

See discussions, stats, and author profiles for this publication at: <https://www.researchgate.net/publication/272009142>

# Structural features of 1,3,5-trifluorobenzene radical anion, as studied by optically detected ESR spectroscopy and quantum chemistry

ARTICLE *in* RUSSIAN CHEMICAL BULLETIN · NOVEMBER 2014

Impact Factor: 0.48 · DOI: 10.1007/s11172-013-0335-3

CITATION

1

READS

12

## 6 AUTHORS, INCLUDING:



**S. V. Blinkova**

Russian Academy of Sciences

4 PUBLICATIONS 6 CITATIONS

SEE PROFILE



**V. A. Bagryansky**

Russian Academy of Sciences

51 PUBLICATIONS 391 CITATIONS

SEE PROFILE



**Yuri N. Molin**

Russian Academy of Sciences

258 PUBLICATIONS 2,172 CITATIONS

SEE PROFILE

## Structural features of 1,3,5-trifluorobenzene radical anion, as studied by optically detected ESR spectroscopy and quantum chemistry\*

S. V. Blinkova,<sup>a\*</sup> M. M. Vyushkova,<sup>a,b</sup> L. N. Shchegoleva,<sup>c</sup> I. V. Beregovaya,<sup>c</sup> V. A. Bagryansky,<sup>a</sup> and Yu. N. Molin<sup>a</sup>

<sup>a</sup>Voevodsky Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Sciences, 3 ul. Institutskaya, 630090 Novosibirsk, Russian Federation.  
Fax: +7 (383) 330 7350. E-mail: s.v.blinkova@gmail.com

<sup>b</sup>Notre Dame Radiation Laboratory,  
Notre Dame, IN, 46556, USA.  
Fax: +1 (574) 631 8068

<sup>c</sup>N. N. Vorozhtsov Novosibirsk Institute of Organic Chemistry, Siberian Branch of the Russian Academy of Sciences, 9 prosp. Lavrentieva, 630090 Novosibirsk, Russian Federation.  
Fax: +7 (383) 330 9752

The ESR spectrum of 1,3,5-trifluorobenzene radical anion was obtained for the first time using optically detected ESR spectroscopy. Experimental data and results of a quantum chemical study of the potential energy surface (density functional theory B3LYP and BHHLYP methods) are indicative of fast interconversions between nonplanar conformations of this radical anion.

**Key words:** radical anions, fluorobenzenes, electronic structure, optically detected ESR spectroscopy, quantum chemical calculations, density functional theory, B3LYP and BHHLYP functionals.

Fluorobenzene radical ions have been a subject of intensive experimental and theoretical research.<sup>1–4</sup> They are of considerable interest as intermediates whose structures and reactivities often govern the pathways of reactions involving fluoroarenes.<sup>5</sup> In particular, a number of synthetically important reactions of polyfluoroarenes, such as nucleophilic  $S_{\text{RN}}1$ -substitution and reductive dehalogenation proceed through formation of a radical anion.<sup>1,6</sup> The regioselectivity of dehalogenation of polyfluoroarenes is determined by the regularities of fluoride ion elimination from corresponding radical anions.<sup>7</sup> In addition, interest in this type of radical ions is due to specific features of their electronic and molecular structures. Radical anions of different polyfluoroarenes have significantly different electronic structures and molecular geometries, lifetimes, and reactivities.

Polyfluorinated benzene radical anions are nonplanar pseudo- $\pi$ -radicals with F atoms deviating from the benzene ring plane.<sup>2,8</sup> Violation of planarity caused by pseudo-Jahn–Teller distortions is reflected in abnormally large values of hyperfine coupling (HFC) constants in ESR spectra.<sup>2</sup> Out-of-plane deviations are due to strong perturbation of the  $\sigma$ -system of benzene by F atoms, lead-

ing to the appearance of low-lying excited radical anion  $\sigma$ -states.

