1218 *Russian Chemical Bulletin, International Edition, Vol. 50, No. 7, pp. 1218—1222, July, 2001*

$S_1 \leftarrow S_0$ Vibronic spectrum and structure of 2,2-difluoroethanal in the S_1 state

I. A. Godunov,★ N. N. Yakovlev, E. K. Dolgov, and A. V. Abramenkov

Department of Chemistry, M. V. Lomonosov Moscow State University,
Leninskie Gory, 119899 Moscow, Russian Federation.
Fax: +7 (095) 932 8846. E-mail: godunov@phys.chem.msu.ru

The vibronic spectrum of the 2,2-difluoroethanal vapor was recorded using a multipass optical cell with an optical length of at least 140 m. The spectrum in the region of 300—364 nm was assigned to the $S_1 \leftarrow S_0$ electronic transition (from the ground S_0 to the first excited singlet S_1 electronic state); the vibrational structure of the spectrum was analyzed. The spectrum bands were assigned to two systems of vibronic transitions, namely, transitions between the levels of the *cis*-conformer (S_0) and of the S_1 conformers, with the origins (0_0^0 transitions between the zero vibrational levels of conformers) at 29192 and 29087 cm^{-1}, respectively. Analysis of the spectrum showed that the $S_1 \leftarrow S_0$ electronic excitation of the *cis*-conformer was followed by rotation of the CHF_2 top and pyramidal distortion of the carbonyl fragment. A number of fundamental frequencies were found for S_1 conformers, in particular, torsion and inversion energy levels. The experimental data are in satisfactory agreement with the results of quantum-chemical calculations for the 2,2-difluoroethanal molecule in the S_0 and S_1 states.

Key words: vibronic spectra, ground and excited electronic states, carbonyl compounds, internal rotation, inversion, conformers, vibration frequencies.

Previously,[1,2] in a study of the conformationally flexible molecules of carbonyl compounds with tops of C_s symmetry in the ground state (S_0) and singlet (S_1) and triplet (T_1) lower electronically excited states, we investigated the $S_1 \leftarrow S_0$ and $T_1 \leftarrow S_0$ vibronic spectra of 2-chloroethanal. The results obtained are generally in good agreement with the data of *ab initio* quantum-chemical calculations.[3,4]

In addition, we studied[5] vibrational and vibromic spectra of 2,2-difluoroethanal (DFE) and performed *ab initio* quantum-chemical calculations for the DFE molecule in the S_0, T_1, and S_1 states.

The *ab initio* calculations[5] for the DFE structure in the S_0 state carried out by various methods showed that the molecule exists as a single stable *cis*-conformer: the H atom of the top occupies the *cis*-position with respect to the O atom (Fig. 1).

The potential energy surface (PES) of DFE in the S_1 state (calculated by the multi-configuration SCF method in the full active space, CASSCF (6e, 5MO), using the AO 6-31G** basis set) has a much more complex shape: six minima correspond to three pairs of enantiomers (see Fig. 1). Thus, excitation of the DFE molecule from the S_0 to the S_1 state should induce a pyramidal distortion of the carbonyl CCHO fragment and rotation of the CHF_2 top. It can be expected that transitions from the vibrational levels of *cis*-DFE (S_0 state) to the vibrational levels of DFE conformers **1** and **3** (S_1 state), designated below for short by **1**,**3**←*cis*, will be manifested in the vibronic spectrum.

The orientations of the top relative to the carbonyl frame in *cis*-DFE (S_0 state) and in conformer **2** (S_1 state) differ by almost 180° (see Fig. 1); therefore, **2**←*cis* vibronic (optical) transitions are very unlikely.

This work is an experimental study of the $S_1 \leftarrow S_0$ vibronic spectrum and the structure of DFE molecule in the S_1 state.

Experimental

2,2-Difluoroethanal was prepared by reduction of 2,2-difluoroacetic acid with lithium hydride using a previously described procedure.[6] Prior to recording the spectrum, the sample was additionally purified by passing through calcium chloride *in vacuo* at ≤100 °C, then through a phosphorus oxide layer at ~20 °C, and, finally, by repeated fractional distillation *in vacuo.* The purity of the product was checked by the IR spectrum in the gas phase.

