# Study of radical cations of *cis*- and *trans*-decalin in nonpolar solutions by the MARY and optically detected ESR spectroscopy

*B. M. Tadjikov, D. V. Stas', and Yu. N. Molin**

*Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Sciences,*
*3 ul. Institutskaya, 630090 Novosibirsk, Russian Federation.*
*Fax: 007 (383 2) 35 2350. E-mail: molin@kinetics.nsk.su*

Radical cations of *cis*- and *trans*-decalin in nonpolar solvents were studied by optically detected ESR and magnetically affected reaction yield (MARY) spectroscopy. The observed differences in the spectra of *cis*- and *trans*-decalin are in agreement with the assumption of the existence of temperature-activated intramolecular dynamic transitions in the radical cation of *trans*-decalin. Using MARY spectroscopy, the signals of the corresponding radical cations were detected at room temperature in diluted solutions containing *cis*- and *trans*-decalin molecules as acceptors. Under these conditions, the total recovery of dynamic transitions in the radical cation of *trans*-decalin is observed. Radical cations of both *cis*- and *trans*-decalin participate in the reaction of the ion-molecular charge transfer to a neutral molecule; the rate constant of this reaction is close to the diffusion-controlled one.

**Key words**: optically detected ESR; magnetic effects, MARY spectroscopy; decalin, *cis*- and *trans*-isomers, radical cations; electron transfer; ion-radical pairs.

Radical cations of *cis*-decalin (*c*-dec$^+$) and *trans*-decalin (*t*-dec$^+$) were investigated in freon matrices by ESR spectroscopy[1—3] as well as in hydrocarbon solutions by the optically detected electron spin resonance (OD ESR) technique in both the continuous-wave[4,5] and time-resolved[6—9] variants. Radical cations of both isomers are stabilized in the low-temperature freon matrices, yielding resolved ESR spectra. However, the pattern of OD ESR signals of *cis*- and *trans*-decalin in hydrocarbon solvents substantially differ. Thus, if the OD ESR spectra of *c*-dec$^+$ can be observed in a diluted solution even at room temperature, were recorded the signals of *t*-dec$^+$ only at the temperatures below 40 K.

Such behavior of the OD ESR signals suggests[8] that the radical cations in the hydrocarbon solvents are capable of fast abstraction of the proton in the ion-molecular reactions of the type

$$\mathrm{RH}^{\cdot+} + \mathrm{RH} \rightarrow \mathrm{R}^{\cdot} + \mathrm{RH_2}^{+}, \qquad (1)$$

and *trans*-decalin reacts much faster than *cis*-isomer. However, it was established by the pulse radiolysis technique[10] that the lifetime of *t*-dec$^+$ exceeds 100 ns even at room temperature and, therefore, deprotonation cannot preclude the registration of its OD ESR spectra.

Two close electronic states with different ESR spectra were found to exist for the cation of *t*-dec$^+$ using ESR spectroscopy in the freon matrices.[3] Intramolecular dynamic transitions between these states can be observed. The same was not detected in the case of *c*-dec$^+$.

In this work it has been shown that the observed temperature dependence of the OD ESR spectrum of *t*-dec$^+$ can be explained by activation of transitions between the two nearly degenerate electronic states. Additional arguments in favor of this statement were obtained when analyzing the effect of magnetic field on the luminescence yield (MARY spectra) upon recombination of the radical ion pairs. Using the MARY spectroscopy, the signals of radical cations of both *cis*- and *trans*-decalin in the cyclohexane solutions were recorded at room temperature and the radical cations were shown to participate in the reaction of resonance ion-molecular charge transfer

$$\underline{\mathrm{C_{10}H_{18}}^{+}} + \mathrm{C_{10}H_{18}} \rightarrow \underline{\mathrm{C_{10}H_{18}}} + \mathrm{C_{10}H_{18}}^{+}, \qquad (2)$$

the rate constant of which is close to the diffusion-controlled value.

