

681 **C₅H₁₅As**
ED, *ab initio*
calculations

Pentamethylarsorane
Pentamethylarsenic(V)

C_{3h}
As(CH₃)₅

| r_a | \AA^a | θ_a | deg^a |
|------------------|----------------|---------------------|----------------|
| As–C(ax) | 2.073(4) | As–C–H ^b | 109.4(5) |
| As–C(eq) | 1.975(3) | | |
| C–H ^b | 1.112(2) | | |

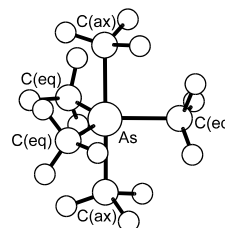
Local C_{3v} symmetry was assumed for the methyl groups. Axial methyl groups were assumed to be in a staggered orientation with respect to the equatorial AsC₃ unit. Equatorial methyl groups were assumed to be oriented in such a manner that one C–H bond of each group was eclipsed with respect to the adjacent As–C(eq) bond.

HF/6-31G* calculations predicted that the C_{3h} conformer was more stable than C_{3v} by 0.58 kJ mol^{–1}.

The nozzle temperature was 25...26 °C.

^a) Estimated standard errors.

^b) Mean value.



Greene, T.M., Downs, A.J., Pulham, C.R., Haaland, A., Verne, H.P., Volden, H.V., Timofeeva, T.V.: *Organometallics* **17** (1998) 5287.