High sensitivity of  $^{19}\text{F}$  HFC constants to structural parameters makes ESR spectroscopy an efficient tool for investigations of the electronic structure of fluoroarene radical anions. However, short lifetimes of radical anions in solutions make it difficult to obtain a stationary concentration that is sufficient for detection of these species. This drawback can be eliminated using optically detected ESR (OD ESR) spectroscopy where the ESR spectrum is detected from the change in the luminescence intensity of recombination products of radical ion pairs. The sensitivity of OD ESR spectroscopy is a few orders of magnitude higher than that of conventional ESR techniques. This enables selective detection of OD ESR spectra of short-lived radical ions (with lifetimes up to  $10^{-8}$  s) in liquid solutions at ambient temperatures.<sup>9,10</sup>

Recently, 1,2,3- and 1,2,4-trifluorobenzene (TFB) radical anions were studied by OD ESR spectroscopy and the theoretically predicted complex, multi-well structure of the potential energy surface (PES) and corresponding structural flexibility of these radicals<sup>11,12</sup> were confirmed experimentally.

Among partially fluorinated benzene molecules, highly symmetric structure of 1,3,5-TFB draws attention. The 1,3,5-TFB radical anion was not studied for long because attempts to detect and record its ESR spectrum by the

\* Dedicated to Academician of the Russian Academy of Sciences M. P. Egorov on the occasion of his 60th birthday.

matrix isolation technique<sup>13</sup> and in cooled squalane solution by OD ESR spectroscopy<sup>14</sup> failed. The ESR spectrum of 1,3,5-TFB radical cation was recorded in a frozen matrix,<sup>4</sup> but only the HFC constants were reported because the signal was very broad and the spectral features were poorly resolved.

Difficulties in recording ESR spectra of 1,3,5-TFB radical ions can be explained by fast paramagnetic relaxation in the highly symmetric system caused by the Jahn–Teller effect.<sup>15</sup> The 1,3,5-TFB radical anion was detected in magnetically affected reaction yield (MARY)<sup>16</sup> experiments in a solution in dodecane at room temperature with radical cations of deuterated *para*-terphenyl (PTP) and deuterobenzene as counterions. The MARY spectra were used to estimate the HFC constant of three equivalent <sup>19</sup>F nuclei ( $a(3\text{ F}) = 7.2\text{--}7.5\text{ mT}$ ) and the lifetime of the species under study (20 ns).

In this work, the ESR spectrum of 1,3,5-TFB radical anion was for the first time detected by OD ESR spectroscopy and a quantum chemical study of the corresponding PES was carried out. The results obtained are indicative of fast interconversions between nonplanar conformers of the 1,3,5-TFB radical anion.

### Experimental

Optically detected ESR spectroscopy makes it possible to detect radical ion pairs that are formed in dilute nonpolar solutions under the action of c.w.<sup>9,10,17</sup> or pulsed<sup>18,19</sup> ionizing radiation. Experiments involve measurements of the dependence of the recombination fluorescence intensity of a solution on the strength of static magnetic field. As in conventional ESR spectroscopy, an oscillating microwave field is applied to a sample. At low microwave power, an OD ESR spectrum is an equal superposition of the ESR spectra of both partners in the radical ion pair.<sup>9</sup>

Measurements were carried out with an OD ESR spectrometer based on a Bruker ER-200D ESR spectrometer<sup>17</sup> equipped with a source of ionizing radiation (X-ray tube), a photomultiplier to measure the fluorescence intensity, and a microwave power amplifier. The microwave power was 2.5 W and the modulation amplitude was 0.36 mT.

To record an OD ESR spectrum of a radical ion pair, it is necessary that at least one partner have a sufficient quantum yield of fluorescence. Luminophores used in this work were PTP (Aldrich, 99%) and durene (Fluka, purity >99%). The former compound is characterized by a near-unity quantum yield of luminescence and exhibits both electron-donating and electron-withdrawing properties (vertical ionization potential<sup>20</sup>  $I_E = 7.83\text{ eV}$ , electron affinity<sup>21</sup>  $E_A = 0.51\text{ eV}$ ) while the latter one is an electron donor ( $I_E = 8.07\text{ eV}$ ,  $E_A < 0.048\text{ eV}$ ).<sup>22,23</sup> The luminophores and 1,3,5-TFB (Aldrich, purity 97%) were used as received.