## Experimental

The OD ESR spectra, obtained under the action of X-ray irradiation, were recorded under steady-state conditions using the setup described previously[11] and modified for performing low-temperature experiments. The samples (~1 mL solutions in quartz cells) were placed into a resonant cavity of a Bruker ER-200D ESR spectrometer equipped with an accessory for optical detection, consisting of an X-ray tube and a photoelectron multiplier (PEM) connected to a quartz light guide. Fluorescence was recorded through a short-wave light filter (λ < 360 nm) cutting the phosphorescence of the sample under modulation of external magnetic field. The PEM signal was fed at the input of a phase-lock detector. The magnetic field was modulated by a small-amplitude alternating component with a frequency of 170 Hz (the base frequency of the

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phase-lock detector). The signals observed were recorded as the first derivative of the spectrum shape. The amplitude of the μw field in the resonant cavity ($H_1 \approx 0.45$ G) corresponded to the operating power of klystron (200 mW).

The procedure for recording the OD ESR spectra at 77 K was described previously.[5] To record the spectra at 4 K, a specially made quartz-jacketed ~2-liter Dewar vessel was used. The outer nitrogen jacket was made of foamed plastic, and the operating end was cooled with a film of gravity-fed liquid nitrogen. The light emission of the samples was transmitted outward using a quartz light guide immersed in liquid helium. The temperature of the sample in the range of 6—40 K was varied by helium flow evaporated from a little helium cryostat mounted directly below the microwave resonant cavity. The temperature of the flow was measured by a calibrated Fe—Au thermocouple.

The MARY spectra, obtained under the action of X-ray irradiation, were recorded under steady-state conditions[12] using modulation of magnetic field at a frequency of 12.5 kHz with the phase-lock detection of the signal. Since the spectra were recorded in a continuous-wave fashion, the signals are the first derivative of the spectrum shape.

The solvents, cyclohexane (99%, Aldrich), squalane (99%, Merck), and *cis*- and *trans*-decalin (99%, Aldrich), were additionally purified on a column with activated silica gel. Cyclohexane was distilled prior to use. Purity of the solvents was controlled by their UV spectra. The solvents used had optical density equal to unity at a wavelength of 215—225 nm. The samples were degassed to ~$10^{-3}$ Torr by repeated freeze—pump—thaw cycle prior to use in the experiments.

## Results and Discussion

### *Study of solutions of cis- and trans-decalin by the OD ESR technique*

The OD ESR spectra of solutions of *cis*- and *trans*-decalin in squalane, containing naphthalene-$d_8$ as scintillator in the temperature range from 4 to 77 K, are shown in Fig. 1. The signals are due to recombination of the singlet radical ion [naphthalene]$^-$/[decalin]$^+$ pairs arising upon X-ray irradiation. An intense line in the central part of the spectrum corresponds to the radical ions of naphthalene-$d_8$, while a quintet with a splitting of about 50 G corresponds to the radical cations of decalin. It can be seen that the amplitude of the quintet of *c*-dec$^+$ remains unchanged (see Fig. 1, curves *1'*—*4'*) as temperature increases from 4 to 77 K, whereas the signals of *t*-dec$^+$ decrease and disappear completely at 77 K.

The data of ESR spectroscopy in the freon matrices and quantum-chemical calculations show[3] that *t*-dec$^+$ can exist in two states with close energies (Fig. 2). The spin density of the $^2A_G$ state is localized along the central C—C bond, which results in large hyperfine interaction (HFI) constants of the equatorial *trans*-β-protons. The spin density in the $^2B_G$ state is delocalized along the side C—C bonds. As a result, the HFI constants of the radical cation are small. Depending on the type of the matrix used,[3] ESR signals of both $^2A_G$ and $^2B_G$ states of *t*-dec$^+$ can be observed. Moreover, dynamic transitions between these states ($^2A_G \leftrightarrow {}^2B_G$) occur under certain conditions (elevated temperature and an appropriate matrix). Only one state, $^2A_G$, is experimentally recorded for *c*-dec$^+$.

