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Microwave spectrum of the axial conformer and potential energy function of the ring puckering motion in fluorocyclobutane[1]

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Abstract

The microwave spectrum of fluorocyclobutane has been investigated in the 26–40 GHz frequency range. The spectrum of the axial conformer has been assigned for the first time, while measurements of the equatorial species, and of several of its puckering vibrational satellites, have been extended. The energy of the axial conformer is 620(30) cm^{-1} higher than that of the equatorial one. Previously reported potential energy functions of the ring puckering have been corrected, interpreting the available vibrational spacings, the shifts of the rotational constants upon puckering excitation and the centrifugal distortion constants with a flexible model.

1. Introduction

In this paper we are studying the dynamic behavior of fluorocyclobutane (FCB), in particular, its ring puckering motion. The ring puckering is a large amplitude motion typical of saturated four membered rings. The prototype molecule of this series is cyclobutane which has been extensively investigated with respect to this motion. The rotational spectra of the 1-*d* and 1,1-d_2 species, obtained with a waveguide Fourier transform spectrometer [1,2], have been very important in describing the dynamics of the ring puckering. Combined with the available vibrational spacings [3], through a flexible model [4], they gave precise values of the W-shaped potential energy surface and of the structural relaxations accompanying the ring puckering.

In mono substituted cyclobutanes the W-shape of the potential energy surface is lost, and an equatorial–axial-type conformational equilibrium takes place.

In the mono haloderivatives of cyclobutane only the equatorial conformer has been clearly identified by microwave spectroscopy [5]. Cyanocyclobutane is an exception: although only the equatorial conformer was assigned in the first stage [6], the axial conformer was also observed in a second microwave investigation [7]. Later on, using the results on cyclobutane as a guide, detailed information has been obtained on the asymmetric potential energy function of the ring puckering and on the main parameters undergoing structural relaxation [8].

Based on far infrared (FIR) and Raman evidence, and on ab initio calculations, the stability of the axial forms of fluoro- and chlorocyclobutane is

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[1] Dedicated to Professor James E. Boggs on the occasion of his 75th birthday.

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Table 1
Experimental transition frequencies of fluorocyclobutane (MHz)

$J'(Ka', Kc') \leftarrow J''(Ka'', Kc'')$	Ground state	$v = 1$	$v = 2$	$v = 3$	$v = 5$ (ax.)
1 (1, 0)–0 (0, 0)[a]	14525.30				
2 (0, 2)–1 (0, 1)[a]	15266.36	15295.41	15333.42	15385.11	
2 (1, 2)–1 (1, 1)[a]	14482.76	14512.22	14550.90	14603.34	
2 (1, 1)–1 (0, 1)[a]	23075.16				
2 (1, 1)–1 (1, 0)[a]	16227.34	16258.50	16298.9	16353.10	
2 (2, 1)–1 (1, 1)	35026.04				
3 (0, 3)–2 (0, 2)[a]	22683.68	22724.29	22777.71	22851.36	
3 (1, 3)–2 (1, 2)[a]	21671.24	21714.65	21771.78		
3 (1, 2)–2 (0, 2)					32688.85
3 (1, 2)–2 (1, 1)[a]	24281.12	24328.20	24387.84	24468.12	27104.40
3 (2, 2)–2 (2, 1)[a]	23032.56	23078.20	23137.32	23217.24	
3 (3, 1)–3 (2, 1)	31673.20				
3 (3, 0)–3 (2, 2)	32116.50				
4 (0, 4)–3 (0, 3)	29873.23	29922.72	29989.12	30081.32	33689.60
4 (1, 4)–3 (1, 3)	28803.88	28860.52	28935.27	29037.39	32897.90
4 (1, 3)–3 (1, 2)	32259.12	32318.26	32395.50	32499.60	35991.19
4 (1, 3)–4 (1, 4)[a]	8683.52				
4 (2, 3)–3 (2, 2)		30700.30	30778.15	30883.75	34577.90
4 (2, 2)–3 (2, 1)	31477.15	31547.75	31638.55	31758.20	35549.40
4 (3, 2)–3 (3, 1)	30871.50	30934.30	31015.90	31125.80	34851.60
4 (3, 1)–3 (3, 0)	30905.40	30968.80	31052.00	31162.80	34906.20
4 (3, 2)–4 (2, 2)	31067.35	30643.43	30165.05	29626.09	
4 (3, 1)–4 (2, 3)	32380.89	31975.44	31518.83	31003.69	
5 (0, 5)–4 (0, 4)	36836.30	36894.15	36972.50	37082.90	
5 (1, 5)–4 (1, 4)		35942.75	36034.45	36160.25	
5 (1, 4)–5 (1, 5)[a]	12928.32				
5 (2, 4)–4 (2, 3)		38263.25	38358.70	38488.40	
5 (3, 3)–4 (3, 2)	38637.07	38715.83	38818.16	38955.47	
5 (3, 2)–4 (3, 1)	38753.65	38835.68	38941.91	39083.66	
5 (4, 2)–4 (4, 1)	38584.19		38765.03	38902.51	
5 (4, 1)–4 (4, 0)	38586.17		38767.49	38904.94	
5 (3, 3)–5 (2, 3)	29965.41			28483.46	
5 (3, 2)–5 (2, 4)	32944.11		32101.78	31599.30	
5 (4, 2)–5 (3, 2)					29610.65
5 (4, 1)–5 (3, 3)					29868.16
5 (5, 1)–5 (4, 1)					38444.50
5 (5, 0)–5 (4, 2)					38450.95
6 (3, 4)–6 (2, 4)	28290.25	27841.28			
6 (3, 3)–6 (2, 5)		33608.90	33183.37		
6 (4, 3)–6 (3, 3)					29125.56
6 (4, 2)–6 (3, 4)					29880.23
6 (5, 2)–6 (4, 2)					38333.76
6 (5, 1)–6 (4, 3)					38363.37
7 (3, 4)–7 (2, 6)		35395.32	35003.58	34563.32	
7 (4, 4)–7 (3, 4)					28232.59
7 (4, 3)–7 (3, 5)					30039.17

