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N. A. Turovskij, E. V. Raksha, Yu. V. Berestneva,
G. E. ZaikovNMR ^{13}C SPECTRA OF THE 1,1,3-TRIMETHYL-3-(4-METHYLPHENYL)BUTYL HYDROPEROXIDE
IN VARIOUS SOLVENTS: MOLECULAR MODELING*Keywords: NMR spectroscopy, 1,1,3-trimethyl-3-(4-methylphenyl)butyl hydroperoxide, chemical shift, magnetic shielding constant, GIAO, molecular modeling.*

GIAO-calculated NMR ^{13}C chemical shifts as obtained at various computational levels are reported for the 1,1,3-trimethyl-3-(4-methylphenyl) butyl hydroperoxide. The data are compared with experimental solution data in chloroform- d , acetonitrile- d_3 , and DMSO- d_6 , focusing on the agreement with spectral patterns and spectral trends. Calculation of magnetic shielding tensors and chemical shifts for ^{13}C nuclei of the 1,1,3-trimethyl-3-(4-methylphenyl) butyl hydroperoxide molecule in the approximation of an isolated particle and considering the solvent influence in the framework of the continuum polarization model (PCM) was carried out. Comparative analysis of experimental and computer NMR spectroscopy results revealed that the GIAO method with MP2/6-31G(d, p) level of theory and the PCM approach can be used to estimate the NMR ^{13}C chemical shifts of the 1,1,3-trimethyl-3-(4-methylphenyl) butyl hydroperoxide.

Ключевые слова: ЯМР-спектроскопия, 1,1,3-триметил-3-(4-метилфенил) бутил гидропероксид, химический сдвиг, константа магнитного экранирования, ГИАО, молекулярное моделирование.

Представлены химические сдвиги ^{13}C ЯМР рассчитанные методом ГИАО на различных вычислительных уровнях для 1,1,3-триметил-3-(4-метилфенил) бутил гидропероксида. Приводится сравнение полученных данных с экспериментальными в растворе хлороформа- d , ацетонитрила- d_3 , и ДМСО- d_6 , ориентируясь на соответствие со спектральными моделями и тенденциями. Приводится расчет тензоров магнитного экранирования и химических сдвигов для ядер ^{13}C молекулы 1,1,3-триметил-3-(4-метилфенил) бутил гидропероксида в приближении изолированной частицы, а также с учетом влияния растворителя в рамках континуальной модели растворителя (PCM). Сравнительный анализ экспериментальных и расчетных результатов ЯМР-спектроскопии показал, что метод ГИАО с уровнем теории MP2/6-31G(d, p) и метод PCM могут быть использованы для оценки химических сдвигов ^{13}C ЯМР 1,1,3-триметил-3-(4-метилфенил) бутил гидропероксида.

Introduction

Arylalkyl hydroperoxides are useful starting reagents in the synthesis of surface-active peroxide initiators for the preparation of polymeric colloidal systems with improved stability [1]. Thermolysis of arylalkyl hydroperoxides was studied in acetonitrile [2]. NMR ^1H spectroscopy has been already used successfully for the experimental evidence of the a complex formation between a 1,1,3-trimethyl-3-(4-methylphenyl) butyl hydroperoxide and tetraalkylammonium bromides in acetonitrile [3-5] and chloroform solution [5]. The aim of this work is a comprehensive study of the 1,1,3-trimethyl-3-(4-methylphenyl) butyl hydroperoxide (ROOH) by experimental NMR ^{13}C spectroscopy and molecular modeling methods.

Experimental

The 1,1,3-trimethyl-3-(4-methylphenyl) butyl hydroperoxide (ROOH) was purified according to Ref. [1]. Its purity (99 %) was controlled by iodometry method as well as by NMR spectroscopy. Experimental NMR ^{13}C spectra of the hydroperoxide solutions were obtained by using the Bruker Avance II 400 spectrometer (NMR ^1H – 400 MHz, NMR ^{13}C – 100 MHz) at 297 K. Solvents, chloroform- d , acetonitrile- d_3 , and DMSO- d_6 , were Sigma-Aldrich reagents and were used without additional purification but were stored above molecular sieves before using. Tetramethylsilane (TMS) was internal standard. The hydroperoxide concentration in solutions was $0.03 \text{ mol}\cdot\text{dm}^{-3}$.