2,2-Difluoroethanal tends to polymerize and is easily hydrolyzable; therefore, the samples synthesized were stored in sealed ampoules at a liquid-nitrogen temperature.

The vibronic absorption spectrum of the DFE vapor in the 300—400 nm range was recorded photographically on a DFS-452 spectrograph equipped with a holographic diffraction grating of 2400 lines mm^{-1} with a theoretical resolving power of 120000. The spectrum was measured using a multipass cell with an optical length from 10 to 140 m at a pressure vapor of 0.5 to 400 Torr. A high-pressure xenon lamp and a Fe—Ne hollow cathode lamp served as the radiation source and reference spectrum, respectively. To prevent photochemical decomposition of DFE during recording the spectrum, a light filter holding radiation with wavelengths of ≤300 nm was used. After

Published in Russian in *Izvestiya Akademii Nauk. Seriya Khimicheskaya,* No. 7, pp. 1161—1165, July, 2001.

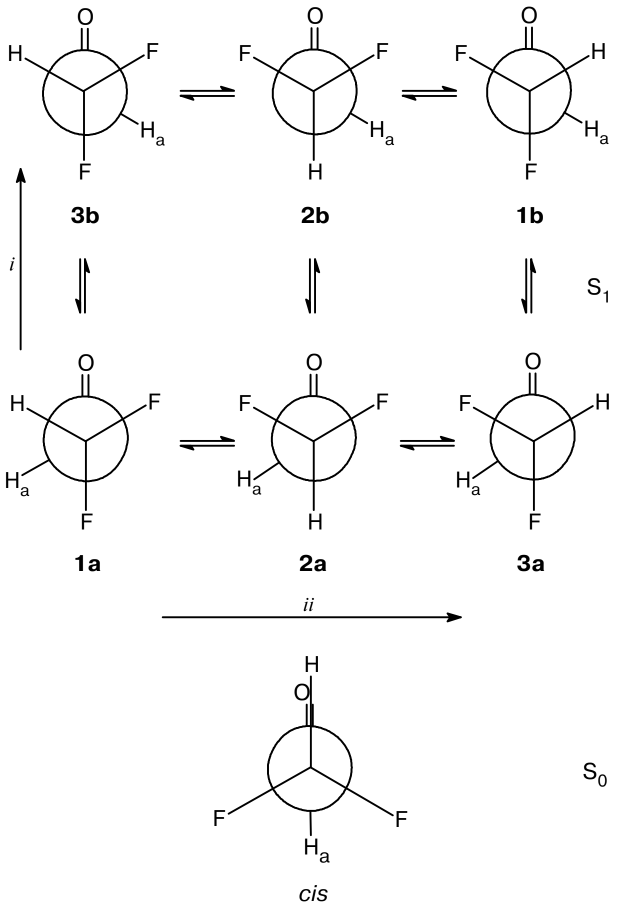

Fig. 1. Newmann projections of DFE conformers in the S_0 and S_1 states. *i*. Inversion. *ii*. Internal rotation.

recording the spectrum, a portion of the DFE vapor was distilled from the multipass cell to a cell for measuring the IR spectrum in order to check the purity of the sample.

The positions of the vibronic bands of the spectrum were measured using an IZA-2 comparator, then the spectrum was obtained as a microdensitometer trace.

The spectrum of DFE has an extended vibrational structure in the region of 33300—25500 cm^{-1} (300—392 nm). The bands in the region of wavenumbers below 30000 cm^{-1} are rather sharp; the error of measurement of the positions of these bands does not exceed 1—2 cm^{-1}. In a higher-frequency region, the bands become diffuse and the accuracy of their measurement gradually decreases to 5 cm^{-1}.

The spectral pattern in the higher-frequency region of 33300—27500 cm^{-1} (300—364 nm), which is partly shown in Fig. 2, differs substantially from the low-frequency region of 28200—25500 cm^{-1} (355—392 nm). In addition, the spectrum in the low-frequency region is markedly less intense than that in the high-frequency region. The low-frequency region was recorded at the maximum optical length and the maximum DFE vapor pressure.