claimed in a recent paper [9]. The axial form of FCB has been indicated to lie 400–500 cm^{-1} higher in energy than the equatorial species. Recently the microwave spectra of both equatorial and axial conformers have been assigned for a related molecule: 1-fluoro-1-silacyclobutane [10]. The equatorial form was found to be more stable by 350 cm^{-1}. All these circumstances have induced us

Table 1 continued

$J'(Ka', Kc') \leftarrow J''(Ka'', Kc'')$	G.S.	$v = 1$	$v = 2$	$v = 3$	$v = 5$ (ax.)
7 (5, 3)–7 (4, 3)					38133.71
7 (5, 2)–7 (4, 4)					38241.62
8 (2, 7)–8 (0, 8)				35359.50	
8 (3, 5)–8 (2, 7)		38175.93			
8 (5, 4)–8 (4, 4)					37783.50
8 (5, 3)–8 (4, 5)					38101.20
9 (2, 8)–9 (0, 9)				39140.65	
9 (5, 5)–9 (4, 5)					37182.20
9 (5, 4)–9 (4, 6)					37981.90
10 (4, 7)–10 (3, 7)		37666.14	36891.14	36017.55	
10 (5, 6)–10 (4, 6)					36189.00
10 (5, 5)–10 (4, 7)					37962.77
11 (2, 9)–11 (2, 10)				30251.55	
11 (4, 8)–11 (3, 8)	35309.40	34595.25	33788.91	32881.68	
11 (5, 7)–11 (4, 7)					34644.65
12 (2, 10)–12 (2, 11)				36683.64	
12 (4, 9)–11 (5, 7)	36739.53				
12 (4, 9)–12 (3, 9)	31693.2	30960.80	30134.71	29207.64	
12 (5, 8)–12 (4, 8)					32429.00
13 (4, 10)–13 (3, 10)	27655.90				
13 (5, 9)–12 (6, 7)	31959.60				
13 (5, 9)–13 (4, 9)					29524.42
13 (5, 8)–12 (6, 6)	32506.50				
14 (3, 11)–14 (3, 12)	28279.10		28922.22	29297.05	
15 (3, 12)–15 (3, 13)	35296.20		35932.91	36297.18	
15 (6, 10)–14 (7, 8)	34870.10				
15 (6, 9)–14 (7, 7)	35037.00				
16 (5, 12)–16 (4, 12)		39164.39	37991.87	36675.23	
17 (4, 13)–17 (4, 14)				26563.38	
17 (5, 13)–17 (4, 13)	35302.80	34249.22	33063.30		
18 (4, 14)–18 (4, 15)	32091.50	32617.18	33210.53	33868.68	
18 (5, 14)–18 (4, 14)	30109.00	29066.76	27898.58		
18 (8, 11)–17 (9, 9)	32237.90	33960.80			
18 (8, 10)–17 (9, 8)	32243.50				
20 (5, 15) 19 (7, 12)		30700.32			
21 (5, 16)–21 (5, 17)			28931.47		
22 (5, 17)–22 (5, 18)	35194.72	35983.5	36876.55		
22 (6, 17)–22 (5, 17)			34222.03		
23 (6, 18)–23 (5, 18)	31056.73	29694.36	28175.99		
25 (6, 19)–25 (6, 20)		30292.88	31429.01		
26 (6, 20)–26 (6, 21)	37680.23	38766.48			
27 (7, 21)–27 (6, 21)	37674.92	35902.76	33927.28		
28 (7, 22)–28 (6, 22)	30793.14	29119.86	27270.38		
29 (7, 22)–29 (7, 23)	30744.12		33492.90		
30 (7, 23)–30 (7, 24)	39616.49				

