

1795
MW

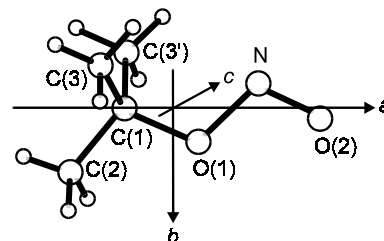
C₄H₉NO₂

***t*-Butyl nitrite**

C_s
O=N=O-C(CH₃)₃

r_s	Å	θ_s	deg
O(2)=N	1.18183(79)	O(2)=N-O(1)	111.59(20)
N-O(1)	1.41751(78)	N-O(1)-C(1)	111.76(17)
O(1)-C(1)	1.43752(62)	O(1)-C(1)-C(2)	103.03(10)
C(1)-C(2)	1.52341(28)	O(1)-C(1)-C(3)	110.09(8)
C(1)-C(3)	1.52902(44)	τ (N-O(1)-C(1)-C(2)) ^a	61.55(10)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(1)	-0.84918	-0.01	0.0
C(2)	-1.81285	1.16988	0.0
C(3,3')	-1.01833	-0.85576	± 1.26253
N	1.49336	-0.32436	0.0
O(1)	0.44057	0.62483	0.0
O(2)	2.55217	0.20065	0.0



^a) Dihedral angle.

Heineking, N., Jäger, W., Gerry, M.C.L.: J. Mol. Spectrosc. **155** (1992) 403.