

1530 **C₄H₃NS**
ED, IR, Ra

3-Thiocyanato-1-propyne
2-Propynyl thiocyanate

C_s(*anti*)
C₁(*gauche*)
HC≡C-CH₂-S-C≡N

r_a	Å ^{a)}	θ_a	deg ^{a)}
C(4)≡N	1.168(4)	C-C-S	112.7(6)
C(1)≡C(2)	1.207(5)	C-S-C	97.4(10)
C(2)-C(3)	1.444(4)	S-C(4)≡N	180 ^{b)}
C(4)-S	1.689(3)	τ (<i>gauche</i>) ^{c)}	53(5)
C(3)-S	1.836(3)	τ (<i>anti</i>) ^{c)}	180 ^{b)}
		δ (<i>gauche</i>) ^{d)}	13(4)
		δ (<i>anti</i>) ^{d)}	20(7)

The molecule exists as a mixture of *anti* (55(6)%) and *gauche* (45(6)%) conformers in the gas phase. Neglecting conformational entropy differences other than the statistical weight of two for *gauche*, this corresponds to an energy difference of 1.24 kJ mol⁻¹, *anti* being marginally the lower-energy form.

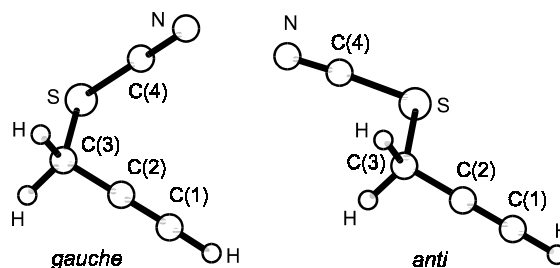
The nozzle temperature was 303 K.

^{a)} 1.4 times the estimated standard errors including the scale error.

^{b)} Assumed.

^{c)} Torsional angle C-C-S-C.

^{d)} The root-mean-square amplitude of the torsional angle.



Midtgaard, T., Gundersen, G., Nielsen, C.J.: J. Mol. Struct. **176** (1988) 159.