Molecular geometry and electronic structure parameters, as well as harmonic vibration frequencies of

the 1,1,3-trimethyl-3-(4-methylphenyl) butyl hydroperoxide molecule were calculated after full geometry optimization in the framework of B3LYP/6-31G(d, p) and MP2/6-31G(d, p) methods. The resulting equilibrium molecular geometry was used for total electronic energy calculations by the B3LYP/6-31G(d, p) and MP2/6-31G(d, p) methods. All calculations have been carried out using the Gaussian03 [6] program.

The magnetic shielding tensors (χ , ppm) for ^{13}C nuclei of the hydroperoxide and the reference molecule were calculated with the MP2/6-31G(d, p) and B3LYP/6-31G(d, p) equilibrium geometries by standard GIAO (Gauge-Independent Atomic Orbital) approach [7]. The calculated magnetic isotropic shielding tensors, χ_{is} , were transformed to chemical shifts relative to TMS molecule, δ_i , by $\delta_i = \chi_{ref} - \chi_{is}$, where both, χ_{ref} and χ_{is} , were taken from calculations at the same computational level. Table 1 illustrates χ values for TMS molecule used for the hydroperoxide ^{13}C nuclei chemical shifts calculations.

χ values were also estimated in the framework of 6-311G(d, p) and 6-311++G(d, p) basis sets on the base of MP2/6-31G(d, p) and B3LYP/6-31G(d, p) equilibrium geometries. The solvent effect was considered in the PCM approximation [8, 9]. χ values for magnetically equivalent nuclei were averaged.

Inspecting the overall agreement between experimental and theoretical spectra RMS errors (σ) were used to consider the quality of the ^{13}C nuclei chemical shifts calculations. Correlation coefficients (R) were calculated to estimate the agreement between spectral patterns and trends.

Table 1 - Magnetic shielding tensors for ^{13}C nuclei of the TMS

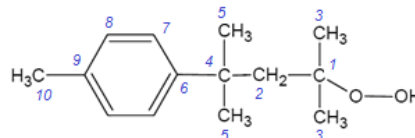
Solvent	MP2		
	1	2	3
-	207.54	199.71	199.37
Chloroform	207.86	200.13	199.79
Acetonitrile	208.01	200.32	199.99
DMSO	208.01	200.33	200.00
B3LYP			
Solvent	1	2	3
-	191.80	184.13	183.72
Chloroform	192.08	184.53	184.13
Acetonitrile	192.19	184.70	184.30
DMSO	192.30	184.81	184.40

Note: 1 - $6-31G(d, p)$; 2 - $6-311G(d, p)$; 3 - $6-311++G(d, p)$

Results and Discussion

Experimental NMR ^{13}C spectra of the 1,1,3-trimethyl-3-(4-methylphenyl) butyl hydroperoxide

Experimental NMR ^{13}C spectra of the 1,1,3-trimethyl-3-(4-methylphenyl) butyl hydroperoxide (ROOH) were obtained from chloroform-d, acetonitrile-d₃, and DMSO-d₆ solutions.



The hydroperoxide concentration in all samples was $0.03 \text{ mol}\cdot\text{dm}^{-3}$. The experimental NMR ^{13}C spectra of the ROOH are presented in Figure 1.

