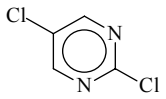
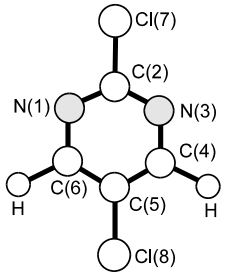
491 **$C_4H_2Cl_2N_2$** **2,5-Dichloropyrimidine** **C_{2v}** assumed

ED, *ab initio* calculations



r_a	Å [a])	θ_α^0	deg [a])
C–C	1.394(11)	N(1)–C(2)–N(3)	127.9(4)
N(1)–C(6)	1.334(4)	C(2)–N(3)–C(4)	116.3(7)
N(1)–C(2)	1.326(4)	N–C–H	117.2(5)
C(2)–Cl(7)	1.733(3)	N(3)–C(4)–C(5) [b])	120.6(8)
C(5)–Cl(8)	1.727(3)	C(4)–C(5)–C(6) [b])	118.3(6)
C–H	1.109(12)		

A new method of ED analysis with restraints based on the results of the *ab initio* calculations was proposed. The calculations were performed at the MP2/6-311G** level of theory.
The nozzle was at 460 K.



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

Blake, A.J., Brain, P.T., McNab, H., Miller, J., Morrison, C.A., Parsons, S., Rankin, D.W.H., Robertson, H.E., Smart, B.A.: J. Phys. Chem. **100** (1996) 12280.