The solvents used were squalane (2,6,10,15,19,23-hexamethyltetracosane, Fluka, purity 99%) and 2,6,10,14-tetramethylpentadecane. They were purified by passing through a chromatographic column filled with alumina activated with 10% AgNO<sub>3</sub>.

Prior to experiments, the samples were degassed to about  $10^{-2}$  Torr by four "freeze—pump—thaw" cycles. To determine

the HFC constants, the measured OD ESR spectra were simulated using the WinSim-2002 program.<sup>24</sup> The signal intensity ratios for different radical ions in the spectra were determined by integrating the simulation curves (the procedure is automatically performed by the program after optimization of parameter values). The *g*-factor values were determined from the shifts of the spectra relative to the signal of PTP radical ions<sup>25</sup> characterized by  $g = 2.0027$ .

Quantum chemical studies of the PES of the 1,3,5-TFB radical anion and calculations of HFC constants for stationary structures were carried out at the second-order Møller–Plesset (MP2) level of perturbation theory and within the framework of density functional theory (DFT) with the B3LYP, M06-2X, and BHHLYP functionals and the 6-31+G\* basis set. All calculations were performed with the GAMESS program.<sup>26</sup>

### Results and Discussion

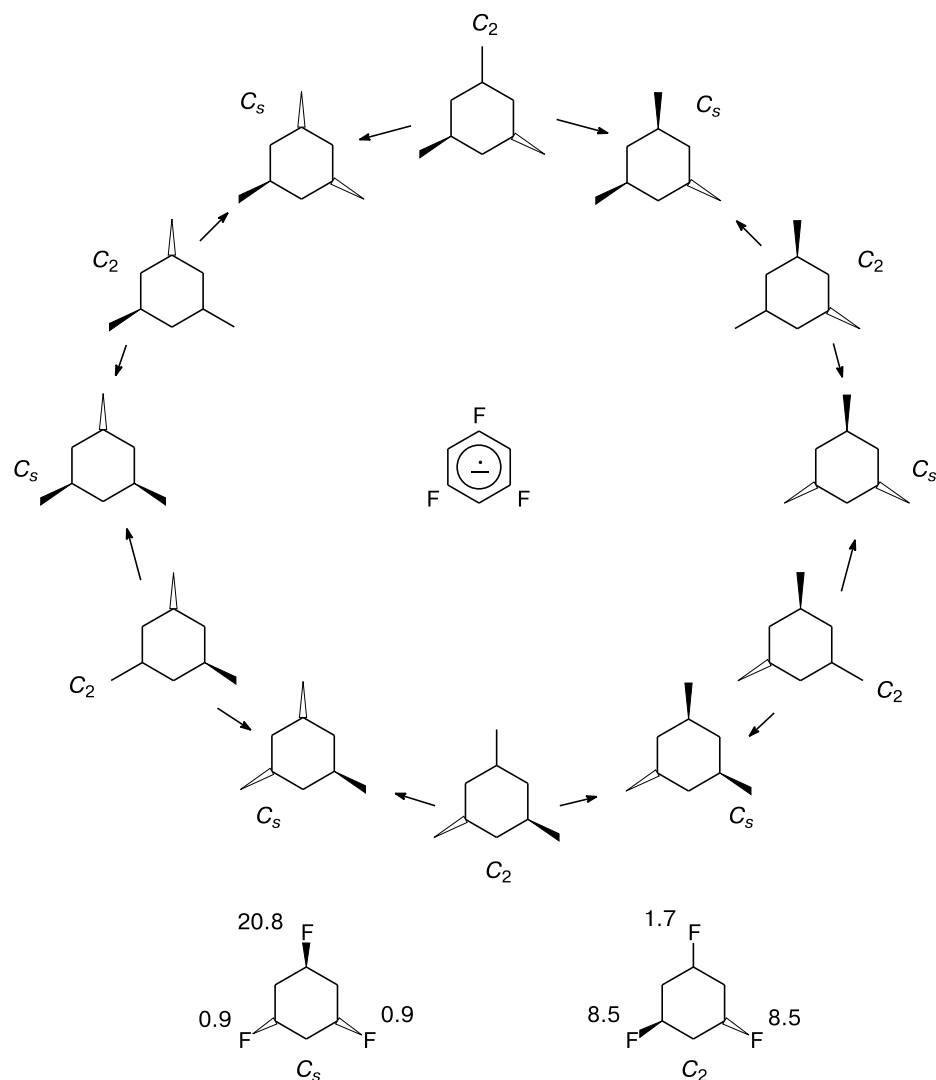
Similarly to hexafluorobenzene radical anion,<sup>2</sup> specific features of the electronic and molecular structure of 1,3,5-TFB radical anion originate from high symmetry of the precursor molecule and from a combination of the Jahn–Teller effect and Jahn–Teller pseudoeffect. For the planar  $D_{3h}$ -structure of this radical anion, the ground state is a <sup>2</sup>E' degenerate  $\pi$ -state; the Jahn–Teller distortion reduces its symmetry to  $C_{2v}$ . Strong vibronic coupling with totally symmetric excited  $\sigma$ -state characteristic of polyfluorobenzene radical anions leads to further symmetry reduction to  $C_s$  and  $C_2$  for the stationary structures with F atoms deviating out of plane.

