

1124
ED

C₃H₃NS

Isothiazole

C_s

r_g	\AA^a	θ_a	deg a
S–N	1.642(5)	C–S–N	96.1(2)
S–C	1.702(5)	S–N=C	112.2(3)
N=C	1.319(3)	N=C–C	111.8(4)
C–C	1.436(3)	C–C=C	113.8(4)
C=C	1.388(3)	C=C–S	106.2(3)
C–H (average)	1.102(3)		



The nozzle temperature was ≈ 30 °C.

^a) Estimated limits of error.

Schultz, G., Hargittai, I., Friedman, P.: J. Mol. Struct. **176** (1988) 61.