[a] From Ref. [5].

to search for the rotational spectrum of axial FCB. Estimates on the dipole moment components and on the conformational energies are looking promising for its assignment.

2. Experimental

FCB has been prepared by mixing CaF_2, AgF and chlorocyclobutane in mass ratios 0.6 : 1.8 : 1,

Table 2
Rotational and centrifugal distortion constants of fluorocyclobutane

	Ground state	$v = 1$	$v = 2$	$v = 3$	$v = 5$ (ax.)
A (MHz)	10250.412 (7)[a]	10175.88 (1)	10093.23 (2)	10002.21 (2)	8628.77(7)
B (MHz)	4274.930 (3)	4282.913 (3)	4293.271 (8)	4307.04 (1)	4726.25(6)
C (MHz)	3402.614 (3)	3409.770 (4)	3419.206 (8)	3434.11 (1)	3939.16(8)
Δ_J (kHz)	0.72 (2)	0.67 (1)	0.8 (2)	0.8 (2)	−2. (2)
Δ_{JK} (kHz)	1.74 (7)	0.87 (9)	0.9 (1)	0.4 (2)	10. (1)
Δ_K (kHz)	4.4 (2)	8.1 (1)	7. (1)	4. (2)	−27. (1)
δ_J (kHz)	0.138 (4)	0.121 (6)	0.156 (6)	0.13 (1)	0.7 (1)
δ_K (kHz)	1.7 (1)	2.3 (2)	1.3 (2)	2.0 (3)	−7. (3)
N[b]	52	40	43	37	30
σ (MHz)	0.10	0.11	0.09	0.12	0.21

[a] Errors in parentheses are expressed in units of the last digit.

[b] Number of transitions in the fit.

as suggested in Ref. [5]. The advancement of the chemical reaction has been monitored through the observation of the microwave spectra of both FCB and chlorocyclobutane. This latter spectrum disappeared completely after a few hours. At this point FCB was separated from the reaction mixture by a trap-to-trap distillation under vacuum.

The microwave (MW) spectra were recorded in the frequency range 26–40 GHz with a computer controlled Stark spectrometer mainly based on Hewlett-Packard components, and the frequency measurements are believed to be accurate to better than 0.1 MHz. Recently a new source (KVARZ microwave synthesizer), which can be particularly useful for long scan searches, has been added to the spectrometer.

The radiofrequency-microwave double resonance (rfmwdr) technique [11] was used for the assignment of some transitions. The absorption cell temperature was kept constant, and measured around −15°C.

3. Results and discussion

3.1. Measurement of the rotational spectra

Just a few rotational transitions were reported for the equatorial form (ground and three excited states belonging to the ring puckering) in the previous MW investigation [5]. For this reason we first extended the measurements of the spectrum of the equatorial form up to $J = 30$. In so doing we determined quartic centrifugal distortion constants, useful in obtaining additional information on the potential energy surface of the ring puckering [12].

Then we considered the axial species. The ab initio geometries given in Ref. [9] have been used to calculate trial values of the rotational constants after apportioning well known empirical correction to the C–H and C–C bond lengths [13]. The rfmwdr technique was used to search for the K_a near degenerate doublet 4(3)–3(3), pumping at about 8 MHz. These lines were very weak and rather far away from the calculated values and were found with some difficulty. Several R- and Q-branch transitions were then measured with the conventional Stark modulation technique.

All the experimental frequencies are listed in Table 1. They have been fitted with quartic Watson Hamiltonian [14], obtaining the spectroscopic constants given in Table 2, together with some statistical parameters of the fits.

