

Structure Data of Free Polyatomic Molecules

 121
MW

 CH_3NSi

 Silyl cyanide
Silanecarbonitrile

 C_{3v}
 $\text{H}_3\text{Si}-\text{C}\equiv\text{N}$

r_0	Å
$\text{C}\equiv\text{N}$	1.1566(9)
$\text{Si}-\text{C}$	1.8495(7)
$\text{Si}-\text{H}$	1.4716(7)

r_s	Å
$\text{C}\equiv\text{N}$	1.1545(17)
$\text{Si}-\text{C}$	1.8502(19)
$\text{Si}-\text{H}$	1.4691(31)

r_z	Å
$\text{C}\equiv\text{N}$	1.1572(8)
$\text{Si}-\text{C}$	1.8497(6)
$\text{Si}-\text{H}$	1.4740(1)

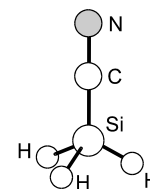
r_e^b	Å
$\text{C}\equiv\text{N}$	1.159(1)
$\text{Si}-\text{C}$	1.848(1) ^{c)}
$\text{Si}-\text{H}$	1.470(2)

θ_0	deg
$\text{H}-\text{Si}-\text{C}$	107.41(3)

θ_s	deg
$\text{H}-\text{Si}-\text{C}$	107.18(64)

θ_z	deg
$\text{H}-\text{Si}-\text{C}$	107.43(1)
$\text{H}-\text{Si}-\text{H}^a$	111.43

θ_e^b	deg
$\text{H}-\text{Si}-\text{C}$	107.4(2)


^{a)} Dependent parameter.

^{b)} Estimated from r_z and *ab initio* results.

^{c)} Uncertainty was not estimated in the original paper.

 Priem, D., Cosleou, J., Demaison, J., Merke, I., Stahl, W., Jerzembeck, W., Bürger, H.:
J. Mol. Spectrosc. **191** (1998) 183.

 Replaces [II/25B\(3, 317\)](#), MW