

1113
MW

C₃H₃NO

Propynamide
Propiolamide

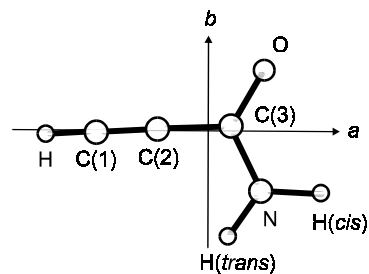
essentially C_s
HC≡C–C(O)–NH₂

r_0	Å	θ_0	deg
C–H	1.055 ^{a)}	H–C≡C	180 ^{a)}
C(1)≡C(2)	1.209 ^{a)}	C≡C–C	180 ^{a)}
C(2)–C(3)	1.47(2)	C–C=O	122.3(20)
C(3)=O	1.219 ^{a)}	O=C–N	124.7 ^{a)}
C(3)–N	1.352 ^{a)}	C–N–H(<i>cis</i>) ^{b)}	118.5 ^{a)}
N–H	1.002 ^{a)}	C–N–H(<i>trans</i>) ^{b)}	120.0 ^{a)}

The molecule has been shown to be essentially planar, with probably zero barrier to NH₂ inversion.

^{a)} Assumed.

^{b)} H(*cis*) is the amido-group hydrogen atom closest to the oxygen; H(*trans*) is the amido-group hydrogen atom farthest from the oxygen.



Little, G.B., Gerry, M.C.L.: J. Mol. Spectrosc. **71** (1978) 321.