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Effect of External Electric Field upon Lower Alkanols

Józef Mazurkiewicz[a]; Piotr Tomasik[b],*

[a] Departament of Chemistry and Physics, University of Agriculture, Mickiewicz Ave., 21, 30149 Cracow, Poland.
[b] Cracow College of the Health Promotion, Krowoderska Street 73, 31159 Cracow, Poland.
* Corresponding author.

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Abstract

Applying the Monte Carlo method, molecules of methanol, ethanol and 1-butanol are brought to temperature of 300 K and under the influence of external electric field of 0.01 a.u their electronic spectra are simulated with HyperChem 8.0 involving ZINDO/S semiempirical method. Particular molecules differently react to the electric field applied as shown by the electronic spectra simulated in the range of 250-2.84 nm. Total energy of the methanol and ethanol molecules turn slightly more negative in the electric field whereas that energy found for 1-butanol more significantly turn to less negative. HyperChem 8.0 software is used together with the AM1 method for optimization of the conformation of the molecules of methanol, ethanol, 1-propanol and 1-butanol. Then polarizability, charge distribution, potential and dipole moment for molecules placed in the external electric field of 0.000, 0.001, 0.01 and 0.05 a.u. are calculated. External field induces a slightly field strength dependent polarizability of the molecules and the electron density redistribution at particular atoms. Total dipole moment (DM) for particular alkanols increases with the strength of the field applied. There is particularly sharp increase in DM at 0.05 a.u. field.

Key words: Butanol; Computer simulations; Ethanol; Methanol; Propanol

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INTODUCTION

There is a considerable experimental evidence for effect of External Electric Field (EEF) with the solid, liquid and gaseous matter. That interaction changes its macrostructure and electron distribution in particular molecular constituents. One of several examples of the influence of EEF upon the solid matter was recently described by Bao *et al.* (2006) who demonstrated how EEF changed microstructural transformation of carbon nanotubes into highly crystalline structures producing the electrostatic force on the carbon surface.

It is known that EEF changes viscosity of electrolytes and this phenomenon is known as electroviscosity (Winslow, 1949; Stangroom, 1983; Monkman, 1995; Stanway *et al.*, 1996; Tam *et al.*, 1997). Also liquid non-electrolytes react to EEF as found in case of 1,4-dioxane. EEF produced a temporary decrease in its viscosity called “the perestroika effect” (Mazurkiewicz & Tomasik, 1996). Electroviscosity can also be observed in suspensions (Wen *et al.*, 2003). Effect of EEF upon gaseous molecules is experienced as so-called St Elmos fires (Wescott *et al.*, 1996) and Kirlian photography (bioelectrophotography) and corona discharges (Goldman *et al.*, 1985; Korotkov, 2007).

These effects imply that EEF can also influence chemical reactivity including physiological processes. Indeed, pulsed EEF stimulated of microorganisms for fermentative production of ethanol (Grosse *et al.*, 1988; Nakanishi *et al.*, 1988). Pulsed EEF appeared to be beneficial in several physiological processes as, for instance, in synthesis of ADNP in respiration inhibited submitochondrial particles (Tiessie *et al.*, 1981) citric acid production by *Aspergillus niger* when an exposure to pulsed electric field increased oxygen consumption of that microorganism (Fiedurek, 1999), and switching of the elevated enzymatic reactions in micelles (Harada & Kataoka, 2003). The effect of EEF influenced also the plant growth under microgravity conditions (Nechitailo & Gordeev, 2001).

The effect of EEF evokes interest in the context of so-called aura and biofield surrounding living organisms. As in such cases the much lower energy of EEF is involved as in case of normally observed corona discharges there are problems with visualization, recording and quantification of biofield and aura. Additionally the role of physiological processes in the organisms and awareness in case of humans should be taken into account (Korotkov, 2007). Thus far experiments do not provide any reliable information on the effect of EEF upon particular molecules. Our former papers described computer simulated structures polarizabilities of bonds and atoms as well as dipole moments of simple gaseous molecules (Mazurkiewicz & Tomasik, 2010) and molecules of selected monosaccharides (MAzurkiewicz & Tomasik, 2012) subjected to the action of EEF. In this paper results of similar approach to the structure dipole moments and polarizabilities of lower alkanols placed in EEF are presented. These results can shed a light upon possible controlling metabolism of ethanol in human organism in EEF, and rationalize, for instance, combustion of alcohols as fuels.

