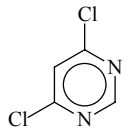
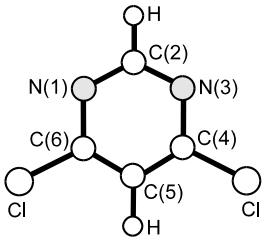
493 **$C_4H_2Cl_2N_2$** **4,6-Dichloropyrimidine** **C_{2v}** assumed

ED, *ab initio* calculations



r_a	Å [a])	θ_α^0	deg [a])
N(1)–C(2)	1.344(2)	N–C–N	127.8(5)
C(4)–N(3)	1.333(3)	C–N–C	114.6(4)
C(4)–C(5)	1.385(6)	N–C–Cl	117.1(4)
C(2)–H	1.104(11)	N–C–C [b])	123.8(3)
C(5)–H	1.103(11)	C–C–C [b])	115.4(7)
C(4)–Cl	1.734(2)		

The structural parameters were determined by supplementing experimental data with restraints based on the results of MP2/6-311G** calculations.
The nozzle was at 400 K.



[a]) Estimated standard errors.
[b]) Dependent parameter.

Morrison, C.A., Smart, B.A., Parsons, S., Brown, E.M., Rankin, D.W.H., Robertson, H.E., Miller, J.: J. Chem. Soc., Perkin Trans. 2 (1997) 857.