Does Tetrazolepentazole exist ?

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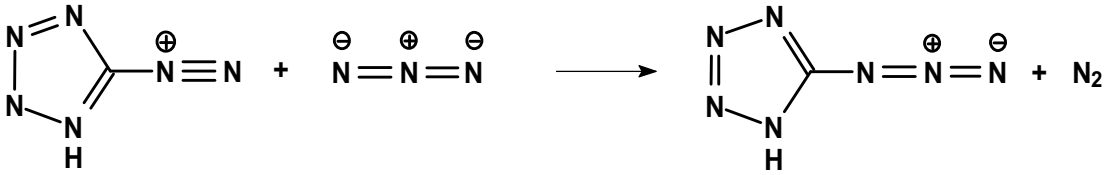
Huisgen and Ugi isolated petazole derivatives from the reaction of substituted benzene diazoniumchlorides with sodium azide. [1] The reaction of tetrazoldiazoniumchloride with sodium azide gave tetrazole azide. [2]



Therefore, tetrazolepentazole may be formed in this reaction.

We optimized the structures of all species involved in this reaction for the 1*H* and 2*H* tautomers of tetrazolepentazole and the anionic species and determined the activation energy for their decomposition at different levels of theory.

[1] a) I. Ugi, R. Huisgen, K. Clusius, M. Vecchi, *Angew. Chem.* **1956**, *68*, 753. b) R. Huisgen, I. Ugi, *Chem. Ber.* **1957**, *90*, 2914-2927. c) I. Ugi, H. Perlinger, L. Behringer, *Chem. Ber.* **1958**, *91*, 2324. d) I. Ugi, *Angew. Chem.* **1961**, *94*, 172.

[2] a) J. A. Cano Gorini, J. Farras, M. Feliz, S. Ollivella, A. Sole, J. Vilarrasa, *J. Chem. Soc. Chem. Comm.* **1986**, 959-961. b) R. M. Claramunt, J. Elguero, A. Fruchier, M. J. Nye, *Afinidad* **1977**, *35*, 545-551.