

1228
ED

$\text{C}_3\text{H}_5\text{N}_3$

Allyl azide
3-Azido-1-propene

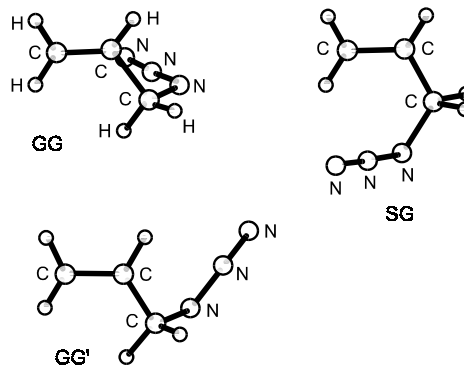
C_1
 $\text{H}_2\text{C}=\text{CH}-\text{CH}_2-\text{N}=\text{N}=\text{N}$

| r_a | \AA^a | θ_α | deg^a |
|--------------------------|----------------|------------------------------|----------------|
| $\text{N}\equiv\text{N}$ | 1.138(4) | $\text{N}=\text{N}=\text{N}$ | 174(5) |
| $\text{N}=\text{N}$ | 1.236(5) | $\text{C}-\text{N}=\text{N}$ | 115.1(14) |
| $\text{C}-\text{N}$ | 1.475(15) | $\text{N}-\text{C}-\text{C}$ | 111.8(34) |
| $\text{C}=\text{C}$ | 1.331(7) | $\text{C}=\text{C}-\text{C}$ | 121.6(30) |
| | | $\tau(\text{C}-\text{N})^b$ | 60(10) |

Analysis of ED data revealed a multiplicity of indistinguishable solutions to the conformational composition consisting of variable amounts of the three conformers SG, GG and GG'; the letters refer to the conformation around the C-C and C-N bonds, respectively. As extremes, the ED data could be interpreted by either a mixture of only two conformers, 73(15)% GG and 27% SG, or a mixture consisting of equal amounts of GG and GG', 87(20)% in total, and 13% SG. A transoid arrangement of the azide chain, $r(\text{C}-\text{C}) = 1.508 \text{ \AA}$, $\theta(\text{C}-\text{C}-\text{H}) = 120.8^\circ$ and torsional angles $\tau(\text{C}-\text{C}) = 0^\circ$ or 120° were assumed. Parameters for the GG conformer assuming the two-conformer model are listed. The nozzle temperature was 293 K.

^a) Unidentified, possibly estimated standard errors.

^b) Torsional angle $\text{C}-\text{C}-\text{N}=\text{N}$.



Possible conformations:

- SG, $\tau(\text{C}-\text{C}) = 0^\circ$,
 $\tau(\text{C}-\text{N}) \approx 60^\circ$;
- GG, $\tau(\text{C}-\text{C}) = 120^\circ$,
 $\tau(\text{C}-\text{N}) \approx 60^\circ$;
- GG', $\tau(\text{C}-\text{C}) = 120^\circ$,
 $\tau(\text{C}-\text{N}) \approx -60^\circ$.

Klaeboe, P., Kosa, K., Nielsen, C.J., Priebe, H., Schei, S.H.: J. Mol. Struct. **176** (1988) 107.