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MW $\text{C}_2\text{H}_3\text{F}_2\text{N}$ **Methyl cyanide – difluorine (1/1)**Acetonitrile – difluorine (1/1)
(weakly bound complex) C_{3v} (effective symmetry class)
(large-amplitude motion) $\text{H}_3\text{C}-\text{C}\equiv\text{N} \cdot \text{F}_2$

Isotopic species	$r_0(R_{\text{cm}})$ [Å]	$r_0(\text{N}\dots\text{F}(\text{i}))^{\text{a)}}$ [Å]	$\theta_0(\alpha)^{\text{b)}}$ [deg]	$\theta_0(\beta)^{\text{b)}}$ [deg]	$k_{\sigma}^{\text{c)}}$ [N m ⁻¹]
$\text{CH}_3\text{C}^{14}\text{N} \cdot \text{F}_2$	4.780(3)	2.748(3)	13.18(14)	20(5) ^{d)}	2.488
$\text{CD}_3\text{C}^{14}\text{N} \cdot \text{F}_2$	4.893(3)	2.747(3)	12.54(15)	20(5) ^{d)}	2.458
$\text{CH}_3\text{C}^{15}\text{N} \cdot \text{F}_2$	4.749(3)	2.749(3)	13.18 ^{e)}	20(5) ^{d)}	2.535

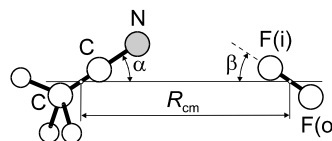
^{a)} F(i) denotes the fluorine atom which is closer to NCCH_3 , of the two.

^{b)} Average values.

^{c)} Intermolecular stretching force constant.

^{d)} Assumed.

^{e)} Assumed unchanged from $\text{CH}_3\text{C}^{14}\text{N} \cdot \text{F}_2$.



Cotti, G., Cooke, S.A., Evans, C.M., Holloway, J.H., Legon, A.C.: Chem. Phys. Lett. **260** (1996) 388.