The high-frequency and low-frequency regions of the spectrum were assigned to the $S_1 \leftarrow S_0$ and $T_1 \leftarrow S_0$ electronic transitions of DFE, respectively, in accordance with the data (the positions and relative intensities of similar electronic transitions) for molecules of other aldehydes.[7—11]

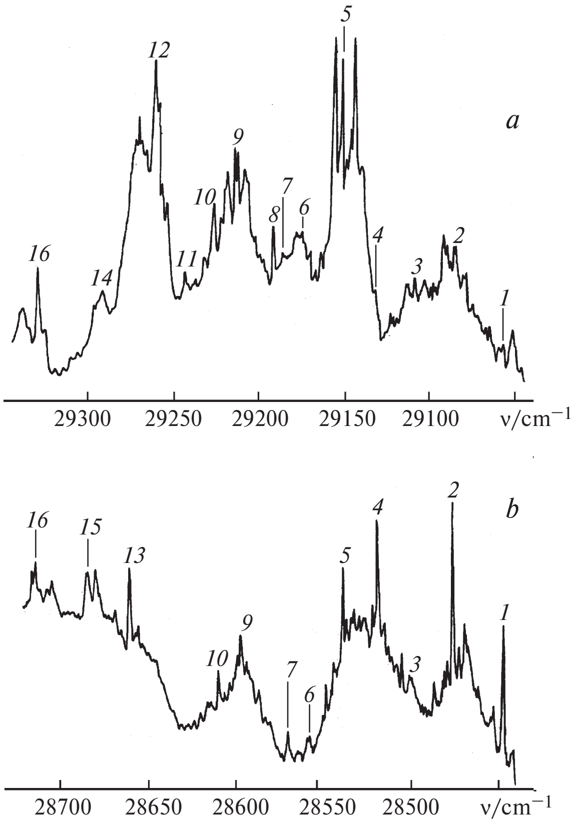

Fig. 2. Microdensitometer traces of sections of the DFE spectrum: (*a*) region of the 0_0^0 transitions of conformers **1** and **3**; (*b*) torsion-inversion transitions common to conformers **1** and **3**. Band numbering coincides with that given in Table 1. The triple bands were measured on the basis of the central peak, while other bands were determined on the basis of the most intense peak.

The results of analysis of the $S_1 \leftarrow S_0$ vibronic spectrum are presented below. The $T_1 \leftarrow S_0$ vibronic spectrum of DFE was published elsewhere.[12]

Results and Discussion

The $S_1 \leftarrow S_0$ spectrum consists of a series of repeating groups of bands of two types (see Fig. 2). The spaces between the bands within the groups mainly coincide (see Fig. 2). However, the first group (see Fig. 2, *a*) contains a number of additional bands absent from the second group (see Fig. 2, *b*); first, this is a very intense band at 29261 cm^{-1} (No. *12*, see Fig. 2, *a*), which does not have an analog in the second group. In addition, the rotational contours of bands in the first and second groups are markedly different.

The above-mentioned differences can be interpreted relying on the results of *ab initio* calculations for the structure of the DFE molecule in the S_1 state and the calculations of the rotational contours of vibronic bands.

The *ab initio* calculations for the DFE molecule in the S_1 state show that conformer **3** has the lowest energy but the energy difference between the zero vibrational levels of conformers **1** and **3** is only 57 cm^{-1}. The energy of the zero level of conformer **1** is somewhat lower than the potential barrier to inversion separating conformers **1** and **3**; however, the region of localization of the corresponding wave function indicates that this level is simultaneously the first inversion level of the system of conformers **1** and **3**. The second inversion level of the system of conformers **1** and **3** (456 cm^{-1}) is located above the inversion barrier.

Thus, according to *ab initio* calculations, the bands corresponding to the **1**←*cis* and **3**←*cis* transitions are expected to occur close to each other and might form one group; the groups of bands related to transitions to high inversion levels (common to conformers **1** and **3**) can comprise only bands common to conformers **1** and **3**. Therefore, the number of bands in these groups should be markedly smaller.