According to quantum chemical calculations, 1,3,5-TFB radical anion has a highly symmetric PES. It includes six equivalent minima and six transition states that form a closed ring; *i.e.*, this PES is a pseudorotation surface. The energy minimum corresponds to the  $C_s$ -structure (Fig. 1) characterized by very large out-of-plane deviation of one F atom (by about 40°) that has a large HFC constant. The other two F atoms lie almost in the ring plane and are magnetically equivalent. The HFC constants for these atoms are relatively small.

The HFC constants for <sup>19</sup>F nuclei obtained from the BHHLYP calculations for structures with  $C_s$  and  $C_2$  symmetry are presented in Fig. 1. The HFC constants for protons are much smaller, namely, 0.75 mT (1 H) and 0.5 mT (2 H) for the lowest-lying  $C_s$ -structures and 1.2 (1 H) and nearly 0 (2 H) mT for the transition states with  $C_2$  symmetry.

The activation barriers to pseudorotation calculated using the B3LYP/6-31+G\* and BHHLYP/6-31+G\* methods are 3.2 and 4.3 kcal mol<sup>-1</sup>, respectively. They are somewhat higher than those obtained for the other two isomers, *viz.*, 2–4 kcal mol<sup>-1</sup> for 1,2,3-TFB radical anion<sup>11</sup> and 1–2 kcal mol<sup>-1</sup> for 1,2,4-TFB radical anion.<sup>12</sup>

The barriers to pseudorotation and the HFC constants calculated using different methods are listed in Table 1. Unlike 1,2,3-TFB radical anion,<sup>11</sup> the results of calcula-



**Fig. 1.** Pseudorotations in 1,3,5-TFB radical anion and symmetries of structures ( $C_s$  and  $C_2$  corresponds to a minimum on the PES and transition state, respectively). The HFC constants for  $^{19}\text{F}$  nuclei are given in mT. Obtained from BHHLYP/6-31+G\* calculations.

tions for 1,3,5-TFB radical anion are strongly dependent on the computational method used. This is due to peculiar features of the mixing of  $\sigma$ -electronic states of the radical anion on lowering the symmetry from  $D_{3h}$  to  $C_s$ . The de-

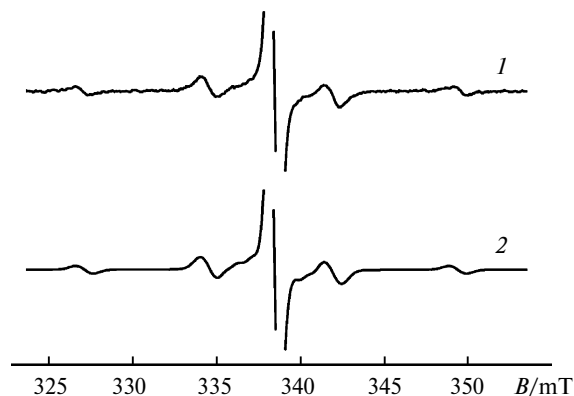
**Table 1.** Barriers to pseudorotation and the HFC constants ( $a_F$ ) calculated for the  $C_s$ -structure of 1,3,5-trifluorobenzene radical anion in the 6-31+G\* basis set

