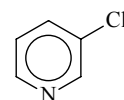


626 **C₅H₄ClN**ED, MW, *ab initio*
calculations**3-Chloropyridine****C_s**, assumed

r_{α}^0	$\text{\AA}^a)$	θ_{α}^0	$\text{deg}^a)$
C–C (average)	1.396(2)	C–C–C (average)	118.7(1)
C–Cl	1.734(2)	C(4)–C(3)–Cl	120.9(4)
C(6)–N	1.339(6)	N–C(6)–H	116.1(9) ^{b)}
C–H (average)	1.102(5) ^{b)}	N–C(6)–C(5)	122.9(3) ^{b)}
C(5)–C(6) ^{c)}	1.400(4)	N–C(2)–C(3) ^{c)}	122.3(3)
C(4)–C(5) ^{c)}	1.399(4)	C(2)–N–C(6) ^{c)}	118.6(5)
C(3)–C(4) ^{c)}	1.391(3)	C(4)–C(5)–C(6) ^{c)}	119.0(3)
C(2)–C(3) ^{c)}	1.395(4)	C(3)–C(4)–C(5) ^{c)}	117.0(2)
N–C(2) ^{c)}	1.326(5)	C(2)–C(3)–C(4) ^{c)}	120.9(4)
C(6)–H ^{c)}	1.102(6)		
C(5)–H ^{c)}	1.102(7)		
C(4)–H ^{c)}	1.100(6)		
C(2)–H ^{c)}	1.102(6)		

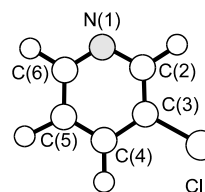
Differences between similar parameters were restrained to the values from MP2/6-311G** calculations.

The nozzle temperature was *ca.* 386 K.

^{a)} Estimated standard errors.

^{b)} Restrained to the value from MP2/6-311G** calculations.

^{c)} 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.