4-DICYANOMETHYLENE-1,4-DIHYDROPYRIMIDINES AND PYRIDO [4,3-d]-PYRIMIDINE-8-CARBONITRILES FROM ENAMINONITRILES

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Reaction of malononitrile dimer (1a) and 3-amino-2-cyano-crotononitrile (1b), resp. with dimethylformamide dimethylacetal gives the biscondensation products 2a-b. Further treatment of 2a with ammonia and 2b with primary aliphatic amines, resp., leads to 4-dicyanomethylene-1,4-dihydro-pyrimidines 3. For the reaction of 2a with primary aliphatic and aromatic amines several isomer structures have to be considered. By X-ray structure analysis it is confirmed that the reaction product from 2a and propylamine is 5,6-dihydro-5-imino-6-propyl-4-propylamino-pyrido-[4,3-d] pyrimidine-8-carbonitrile (4c). Cyclization occurs by substitution of the dimethylamino groups, reaction of both nitriles and Dimroth-rearrangement in the pyrimidine part of the molecule. Hydrolysis of the imino group leads to the 5,6-dihydro-5-oxo-pyrido[4,3-d]pyrimidines 5.