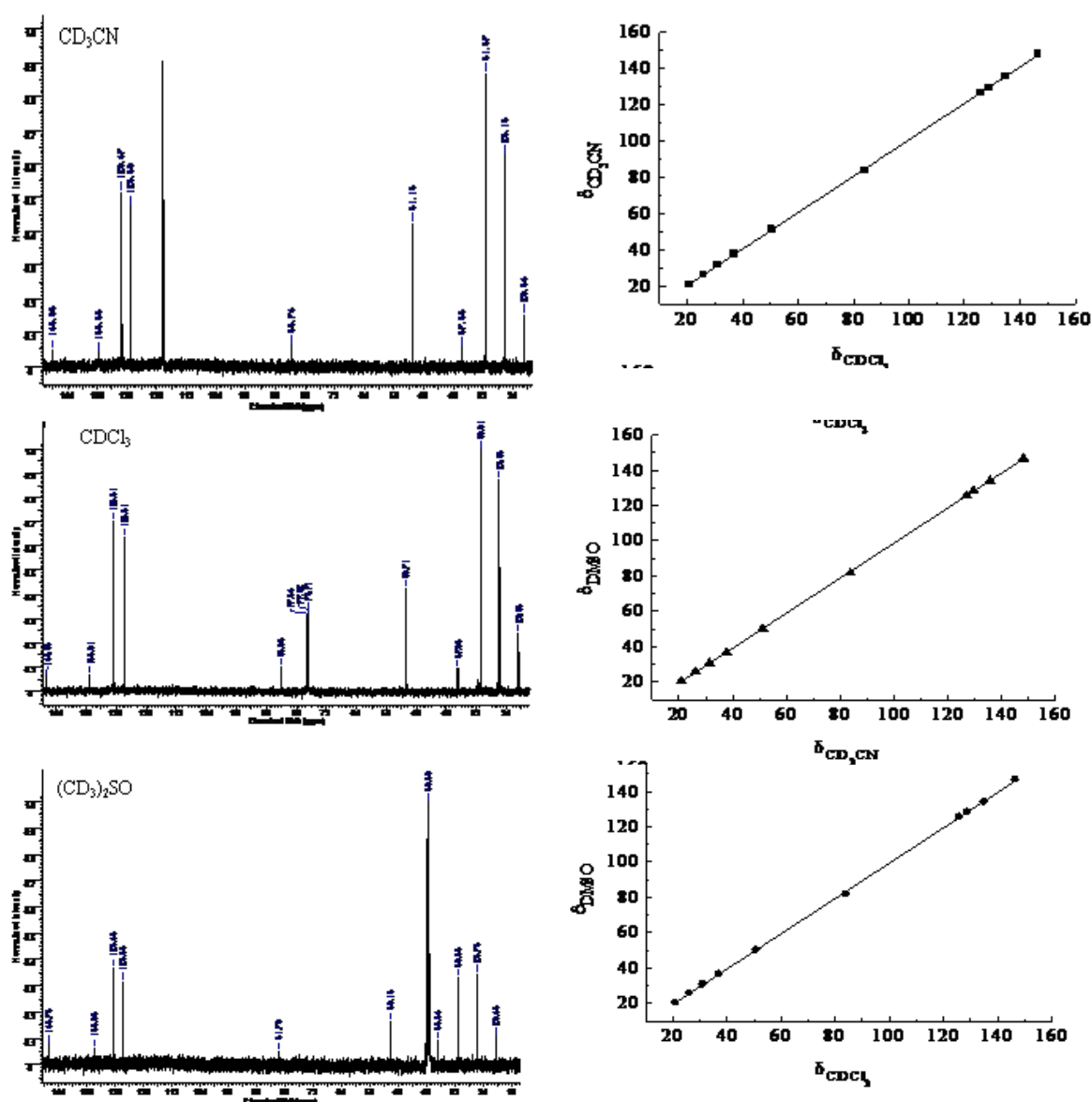


Fig. 1 - The relationship between the experimental NMR ^{13}C chemical shifts (relative to TMS) of the 1,1,3-trimethyl-3-(4-methylphenyl)butyl hydroperoxide in different solvents

Ten signals for the hydroperoxide carbon atoms are observed in the ROOH ^{13}C NMR spectrum. Signal of the carbon atom bonded with a hydroperoxide group shifts slightly to the stronger fields with the solvent polarity increasing, while the remaining signals are shifted to weak fields. A linear dependences between the ^{13}C chemical shifts values of the hydroperoxide are observed in the studied solvents (Fig. 1). This is consistent with authors [11], who showed linear correlation between the chemical shifts values in chloroform-d and dimethylsulphoxide-d₆ for a large number of organic compounds of different classes. Equations corresponded to the obtained relationships (Fig. 1) are listed below.