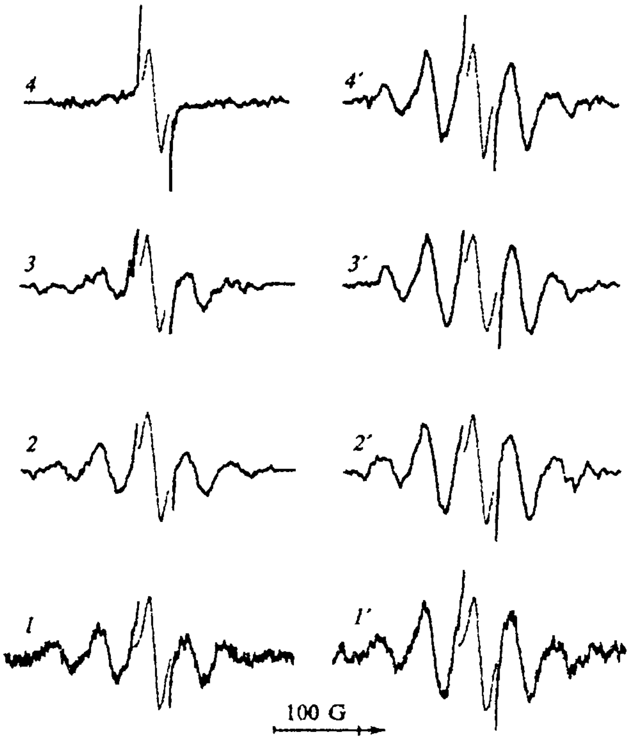

**Fig. 1.** Effect of temperature on the OD ESR spectra of glassy solutions of naphthalene-$d_8$ ($8 \cdot 10^{-3}$ mol L$^{-1}$) in squalane containing 0.3 mol L$^{-1}$ of *trans*-decalin (*1*—*4*) and *cis*-decalin (*1'*—*4'*): *T*/*K* = 4 (*1*, *1'*); 6—7 (*2*); 8—10 (*2'*); 21 (*3*, *3'*); 77 (*4*, *4'*). The central component of the spectrum was recorded at weaker amplification than the rest of the spectrum.

It can be assumed that the differences observed in the OD ESR spectra of *cis*- and *trans*-decalin (see Fig. 1) are due to a quasi-degeneracy in the system of electronic levels of *t*-dec$^+$, which results in a dynamic averaging of the structure of the spectrum and an increase in the rate of the spin-lattice relaxation.

The temperature dependence of the OD ESR spectra of a solution of *trans*-decalin in squalane is shown in Fig. 3. Curves *1*—*4* were obtained by numerical integration of the corresponding experimental spectra (*1*—*4*), shown in Fig. 1, and their amplitudes are normalized with respect to the central line. It can be seen that the intensities of the outermost lines in the spectrum of *t*-dec$^+$ ($M_I = \pm 2$) decrease relative to those nearest to the center ($M_I = \pm 1$) (see Fig. 3, spectra *1*—*3*) as temperature increases from 4 to 21 K. Simultaneously, the gaps between the lines disappear. The resolved structure disappears at 77 K, and the observed signal of *t*-dec$^+$ appears as a broad diffuse line (see Fig. 3, spectrum *4*). Figure 3 (spectrum *1*, see also Fig. 1, curve *1*) shows that the ratio of amplitudes of the lines of *t*-dec$^+$ at 4 K appreciably

