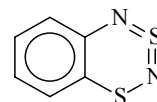


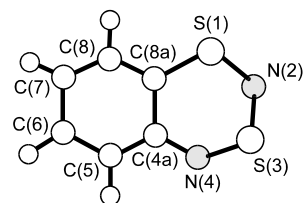
704 **C₆H₄N₂S₂**
ED, *ab initio* and DFT
calculations

1,3,2⁴δ²,2,4-Benzodithiadiazine**C₁**

r_{hl} ^{a)}	Å ^{b)}	θ_{hl} ^{a)}	deg ^{b)}
C(4a)–C(8a)	1.391(6)	C(5)–C(4a)–C(8a)	119.4(6)
C(8a)–C(8)	1.392(8)	C(6)–C(5)–C(4a)	120.9(7)
C(8)–C(7)	1.388(8)	C(5)–C(6)–C(7)	120.1(5)
C(7)–C(6)	1.395(8)	H–C(5)–C(4a)	117.8(6)
C(6)–C(5)	1.402(7)	H–C(6)–C(5)	119.67(12)
C(5)–C(4a)	1.378(7)	H–C(7)–C(6)	120.4(6)
C(4a)–N(4)	1.393(6)	H–C(8)–C(7)	120.4(12)
C(8a)–S(1)	1.784(5)	N–C(4a)–C(8a)	123.3(7)
N(2)–S(1)	1.697(5)	S(1)–N(2)=S(3)	119.9(5)
S(3)=N(2)	1.548(3)	N(2)–S(1)–C(8a)	101.5(7)
N(4)=S(3)	1.543(3)	S(1)–C(8a)–C(4a)	122.7(6)
C–H ^{c)}	1.087(2)	N–C(4a)–C(8a)–S(1)	–17(3)
		S(3)=N(2)–S(1)–C(8a)	–41(3)
		N(2)–S(1)–C(8a)–C(4a)	26.2(23)
		S(1)–C(8a)–C(4a)–C(5)	174.6(12)

The C₆H₄ fragment was assumed to be planar.
Differences between similar parameters were
restrained to the values from quantum chemical
calculations.

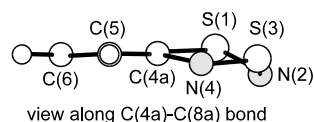
The nozzle temperature was 154...162 °C.



^{a)} Nonlinear kinematic effects were taken into
account.

^{b)} Estimated standard errors.

^{c)} Average value.



Blockhuys, F., Hinchley, S.L., Marakov, A.Yu., Gatilov, Yu.V.,
Zibarev, A.V., Woollins, J.D., Rankin, D.W.H.: Chem. Eur. J. **7** (2001) 3592.