$$\delta_{\text{CD}_3\text{CN}} = (0.02 \pm 0.23) + 1.006 \pm 0.002 \delta_{\text{CDCl}_3}$$

$$\delta_{\text{DMSO-d}_6} = (-0.46 \pm 0.41) + 0.999 \pm 0.004 \delta_{\text{CDCl}_3}$$

$$\delta_{\text{DMSO-d}_6} = (-0.48 \pm 0.24) + 0.993 \pm 0.003 \delta_{\text{CD}_3\text{CN}}$$

Molecular modeling of the 1,1,3-trimethyl-3-(4-methylphenyl) butyl hydroperoxide NMR ^{13}C spectra by MP2 and B3LYP methods

The hydroperoxide molecule geometry optimization in the framework of MP2/6-31G(d, p) and B3LYP/6-31G(d, p) methods was carried out as the first step of the hydroperoxide NMR ^{13}C spectra modeling. Initial hydroperoxide configuration chosen for calculations was those one obtained by semiempirical AM1 method and used recently for the hydroperoxide O-O bond homolysis [2] as well as complexation with Et₃NBr [4, 12] modeling. The main parameters of the hydroperoxide fragment molecular geometry obtained in the isolated particle approximation within the framework of MP2/6-31G(d, p) (Fig. 2) and B3LYP/6-31G(d, p) levels of theory are presented in Table 2. Peroxide bond O-O is a reaction centre in this type of chemical initiators thus the main attention was focused on the geometry of -CO-OH fragment. The calculation results were compared with known experimental values for the *tert*-butyl hydroperoxide [13], and appropriate agreement between calculated and experimental parameters can be seen in the case of MP2/6-31G(d, p) method.

Table 2 - Molecular geometry parameters of the 1,1,3-trimethyl-3-(4-methylphenyl) butyl hydroperoxide -CO-OH moiety

parameter	MP2/6-31G(d, p)	B3LYP/6-31G(d, p)	Experiment*
$l_{\text{O-O}}$, Å	1.473	1.456	1.473
$l_{\text{C-O}}$, Å	1.459	1.465	1.443
$l_{\text{O-H}}$, Å	0.970	0.971	0.990
C-O-O, °	108.6	110.0	109.6
O-O-H, °	98.2	99.9	100.0
C-O-O-H, °	112.4	109.1	114.0

*Note: experimental values are those for *tert*-butyl hydroperoxide from [13]

Calculation of ^{13}C chemical shifts of the hydroperoxide was carried out by GIAO method in the approximation of an isolated particle as well as in

studied solvents within the PCM model, which takes into account the nonspecific solvation. Equilibrium hydroperoxide geometries obtained in the framework of MP2/6-31G(d, p) and B3LYP/6-31G(d, p) levels of theory for the isolated particle approximation were used in all cases.

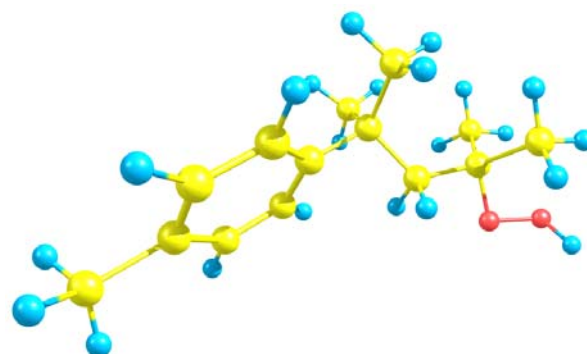


Fig. 2 - The 1,1,3-trimethyl-3-(4-methylphenyl) butyl hydroperoxide structural model (MP2/6-31G(d, p) method)

The chemical shift values (δ , ppm) for ^{13}C nuclei in the hydroperoxide molecule were evaluated on the base of calculated magnetic shielding constants (χ , ppm). TMS was used as standard, for which the molecular geometry optimization and χ calculation were performed using the same level of theory and basis set. Values of the ^{13}C chemical shifts were found as the difference of the magnetic shielding tensors of the corresponding TMS and hydroperoxide nuclei (Tabl. 3 and 4).

