

554 **C₄H₇N**
MW, IR, *ab initio*
calculations

2,5-Dihydro-1H-pyrrole
3-Pyrroline

C_s (axial)
C_s (equatorial)



θ_0	deg	
	axial ^{a)}	equatorial ^{b)}
α_0 ^{c)}	57.89(55)	-56.1(8)
β_0 ^{d)}	21.91(35)	15.8(5)
θ_0 ^{e)}	110.08(4)	110.80(8)
$\Delta\theta$ ^{f)}	0.848(12)	

Ring puckering was analyzed by two-dimensional flexible model calculations. The observed molecular properties were reproduced by a model which involved adjustable parameters for the potential energy surface and the structural relaxation of the C–C–C valence angles. Additional parameters were transferred from *ab initio* calculations. The adjustment of the model to the experimental data yielded an equatorial equilibrium conformation with slightly larger C–C–C valence angle than in the most stable axial conformation.

The potential function used for the flexible model is

$$V(\xi, \eta) = c_{40}(\xi^2 - 1)^2 + c_{04}(\eta^2 - 1)^2 + c_{22}(\xi^2 - 1)(\eta^2 - 1) - c_{11}[(1/4)(\xi^3\eta + \xi\eta^3 - 2) - \xi\eta + 1] \\ - c_{20}[(1/4)(3\xi^3\eta - \xi\eta^3 - 2) - \xi^2 + 1] - c_{02}[(1/4)(3\xi\eta^3 - \xi^3\eta - 2) - \eta^2 + 1],$$

where $\xi = \alpha/\alpha_0$ and $\eta = \beta/\beta_0$. The valence angle C–C–C is assumed to depend on the inversion and puckering angles as follows: $\theta(\text{CCC}) = \theta_0 + (1/2)\Delta\theta(1 - \xi\eta)$. The change in the parameters on deuterium substitution in the imino group is given, for example, by $\delta c_{40} = c_{40}(\text{N-d}) - c_{40}(\text{parent})$.

^{a)} Estimated standard errors.

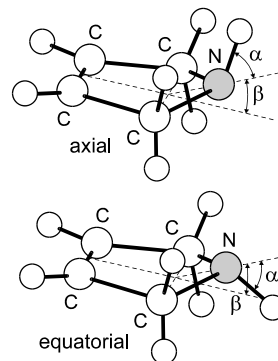
^{b)} Uncertainties were not directly calculated in the original paper.

^{c)} Imino group inversion angle, see figure.

^{d)} Ring puckering angle, see figure.

^{e)} C–C=C bond angles.

^{f)} Relaxation of the C–C=C valence angles.



Dommen, J., Caminati, W., Hollenstein, H., Ha, T.-K.,
Meyer, R., Bauder, A.: J. Mol. Spectrosc. **180** (1996) 369.