3.2. Dipole moments of the axial conformer

The dipole moment of the equatorial conformer has already been reported [5]. In order to obtain the conformational energy difference from MW relative intensities we measured the dipole moment also for the axial conformer. Displacements of some Stark lobes which showed a second order Stark effect have been measured as a function of

Table 3
Stark coefficients (Hz cm^2 V^{-2}) and dipole moment components (D) of the axial conformer of fluorocyclobutane

$J'(Ka', Kc') \leftarrow J''(Ka'', Kc'')$	$\|M\|$	$\Delta\nu/E^2$	
		Obs.	Calc.
4 (0, 4) ← 3 (0, 3)	1	−0.34	−0.30
	2	0.99	0.82
4 (1, 3) ← 3 (1, 2)	1	−0.82	−0.91
	2	−1.96	−1.93

$\mu_a = 1.61\ (5)$, $\mu_b = 0^a$, $\mu_c = 1.22\ (22)$ $\mu_{tot} = 2.02\ (17)$

[a] Assumed.

the applied electric field for the transitions. The cell was calibrated with the 3 ← 2 line of OCS ($\mu = 0.71521$ D [15]). The transitions used, their Stark coefficients, and the resulting dipole moment components are listed in Table 3.

3.3. Conformational equilibrium and vibrational spacing

The values of the μ_a dipole moment components, the measured peak intensities (I) and the half widths ($\Delta\nu$) of similar lines of the two conformers have been used to determine the energy difference between the equatorial and axial vibrational ground states:

$$\Delta E_{0,0} = E_{0,0}(\mathrm{Ax}) - E_{0,0}(\mathrm{Eq}) \tag{1}$$

The following formula has been used:

$$\Delta E_{0,0} = KT \cdot \ln\left(\frac{I_{\mathrm{Eq}} \cdot \Delta\nu_{\mathrm{Eq}} \cdot \mu^2_{a,\mathrm{Ax}} \cdot \gamma_{\mathrm{Ax}} \cdot \nu^2_{\mathrm{Ax}}}{I_{\mathrm{Ax}} \cdot \Delta\nu_{\mathrm{Ax}} \cdot \mu^2_{a,\mathrm{Eq}} \cdot \gamma_{\mathrm{Eq}} \cdot \nu^2_{\mathrm{Eq}}}\right) \tag{2}$$

where γ and ν are the line strength and transition frequency respectively. The degeneracy has not been considered in Eq. (1) since it is the same for the two conformers. The value $\Delta E_{0,0} = 610\,(30)$ cm^{-1} has been obtained.

3.4. Potential energy surface for the ring puckering

The experimental data attributed to the ring puckering motion were interpreted by the flexible model approach [12]. This scheme allows the calculation of the rotational and centrifugal distorsion constants, the energies, and the wavefunctions for the overall momentum quantum numbers $J = 0$, 1, 2 in the vibrational excited states. Some of these calculated values can be fitted to reproduce the experimental ones.

The leading coordinate of the ring puckering motion is the angle τ (see Fig. 1) which is zero at the planar configuration of the ring and negative for the equatorial conformation. The potential function which has been assumed is:

$$V(\tau) = \tfrac{1}{2}\Delta E \cdot \frac{\tau}{\tau_0} + B_0 \cdot \left[1 - \left(\frac{\tau}{\tau_0}\right)^2\right]^2 \tag{3}$$

where B_0 and τ_0 are the barrier to ring puckering and the ring puckering angle in the limit of the symmetric double minimum, while the ΔE parameter approximates the energy difference between the two minima.

The relaxation of several structural parameters upon the ring puckering motion was taken into account. We chose the ones that showed a significant variation in the two conformational minima as predicted by ab initio calculations. For $C_2C_1C_4$ angle (α) and for the θ angle between the bisector of α and the C–F bond the dependence on τ was assumed as:

$$\begin{aligned} \alpha(\tau) &= \alpha_0 + \Delta\alpha_1 \cdot \left(\frac{\tau}{\tau_0}\right)^2 + \Delta\alpha_2 \cdot \frac{\tau}{\tau_0} \\ \theta(\tau) &= \theta_0 + \Delta\theta \cdot \frac{\tau}{\tau_0} \end{aligned} \tag{4}$$

These expressions involve the parameters α_0, $\Delta\alpha_1$, $\Delta\alpha_2$, θ_0 and $\Delta\theta$, which together with B_0, τ_0 and ΔE were adjusted to reproduce the experimental data (see above).