Table 3 - NMR ^{13}C chemical shifts (δ , ppm) of the 1,1,3-trimethyl-3-(4-methylphenyl)butyl hydroperoxide (the isolated particle approximation)

nuclei	MP2		
	1	2	3
C1	83.61	86.87	88.24
C2	53.50	57.48	57.42
C3	26.46	26.71	26.62
C4	37.04	40.23	40.37
C5	30.10	30.93	31.03
C6	141.39	153.47	153.93
C7	116.91	125.90	126.29
C8	127.07	137.37	137.97
C9	121.55	130.79	131.41
C10	22.98	23.82	23.75
nuclei	B3LYP		
	1	2	3
C1	85.77	90.90	92.04
C2	53.23	57.70	57.00
C3	24.62	25.27	24.93
C4	41.14	44.66	44.49
C5	28.57	29.78	29.75
C6	144.46	158.38	158.37
C7	119.80	130.58	131.03
C8	130.75	142.40	143.32
C9	123.68	134.44	135.07
C10	21.84	23.25	22.84

Note: 1 - 6-31G(d, p); 2 - 6-311G(d, p); 3 - 6-311++G(d, p)

The correct spectral pattern for the hydroperoxide NMR ^{13}C spectrum was obtained for all methods and basis sets used within the isolated molecule approximation (See Table 3) as well as solvation accounting (See Table 4). Exceptions are aromatic C8 and C9 carbons, which signals are interchanged for all calculations.

The best reproduced experimental chemical shift value for the carbon atom of the CO-OH group is observed in the case of MP2/6-31G(d, p) approximation in all used solvents whereas B3LYP with the same basis set gives slightly worse values. Basis set extension to 6-311++G(d, p) leads to a deterioration of the calculation results. Calculated value for the carbon of CO-OH group (83.61 ppm) within the isolated molecule approximation is closest to experimental one in

acetonitrile (83.74 ppm). When passing to the calculations in the PCM mode solvation accounting leads to more correct results for the MP2 and B3LYP methods. The lowest σ values for all solvents are obtained with 6-31G(d, p) basis set. Linear relationships between the experimental NMR ^{13}C chemical shifts and the calculated values δ_{calc} for the hydroperoxide ^{13}C nuclei (see Fig. 3) have been obtained for both methods and all basis sets. The correlation coefficients (R) corresponding to obtained dependences are shown in Table 4. Joint account of σ and R values indicates possibility of MP2 method with 6-31G(d, p) basis set using for the calculation of the hydroperoxide ^{13}C nuclei chemical shifts.

