

1070
MW

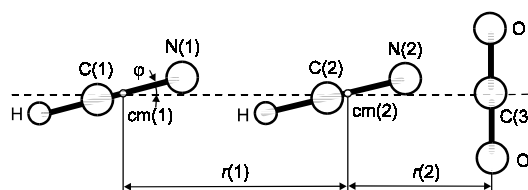
$\text{C}_3\text{H}_2\text{N}_2\text{O}_2$

Carbon dioxide – hydrogen cyanide (1/2)
(weakly bound complex)

C_{2v}
(effective symmetry class)
 $\text{CO}_2 \cdot (\text{HC}\equiv\text{N})_2$

r_0	\AA^{a}	θ_0	deg^{a}
$\text{C}(1)\equiv\text{N}(1)$	1.1238(10)	φ^{b}	13.37(30)
$\text{C}(2)\equiv\text{N}(2)$	1.2841(10)		

Atom	Position [\AA]
C(1)	-5.3515
N(1)	-4.2277
C(2)	-0.9557
N(2)	0.3284
C(3)	3.1714



Isotopic species employed	12-12-CO ₂ ^{c)}	14-14-CO ₂ ^{d)}	all eight species
	12-13-CO ₂	14-15-CO ₂	
	13-12-CO ₂	15-14-CO ₂	
	13-13-CO ₂	15-15-CO ₂	
	12-12- ¹³ CO ₂		

$r_0(1)$ [\AA]	4.3829	4.4875	4.4365(30) ^{a)}
$r_0(2)$ [\AA]	3.6012	3.5042	3.5516(30) ^{a)}

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

^{b)} Average deviations of the $\text{H}-\text{C}(1)\equiv\text{N}(1)$ axis from the principal inertial axis of the trimer.

^{c)} Only carbon isotopes are specified (all nitrogens are ¹⁴N).

^{d)} Only nitrogen isotopes are specified (all carbons are ¹²C).

Ruoff, R.S., Emilsson, T., Chuang, C., Klots, T.D., Gutowsky, H.S.: J. Chem. Phys.

90 (1989) 4069.