COMPUTATIONS

Applying the Monte Carlo method (Brzozowski *et al.*, 2002) molecules of methanol, ethanol and 1-butanol were brought to temperature of 300 K and with influence of electric field of 0.01 a.u. (1 a.u. = 1.49×10^{-10} J = 931 MeV) and electronic spectra were simulated with HyperChem 8.0 involving ZINDO/S semiempirical method.

HyperChem 8.0 software was used together with the AM1 method for optimization of the conformation of the molecules of alkanols under study. Then polarizability, charge distribution, potential and dipole moment for molecules placed in the external electric field of 0.000, 0.001, 0.01 and 0.05 a.u. were calculated. For the computations of the polarizability the field of 10^{-10} a.u. has to be adapted as the no field condition. In the computations of polarizability, every molecule was oriented against the external electric field in an identical manner.

Figure 1 presents numbering of the atoms applied in the computations and their orientation in the Cartesian system. The molecule is situated along the x-axis. The y- and z-axes are perpendicular in plane and perpendicular to plane containing this structure, respectively.

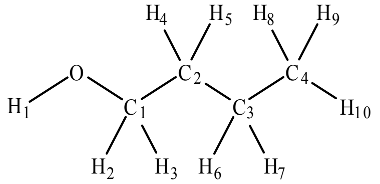


Figure 1
Numbering of Atoms in the Molecules of Alkanols. In the Methanol Ethanol and 1-Propanol Molecules H4, H5 and H8 Atoms Take Positions of C2, C3 and C4, Respectively

REULTS AND DISCUSSION

The spectral transitions of alkanols computed in the rage from 2.82 to 250 nm are given in Table 1. In the spectra only one active transition could be seen in the region above 200 nm. One could also see that particular alcohols differently reacted to the electric field applied. Total energy of the methanol and ethanol molecules turned slightly more negative in the electric field whereas that energy found for 1-butanol more significantly turned oppositely, that is, to less negative. The application of external electric field resulted in vanishing some transitions and some new transitions, mainly in the region of 65-75 nm appeared. In the consequence the spectrum of methanol became richer totally by one transitions whereas in the spectrum of ethanol in the electric field two transitions ceased. In the electric field, the spectrum of 1-butanol became richer by 20 transitions. In all spectra the electric field produced bathochromic shift of the bands. This effect fairly prominent in the longwavelength region of the spectra gradually became less significant in moving towards shorter wavelength region. Intensities of the transitions changed chimerically but mostly they decreased.

Table 1
Simulated Electronic Spectra of Molecules of Methanol, Ethanol and 1-Butanol Without Exposure and with Exposure to External Electric Field[a]

Molecule and total number of transitions	Transition energy (E) [nm] and its characteristics					
	Without electric field			**With electric field**		
	E	f^b	HOMO→LUMO and **total energy** [a.u.]	E	f^b	HOMO→LUMO and **total energy** [a.u.]
Methanol 91	237.03	0.0028	1→5	254.42	0.0023	1→5
	134.10	0.0032	1→8	135.27	0.0054	1→9
	122.80	0.0017	1→9	126.74	0.0003	1→10
	116.12	0.0002	1→10	109.85	0.0002	1→14
	105.05	0.0006	1→13	108.91	0.0016	1→15
	102.26	0.0012	1→15	105.33	0.0051	1→17
	99.88	0.0031	1→17	98.53	0.0004	1→20
	92.01	0.0006	1→20	92.06	0.0003	1→22
	84.86	0.0011	1→22	87.63	0.0014	1→23

