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Andreas S. Kalogirou, Maria Manoli, Panayiotis A. Koutentis

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Reaction of 3,4,4,5-tetrachloro-4*H*-1,2,6-thiadiazine with benzyltriethylammonium chloride

Andreas S. Kalogirou,[a,b,*] Maria Manoli[b] and Panayiotis A. Koutentis[b]

[a] Department of Life Sciences, School of Sciences, European University Cyprus, 6 Diogenis Str., Engomi, P.O. Box 22006, 1516 Nicosia, Cyprus

[b] Department of Chemistry, University of Cyprus, P. O. Box 20537, 1678 Nicosia, Cyprus

e-mail: a.kalogirou@external.euc.ac.cy, tel.: +357-22892804

Abstract. 3,4,4,5-Tetrachloro-4*H*-1,2,6-thiadiazine was reacted with $BnEt_3NCl$ (10 mol%) to give perchloro-9-thia-1,5,8,10-tetraazaspiro[5.5]undeca-1,4,7,10-tetraene (up to 18% yield), 4,5,6-trichloropyrimidine-2-carbonitrile (up to 44% yield) and four minor side products: 2,7-dichlorothiazolo[5,4-*d*]pyrimidine-5-carbonitrile, 2-(4-chloro-6*H*-thiazolo[5,4-*c*][1,2,6]thiadiazin-6-ylidene)malononitrile, 4,8-dichloropyrrolo[2',1':2,3]imidazo[4,5-*c*][1,2,6]thiadiazine-6,7-dicarbonitrile and 4,7-dichloro-[1,2,6]thiadiazino[3,4-*b*]thiazolo[5,4-*e*][1,4]diazepin-9(10*H*)-one. Single crystal X-ray studies support the structures of the minor products. Tentative rationale for the formation of these minor products and the synthesis of 8-bromo-4-chloropyrrolo[2',1':2,3]imidazo[4,5-*c*][1,2,6]thiadiazine-6,7-dicarbonitrile are presented.

Keywords: sulfur-nitrogen heterocycles; ring transformations; pyrimidine; thiazole; diazepine; pyrrole; thiophile; spirocycle