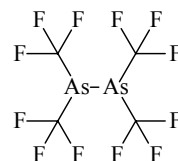


**471**      **C<sub>4</sub>As<sub>2</sub>F<sub>12</sub>**ED, *ab initio*  
calculations**Tetrakis(trifluoromethyl)diarsine**

Tetrakis(trifluoromethyl)diarsane

**C<sub>2h</sub>** assumed (*anti*)

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
As–As	2.452(6)	As–As–C	94.6(7)
As–C	2.012(4)	C–As–C	94.5(17)
C–F	1.336(2)	F–C–F	107.2(3)
		tilt(CF <sub>3</sub> ) <sup>b)</sup>	4.2(15)
		$\tau^c$	–175.7(34)



The molecule was found to exist as *anti* (100(10)%) conformer. A small amount of *gauche* conformer could not be excluded.

Local C<sub>3v</sub> symmetry was assumed for the CF<sub>3</sub> groups.

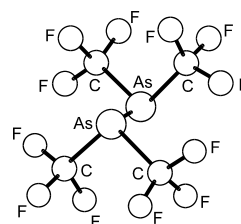
According to results of HF/6-311+G\* calculations, the *anti* conformer is lowest in the energy.

The nozzle was at room temperature.

<sup>a)</sup> Three times the estimated standard errors.

<sup>b)</sup> Angle between the C<sub>3</sub> axis of the CF<sub>3</sub> group and the As–C vector towards the lone pair of the As atom.

<sup>c)</sup> C–As–C–F torsional angle,  $\tau = 0^\circ$  for the *syn* position.



Becker, G., Golla, W., Grobe, J., Klinkhammer, K.W., Le Van, D., Maulitz, A.H., Mundt, O., Oberhammer, H., Sachs, M.: Inorg. Chem. **38** (1999) 1099.