Additional information useful for the assignment of bands in groups (see Fig. 2) can be gained from calculations of rotational contours.

Figure 3 presents the rotational contours of *A*, *B*, and *C* types for the **1**←*cis* and **3**←*cis* systems of the DFE molecule calculated using a program similar to that described previously.[13] The equilibrium geometric parameters of DFE conformers in the S_0 and S_1 states found using the CASSCF method were employed in the calculations.[5]

Since conformers **1** and **3** contain no elements of symmetry, the spectrum should exhibit hybrid ($A + B + C$) bands. The experimental rotational contours of the first-group bands (with three peaks) bear resemblance to the ($A + B + C$)-type bands calculated for the **1**←*cis* and **3**←*cis* transitions; in addition, the very intense band No. *12* of the first group (29261 cm^{-1}) is similar to the *A*-type band observed for conformer **1**. Earlier,[1] good agreement between the calculated and experimental rotational contours of the bands of the $S_1 \leftarrow S_0$ spectrum of 2-chloroethanal conformers was attained when the geometric parameters in the S_1 state ($q(S_1)$) were estimated using the formula $q(S_1) = q(S_0) + \Delta q$, where $q(S_0)$ are the experimental geometric parameters of the conformers in the S_0 state and Δq are the difference between the corresponding geometric parameters of conformers in the S_1 and S_0 states calculated by the CASSCF method. However, in the case of DFE, we were unable to attain a good agreement between the calculated and experimental values, apparently, due to the lack of experimental geometric parameters of DFE conformers in the S_0 state.

In view of the aforesaid, we assigned the bands of the first group (see Fig. 2, *a*) to the torsion transitions of conformers **1** and **3**, while the bands of the second group (see Fig. 2, *b*) were assigned to transitions to the torsion-inversion levels common to conformers **1** and **3** (Table 1*; the reasons for assigning the band at 28477 cm^{-1} to the 13_2^4 inversion transition are considered below). When assigning the bands listed in Table 1, we used the energies of the 15_1, 15_2, 15_3, 15_4, and 15_5 torsion levels of the *cis*-conformer found[12] in analysis of the $T_1 \leftarrow S_0$ spectrum of DFE, namely, 80, 155, 224, 284, and 340 cm^{-1}, respectively.