For all the other internal coordinates we assumed a linear dependence on τ which reproduces the ab initio values given in Ref. [9] in the two conformational minima.

For this model ten vibrational states were calculated on a grid of 41 mesh points in the range $-70 \leqslant \tau \leqslant 70$ deg [12]. The model parameters were adjusted to fit 22 experimental data: five vibrational energies, three second moments of inertia of the ground state (equatorial conformer), 12 shifts of second moments of inertia and two quartic centrifugal distorsion constants (the ones

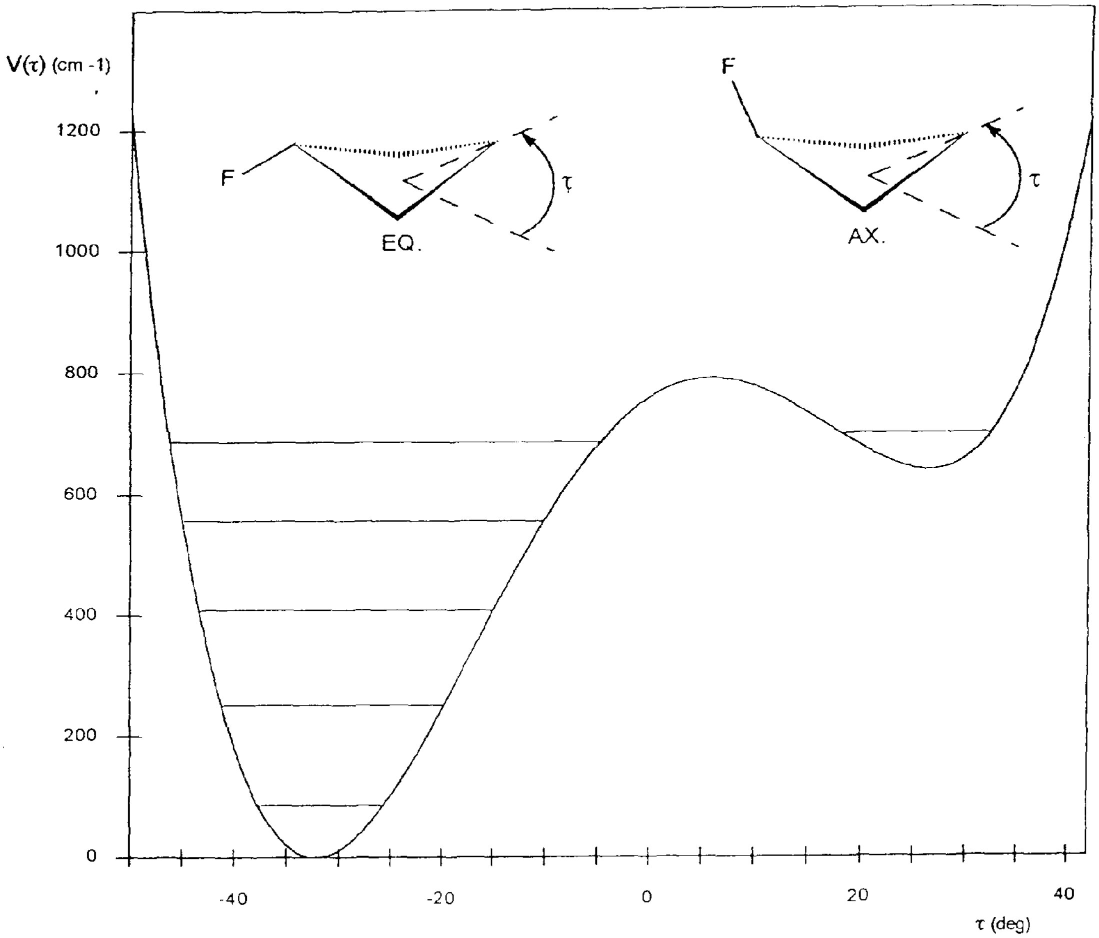

Fig. 1. Ring puckering potential energy function for FCB.

for which the contribution due to the ring puckering is significant).

The second moments of inertia:

$$M_{aa} = \frac{h}{16\pi^2} \cdot \left(-\frac{1}{A} + \frac{1}{B} + \frac{1}{C}\right) \quad \text{etc.} \qquad (5)$$

and their shifts in the excited states relative to the ground state:

$$\Delta M_{gg} = M_{gg}(\nu) - M_{gg}(0) \qquad (g = a, b, c) \qquad (6)$$

have been chosen to refine the model because they reflect the changes in molecular extension along the principal axes and suggest that the structural parameters are relaxed upon ring puckering excitation.