Method	$E(C_s) - E(C_2)$ /kcal mol $^{-1}$	$a_F$		
		mT		
MP2	9.1	24.1 (1 F), 2.3 (2 F)	9.6	
B3LYP	3.2	23.0 (1 F), 1.9 (2 F)	8.9	
M06-2X	3.6	17.3 (1 F), 1.2 (2 F)	6.6	
BHHLYP	4.3	20.8 (1 F), 0.9 (2 F)	7.5	

gree of mixing depends on the energy splitting of the  $\sigma$ -states which in turn depends on the approximation level.

The room-temperature OD ESR spectrum of 1,3,5-TFB radical anion in a solution in squalane containing deuterated PTP as luminophore is shown in Fig. 2. The spectrum exhibits a signal corresponding to a HFC for three equivalent nuclei with the spin 1/2, a HFC constant of 7.4 mT, and a  $g$ -factor of 2.0039. The large HFC constant can be assigned to  $^{19}\text{F}$  nuclei only. The rather large individual linewidth (0.77 mT) masks the proton HFC.

It should be noted that this signal may originate from both the 1,3,5-TFB radical anion and radical cation. However, the isotropic HFC constant for  $^{19}\text{F}$  nuclei in the 1,3,5-TFB radical cation determined in a frozen matrix<sup>4</sup> is 1.7 mT, being much smaller than the value we obtained. The value  $a(3\text{ F}) = 7.4$  mT agrees with the estimated HFC constant of the radical anion in the MARY experiments<sup>16</sup>



**Fig. 2.** OD ESR spectrum (1) of a solution of a mixture of 1,3,5-TFB ( $10^{-2}$  mol L $^{-1}$ ) with PTP ( $1.5 \cdot 10^{-3}$  mol L $^{-1}$ ) in squalane at  $T = 309$  K and the simulated spectrum (2) with the parameters  $a(3\text{ F}) = 7.4$  mT,  $g = 2.0039$ ,  $\Delta H_{\text{peak-to-peak}} = 0.77$  mT (Lorentzian line) of 1,3,5-TFB radical anion,  $\Delta H_{\text{peak-to-peak}} = 4.6$  mT (Gaussian line) for the unresolved signal, HFC = 0,  $\Delta H_{\text{peak-to-peak}} = 0.27$  mT (Lorentzian line) for PTP radical ions.

(7.2–7.5 mT). The spectrum also exhibits a single central line of PTP radical ions and a broad unresolved signal at the center. In the text below, we will show that this is a signal of 1,3,5-TFB radical cation.

Clearly, the experimentally observed equivalence of F atoms (see Fig. 2) is a result of averaging of the HFC constants over three positions through fast pseudorotation because the energy minimum corresponds to the structure characterized by one large and two small HFC constants. Assuming fast interconversion between  $C_s$ -structures, the averaged HFC constant values are 8.9 mT (B3LYP) and 7.5 mT (BHHLYP). The latter value is close to the experimental one (7.4 mT).