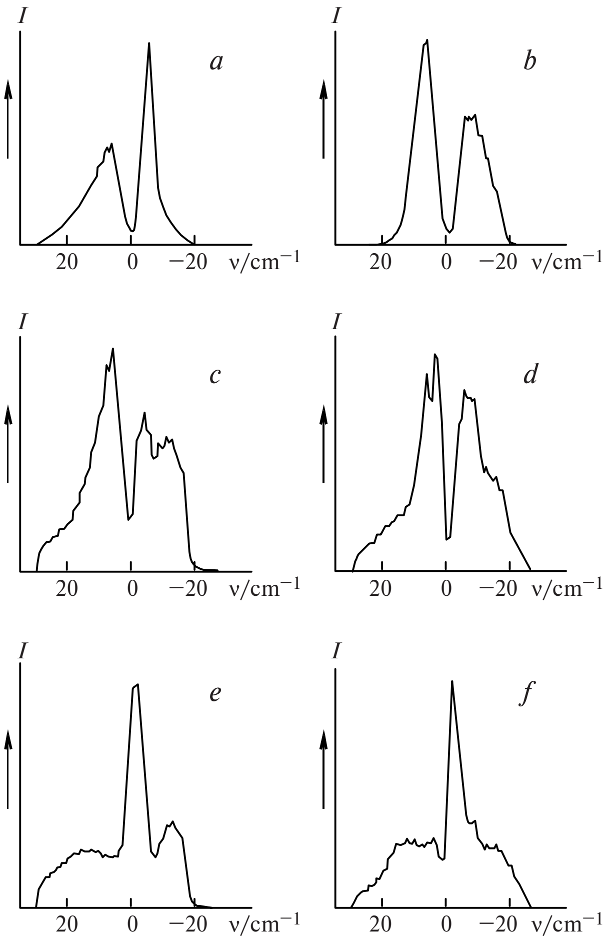

Fig. 3. Calculated rotational contours of the vibronic bands of the *A* (*a*, *b*), *B* (*c*, *d*), and *C* types (*e*, *f*) for **1**←*cis* (*a*, *c*, *e*) and **3**←*cis* (*b*, *d*, *f*) systems. Slit width 0.8 cm^{-1}, temperature 298 K, rotational constants: $A'' = 0.320768$, $B'' = 0.130217$, $C'' = 0.101778$ cm^{-1} (*cis*); $A' = 0.327198$, $B' = 0.133886$, $C' = 0.100109$ cm^{-1} (**1**) and $A' = 0.325963$, $B' = 0.129633$, $C' = 0.100254$ cm^{-1} (**3**).

The assignment of bands at 29192 and 29087 cm^{-1} to the origins of the **1**←*cis* and **3**←*cis* electronic transitions (*i.e.*, to the 0_0^0 transitions between the zero vibra-

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* Six minima in the PES of DFE in the S_1 state correspond to three pairs of enantiomers (see above, Fig. 1). Therefore, all vibrational levels are doubly degenerate; for some levels, the degeneracy is eliminated, and the inversion splitting of levels into even (+) and odd (−) components takes place. Below, in assigning the levels, we will use the signs "+" and "−" only in those cases where splitting takes place; otherwise, these signs are omitted for short.

Table 1. Wavenumbers (reduced to vacuum) (ω_i/cm^{-1}) and assignment of vibronic bands of DFE of the first (*A*) and second (*B*) type characteristic groups

Band	*A*			*B*		
	ω_i	$\omega_i - \omega_0$	Assignment	ω_i	$\omega_i - \omega_0$	Assignment
1	29058	−29	15_2^1(**3**)	28448	−29	$13_2^4 15_2^1$(**1**, **3**)
2	29087	0	0_0^0(**3**)	28477	0	13_2^4(**1**, **3**)
3	29110	23	15_3^2(**3**)	28502	25	$13_2^4 15_3^2$(**1**, **3**)
4	29132	45	15_1^1(**3**)	28521	44	$13_2^4 15_1^1$(**1**, **3**)
5	29153	66	15_4^3(**3**)	28541	64	$13_2^4 15_4^3$(**1**, **3**)
6	29176	89	15_2^2(**3**)	28560	83	$13_2^4 15_2^2$(**1**, **3**)
7	29186	99	15_5^4(**3**)	28573	96	$13_2^4 15_5^4$(**1**, **3**)
8	29192	105	0_0^0(**1**)	—	—	—
9	29213	126	$\left.\begin{matrix}15_0^1\\15_3^3\end{matrix}\right\}$(**3**)	28600	123	$\left.\begin{matrix}13_2^4 15_0^1\\13_2^4 15_3^3\end{matrix}\right\}$(**1**,**3**)
10	29227	140	15_6^5(**3**)	28614	137	$13_2^4 15_6^5$(**1**, **3**)
11	29243	156	15_1^1(**1**)	—	—	—
12	29261	174	15_4^3(**1**)	—	—	—
13	—	—	—	28665	188	$13_2^4 15_2^3$(**1**, **3**)
14	29291	204	15_5^4(**1**)	—	—	—
15	—	—	—	28690	213	$13_2^4 15_3^4$(**1**, **3**)
16	29329	242	15_0^2(**3**)	28720	243	$13_2^4 15_0^2$(**1**, **3**)

Note. The standard designations of the vibronic transitions are used: $N_{v''}^{v'}$, where *N* is the number of vibration, and v'' and v' are vibrational quantum numbers of the ground and excited electronic states; *N* = 13 and 15 correspond to inversion (out-of-plane vibration of the carbonyl fragment) and the torsion vibrations, respectively;[5] 0_0^0 is the transition between the zero vibrational levels of the ground and excited electronic states; the numerals in parentheses denote the number of the conformer (see Fig. 1). Band numbering corresponds to that in Fig. 2.