To be continued

Continued

Molecule and total number of transitions	**Transition energy (E) [nm] and its characteristics**					
	Without electric field			**With electric field**		
	E	f^b	HOMO→LUMO and **total energy** [a.u.]	E	f^b	HOMO→LUMO and **total energy** [a.u.]
Methanol 91	82.69	0.0018	1→23	82.09	0.0012	1→26
	79.75	0.0209	1→25	81.00	0.0208	1→27
	78.49	0.0050	1→27	79.84	0.0001	1→28
	77.13	0.0004	1→29	79.33	0.0023	1→29
	76.02	0.0001	1→30	78.31	0.0060	1→32
	74.81	0.0077	1→33	76.65	0.0110	1→34
	68.72	0.1390	1→39	69.12	0.0004	1→40
	67.41	0.0006	1→40	68.99	0.1353	1→41
	66.54	0.0256	1→43	68.29	0.0010	1→42
	64.99	0.0003	1→45	67.33	0.0427	1→45
	64.54	0.0019	1→47	66.07	0.0247	1→47
	62.62	0.0051	1→49	64.89	0.0077	1→49
	60.52	0.0022	1→51	61.34	0.0032	1→52
	57.65	0.0001	1→53	59.81	0.0001	1→53
	57.62	0.0005	1→54	58.69	0.0012	1→54
	56.81	0.0007	1→55	58.64	0.0001	1→55
	54.49	0.0010	1→58	55.28	0.0018	1→59
	50.20	0.0007	1→62	49.99	0.0004	1→62
	41.58	0.0007	1→65	43.21	0.0009	1→65
	39.18	0.0001	1→70	40.11	0.0001	1→70
	5.60	0.0002	1→72	5.61	0.0001	1→72
	5.57	0.0002	1→76	5.61	0.0002	1→73
	5.38	0.0021	1→80	5.58	0.0005	1→76
	2.84	0.0654	1→82	5.38	0.0025	1→80
	2.82	0.0003	1→84	2.84	0.0641	1→82
			-98.883514877	2.82	0.0004	1→84
						-98.887900084
Ethanol 208	236.01	0.0028	1→5	252.84	0.0021	1→5
	134.50	0.0030	1→8	143.70	0.0002	1→7
	125.02	0.0015	1→9	138.43	0.0046	1→9
	118.59	0.0001	1→10	132.22	0.0006	1→10
	117.62	0.0005	1→11	128.12	0.0001	1→11
	108.31	0.0012	1→15	119.18	0.0001	1→13
	106.70	0.0003	1→16	116.14	0.0012	1→15
	104.25	0.0003	1→18	111.89	0.0001	1→17
	100.48	0.0025	1→20	106.63	0.0039	1→20
	94.49	0.0023	1→23	103.56	0.0019	1→23
	86.07	0.0009	1→25	94.48	0.0002	1→25
	85.78	0.0009	1→26	91.15	0.0009	1→26
	85.52	0.0011	1→28	89.98	0.0060	1→27
	81.75	0.0038	1→33	88.36	0.0012	1→31
	81.25	0.0023	1→35	86.94	0.0006	1→35
	81.04	0.0067	1→36	85.64	0.0013	1→36
	80.31	0.0092	1→37	85.23	0.0008	1→37
	79.89	0.0020	1→38	83.14	0.0053	1→40
	78.54	0.0099	1→41	82.19	0.0009	1→41
	77.62	0.0003	1→43	81.55	0.0181	1→43
	76.20	0.0001	1→45	80.34	0.0049	1→46
	75.22	0.0002	1→47	79.42	0.0025	1→47
	74.72	0.0005	1→48	78.41	0.0022	1→48
	74.14	0.0004	1→50	78.40	0.0001	1→49
	73.60	0.0005	1→53	76.31	0.0014	1→54
	73.26	0.0006	1→55	75.87	0.0011	1→56
	72.22	0.0012	1→57	75.02	0.0001	1→58
	69.86	0.1161	1→63	71.16	0.0009	1→63
	68.53	0.0373	1→64	70.91	0.0755	1→64
	68.14	0.0320	1→67	70.71	0.0289	1→66
	66.68	0.0004	1→72	69.62	0.0405	1→70
	66.39	0.0020	1→73	69.29	0.0251	1→72
	65.71	0.0002	1→75	68.78	0.0104	1→74
	65.04	0.0001	1→78	68.12	0.0048	1→77
	64.39	0.0041	1→79	67.20	0.0129	1→82
	63.63	0.0023	1→83	64.23	0.0025	1→85
	62.32	0.0019	1→84	63.10	0.0002	1→86
	61.55	0.0061	1→86	62.52	0.0056	1→87
	61.07	0.0126	1→88	62.29	0.0003	1→89
	60.05	0.0013	1→90	61.88	0.0001	1→90