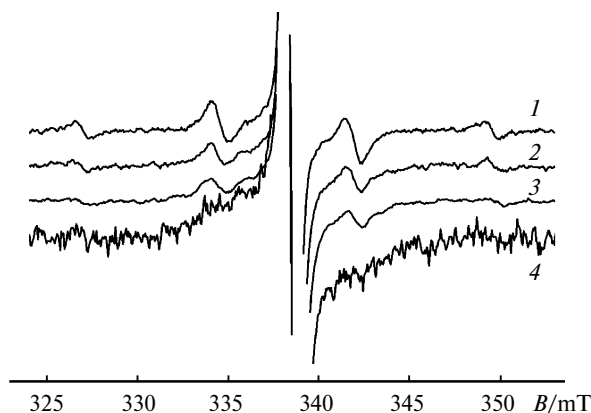
For two isomeric radical anions, 1,2,3-TFB<sup>11</sup> and 1,2,4-TFB,<sup>12</sup> the room-temperature HFC constants differ appreciably from the value obtained by averaging over the structures corresponding to global energy minima and approach this value on lowering the temperature. Temperature variations of the HFC constants of these radical anions are in good agreement with the model for fast classical motion of nuclei along a pseudorotation path, according to which the observed HFC constant is a weighed mean taken over the pseudorotation path, with statistical weights determined by the Boltzmann distribution. As temperature decreases, the statistical weight of high-energy structures is reduced and therefore the observed mean HFC constant approaches the mean value taken over the minimum-energy points only. In this model, coincidence of the HFC constants obtained by averaging over all points and over the energy minima points indicate that the mean value taken over all structures with potential energies exceeding the minimum energy by about  $kT$  differs only slightly from the mean taken over the energy minima. This is the case for 1,3,5-TFB radical anion, where mean

$a_F$  values taken over transition states and over energy minima differ by only 20%. Clearly, the observed HFC should depend only slightly on temperature.

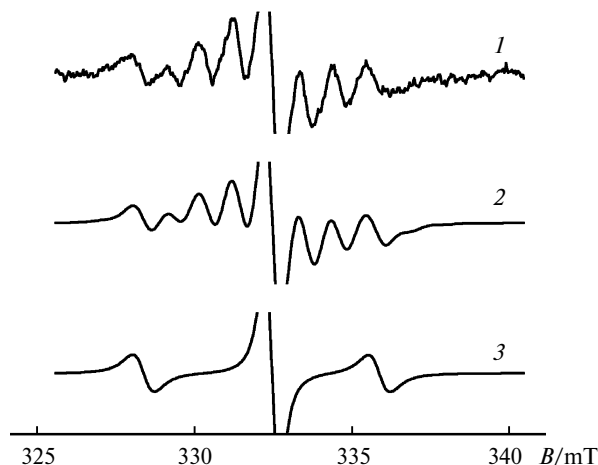
To check this assumption, we studied the temperature dependence of the OD ESR spectrum in the range from 257 to 309 K (Fig. 3). Indeed, the observed HFC constant remained unchanged in this temperature range. There is an interesting feature of the temperature variations of the OD ESR spectrum of the 1,3,5-TFB radical anion only, *viz.*, lowering the temperature causes so great decrease in the spectral line intensities that they become indistinguishable below 260 K (see Fig. 3).

Disappearance of the signal of 1,3,5-TFB radical anion on lowering the temperature can be associated with slowing down thermally activated interconversions between different structures to a rate at which the fast spectral exchange condition is no longer valid and the observed lines are broadened which leads to a decrease in their amplitudes.<sup>27</sup> Estimates of the temperature dependence of the transition frequency using the calculated barrier values of 4.3 kcal mol $^{-1}$  (BHHLYP) and 3.2 kcal mol $^{-1}$  (B3LYP) suggest that such broadening may occur in the temperature range studied in this work. Unfortunately, measurements of the temperature dependence of the linewidth were impossible owing to low intensity of OD ESR signals below 270 K.

The width of the broad unresolved signal at the center of the spectrum, which is particularly pronounced at low temperatures, is close to the value characteristic of 1,3,5-TFB radical cation (HFC constants of 1.7 mT for three F atoms<sup>4</sup>). To confirm the assignment of this signal to 1,3,5-TFB radical cation, we carried out experiments under conditions where the generation of the 1,3,5-TFB radical cation was suppressed. To this end, a solution of durene (good electron donor) ( $C = 2.5 \cdot 10^{-2}$  mol L $^{-1}$ ) was added to the solution of 1,3,5-TFB ( $C = 10^{-2}$  mol L $^{-1}$ ). Durene has a very low electron affinity and therefore does



**Fig. 3.** OD ESR spectra of a solution of a mixture of 1,3,5-TFB ( $10^{-2}$  mol L $^{-1}$ ) with PTP ( $1.5 \cdot 10^{-3}$  mol L $^{-1}$ ) in squalane at 309 (1), 283 (2), 271 (3), and 257 K (4).



