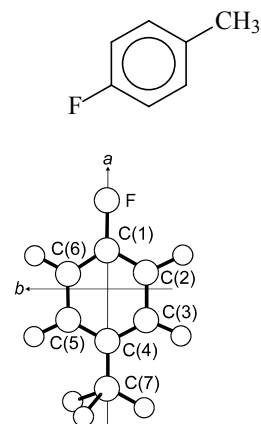


794
MW C_7H_7F **1-Fluoro-4-methylbenzene**
p-Fluorotoluene**G₁₂**
(effective symmetry class)

r_s	Å	θ_s	deg
C(1)–C(2)	1.384(1)	C(6)–C(1)–C(2)	122.2(1)
C(2)–C(3)	1.389(1)	C(1)–C(2)–C(3)	118.4(1)
C(3)–C(4)	1.398(1)	C(2)–C(3)–C(4)	121.3(1)
C(4)–C(7)	1.510(1)	C(3)–C(4)–C(5)	118.3(1)
C(1)...C(4)	2.774(1)	C(7)–C(4)–C(3)	120.9(1)

Atom	$ a_s $ [Å]	$ b_s $ [Å]
C(1)	1.309	0.0
C(2),C(6)	0.640	1.211
C(3),C(5)	0.748	1.200
C(4)	1.465	0.0
C(7)	2.9754	0.0



The barrier V_6 to internal rotation was redetermined to be $57.777 \text{ J mol}^{-1}$.

Rottstegge, J., Hartwig, H., Dreizler, H.: J. Mol. Struct. **478** (1999) 37.