363 **C_3H_3NS** **1,3-Thiazole** **C_s** assumed

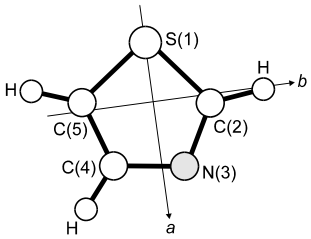
ED, MW, *ab initio* calculations

r_α^0	Å [a])
S–C(2)	1.7237(11)
S–C(5)	1.7138(13)
C(2)=N	1.310(2)
C(4)=C(5)	1.3690(19)
N–C(4)	1.372(2)
C(2)–H	1.098(4)
C(4)–H	1.099(4)
C(5)–H	1.097(4)

θ_α^0	deg [a])
C(2)–S–C(5)	89.41(4)
S–C(2)=N	115.16(6)
S–C(5)=C(4)	109.52(8)
C(2)=N–C(4)	109.97(9)
N–C(4)=C(5)	115.95(11)
S–C(2)–H	120.7(2)
C(5)=C(4)–H	125.0(4)
C(4)=C(5)–H	128.8(2)
S–C(5)–H	121.7(2)
N=C(2)–H	124.2(2)
N–C(4)–H	119.0(4)

Flexible restraints derived from results of MP2/6-311G(2df,2dp) calculations were employed on the differences in the C–H bond lengths and in the S–C–H bond angles and on the C(5)=C(4)–H bond angle.
The nozzle temperature was 290 K.

[a]) Estimated standard errors.



Bone, S.F., Smart, B.A., Gierens, H., Morrison, C.A., Brain, P.T., Rankin, D.W.H.: Phys. Chem. Chem. Phys. **1** (1999) 2421.

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