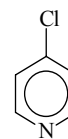


627 **C₅H₄ClN**ED, MW, *ab initio*
calculations**4-Chloropyridine****C_{2v}** assumed

r_{α}^0	Å ^{a)}	θ_{α}^0	deg ^{a)}
C–C (average)	1.392(2)	N...C(4)–C(3)	60.7(2)
C–Cl	1.742(3)	C(2)–C(3)–C(4)	116.2(3)
C(4)...N	2.782(4)	C(3)–C(4)–C(5) ^{b)}	121.3(3)
C–H (average)	1.098(6) ^{c)}	C(3)–C(4)–Cl ^{b)}	119.4(2)
C(2)–N ^{b)}	1.336(3)	N–C(2)–C(3) ^{b)}	125.1(3)
C(3)–C(4) ^{b)}	1.389(2)	C(2)–N–C(6) ^{b)}	116.1(4)
C(2)–C(3) ^{b)}	1.396(3)	C(4)–C(3)–H ^{b)}	122.1(4)
C(2)–H ^{b)}	1.099(6)	C(3)–C(2)–H ^{b)}	120.9(12)
C(3)–H ^{b)}	1.097(6)		

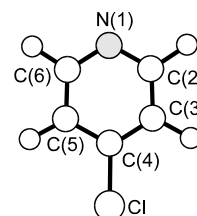
Differences between similar parameters were restrained to the values from MP2/6-311G** calculations.

The nozzle temperature was *ca.* 386 K.

^{a)} Estimated standard errors.

^{b)} Dependent parameter.

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



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.