

110 **CH₃AsF₂**ED, MW, *ab initio*
calculations**Difluoromethylarsine**

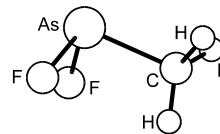
Methylarsonous difluoride

C_sF₂As–CH₃

r_g	Å ^{a)}
As–C	1.949(4)
As–F	1.734(1)

r_a^0	Å ^{a)}
As–C	1.946(4)
As–F	1.731(1)
C–H	1.114(10)

θ_a^0	deg ^{a)}
C–As–F	95.2(1)
F–As–F	97.0(1)
As–C–H	106.5(17)



Local C_{3v} symmetry was assumed for the methyl group. The molecule was described by a model with large-amplitude torsional motion of CH₃ group about staggered conformation with respect to the AsF₂ group. The three-fold barrier to rotation was estimated to be 5.85 kJ mol^{–1} at the MP2/6-31G** level of theory.

The nozzle was at about 293 K.

^{a)} Estimated standard errors.

Downs, A.J., Greene, T.M., McGrady, G.S., Townson, N., Brain, P.T., Pulham, C.R., Rankin, D.W.H., Robertson, H.E., Smart, B.A., Alberts, I.L.: *Inorg. Chem.* **35** (1996) 6952.

[II/25B\(3, 243\)](#)