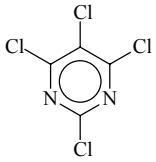
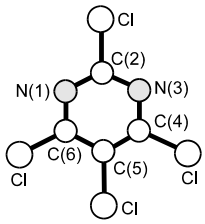
474 **$C_4Cl_4N_2$** **2,4,5,6-Tetrachloropyrimidine** **C_{2v}** assumed

ED, *ab initio* calculations



r_α	Å [a])	θ_α	deg [a])
r [b])	1.342(1)	N–C–N	127.1(4)
C–Cl (average)	1.709(1)	C–N–C	116.2(3)
C–C [c])	1.393(2)	N–C–Cl	116.2(2)
N(1)–C(2) [c])	1.318(2)	N–C–C [c])	122.8(1)
N(1)–C(6) [c])	1.316(2)	C–C–C [c])	114.9(2)
C(2)–Cl [c])	1.716(1)		
C(4)–Cl [c])	1.711(1)		
C(5)–Cl [c])	1.702(1)		

Differences between similar parameters were restrained to the values from MP2/6-311G** calculations.
The nozzle temperature was *ca*. 470 K.



[a]) Estimated standard errors.
[b]) Average ring bond distance.
[c]) Dependent parameter.

Navarro, A., Fernández-Gómez, M., Fernández-Liencres, M.P., Morrison, C.A., Rankin, D.W.H., Robertson, H.E.: Phys. Chem. Chem. Phys. **1** (1999) 3453.