

1693  
MW

**C<sub>4</sub>H<sub>7</sub>F**

**Fluorocyclobutane**

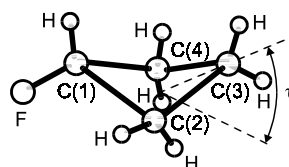
Flexible model parameters <sup>a)</sup>

	cm <sup>-1</sup>	$\theta_0$	deg
$B_0$	425.9(20)	$\tau_0$	29.73(12)
$\Delta E$	642.6(4)	$\alpha_0$	92.4(5)
		$\Delta\alpha_1$	-3.4(5)
		$\Delta\alpha_2$	-0.72(17)
		$\varphi_0$	125.6(4)
		$\Delta\varphi$	-4.4(2)

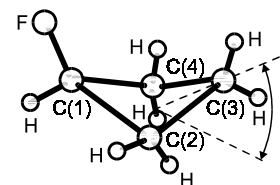
C<sub>s</sub> (axial)  
C<sub>s</sub> (equatorial)



Both the equatorial and the axial forms were detected.



equatorial



axial

<sup>a)</sup> The potential function was assumed to be  $V(\tau) = (1/2) \Delta E (\tau/\tau_0) + B_0 [1 - (\tau/\tau_0)^2]^2$ , where  $\tau$  denotes the puckering angle defined in the figure. The angle  $\alpha(C(2)-C(1)-C(4))$  and the angle  $\varphi$  between the bisector of  $\alpha$  and C(1)-F were both assumed to depend on  $\tau$  as follows:  $\alpha(\tau) = \alpha_0 + \Delta\alpha_1(\tau/\tau_0)^2 + \Delta\alpha_2(\tau/\tau_0)^4$ ,  $\varphi(\tau) = \varphi_0 + \Delta\varphi(\tau/\tau_0)$ .

Caminati, W., Favero, L.B., Maris, A., Favero, P.G.: J. Mol. Struct. **376** (1996) 25.