To be continued

Continued

Molecule and total number of transitions	**Transition energy (E) [nm] and its characteristics**					
	Without electric field			**With electric field**		
	E	f^b	HOMO→LUMO and **total energy** [a.u.]	E	f^b	HOMO→LUMO and **total energy** [a.u.]
Ethanol 208	59.71	0.0003	1→91	61.56	0.0138	1→92
	58.65	0.0002	1→93	61.37	0.0005	1→94
	58.02	0.0005	1→96	60.56	0.0005	1→96
	57.98	0.0006	1→97	60.31	0.0002	1→99
	57.57	0.0013	1→100	60.10	0.0004	1→100
	57.08	0.0001	1→104	59.81	0.0003	1→102
	56.88	0.0002	1→105	57.54	0.0027	1→115
	56.69	0.0001	1→107	56.60	0.0009	1→116
	55.86	0.0011	1→114	56.41	0.0006	1→119
	55.15	0.0003	1→115	55.18	0.0001	1→125
	54.89	0.0005	1→118	54.57	0.0002	1→127
	53.51	0.0001	1→124	52.50	0.0005	1→131
	51.87	0.0006	1→130	43.84	0.0009	1→149
	41.83	0.0007	1→149	41.17	0.0001	1→153
	39.71	0.0001	1→154	5.62	0.0002	1→163
	5.61	0.0001	1→162	5.59	0.0004	1→170
	5.60	0.0002	1→163	5.39	0.0028	1→178
	5.57	0.0002	1→169	2.84	0.0639	1→194
	5.38	0.0021	1→178	2.82	0.0004	1→196
	2.84	0.0653	1→194			**-131.672971257**
	2.82	0.0003	1→196			
			-131.668628141			
1-Butanol 588	235.55	0.0028	1→5	273.08	0.0007	1→5
	134.40	0.0031	1→8	192.83	0.0002	1→6
	125.10	0.0011	1→9	178.91	0.0010	1→8
	122.97	0.0004	1→10	174.85	0.0001	1→10
	117.56	0.0006	1→11	154.94	0.0007	1→15
	108.97	0.0006	1→16	151.64	0.0043	1→16
	107.35	0.0003	1→18	150.04	0.0001	1→17
	100.45	0.0026	1→26	138.51	0.0001	1→21
	94.28	0.0032	1→29	128.67	0.0035	1→23
	86.25	0.0013	1→36	121.96	0.0007	1→25
	86.17	0.0010	1→37	117.31	0.0025	1→27
	85.82	0.0010	1→38	116.22	0.0033	1→28
	83.20	0.0009	1→40	108.67	0.0012	1→32
	82.07	0.0001	1→43	108.29	0.0001	1→34
	81.42	0.0005	1→44	107.38	0.0001	1→37
	80.70	0.0146	1→45	101.92	0.0013	1→44
	79.74	0.0008	1→48	101.16	0.0002	1→47
	79.73	0.0026	1→49	100.89	0.0033	1→50
	79.50	0.0001	1→50	100.38	0.0015	1→52
	79.41	0.0013	1→51	99.82	0.0004	1→53
	79.19	0.0057	1→53	95.39	0.0001	1→65
	78.49	0.0012	1→54	95.21	0.0006	1→67
	78.12	0.0022	1→59	94.94	0.0003	1→68
	78.03	0.0002	1→61	93.14	0.0001	1→77
	77.99	0.0003	1→62	92.22	0.0013	1→81
	77.28	0.0001	1→65	91.54	0.0001	1→83
	75.18	0.0005	1→74	91.02	0.0006	1→86
	75.08	0.0005	1→75	90.06	0.0002	1→93
	74.56	0.0001	1→78	89.83	0.0345	1→95
	74.32	0.0004	1→79	88.59	0.0008	1→99
	73.96	0.0002	1→82	88.50	0.0022	1→100
	73.59	0.0004	1→85	87.80	0.0041	1→102
	72.94	0.0001	1→91	86.74	0.0008	1→104
	72.50	0.0005	1→93	86.24	0.0011	1→107
	72.41	0.0001	1→96	85.03	0.0005	1→111
	71.99	0.0001	1→99	84.77	0.0002	1→114
	70.68	0.0001	1→106	81.94	0.0001	1→122
	70.30	0.0906	1→109	81.21	0.0003	1→124
	68.71	0.0367	1→115	80.78	0.0001	1→127
	68.62	0.0464	1→116	80.18	0.0001	1→130
	67.70	0.0008	1→122	79.93	0.0001	1→132
	67.65	0.0006	1→123	79.04	0.0439	1→135
	65.93	0.0006	1→131	78.59	0.0026	1→137
	65.55	0.0001	1→133	78.28	0.0020	1→138
	64.44	0.0021	1→136	78.24	0.0003	1→139