tional levels of the *cis*-conformer and those of conformers **1** and **3**) (see Table 1) is confirmed by the presence of pseudo-origins at 1200 and 2390 cm^{-1} for conformer **1** and at 1207, 2399, and 3582 cm^{-1} for conformer **3**, which can be unambiguously assigned to the stretching C=O modes (ν'_3 and the $2\nu'_3$ and $3\nu'_3$ overtones) because these frequencies are highly typical of n→π* electron transitions in the molecules of carbonyl compounds.[8] The other pseudo-origins, observed from the origins at 29192 and 29087 cm^{-1}, can be ascribed to the fundamental frequencies of conformers **1** and **3**: ν'_6 (the CC stretching mode), ν'_8 (CF$_2$ scissoring mode), ν'_{10} (CCO bending mode), and ν''_{10} (CCO bending mode) of the *cis*-conformer (Table 2) and to some frequency combinations (not given in Table 2). The band at 29192 cm^{-1}, assigned to the 0_0^0 transition of conformer **1**, has a low intensity (see Fig. 2); therefore, the fundamental modes of conformer **1** listed in Table 2 (except for the torsion mode) were calculated as the differences between the most intense bands $N_0^{v'}15_4^3 - 15_4^3$ (v' = 1, 2).

Comparison of the corresponding experimental frequencies for *cis*-DFE and the calculated frequencies for all conformers (see Table 2) shows a satisfactory agreement between the calculated and experimental values.

Table 2. Experimental (I) and calculated (II) frequencies (ν_i/cm^{-1}) of the vibrations of DFE conformers in the S$_1$ and S$_0$ states

Vibration number and form[b]	**1** (S$_1$)[a]		**3** (S$_1$)[a]		*cis*-DFE (S$_0$)[5]	
	I[c]	II[d]	I	II[d]	I	II
ν_3(CO str.)	1200	1137	1207	1108	1770	1797
ν_6(CC str.)	875	1089	840	1190	946	1172
ν_8(CF$_2$ sciss.)	542	622	564	614	605	611
ν_{10}(CCO pl.bend)	258	255	285	261	323 [a]	374
ν_{15}(tors.)	131 [e]	106	126	102	80 [f]	69

[a] This work.

[b] Designations of the vibration forms: str. is stretching, sciss. is scissoring, pl. bend is in-plane bending, tors. is torsion.

[c] The $N_0^1 15_4^3 - 15_4^3$ range, where *N* = 3, 6, 8, and 10 (see the text).

[d] Solution of the vibration problem on the basis of PES calculated by the CASSCF method (6e,5MO) using the AO 6-31G** basis set.

[e] Calculated with allowance for the wavenumbers of the 15_1^1 (see Table 1) and 15_1^0 transitions of *cis*-DFE (see Ref. 12 and the text).

[f] See Ref. 12.

The experimental and calculated energies of the torsion levels of conformers **1** and **3**, together with the $13^4 15^{v'}$ torsion-inversion levels, v' = 1, 2, 3, 4, common to conformers **1** and **3** are presented in Table 3. The agreement between the calculated and experimental values is not very good even for lower torsion levels,

Table 3. Experimental and calculated energy differences (*E*) of the torsion levels (Δ_i) of DFE conformers in the S$_1$ state

Conformer	Δ_i	*E*/cm^{-1}	
		Experiment	Calculation[a]
1	$15^1 - 15^0$	131 [b]	89.1
	$15^2 - 15^0$	–	172.9
	$15^3 - 15^0$	353	250.1(−), 250.4(+)
	$15^4 - 15^0$	439	317.1(−), 320.8(+)
3	$15^1 - 15^0$	126	85.1
	$15^2 - 15^0$	242	165.7
	$15^3 - 15^0$	350	240.6(+), 241.1(−)
	$15^4 - 15^0$	439	304.9(+), 310.9(−)
1, **3** [c]	$13^4 15^1 - 13^4$	123	84.7
	$13^4 15^2 - 13^4$	243	164.7(+), 164.9(−)
	$13^4 15^3 - 13^4$	348	238.5(+), 239.5(−)
	$13^4 15^4 - 13^4$	437	299.3(+), 309.1(−)

[a] Solution of the vibration problem on the basis of PES calculated by the GASSCF method (6e,5MO) using the AO 6-31G** basis set; the signs "+" and "−" designate the even and odd components of the inversion splitting of levels (see the text).

