

120 MW	CH₃N	Hydrogen cyanide – dihydrogen (1/1) (weakly bound complex)	C_{∞v} (effective symmetry class) (large-amplitude motion) H–C≡N · H ₂
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r_0	Å
R_{cm}	3.9613(35) ^{a)}
R_{cm}	4.229(11) ^{b)}

Totally different configurations are taken in the *ortho* and *para* species: H₂ is attached to the hydrogen end of HCN in the *para* species, while to the nitrogen end in the *ortho* species. The nuclear quadrupole interaction constants show that the HCN part executes a floppy motion with a large mean amplitude of about 30° in the *ortho*, as well as *para*, species.

^{a)} For the complex with *ortho* H₂.

^{b)} For the complex with *para* H₂.

Ishiguro, M., Tanaka, T., Harada, K., Whitham, C.J., Tanaka, K.: J. Chem. Phys. **115** (2001) 5155.