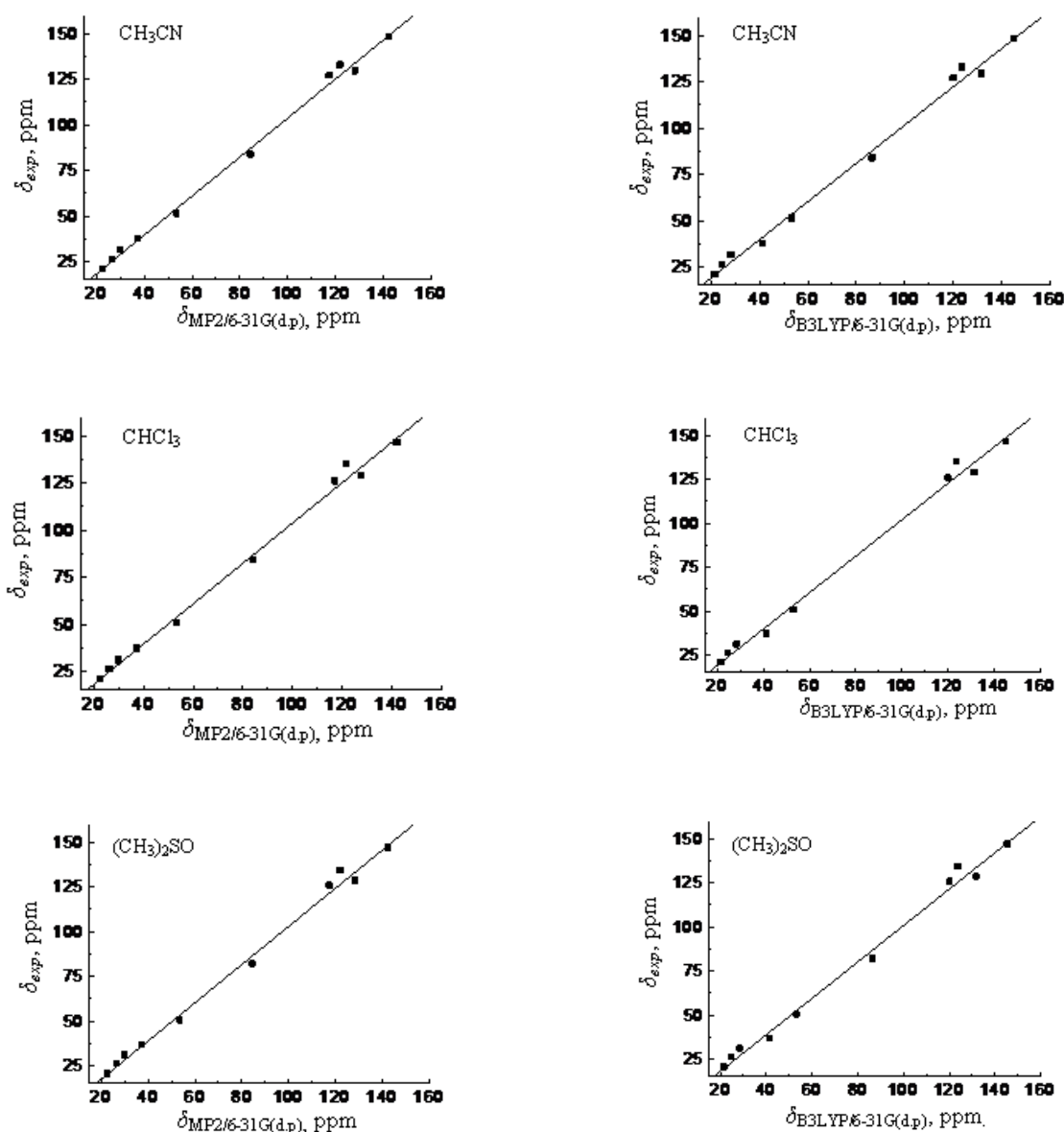


Fig. 3 - Experimental (δ_{exp}) versus GIAO calculated ^{13}C chemical shifts (relative to TMS) of the 1,1,3-trimethyl-3-(4-methylphenyl) butyl hydroperoxide

Table 4 - NMR ^{13}C chemical shifts (δ , ppm) of the 1,1,3-trimethyl-3-(4-methylphenyl)butyl hydroperoxide in different solvents

nuclei	MP2			4
	1	2	3	
	Chloroform			
C1	84.29	87.74	89.27	83.93
C2	53.69	57.73	57.64	50.71
C3	26.62	26.99	26.89	25.98
C4	37.46	40.74	40.92	37.03
C5	30.18	31.10	31.20	30.91
C6	142.14	154.40	154.90	146.55
C7	117.33	126.51	126.91	125.81
C8	127.92	138.43	139.03	128.81
C9	121.90	131.35	131.91	135.01
C10	23.01	23.96	23.88	20.86
σ	27.86	25.63	28.66	
R	0.997	0.997	0.997	

