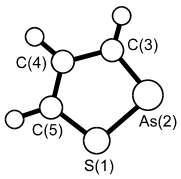
351 **C_3H_3AsS** **1,2-Thiarsole** **C_s** assumed

ED, DFT calculations

r_g	Å [a])	θ_α	deg [a])
C–H (average)	1.078(14)	C–C=C	118.0(12)
C(4)=C(5)	1.382(9) [b])	As=C–C	117.7(10)
C(3)–C(4)	1.414(10) [b])	S–C=C	117.9(9)
S–C	1.711(5)	As–S–C	96.6(4)
As=C	1.829(4)	S–As=C	89.8(5)
As–S	2.198(3)	C(4)–C(3)–H	123.8(61) [b])
		C(3)–C(4)–H	121.7(82) [b])
		C(4)=C(5)–H	123.4(92) [b])

The nozzle temperature was 24 °C.



[a]) Twice the estimated standard errors.
[b]) Differences between the C–C bond lengths and between the C–C–H bond angles were constrained to the values from B3LYP/6-31G* calculations.

Ashe, A.J., Fang, X., Schiesher, M., Richardson, A.D., Hedberg, K.: J. Am. Chem. Soc. **122** (2000) 7012.