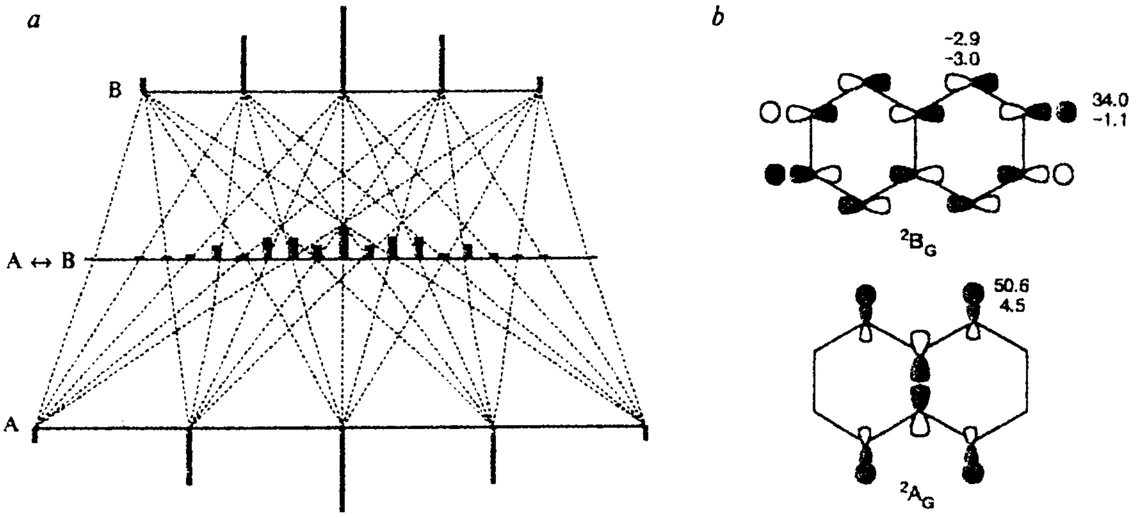

**Fig. 2.** Diagrams of ESR spectra (*a*) and schematic picture of molecular orbitals (*b*) for the pair of degenerated states of *t*-dec$^+$. The HFI constants (G) calculated by quantum-chemical methods[3] are given; only the largest HFI constants were taken into account when constructing the diagram.

differs from the statistical one. This fact is reflected in the increased amplitudes of the outermost components of the spectrum. A similar phenomenon was previously observed in the OD ESR spectra of the cations of the alkane matrices,[13—15] and it was shown to be due to "spectral migration" (or "spectral diffusion" according to Refs. 14 and 15) between components of the hyperfine structure and to occur under conditions of strong microwave pumping. In the alkane matrices such migration is due to the ion-molecular charge transfer of the holes over the molecules of solution. In the diluted solutions we studied the positive charge is stabilized on the acceptor molecule, and no ion-molecular charge transfer occurs. Thus, the abnormal ratio of amplitudes of the lines of the hyperfine structure of *t*-dec$^+$ confirms the assumption of the presence of intramolecular dynamic transitions. For comparison, no anomalies are observed in the spectrum of *cis*-decalin (see Fig. 1, curve *1'*), where no similar transitions are observed.

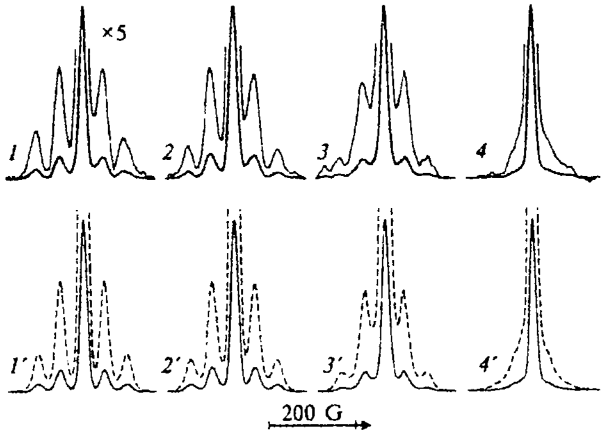

**Fig. 3.** Effect of temperature on the OD ESR spectra of glassy solutions of *trans*-decalin (0.3 mol L$^{-1}$) in squalane: $T/K$ = 4 (*1, 1'*), 6—7 (*2, 2'*), 21 (*3, 3'*), and 77 (*4, 4'*); *1—4*, integral representation of experimental spectra; *1'—4'*, simulated spectra taking into account the exchange over two states calculated using the following parameters: $k_{AB} = 10^6$ s$^{-1}$, $k_{BA} = 5 \cdot 10^7$ s$^{-1}$, $t_1 = 8$ μs (*1'*); $k_{AB} = 10^7$ s$^{-1}$, $k_{BA} = 1.25 \cdot 10^8$ s$^{-1}$, $t_1 = 2$ μs (*2'*); $k_{AB} = 1.7 \cdot 10^8$ s$^{-1}$, $k_{BA} = 3.3 \cdot 10^8$ s$^{-1}$, $t_1 = 1$ μs (*3'*); $k_{AB} = 5 \cdot 10^8$ s$^{-1}$, $k_{BA} = 5 \cdot 10^8$ s$^{-1}$, $t_1 = 0.1$ μs (*4'*). The central line of the naphthalene ions added for clarity.

