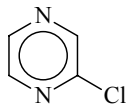
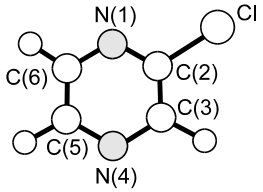
501 **$C_4H_3ClN_2$** **Chloropyrazine** **C_s** assumed

ED, MW, *ab initio* calculations



r_α^0	Å [a])	θ_α^0	deg [a])
C(2,3,5)–N (average)	1.331(2)	N(1)–C(2)–Cl	118.2(3)
C(2)–Cl	1.736(2)	α [b])	120.8(1)
C–C (average)	1.390(3)	(N,C)–C–H (average)	120.6(8) [c])
C–H (average)	1.080(7) [c])	N(1)–C(2)–C(3) [d])	123.8(2)
N(1)–C(2) [d])	1.322(3)	N(1)–C(6)–C(5) [d])	121.8(4)
N(1)–C(6) [d])	1.351(3)	N(4)–C(3)–C(2) [d])	121.0(3)
N(4)–C(3) [d])	1.332(4)	N(4)–C(5)–C(6) [d])	122.2(3)
N(4)–C(5) [d])	1.340(3)	C(2)–N(1)–C(6) [d])	115.0(4)
C(2)–C(3) [d])	1.392(4)	C(3)–N(4)–C(5) [d])	116.2(3)
C(5)–C(6) [d])	1.389(4)	C(2)–C(3)–H [d])	122.2(7)
C(3)–H [d])	1.080(7)	C(6)–C(5)–H [d])	120.2(10)
C(5)–H [d])	1.080(8)	C(5)–C(6)–H [d])	122.1(9)
C(6)–H [d])	1.081(8)		

Differences between similar parameters were restrained to the values from MP2/6-311G** calculations.
The nozzle temperature was *ca*. 386 K.



[a]) Estimated standard errors.
[b]) Average ring angle.
[c]) Restrained to the value from MP2/6-311G** calculations.
[d]) Dependent parameter.

Smart, B.A., Morrison, C.A., Papathomas, P.M., Brookman, C.A., Robertson, H.E., Rankin, D.W.H.: J. Chem. Soc., Perkin Trans. 2 (1999) 745.