

1499
MW

C_4HNO_6

Hydrogen cyanide – carbon dioxide (1/3)
(weakly bound complex)

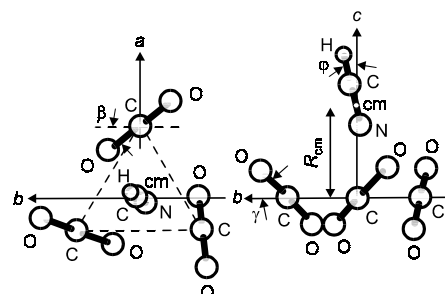
C_3
(effective symmetry class)

$\text{HCN} \cdot (\text{CO}_2)_3$

r_s	$\text{\AA}^a)$	θ_s	$\text{deg}^a)$
C–H	1.074(1)	φ	10.30(30)
C \equiv N	1.1365(30)	γ	$\pm 36.9(5)$
R_{cm}	2.7588(30)		
C...C	3.7968(50)		

Atom or center of mass	$a_s [\text{\AA}]$	$c_s [\text{\AA}]$
H		3.914
C(HCN)		2.8403
cm(HCN)		2.2901
N		1.7038
cm($(\text{CO}_2)_3$)		-0.4687
C(CO_2)	2.1921	

^{18}O species			
r_0	$\text{\AA}^a)$	θ_0	$\text{deg}^a)$
R_{cm}	2.797(17)	β	32.5(10)
C...C	3.814(6)	γ	-28.9(11)



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

Gutowsky, H.S., Hajduk, P.J., Chuang, C., Ruoff, R.S.: J. Chem. Phys. **92** (1990) 862.