nuclei	B3LYP			4
	1	2	3	
	Chloroform			
C1	86.44	91.86	93.14	83.93
C2	53.37	57.89	57.17	50.71
C3	24.73	25.52	25.17	25.98
C4	41.54	45.20	45.07	37.03
C5	28.59	29.90	29.88	30.91
C6	145.12	159.23	159.25	146.55
C7	120.11	131.14	131.60	125.81
C8	131.56	143.43	144.34	128.81
C9	123.85	134.81	135.37	135.01
C10	21.81	23.36	22.93	20.86
σ	20.82	59.16	63.32	
R	0.996	0.996	0.996	

nuclei	MP2			4
	1	2	3	
	Acetonitrile			
C1	84.58	88.13	89.73	83.74
C2	53.80	57.88	57.78	51.15
C3	26.70	27.13	27.02	26.13
C4	37.64	40.99	41.18	37.65
C5	30.22	31.19	31.29	31.37
C6	142.50	154.84	155.37	148.03
C7	117.52	126.80	127.20	126.89
C8	128.29	138.90	139.49	129.47
C9	122.08	131.63	132.17	132.66
C10	23.03	24.04	23.96	20.84
σ	24.571	22.325	25.741	
R	0.998	0.998	0.998	

nuclei	B3LYP			4
	1	2	3	
	Acetonitrile			
C1	86.72	92.27	93.61	83.74
C2	53.44	57.98	57.27	51.15
C3	24.77	25.63	25.28	26.13
C4	41.71	45.43	45.32	37.65
C5	28.59	29.95	29.93	31.37
C6	145.42	159.62	159.66	148.03
C7	120.24	131.37	131.84	126.89
C8	131.88	143.85	144.75	129.47
C9	123.94	135.00	135.52	132.66
C10	21.80	23.41	22.97	20.84
σ	17.395	55.560	60.243	
R	0.997	0.997	0.996	

nuclei	MP2			4
	1	2	3	
	DMSO			
C1	84.60	88.15	89.75	81.79
C2	53.80	57.88	57.78	50.18
C3	26.70	27.13	27.03	25.76
C4	37.65	41.00	41.19	36.64
C5	30.22	31.19	31.30	30.85
C6	142.52	154.86	155.39	146.73
C7	117.53	126.81	127.22	125.65
C8	128.31	138.92	139.52	128.43
C9	122.09	131.64	132.18	133.98
C10	23.03	24.04	23.96	20.45
σ	25.496	31.656	35.949	
R	0.997	0.997	0.997	

nuclei	B3LYP			4
	1	2	3	
	DMSO			
C1	86.84	92.38	93.72	81.79
C2	53.54	58.09	57.37	50.18
C3	24.87	25.74	25.37	25.76
C4	41.82	45.54	45.43	36.64
C5	28.69	30.06	30.03	30.85
C6	145.54	159.74	159.77	146.73
C7	120.35	131.48	131.94	125.65
C8	131.99	143.97	144.86	128.43
C9	124.05	135.11	135.62	133.98
C10	21.90	23.51	23.06	20.45
σ	21.206	70.994	76.092	
R	0.995	0.996	0.995	

Note: 1 - 6-31G(d, p); 2 - 6-311G(d, p); 3 - 6-311++G(d, p); 4 - experimental data

Conclusions

A comprehensive study of the 1,1,3-trimethyl-3-(4-methyl-phenyl) butyl hydroperoxide by experimental NMR ^{13}C spectroscopy and molecular modeling methods was performed. A comparative assessment of the ^{13}C nuclei chemical shifts calculated by GIAO in various approximations. For NMR ^{13}C spectra of the hydroperoxide in different solvents MP2 and B3LYP methods approximations with 6-31G(d, p), 6-311G(d, p), and 6-311++G(d, p) basis sets allow to obtain the correct spectral pattern. A linear correlations between the calculated and experimental values of the ^{13}C chemical shifts for the studied hydroperoxide molecule were obtained for all solvents studied. In all cases, the MP method combined with 6-31G(d, p) basis set allows to get a better agreement between the calculated and experimental data as compared to the B3LYP results.

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