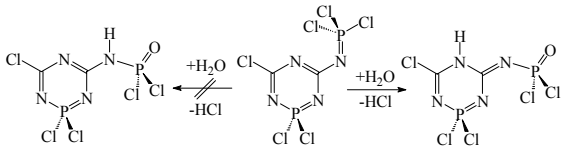
Gentle Hydrolysis of a Trichlorophosphazeno-1,3,5,2λ^5-triazaphosphorine

Ferdinand Belaj, *Institut für Chemie, Karl-Franzens-Universität Graz, Schubertstr. 1, Austria.* E-mail: ferdinand.belaj@uni-graz.at

The reaction product of dicyanodiamide with PCl_5 (1:2) was determined to have structure **I** [1]. By a gentle hydrolysis of **I** not the expected aromatic compound **II**, but the hitherto unknown compound **III** was obtained.



II I III

The crystal structure determination of compound **III** was performed at 100K and shows unambiguously that the H atom is bonded to the ring N atom at position 5 and not to the exocyclic N atom: at first by the isotropic refinement of the H atom, then by the observed bonding distances [for example $N_{exocyclic}$–C = 1.361(3)Å in **I** and 1.310(4)Å in **III**, resp.], and finally by the packing of the molecules: two molecules lying around a center of symmetry are held together by two presumably strong N–H···O hydrogen bonds [N···O 2.732(4)Å, N–H···O 166.5(2)°].

The single crystal X-ray refinement of the structure of compound III reported here is the first for a member of this hydrogenated 1,3,5,2λ^5-triazaphosphorine ring system.

[1] Belaj F., *Z. Naturforsch.*, 1996, **51b**, 1428.

Keywords: phosphazene, triazaphosphorine, aromaticity