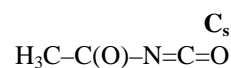
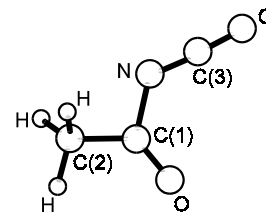


1120 C₃H₃NO₂**Acetyl isocyanate**ED, MW, *ab initio* calculations
(HF/6-31G*, MP2/6-31G*)

r_α	Å ^{a)}	θ_α	deg ^{a)}
C=O (mean)	1.179(3)	C(1)–N=C(3)	128.2(13)
$\Delta(\text{C}=\text{O})$ ^{b)}	0.040 ^{c)}	N–C(1)–C(2)	111.5(4)
C(3)=O	1.159(6)	C(2)–C(1)=O	124.0(23)
C(1)=O	1.199(6)	N–C(1)=O ^{d)}	124.5(23)
N=C(3)	1.199(7)	N–C(3)=O ^{e)}	173.0 ^{c)}
N–C(1)	1.413(7)	H–C(2)–H	107.2(22)
C(1)–C(2)	1.499(11)		
C–H	1.090 ^{c)}		



Only the *cis* conformer (with respect to the C(1)=O and N=C bonds) was observed.
The nozzle was at room temperature.

^{a)} Twice the estimated standard errors.

^{b)} $\Delta(\text{C}=\text{O}) = (\text{C}(1)=\text{O}) - (\text{C}(3)=\text{O})$.

^{c)} Assumed from *ab initio* calculations.

^{d)} Dependent parameter.

^{e)} C(3)=O is bent away from the C(1)=O bond.

Mack, H.-G., Oberhammer, H., Della Védova, C.O.: J. Mol. Struct. **265** (1992) 359.

MW

r_0	Å ^{a)}	θ_0	deg ^{a)}
C(3)=O	1.171 ^{b)}	C(1)–N=C(3)	126.1(20)
C(1)=O	1.226 ^{b)}	N–C(1)–C(2)	114 ^{b)}
N=C(3)	1.207 ^{b)}	C(2)–C(1)=O	124 ^{b)}
N–C(1)	1.460(20)	N–C(3)=O	180 ^{b)}
C(1)–C(2)	1.497 ^{b)}	H–C(2)–H	110.5 ^{b)}
C–H	1.086 ^{b)}		

^{a)} Uncertainties were not estimated in the original paper.

^{b)} Assumed.

Landsberg, B. M., Iqbal, K.: J. Chem. Soc., Faraday Trans. II **76** (1980) 1208.