The theoretical OD ESR spectra calculated taking into account the process of intramolecular $^2A_G \leftrightarrow {}^2B_G$ exchange (spectra *1'—4'*) are also shown in Fig. 3. The calculations were performed assuming that the exchange occurs between two groups of the protons with HFI constants close to those obtained by quantum-chemical methods and that the ratio of the rates of direct and inverse reactions exponentially depends on temperature. The procedure of calculations was described previously.[13] It was also assumed that the decrease in the amplitudes of the signals is due to decreasing the relaxation time with increasing temperature.

As can be seen in Fig. 3, taking into account the intramolecular dynamic transitions allows one to describe the key features of transformation of the shape of the spectrum of *t*-dec$^+$, while the assumption of increasing the rate of the spin relaxation due to degeneracy in the system of electronic levels explains the distinctions between the intensities of the OD ESR spectra of *cis*- and *trans*-decalin. It follows from the data obtained that complete dynamic averaging of the HFI constant in the *t*-dec$^+$ cation should occur with increasing temperature of the solution up to room temperature and the resultant spectrum will contain the signals of the protons of two groups, $a_1$(4 H) ≈ 25 G and $a_2$(4 H) ≈ 17 G (see

Fig. 2). However, a short relaxation time of *t*-dec$^+$ at these temperatures likely prevents its registration by the OD ESR method. Assuming that in the high-temperature limit the degenerate terms have nearly equal populations, the expected second moment of the spectrum of *t*-dec$^+$ is readily calculated. Its value is in good agreement with the experimental one obtained from the MARY spectrum of *t*-dec$^+$ recorded at room temperature (see below).

### *Study of solutions of cis- and trans-decalin by MARY spectroscopy*

As has been shown recently,[12,16,17] the coherent nature of the radical ion pairs can result in local extrema appearing on the curve of the dependence of the yield of recombination products on the external magnetic field (the MARY spectrum). In particular, a narrow line in the MARY spectrum must appear in zero field (at $H^* = 0$) for any set of magnetic nuclei in one of the radicals of the pair, if the HFI constants of the second partner are negligible.[12] For the radical pairs with equivalent nuclei the appearance of narrow lines in nonzero fields is also possible. For instance, for a system with an integer total nuclear spin the most intense line must appear in a field equal to the triple HFI constant[16,18,19] (at $H^* = 3a$). Apart from the narrow resonance lines, the MARY spectra contain a broad diffuse line, in which width ($\Omega$) is determined by the second moment ($\Delta$) of the spectrum of the "broad" partner:

$$\Omega = [2\sum a_i^2 I_i(I_i+1)/3]^{1/2} = \sqrt{2\Delta^2}\,.$$

The experimental MARY spectra of *trans*- (curves *1—5*) and *cis*-decalin (curves *1'—5'*) cyclohexane solutions of different concentrations obtained at room temperature are shown in Fig. 4. Since the coherence effects are particularly large in the pairs with small HFI constants of one of the partners, *para*-terphenyl-d$_{14}$ (PTP) was chosen as the electron acceptor and luminophore. Since the spectra were recorded under the continuous-wave mode, the signals are the first derivatives of the spectrum shape. In the absence of decalin in solution (see Fig. 4, curves *1* and *1'*) only a narrow zero-field line corresponding to the PTP$^+$/PTP$^-$ pairs is observed in the MARY spectrum. The width of the zero-field line corresponds to the second moment of the spectrum of PTP-d$_{14}$ ions, while the phase reflects the increasing fluorescence due to the increasing magnetic field strength. Thus, there are no coherence effects and broad signals in pure cyclohexane, which allows one to use it as a solvent for spectral recording.

If *cis*-decalin is added to the solution, the signals of its radical cation appear in the spectrum (see Fig. 4, curve *2'*) as an intense inverted zero-field line and a satellite line in the field $H^* = 150$ G against the background of the whole contour, in which total width corresponds to the second moment of the ESR spectrum of *c*-dec$^+$. Since the spin evolution of the radical cation of *cis*-decalin is mainly due to the hyperfine interaction with four equivalent protons $a(4\ \mathrm{H}) = 50$ G, its MARY spectrum is unambiguously identified[16] by a line in the field $H^* = 3a$. For clarity the corresponding segment of the spectrum (see curve *2'* in Fig. 4) is shown framed.