**Fig. 4.** OD ESR spectrum (1) of a solution of a mixture of 1,3,5-TFB ( $10^{-2}$  mol L $^{-1}$ ) with durene ( $2.5 \cdot 10^{-2}$  mol L $^{-1}$ ), and PTP ( $6.7 \cdot 10^{-5}$  mol L $^{-1}$ ) in 2,6,10,14-tetramethylpentadecane at 233 K; the simulated spectrum (2) with the parameters  $a(3\text{ F}) = 7.4$  mT,  $g = 2.0039$ ,  $\Delta H_{\text{peak-to-peak}} = 0.77$  mT for 1,3,5-TFB radical anion,  $a(12\text{ H}) = 1.1$  mT for durene radical cation,  $\text{HFC} = 0$ ,  $\Delta H_{\text{peak-to-peak}} = 0.27$  mT for PTP radical ions; (3) — the same as (2) but the contribution of durene radical cation was excluded.

not suppress the generation of 1,3,5-TFB radical anion. When acting as luminophore, durene is characterized by low quantum yield of recombination fluorescence. Therefore, a small amount of PTP ( $6.7 \cdot 10^{-5}$  mol L $^{-1}$ ) was also added to this solution; PTP can not compete with durene and 1,3,5-TFB in charge trapping but significantly improves the OD ESR signal.

The OD ESR spectrum of this sample at 233 K is shown in Fig. 4. It exhibits a narrow central line of PTP radical ions, a multiplet with a HFC constant of 1.1 mT for 12 protons in the durene radical cation, and a quartet with a HFC constant of 7.4 mT for three equivalent F nuclei in the 1,3,5-TFB radical anion. To give a clear idea of the contribution of 1,3,5-TFB radical anion, Fig. 4 also presents the simulated ESR spectrum obtained with the optimum parameter values where the contribution of the durene radical cation has been excluded. The absence of the broad central singlet confirms the assignment of this feature to 1,3,5-TFB radical cation. We assume that unresolved HFS in the ESR spectrum of 1,3,5-TFB radical cation is due to fast spin-lattice paramagnetic relaxation characteristic of radical cations of symmetrical molecules.<sup>28</sup>

Summing up, the OD ESR spectrum of 1,3,5-TFB radical anion was obtained for the first time. The shape of the spectrum and the results of quantum chemical calculations are indicative of fast interconversions between non-planar conformations of the radical anion. Ionizing irradiation of solutions of 1,3,5-TFB in alkanes also produces radical cations of this compound that appear in the OD ESR spectrum as a single unresolved line whose width is consistent with the published data.

The authors express their gratitude to N. E. Ivanova (Voevodsky Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Sciences) for help with purifying the solvents used in this work.

This work was financially supported by the Russian Foundation for Basic Research (Project No. 08-03-00495) and the Council on Grants at the President of the Russian Federation (Program of State Support of Leading Scientific Schools in the Russian Federation, Grant NSh-2272.2012.3).

