyl-2(3H)thiazolylidene)thiourea as the main product. The pyrolysis proceeded smoothly without any solvent. In the pyrolysis of other N,N-dialkyl-N'-(2-thiazolyl)-S-methylisothioureas, a similar migration of the methyl group from the isothiourea sulfur atom to the thiazole nitrogen atom was observed.

In contrast, the pyrolysis of an N-nonomethyl analog, N-methyl-N'-(4-methyl-2-thiazolyl)-S-methylisothiourea (1a), under the same conditions gave N-methyl-N',N''-bis-(4-methyl-2-thiazolyl)guanidine (2a) as a product. The S \rightarrow N methyl migrated compounds such as N-methyl-N'-(3,4-dimethyl-2(3H)thiazolylidene)thiourea and N-methyl-N'-(3,4-dimethyl-2-thiazolyl)guanidine (6a) were not formed in the pyrolysis. Similarly, a pyrolytic procuct of an N-ethyl analog of 1a, N-ethyl-N'-(4-methyl-2-thiazolyl)-S-methylisothiourea (1a), was identified as an N-ethyl analog of 1a, N-ethyl-N',N''-bis(4-methyl-2-thiazolyl)guanidine (1a).

The difference in the pyrolytic behavior between the N,N-dialkyl- and N-monoalkyl-N'-(2-thiazolyl)-S-methylisothioureas were interpreted in terms of the basicity of the thiazole nitrogen atom and the predominant chemical species.

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