

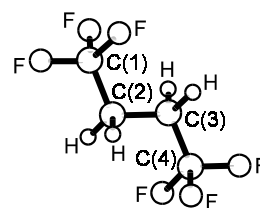
1548
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C₄H₄F₆

1,1,1,4,4,4-Hexafluorobutane

C_{2h} (*trans*)
F₃C–CH₂–CH₂–CF₃

| r_g | Å ^{a)} | θ_α | deg ^{a)} |
|---------------------------|-----------------|-----------------|---------------------|
| C–H | 1.090(14) | C–C–C | 110.6(6) |
| C–F | 1.340(2) | F–C–F | 107.2(2) |
| C–C (mean) ^{b)} | 1.509(3) | H–C–H | 108.5 ^{d)} |
| ΔCC ^{c)} | 0.028(16) | | |
| C(1)–C(2) | 1.501(7) | | |
| C(2)–C(3) | 1.529(11) | | |



Local C_{3v} and C_{2v} symmetry was assumed for the CF₃ and CH₂ groups, respectively. The tilt angle of the CF₃ group was found to be essentially zero. The contribution of a *gauche* conformer is zero or very small.

The nozzle was at room temperature.

^{a)} Three times the estimated standard errors including a systematic error.

^{b)} C–C (mean) = (1/3)[2(C(1)–C(2)) + (C(2)–C(3))].

^{c)} $\Delta CC = [C(2)–C(3)] - [C(1)–C(2)]$.

^{d)} Assumed.

Mack, H.-G., Oberhammer, H., Bielefeldt, D.: J. Mol. Struct. **273** (1992) 317.