A NOVEL SYNTHESIS OF v-TRIAZOLO[4,5-d]PYRIMIDINES

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Treatment of 6-azido-1,3-dimethyluracil with alkyl halides in dimethylformamide containing potassium carbonate gave the corresponding 1-alkyl-4,6-dimethyl-v-triazolo[4,5-d]-pyrimidine-5,7(4H,6H)-diones via 4,6-dimethyl-v-triazolo-[4,5-d]pyrimidine-5,7(4H,6H)-dione.

In recent years considerable interest has been devoted on the derivatives of v-triazolo[4,5-d]pyrimidine as potential purine antagonists,[1] and several synthetic routes to this ring system have been developed.[2] We now report a novel synthesis of 1-alkyl-4,6-dimethyl-v-triazolo[4,5-d]pyrimidine-5,7(4H,6H)-diones (IIa-f) from 6-azido-1,3-dimethyluracil (I).[3]

Refluxing (I)(0.001 mol) with alkyl halides (0.001 mol) in dimethylformamide (3 ml) containing potassium carbonate (0.001 mol) for 1 hr afforded the corresponding 1-alkyl-4,6-dimethyl-v-triazolo-[4,5-d]pyrimidine-5,7(4H,6H)-diones (IIa-f). An intermediate of these reactions is 4,6-dimethyl-v-triazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione (IIg),[4] which was obtained by treatment of (I) with di-

methylformamide containing potassium carbonate under the same conditions[5,6] (Table). The formation of (IIg) involves the intramolecular cyclization of a vinyl azide[7] to a triazole. Numerous examples have been reported on the cyclization of imidoyl azides to tetrazoles and of thiocarbonyl azides to thiatriazoles,[8] however, only one paper has hitherto been recorded on the conversion of a vinyl azide to a triazole.[9]

(I) (IIa-g)

Table Formation of v-Triazolo[4,5-d]pyrimidine Derivatives

Alkyl halide	Product	R	$\lambda_{max}^{H_2O}$ nm(log ε)	Mp(°C) (Recrystn. solvent)	Yield(%)
MeI	IIa	Me	230sh(3.64) 280(3.94)[a]	202-203[c] (EtOH)	77
EtI	IIb	Et	230sh(3.71) 277(4.07)	83-84 (EtOH)	56
n-PrI	IIc	n-Pr	230sh(3.63) 278(4.49)	78-79 (EtOH)	26
$EtOOCCH_2Cl$	IId	$EtOOCCH_2$	235sh(3.67) 280(4.07)	164-166[d] (MeOH)	21
CH_2=CH-CH_2Br	IIe	CH_2=CH-CH_2	306(3.80)	183-184 (MeOH-H_2O)	24
Ph-CH_2Cl	IIf	Ph-CH_2	240sh(3.74) 280(4.10)	119-120 (EtOH)	38
None	IIg	H	230sh(3.83) 268(3.98)	259-260[e] (H_2O)	30

a) Lit.[4] 230sh(3.56), 280(3.74). b) Lit.[4] 230sh(3.62), 269(3.93). c) Lit.[4] mp 223-224°. d) Lit. mp 157-159°: D.S. Bariana, J. Med. Chem., 1971, 14, 543. e) Lit. mp 260°.

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5 Compounds (IIa-g) were isolated by evaporation of the reaction mixtures, followed by addition of 5% hydrochloric acid, and subsequent extraction with chloroform. Satisfactory analytical and spectral data were obtained for all products.

6 Compound (IIg) could not be obtained by refluxing (I) with dimethylformamide alone for 1 hr.

7 The starting material (I) possesses a vinyl azide structure.

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