[b] Calculated with allowance for the wavenumbers of the 15_1^1 (see Table 1) and 15_1^0 transitions of *cis*-DFE (see Ref. 12 and the text).

[c] Torsion progression from the 13^4 inversion level common to conformers **1** and **3**.

Table 4. Experimental and calculated energies (E) of the inversion levels of DFE conformers **1** and **3**

Number of the level	E/cm^{-1}	
	Experiment	Calculation[a]
0[b]	0	0
1[c]	105	57.5
2	—	456.0
3	680	674.5(+), 674.6(−)
4	1090	1029.2(+), 1029.3(−)
5	—	1406.4(−), 1406.5(+)
6	1866 (?)	1822.4

[a] See the note[a] to Table 2.

[b] The zero vibration level of conformer **3**.

[c] The zero vibrational level of conformer **1** is simultaneously the first inversion level of the system of conformers **1** and **3**.

although the differences between them are relatively small in magnitude. However, substantially better results have been obtained previously for the torsion levels of the 2-chloroethanal molecule.[1]

The group of bands of the second type is encountered three times in the spectrum and forms pseudo-origins from the 29087 cm^{-1} band (corresponding to the transition from the zero vibrational level of the *cis*-conformer to the zero vibrational level of the conformer **3** lowest in energy): −610 cm^{-1} (the band at 28477 cm^{-1}, see Table 1), −1020 cm^{-1} (the band at 28067 cm^{-1}), and −1534 cm^{-1} (the band at 27553 cm^{-1}). These bands should be assigned to the $13_{v''}^{v'}$ transitions from the excited levels of the out-of-plane CH$_a$ vibration of *cis*-DFE to the high inversion levels common to conformers **1** and **3**. Previously, a value of 850 cm^{-1} has been found[5] in the IR spectrum of DFE for the ν''_{13} mode of the *cis*-conformer. By taking into account also the calculated energies of the inversion levels of DFE conformers **1** and **3** and by performing trial determinations of one-dimensional potentials for the **1**↔**3** inversion from experimental inversion energy levels (using a method reported previously[14]), we assigned the bands at 28477 and 28067 cm^{-1} to the 13_2^4 and 13_2^3 transitions, while the band 27553 cm^{-1} was (tentatively) assigned to the 13_4^6 transition. The experimental energies of the inversion levels calculated from this, together with the values found by *ab initio* calculations, are listed in Table 4. The agreement between calculated and experimental values is quite satisfactory even for relatively high levels (see Table 4). Previously, noticeably greater deviations have been obtained for the corresponding inversion levels of the 2-chloroethanal molecule. It is noteworthy that no bands that could be assigned to transitions of *gauche*-DFE (S_0 state) were found in the spectrum.

The intensity distribution of the bands of torsion transitions in the **1**←*cis* and **3**←*cis* systems (see Fig. 2) as well as the presence of pseudo-origins that could be assigned only to inversion transitions indicate that the $S_1 \leftarrow S_0$ electronic excitation of *cis*-DFE induces rotation of the CHF$_2$ top relative to the carbonyl frame and a pyramidal distortion of the carbonyl fragment.

Thus, experimental study of the $S_1 \leftarrow S_0$ vibronic spectrum of the DFE molecule generally confirmed the results of *ab initio* calculations performed for this molecule in the S_0 (see Ref. 5) and S_1 states and, thus, it demonstrated the applicability of the calculation methods used to the description of fine conformation effects in the molecules of carbonyl compounds in the ground S_0 and excited S_1 electronic states.

The authors are grateful to E. B. Averina for the synthesis of the DFE sample.

This work was supported by the Russian Foundation for Basic Research (Projects No. 98-03-33233a and No. 00-15-97346).

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Received December 26, 2000;
in revised form March 15, 2001