79 **CHHeN** **Hydrogen cyanide – helium (1/1)** **$C_{\infty v}$** (quasilinear)
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)
H–C≡N · He

r_0	Å [a])
R_{cm} [b])	4.23(5)

The global minimum occurs at the linear He...H–C–N configuration, and the minimum energy rises monotonically, with large angular-radial coupling, as the HCN orientation angle θ increases from 0 to π. Very large-amplitude radial motion results from zero-point energy that is 75% of the 25 cm^{-1} well depth. The hyperfine data reflect very weak anisotropy in the potential, with $\langle P_2(\cos\theta)\rangle = 0.092$ ($J = 1$) and $\langle P_2(\cos\theta)\rangle = 0.115$ ($J = 2$).

[a]) Uncertainty was not estimated in the original paper.
[b]) Value for $\langle R_{cm}^{-2}\rangle^{-1/2}$, which was derived from an analysis of the Coriolis interaction.

Drucker, S., Tao, F.-M., Klemperer, W.: J. Phys. Chem. **99** (1995) 2646.

The potential surface obtained has a global minimum in the linear configuration (He...H–C≡N) with a well depth of 30.2 cm^{-1}, and a saddle point located in the antilinear configuration (H–C≡N...He), which is higher by 8.91 cm^{-1} in energy than the global minimum. The distance R_{cm} along the minimum energy path shows a strong angular dependence; R_{cm} is 4.169 and 4.040 Å in the linear and antilinear forms, respectively, while it is 3.528 Å in a T-shaped configuration.

Harada, K., Tanaka, K., Tanaka, T., Nanbu, S., Aoyagi, M.: J. Chem. Phys. **117** (2002) 7041.