## References

1. V. D. Shteingarts, L. S. Kobrina, I. I. Bil'kis, V. F. Starichenko, *Khimiya poliflorarenov. Mekhanizm reaktsii, intermediaty* [The Chemistry of Polyfluoroarenes. Reaction Mechanisms and Intermediates], Nauka, Sib. Otd., Novosibirsk, 1991, 272 (in Russian).
2. P. V. Schastnev, L. N. Shchegoleva, *Molecular Distortions in Ionic and Excited States*, CRC Press, Boca Raton, 1995, 192.
3. A. Hasegawa, M. Shiotani, Y. Hama, *J. Phys. Chem.*, 1994, **98**, 1834.
4. A. Hasegawa, Y. Itagaki, M. Shiotani, *J. Chem. Soc., Perkin Trans. 2*, 1997, 1625.
5. G. M. Brooke, *J. Fluor. Chem.*, 1997, **86**, 1.
6. R. A. Rossi, R. M. de Rossi, *Aromatic Substitution by the  $S_{\text{RN}}1$  Mechanism*, American Chemical Society, Washington, DC, 1983, 300 pp.
7. S. S. Laev, V. D. Shteingarts, *J. Fluorine Chem.*, 1999, **96**, 175.
8. I. V. Beregovaya, L. N. Shchegoleva, *Inter. J. Quant. Chem.*, 2002, **88**, 481.
9. Yu. N. Molin, O. A. Anisimov, V. I. Melekhov, S. N. Smirnov, *Faraday Discuss. Chem. Soc.*, 1984, **78**, 289.
10. Yu. N. Molin, R. Z. Sagdeev, O. A. Anisimov, *Khim. Fiz.*, 1983, **4**, 437 [*Russ. J. Phys. Chem. B*, 1983, **4**].
11. M. M. Barlukova, I. V. Beregovaya, V. P. Vysotsky, L. N. Shchegoleva, V. A. Bagryansky, Yu. N. Molin, *J. Phys. Chem. A*, 2005, **109**, 4404.
12. S. V. Blinkova, L. N. Shchegoleva, I. V. Beregovaya, M. M. Vyushkova, V. A. Bagryansky, Yu. N. Molin, *Appl. Magn. Reson.*, 2011, **41**, 229.
13. M. B. Yim, D. E. Wood, *J. Am. Chem. Soc.*, 1976, **98**, 2053.
14. V. V. Lozovoy, V. M. Grigoryants, O. A. Anisimov, Yu. N. Molin, P. V. Schastnev, L. N. Shchegoleva, I. I. Bilkis, V. D. Shteingarts, *Chem. Phys.*, 1987, **112**, 463.
15. V. I. Borovkov, I. V. Beregovaya, L. N. Shchegoleva, P. A. Potashov, V. A. Bagryansky, Y. N. Molin, *J. Chem. Phys.*, 2012, **137**, 104305.
16. E. V. Kalneus, D. V. Stass, K. L. Ivanov, Yu. N. Molin, *Mol. Phys.*, 2006, **104**, 1751.
17. Yu. N. Molin, O. A. Anisimov, *Radiation Phys. Chem.*, 1983, **21**, 77.
18. D. W. Werst, A. D. Trifunac, *J. Phys. Chem.*, 1988, **92**, 1093.
19. A. D. Trifunac, D. W. Werst, in *Radical Ionic Systems: Properties in Condensed Phase*, Eds A. Lund, M. Shiotani, Kluwer Academic Publishers, Dordrecht, 1991, p. 195.
20. S. Hino, K. Seki, H. Inokuchi, *Chem. Phys. Lett.*, 1975, **36**, 335.

21. *Energii razryva khimicheskikh svyazei, potentsialy ionizatsii i srodstva k protonu* [Bond Dissociation Energies, Ionization Potentials, and Proton Affinity Energies], Ed. V. I Kondratiev, Nauka, Moscow, 1974, 351 pp. (in Russian).
22. L. Wojnarovits, G. Foldiac, *J. Chromatogr. A*, 1981, **206**, 511.
23. C. Santiago, R. W. Gandour, K. N. Houk, W. Nutakul, W. E. Gravey, R. P. Thummel, *J. Am. Chem. Soc.*, 1978, **100**, 3730.
24. D. R. Duling, *J. Magn. Reson. B*, 1994, **104**, 105.
25. *Landolt-Bornstein. Numerical Data and Functional Relationships in Science and Technology: New Series Gruppe/Group 2*, Eds H. Fischer, K.-H. Hellwege, Springer-Verlag, Berlin, 1987, 608 pp.
26. M. W. Schmidt, K. K. Baldridge, J. A. Boatz, S. T. Elbert, M. S. Gordon, J. H. Jensen, S. Koseki, N. Matsunaga, K. A. Nguyen, S. J. Su, T. L. Windus, M. Dupuis, J. A. Montgomery, *J. Comput. Chem.*, 1993, **14**, 1347.
27. A. Carrington, A. D. McLachlan, *Introduction to Magnetic Resonance*, Chapman and Hall, London, 1967, 266 pp.
28. V. I. Borovkov, Yu. N. Molin, *Chem. Phys. Lett.*, 2004, **398**, 422.

*Received May 31, 2013;  
in revised form September 10, 2013*