

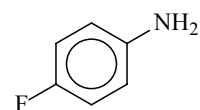
**718**      **C<sub>6</sub>H<sub>6</sub>FN**MW, *ab initio* calculations**4-Fluoroaniline**

4-Fluorobenzenamine

**C<sub>s</sub>**

$$\frac{r_0}{\Delta r(\text{C-N})^{\text{a})}} \quad \text{\AA} \quad 0.177(8)$$

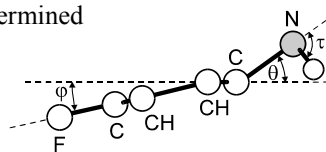
$$\begin{array}{ll} \theta_0 & \text{deg} \\ \Delta\theta^{\text{a})} & 3.34(32) \\ \tau_0^{\text{a})} & 47.39(20) \\ \Delta\alpha^{\text{a})} & 9.16(27) \\ \Delta\varphi^{\text{a})} & 0.67^{\text{b})} \end{array}$$



The potential energy surface and the associated structural relaxation for the amino inversion were determined for the three vibrational modes with lowest energies by combining the observed spectra with *ab initio* and flexible-model quantum calculations. The suitable flexible model was assumed to have the following potential function:  $V(\tau) = B[1 - (\tau/\tau_0)^2]^2$ ,  $\alpha(\text{H-C-H})(\tau) = \alpha_0 + \Delta\alpha(\tau/\tau_0)^2$ ,  $\theta(\tau) = \Delta\theta(\tau/\tau_0)$ ,  $\varphi(\tau) = \Delta\varphi(\tau/\tau_0)$ , and  $r(\text{C-N})(\tau) = r(\text{C-N})(0) + \Delta r(\text{C-N})(\tau/\tau_0)^2$ .  $B$  was determined to be  $599.8 \text{ cm}^{-1}$ .

<sup>a)</sup> See figure and comments for the definition.

<sup>b)</sup> Assumed.



Favero, L.B., Moreschini, P., Caminati, W., Becucci, M., López-Tocón, I., Pietraperzia, G.: Phys. Chem. Chem. Phys. **2** (2000) 1351.

[II/25D \(3, 2236\)](#)