To be continued

Continued

Molecule and total number of transitions	Transition energy (E) [nm] and its characteristics					
	Without electric field			With electric field		
	E	f^b	HOMO→LUMO and **total energy** [a.u.]	E	f^b	HOMO→LUMO and **total energy** [a.u.]
1-Butanol 588	63.83	0.0220	1→138	78.12	0.0012	1→141
	63.39	0.0064	1→139	77.96	0.0018	1→143
	63.04	0.0033	1→142	77.67	0.0003	1→146
	62.12	0.0001	1→149	77.07	0.0210	1→149
	61.39	0.0016	1→150	76.34	0.0001	1→150
	61.05	0.0001	1→153	76.20	0.0001	1→152
	60.93	0.0001	1→154	76.19	0.0764	1→153
	60.71	0.0006	1→156	76.06	0.0218	1→154
	60.50	0.0015	1→157	75.71	0.0002	1→156
	60.34	0.0004	1→158	74.86	0.0007	1→162
	60.03	0.0003	1→164	74.50	0.0143	1→163
	59.85	0.0001	1→165	74.16	0.0002	1→164
	59.78	0.0001	1→166	74.00	0.0002	1→166
	59.63	0.0002	1→170	73.78	0.0047	1→167
	59.54	0.0004	1→172	73.53	0.0005	1→170
	59.49	0.0003	1→173	73.17	0.0011	1→173
	59.19	0.0001	1→176	72.94	0.0001	1→174
	58.88	0.0003	1→181	72.65	0.0003	1→178
	58.75	0.0003	1→186	72.51	0.0006	1→181
	58.62	0.0001	1→189	72.35	0.0001	1→182
	58.60	0.0002	1→190	71.93	0.0001	1→187
	58.44	0.0002	1→195	71.64	0.0001	1→192
	58.43	0.0001	1→196	71.40	0.0003	1→195
	57.95	0.0002	1→204	70.99	0.0002	1→199
	57.42	0.0001	1→213	70.61	0.0011	1→205
	57.40	0.0004	1→214	70.37	0.0002	1→209
	57.18	0.0001	1→218	69.75	0.0001	1→215
	57.15	0.0001	1→219	69.68	0.0008	1→216
	56.89	0.0003	1→227	69.54	0.0018	1→217
	56.35	0.0003	1→237	69.38	0.0001	1→220
	56.28	0.0002	1→239	69.32	0.0021	1→221
	55.76	0.0001	1→243	69.11	0.0037	1→224
	55.19	0.0001	1→251	68.99	0.0017	1→227
	55.04	0.0001	1→254	68.49	0.0002	1→232
	54.45	0.0001	1→261	68.46	0.0051	1→234
	54.26	0.0001	1→265	68.06	0.0121	1→239
	52.97	0.0001	1→285	67.82	0.0009	1→241
	52.89	0.0001	1→287	67.53	0.0001	1→243
	52.76	0.0001	1→292	67.40	0.0009	1→245
	51.42	0.0001	1→312	66.62	0.0002	1→252
	49.47	0.0003	1→325	66.31	0.0002	1→254
	41.83	0.0006	1→406	65.14	0.0032	1→266
	39.66	0.0001	1→426	64.33	0.0002	1→271
	5.60	0.0002	1→451	63.96	0.0002	1→275
	5.57	0.0001	1→463	63.75	0.0006	1→279
	5.38	0.0021	1→482	63.15	0.0021	1→282
	2.84	0.0654	1→562	62.66	0.0001	1→287
	2.82	0.0003	1→564	62.57	0.0002	1→289
			-197.238574662	62.48	0.0001	1→291
				62.20	0.0001	1→293
				61.85	0.0001	1→299
				61.75	0.0009	1→301
				61.46	0.0009	1→303
				60.79	0.0004	1→311
				60.34	0.0002	1→316
				58.46	0.0002	1→331
				58.22	0.0015	1→333
				57.73	0.0001	1→334
				56.72	0.0001	1→340
				56.01	0.0001	1→354
				53.97	0.0005	1→368
				47.76	0.0011	1→409
				44.11	0.0001	1→427
				5.67	0.0003	1→456
				5.63	0.0007	1→479
				5.44	0.0045	1→482
				2.84	0.0614	1→562
				2.82	0.0004	1→564
						-197.066354923