The estimated errors σ on the experimental data were used so as to define the relative weights in the least squares fit.

The results of the flexible model calculations are given in Table 4. In Fig. 1 the potential energy function and the energy levels are illustrated. This function is quite different from that of Ref. [9]. Our model sets four vibrational excitated states in the equatorial well of energy lower than

Table 4
Flexible model results for fluorocyclobutane

$v_u \leftarrow v_l$	Exptl.	Calc.
Vibrational transitions (cm^{-1})		
1–0	166.44[a]	166.48
2–1	157.25[a]	157.39
3–2	146.50[a]	146.24
4–3	130.94[a]	131.06
5–0	610 (30)	614.42

g	Exptl.	Calc.
Second moments of inertia M_{gg} (u Å^2) ($v = 0$, equatorial)		
a	108.721	108.728
b	39.805	39.767
c	9.498	9.376

v	g	Exptl.	Calc.
Shifts of second moments $M_{gg}(v) - M_{gg}(0)$ (u Å^2)			
1	a	−0.447	−0.540
	b	0.135	0.135
	c	0.226	0.138
2	a	−0.996	−1.193
	b	0.276	0.286
	c	0.492	0.314
3	a	−1.690	−2.038
	b	0.414	0.462
	c	0.809	0.557
5 (Ax.)	a	−20.392	−20.357
	b	0.163	0.070
	c	9.104	8.917

v		Exptl.	Calc.
Centrifugal distortion constants (kHz)			
Axial	Δ_{JK}	10.5	10.38
	Δ_K	−27.1	−29.58

Flexible model parameters			
B_0 (cm^{-1})	425.9 (20)	$\Delta\alpha_1$ (deg)	−3.4 (5)
ΔE (cm^{-1})	642.6 (4)	$\Delta\alpha_2$ (deg)	−0.72 (17)
τ_0 (deg)	29.73 (12)	θ_0 (deg)	125.6 (4)
α_0 (deg)	92.4 (5)	$\Delta\theta$ (deg)	−4.4 (2)

[a] From Ref. [9].

that of the axial state. The axial well is higher in energy and very small, so only the axial ground state ($v = 5$) is localized there.

For these reasons we had to reassign the $5 \leftarrow 3$ vibration transition of Ref. [9] as $4 \leftarrow 3$. We did not locate the $6 \leftarrow 4$ transition reported in Ref. [9], but in the FIR spectrum of Fig. 2 of Ref. [9] the corresponding peak is very small.

Our model takes into account some new and very important pieces of information: the rotational and centrifugal distortion constants of the axial conformer. Furthermore the rotational and centrifugal constants of the assigned states in the equatorial well have been considered in the fitting. In addition the reduced masses of our model are functions of τ in a dynamic way.

4. Conclusions

The spectrum of the axial conformer of FCB has been assigned. The corresponding spectroscopic constants allowed a considerable improvement of the description of the potential energy function of the ring puckering.

A flexible model has been used to describe the ring puckering motion. Three potential energy parameters and five parameters connected to the structural relaxation upon the motion were determined. The observed vibrational spacings, the variations of rotational constants upon vibrational excitation and conformational change, and the centrifugal distortion constants have been satisfactorily reproduced.

Important structural differences with respect to the ab initio geometries [9] have been observed. For instance the equilibrium puckering angles τ_0 for the equatorial and axial conformers were determined to be 32.13° and 26.37° respectively, so that $\Delta\tau_0$ (the change in going from axial to equatorial) is 5.76°. The theory on the 6-31G* level predicts only 4° for this difference.

The potential energy parameter B (454.9 cm^{-1}) is similar to that of cyclobutane (504.7 cm^{-1}, Ref. [2]), but the barrier heights in going from the axial and from the equatorial wells to the planar configuration are very different (152.4 and 792.0 cm^{-1}, respectively). The corresponding values for the related molecule 1-fluoro-1-silacyclobutane [10] are significantly lower, but the shape of the potential energy function, apart the vibrational spacings, is very similar for the two molecules.

Based on the results discussed in the present paper it seems interesting to reinvestigate the MW spectrum of chlorocyclobutane since observation of the axial conformer should be possible.

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