

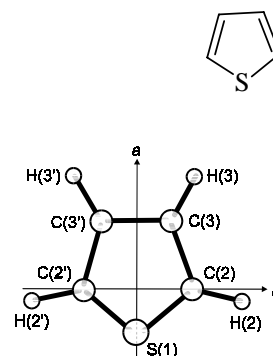
**1570 C<sub>4</sub>H<sub>4</sub>S****Thiophene****C<sub>2v</sub>**

ED, MW,

liquid-crystal NMR

$r_\alpha$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C(2)–H	1.0688(6)	H–C–S	120.24(8)
C(3)–H	1.0812(11)	H–C(3)–C(3')	124.06(6)
C(2)=C(3)	1.3783(15)	C–S–C	92.56(8)
S–C	1.7136(11)		
C(3)–C(3')	1.4274(11)		

The nozzle temperature was 300 K.

<sup>a)</sup> Estimated standard errors.Liescheski, P.B., Rankin, D.W.H.: J. Mol. Struct. **178** (1988) 227.See also: Bonham, R.A., Momany, F.A.: J. Phys. Chem. **67** (1963) 2474.Harshberger, W., Bauer, S.H.: Acta Cryst. B **26** (1970) 1010.**MW**

$r_s$	Å	$\theta_s$	deg
C(2)–H	1.0776(50)	H–C–S	119.9(5)
C(3)–H	1.0805(50)	H–C(3)–C(3')	124.3(5)
C(2)=C(3)	1.3696(30)	C–S–C	92.2(2)
S–C	1.7140(20)	S–C=C	111.5(2)
C(3)–C(3')	1.4232(30)	C(2)=C(3)–C(3')	112.5(2)

Atom	$a_s$ [Å]	$b_s$ [Å]
S	–1.1426	0.0
C(2)		±1.2346
C(3)	1.3121	±0.7116
H(2)	–0.2550	±2.2692
H(3)	2.2050	±1.3201

Bak, B., Christensen, D., Hansen-Nygaard, L., Rastrup-Andersen, J.: J. Mol. Spectrosc. **7** (1961) 58.

See also:

Bak, B., Christensen, D., Rastrup-Andersen, J., Tannenbaum, E.: J. Chem. Phys. **25** (1956) 892.