

1119
MW

C₃H₃NO₂

2-Propynyl nitrite
Propargyl nitrite

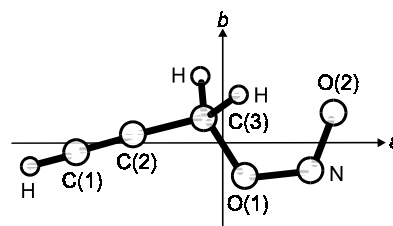
C_s
HC#C-CH2-O-N=O

r_0	Å	θ_0	deg
C(1)–H	1.0562 ^{a)}	H–C(3)–C(2)	109.5 ^{a)}
C(1)≡C(2)	1.2062 ^{a)}	H–C(3)–H	109.5 ^{a)}
C(3)–H	1.1054 ^{a)}	O(1)–N=O(2)	114.8 ^{a)}
O(1)–N	1.398 ^{a)}	C(2)–C(3)–O(1)	107.9(5)
N=O(2)	1.182 ^{a)}	C(3)–O(1)–N	113.6(5)
C(2)–C(3)	1.472(8)	C(3)–O(1)–N=O(2)	0 (<i>cis</i>)
C(3)–O(1)	1.437(4)	C(2)–C(3)–O(1)–N	180 (<i>trans</i>)

Atom	a_s [Å]	b_s [Å]
N	1.776	–0.536

The C(3)–C(2)≡C(1)–H skeleton is linear.

^{a)} Assumed.



Endo, K., Furuhashi, A.: Nippon Kagaku Kaishi (1988) 1925.