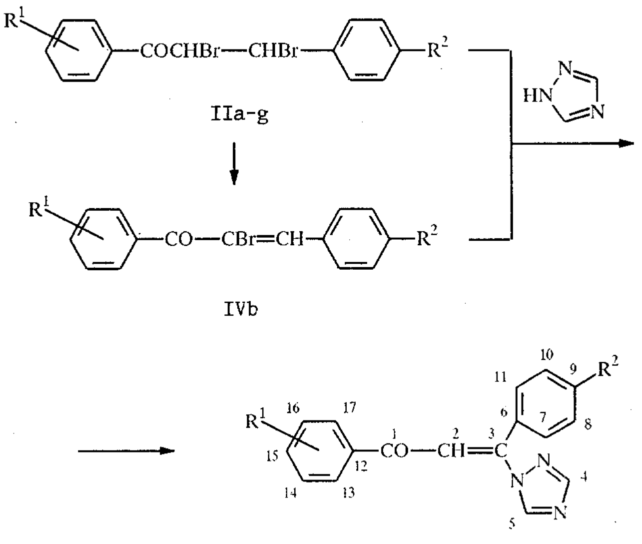
LETTERS TO THE EDITOR

1,3-DIARYL-3-(1H-1,2,4-TRIAZOL-1-YL)PROP-2-EN-1-ONES

M. A. Rekhter, G. N. Grushetskaya, A. A. Panasenko,
and M. Z. Krimer

In recent years research teams have shown much interest in N-vinyltriazoles — 1,3-diaryl-2-(1H-1,2,4-triazol-1-yl)prop-2-en-1-ones (I), which show fungicidal and growth-regulating activities [1, 2].

We have, for the first time, prepared representatives of a new type of compound of this class — 1,3-diaryl-3-(1H-1,2,4-triazol-1-yl)prop-2-ene-1-ones (IIIa-g) which are regioisomers of N-vinyltriazoles I.



IIIa-g

II, IIIa $R^1 = R^2 = H$; b R^1 = 4-Cl, $R^2 = H$; c R^1 = 4-Cl, $R^2 = Cl$; d $R^1 = 2,4\text{-}Cl_2$, $R^2 = NO_2$; e $R^1 = H$, $R^2 = OMe$; f R^1 = 4-Cl, $R^2 = OMe$; g R^1 = 4-Cl, $R^2 = NO_2$

As it proved, condensation of chalcone dibromides IIa-g with 1,2,4-triazole in DMSO led exclusively to the formation of compounds IIIa-g in the form of a mixture of E and Z isomers. From these mixtures the E isomers of IIIa-g were isolated by crystallization from methanol. The structure of compounds IIIa-g and their isomeric composition were established by means of ^{13}C NMR spectroscopy and the structure of the E isomers of IIIb (mp 177-178°C) and IIId (mp 157-159°C) were confirmed by x-ray structural studies.

The regiospecific formation of N-vinyltriazoles IIIa-g from chalcone dibromides IIa-g is evidence that in contrast to the known reactions of chalcone dibromides [3] the direction of the present reaction is independent of the nature of the radical R^2 and we have confirmed this by preparing, under the conditions described, N-vinyltriazole IIIb (80% yield) from the monobromoketone IVb. Further studies will be devoted to clarifying the mechanism of this reaction.

Thus, a solution of 4.82 g (10 mmoles) chalcone dibromide IId and 2.76 g (40 mmoles) 1,2,4-triazole in 50 ml DMSO was heated 4 h at 110-130°C, cooled to room temperature, poured into 500 ml water and extracted with 4 × 100 ml benzene. The benzene extract was washed with water and dried over Na_2SO_4. The residue obtained after removing the benzene was

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Institute of Chemistry, Moldavian Academy of Sciences, Kishinev 277028. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 2, pp. 266-267, February, 1993. Original article submitted February 5, 1993.

separated chromatographically (Silpearl, 3:2 ethyl acetate–hexane) to give 3.31 g (85%) (E,Z)-3-(4-nitrophenyl)-3-(1H-1,2,4-triazol-1-yl)-1-(2,4-dichlorophenyl)-prop-2-en-1-one (III, $C_{17}H_{10}Cl_2N_4O_3$). ^{13}C NMR spectrum (DMSO-D_6): E isomer (50%): 189.7 ($C_{(1)}$), 117.7 ($C_{(2)}$), 144.7 ($C_{(3)}$), 153.2 ($C_{(4)}$), 145.7 ($C_{(5)}$), 136.8 ($C_{(6)}$), 131.5 ($C_{(7)}$, $C_{(11)}$), 123.4 ($C_{(8)}$, $C_{(10)}$), 148.2 ($C_{(9)}$), 136.6 ($C_{(12)}$), 136.9 ($C_{(13)}$), 129.7 ($C_{(14)}$), 137.8 ($C_{(15)}$), 127.5 ($C_{(16)}$), 131.6 ($C_{(17)}$); Z isomer (50%): 189.0 ($C_{(1)}$), 124.8 ($C_{(2)}$), 141.0 ($C_{(3)}$), 152.6 ($C_{(4)}$), 146.7 ($C_{(5)}$), 139.9 ($C_{(6)}$), 129.1 ($C_{(7)}$, $C_{(11)}$), 123.9 ($C_{(8)}$, $C_{(10)}$), 148.6 ($C_{(9)}$), 132.2 ($C_{(12)}$), 135.3 ($C_{(13)}$), 130.2 ($C_{(14)}$), 136.8 ($C_{(15)}$), 127.3 ($C_{(16)}$), 131.9 ($C_{(17)}$).

The remaining N-vinyltriazoles IIIa-c, e-g were prepared similarly; their yields were 50, 72, 96, 41, 48, and 72%, respectively.

The results of elemental analyses of the compounds prepared corresponded to those calculated.

REFERENCES

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3. R. Elderfield, Heterocyclic Compounds, Wiley, New York (1957), p. 185.