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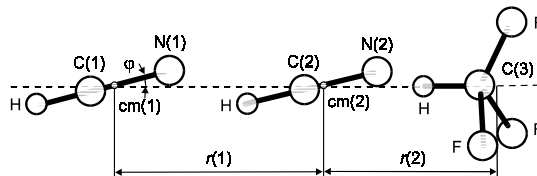
$\text{C}_3\text{H}_3\text{F}_3\text{N}_2$

Fluoroform – hydrogen cyanide (1/2)
(weakly bound complex)

C_{3v}
(effective symmetry class)
 $\text{HCF}_3 \cdot (\text{HC}\equiv\text{N})_2$

r_0	\AA^a	θ_0	deg^a
$\text{C}(1)\equiv\text{N}(1)$	1.1268(10)	φ^b	12.71(30)
$\text{C}(2)\equiv\text{N}(2)$	1.0706(10)		

Atom	Position [\AA]
C(1)	-6.4603
N(1)	-5.3335
C(2)	-2.0822
N(2)	-1.0116



Isotopic species employed	12–12– HCF_3^c	14–14– HCF_3^d	all seven species
	12–13– HCF_3	14–15– HCF_3	
	13–12– HCF_3	15–14– HCF_3	
	13–13– HCF_3	15–15– HCF_3	
$r_0(1)$ [\AA]	4.3731	4.4378	4.3982(30) ^a
$r_0(2)$ [\AA]	4.3962	4.3451	4.3765(20) ^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 ^{14}N).

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

Ruoff, R.S., Emilsson, T., Chuang, C., Klots, T.D., Gutowsky, H.S.: J. Chem. Phys.
90 (1989) 4069.