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# A NOVEL RING-CLEAVAGE OF 2-PHENYL-1,2,3-TRIAZOLE-4-CARBOXYLIC ACID

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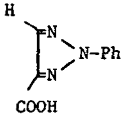
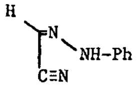
2-Phenyl-1,2,3-triazole systems are noted for the stability of the aromatic triazole ring (1).

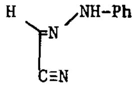
Distillation of 2-phenyl-1,2,3-triazole-4-carboxylic acid (I) from barium hydroxide gave in high yield the two ring-cleavage products II and III. The same two products are obtained by heating the hydrated barium salt of the acid I. The isomer II is thermally unstable and on further heating gives III.



I



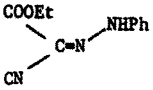
II



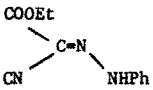
III

The structures of II and III follow from infrared, ultraviolet and p.m.r. spectroscopy. Both isomers have been synthesised by attack of phenyldiazonium chloride upon the anion from cyanoacetic ester, followed by alkaline hydrolysis of the two stereoisomeric esters IV and V and either acid or thermal decarboxylation.

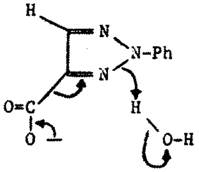
A rational mechanistic route for the cleavage I→II involves electronic rearrangement as shown in VI. Compound III is then derived from II by thermal rearrangement.



IV



V



VI

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## References

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