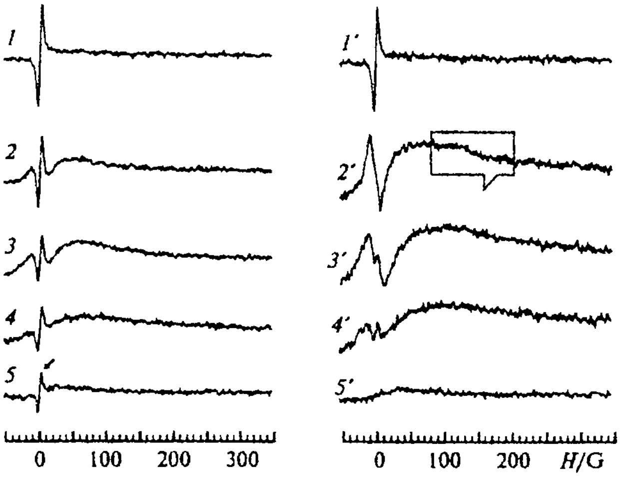

**Fig. 4.** Experimental MARY spectra of solutions of *trans*-decalin (*1—5*) and *cis*-decalin (*1'—5'*) in cyclohexane obtained at room temperature at different concentrations of decalin: 100% *cyclo*-hex (*1, 1'*); [*t*-dec] = [*c*-dec]/mol L$^{-1}$ = 0.02 (*2, 2'*), 0.1 (*3, 3'*), and 0.5 (*4, 4'*); 100% *t*-dec (*5*); 100% *c*-dec (*5'*). PTP-d$_{14}$ ($10^{-3}$ mol L$^{-1}$) was added in the solution as luminophore, the narrow line of the PTP$^+$/PTP$^-$ pair is indicated by an arrow. The satellite line of the radical cation of *c*-dec$^{\cdot+}$ at $H^* = 3a$ is shown framed.

The MARY spectra of *cis*-decalin in cyclohexane and their concentration-dependent changes are, on the whole, similar to those observed for its solutions in hexane.[17] Transformations of the shape of the MARY spectra (see Fig. 4, curves *2'—4'*) are caused by the ion-molecular charge transfer of the radical cations of *cis*-decalin (see reaction (2)). The charge transfer accelerates resulting in the corresponding broadening of individual spectral components and their decreasing intensities as the concentration of *cis*-decalin increases. The rate constant for the charge transfer according to reaction (2), obtained by numerical simulation in diluted solutions, is equal to ~$6 \cdot 10^9$ L mol$^{-1}$ s$^{-1}$, *i.e.*, it is close to the diffusion-controlled value.

The MARY spectra of solutions of *trans*-decalin in cyclohexane (see Fig. 4, curves *1—5*) are in general similar to the corresponding spectra of *cis*-decalin, however, there are appreciable distinctions between them. A broad diffuse line in the spectrum of *trans*-decalin is more narrow, while the satellite line in the non-zero fields is absent. Because of superimposition of a more strong narrow signal of PTP$^+$/PTP$^-$ (normal phase) the

