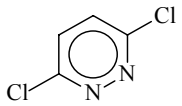
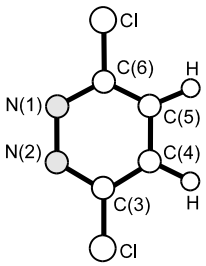
490 **$C_4H_2Cl_2N_2$** **3,6-Dichloropyridazine** **C_{2v}** assumed

ED, MW, *ab initio* calculations



r_a	Å [a])	θ_α^0	deg [a])
N(1)–N(2)	1.343(3)	N–N–C	118.4(2)
C(3)–N(2)	1.331(3)	N–C–C	124.7(4)
C(3)–C(4)	1.401(3)	C–C–Cl	119.1(14)
C(4)–C(5)	1.383(3)	C–C–H	122.8(13)
C–Cl	1.736(2)	C–C–C [b])	116.9(3)
C–H	1.085(13)		

The structural parameters were determined by supplementing ED data with rotational constants and restraints based on the results of MP2/6-311G** calculations.
The nozzle was at 442 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.

Replaces II/25C (**3**, 1502)