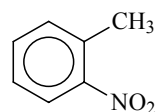


800 **C₇H₇NO₂**
ED, *ab initio* and DFT
calculations

1-Methyl-2-nitrobenzene
2-Nitrotoluene

C₁



r_g	Å ^{a)}	θ_a	deg ^{a)}
C(1)–C(2)	1.405(8)	C(7)–C(1)–C(2)	127.3(7)
C(1)–C(7) ^{b)}	1.508(8)	N–C(2)–C(3)	113.8(6)
C–C (ring) ^{b) c)}	1.399(9)	C(6)–C(1)–C(2)	114.8(6)
N=O	1.231(3)	C(1)–C(2)–C(3)	124.2(9)
C–N	1.490(9)	C(2)–C(3)–C(4)	118.6(9)
C–H (methyl) ^{b) c)}	1.103(4)	C(3)–C(4)–C(5)	119.8(5)
C–H (ring) ^{b) c)}	1.097(4)	C(4)–C(5)–C(6)	119.6(10)
		C(5)–C(6)–C(1)	123.1(10)
		O=N=O	124.9(3)
		τ (N–C) ^{d)}	38(1)
		τ (CH ₃) ^{e)}	–75.3 ^{f)}

It was assumed that the NO₂ group has local C_{2v} symmetry and the CH₃ group has local C_{3v} symmetry. The aromatic C–H bonds were assumed to lie in the plane of the benzene ring bisecting the adjacent C–C–C angle.

The nozzle temperature was 421 K.

^{a)} Estimated total errors.

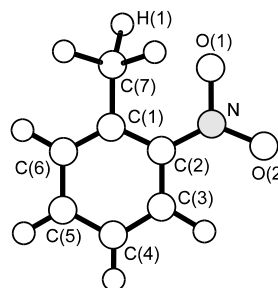
^{b)} Differences in the C–C and C–H bond lengths were assumed at the values from MP2/6-31G* calculations.

^{c)} Mean value.

^{d)} Torsional angle around the N–C bond, O(1)–N–C(2)–C(1); zero degree for the eclipsed position.

^{e)} Torsional angle of CH₃ group around the C(1)–C(7) bond, H(1)–C(7)–C(1)–C(2); zero degree for the eclipsed position.

^{f)} Assumed at the value from MP2/6-31G* calculations.



Shishkov, I.F., Vilkov, L.V., Kovács, A., Hargittai, I.: J. Mol. Struct. **445** (1998) 259.