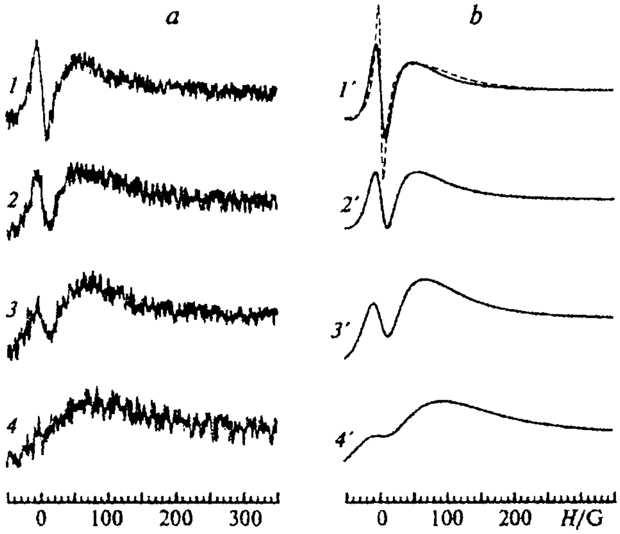

**Fig. 5.** *a.* The MARY spectra of solutions of *trans*-decalin in cyclohexane obtained at room temperature at different concentrations of decalin: [*t*-dec]/mol $L^{-1}$ = 0.018 (*1*), 0.036 (*2*), 0.072 (*3*), and 0.18 (*4*); [PTP-$d_{14}$] = $10^{-4}$ mol $L^{-1}$. *b.* Calculated for different rates of the charge transfer ($k_0 = 1/\tau_0$) at the initial width of the ESR spectrum of *t*-dec$^+$ $\Omega$ = 44 G: $k_0$/$s^{-1}$ = $10^8$ (*1*), $2.1 \cdot 10^8$ (*2*), $4.4 \cdot 10^8$ (*3*), and $1.1 \cdot 10^9$ (*4*). The spin relaxation time in the cation ($t_1$ = 7 ns), the nature of which is not related to the charge transfer, was taken into account; dashed line — calculated with no consideration for this relaxation.

inverted zero-field line is appreciably suppressed. To suppress the first signal caused by the hole capture by the PTP molecules, the measurements were performed at a decreased ($10^{-4}$ mol $L^{-1}$) concentration of PTP in solution (Fig. 5). In a diluted solution of *trans*-decalin, where virtually no charge transfer occurs (see Fig. 5, curve *1*), an intense central line (at $H^* = 0$) appears in the MARY spectrum.

The observed spectrum can be assigned to the radical cations of *trans*-decalin because of the following reasons: (1) the shape of the spectrum is independent of the solvent; (2) the change of the spectrum with increasing concentration of *t*-dec$^+$ points to the fact that this spectrum is not consistent with the products of monomolecular decay of the radical cations of *trans*-decalin (*i.e.*, olefins):

$$C_{10}H_{18}^+ \rightarrow C_{10}H_{16}^+ + H_2; \qquad (3)$$

(3) the spectrum corresponds to the second moment of the spectrum of *t*-dec$^+$ (with $\Omega$ = 44 G) calculated using the OD ESR data. A satellite non-zero-field line does not appear, as it should be in the absence of equivalency of the protons in the high-temperature limit.

In the total accord with theoretical predictions the increase in the concentration of *trans*-decalin (as in the case of *cis*-decalin) results in destroying the spin coherence in the pairs, which is followed by broadening the zero-field MARY line and a corresponding decrease in its amplitude (see Fig. 5, curves *1*—*4*). The observed transformation of the shape of the MARY spectrum of *t*-dec$^+$ is well described by the theory under the assumption that the HFI constant in the cation is due to interaction with a large number of nonequivalent nuclei[12] (quasi-classical approximation) at a constant width of the spectrum ($\Omega$ = 44 G).

To complete agreement between the simulated and experimental MARY spectra it was necessary to additionally take into account the short spin relaxation time ($t_1$ ~7 ns) of the cation, the nature of which was not associated with the charge transfer (see Fig. 5, *b*, curve *1′*, solid and dashed lines, respectively). The observed dependence of the shape of the MARY spectrum of *t*-dec$^+$ on concentration (see Fig. 5, *a*, curves *1*—*4*) is well described by the theory taking into account these assumptions while the value of the rate constant for charge transfer according to reaction (2) ($k \approx 5.9 \cdot 10^9$ L $mol^{-1}$ $s^{-1}$) obtained in this way is close to the diffusion-controlled value in cyclohexane.

The analysis performed has shown that the peculiarities of the OD ESR and MARY spectra of the radical cations of *trans*-decalin at elevated temperatures are due to quasi-degeneracy of the system of electronic levels and related dynamic transitions. Note that a short time $t_1$ which should be taken into account when modeling both the OD ESR and MARY spectra of the radical cation of *trans*-decalin might also be associated with the quasi-degeneracy of electronic levels of this radical. The unsuccessful attempts in recording the OD ESR spectra of the radical cations of other cyclic alkanes where electronic degeneracy is due to the molecular symmetry can likely be explained by short $t_1$ times.

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