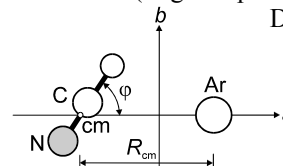


58
MW

CHArN

Hydrogen cyanide – argon (1/1)
(weakly bound complex) C_s
(effective symmetry class)
(large-amplitude motion)
 $D-C\equiv N \cdot Ar$

State	$r_0(R_{cm})$ [\AA] ^{a)}	$\theta_0[\langle\varphi^2\rangle^{1/2}]$ [deg] ^{a) b)}
Σ_0	4.327915(12)	28.03(2)
Σ_1	3.92584(21)	62.82(31)
Π_1	3.88203(15)	61.14(20)



Structural parameters were given for $Ar \cdot DCN$. The intermolecular bending bands $\Sigma_1 - \Sigma_0$ and $\Pi_1 - \Sigma_0$ were observed for $Ar \cdot DCN$, which showed anomalous isotope effects (larger in frequency than those of $Ar \cdot HCN$) on the vibrational frequencies and were attributed to the presence of two minima in the potential function, one corresponding to a linear configuration and the other to a much shallower T-shaped one. The observed rotational constants indicate the shrinkage of the bond length of the complex by $0.402 \sim 0.440 \text{ \AA}$ on the excitation of the van der Waals bending mode, together with the change from the linear form in the ground state to the T-shaped form in the first excited state.

^{a)} Estimated standard errors.

^{b)} See figure for the definition of φ .

Tanaka, K., Bailleux, S., Mizoguchi, A., Harada, K., Baba, T., Ogawa, I., Shirasaka, M.:
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