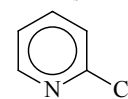


625 **C₅H₄ClN**ED, MW, *ab initio*
calculations**2-Chloropyridine****C_s assumed**

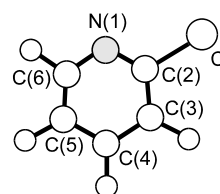
r_{α}^0	\AA^a	θ_{α}^0	deg ^{a)}
C–C (average)	1.395(2)	C–C–C (average)	118.1(1)
C–Cl	1.738(2)	C–C–Cl	118.1(3)
C(6)–N	1.345(4)	N–C(2)–C(3)	125.3(2) ^{b)}
C–H (average)	1.088(4) ^{b)}	C–C–H (average)	121.6(6) ^{b)}
C(5)–C(6) ^{c)}	1.395(3)	C(2)–N–C(6) ^{c)}	117.0(4)
C(4)–C(5) ^{c)}	1.400(4)	C(2)–C(3)–C(4) ^{c)}	117.3(3)
C(3)–C(4) ^{c)}	1.393(3)	C(3)–C(4)–C(5) ^{c)}	119.0(3)
C(2)–C(3) ^{c)}	1.392(4)	C(4)–C(5)–C(6) ^{c)}	118.2(1)
N–C(2) ^{c)}	1.319(3)	C(5)–C(6)–N ^{c)}	123.3(3)
C(6)–H ^{c)}	1.089(5)	C(6)–C(5)–H ^{c)}	120.7(8)
C(5)–H ^{c)}	1.087(6)	C(5)–C(4)–H ^{c)}	121.5(7)
C(4)–H ^{c)}	1.089(5)	C(4)–C(3)–H ^{c)}	122.7(9)
C(3)–H ^{c)}	1.087(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.



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Rankin, D.W.H.: J. Chem. Soc., Perkin Trans. 2 (1999) 745.

[II/25D \(3, 1910\)](#)