Note: [a]Only transitions of $f > 0.0000$ are quoted.
[b]The oscillator strength.

Situating alkanols in external electric field induced a field strength dependent reorientation of the molecules as shown in Figure 2.

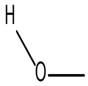
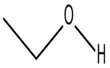
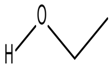
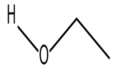
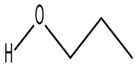
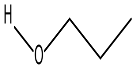
	0.000 a.u	**0.001 a.u**	**0.01 a.u**	**0.05 a.u**
Methanol		no change	no change	no change
Ethanol				no change
1-Propanol		no change		no change
1-Butanol			no change	no change

Figure 2
Changes of the Orientation of the Alkanol Molecules in the External Electric Field

Molecule of methanol behaved passively in the external field and did not change its original position as the strength of the field increased even to 0.05 a.u. The 0.001 a.u., field rotated the molecule of ethanol by 180° around the ordinate y axis but the field of 0.01 a.u. additionally rotated that molecule by 180° around the coordinate x-axis and that position remained unchanged in the 0.05 a.u. field. The molecule of 1-propanol was inert at 0.001 a.u. field and just at the 0.01 a.u. field rotated by 180° around both x- and y-axes. It remained stable in the resulting position at the 0.05 a.u. field. The similar rotation around both axes performed molecule of 1-butanol already in the 0.001 a.u. field and then did not change its orientation as the strength of field increased to 0.05 a.u.

Application of the external induced polarizability of the molecules and the electron density redistribution at particular atoms as shown in Table 2.

Table 2
Electric Field Induced Charge Distribution on the Atoms of Alkanols

Alkanol	Field strength [a.u.]	Charge distribution at particular atoms[a]													
		O	C1	C2	C3	C4	H1	H2	H3	H4	H5	H6	H7	H8	H9	H10
Methanol	0.000	-.326	-.073				.195	.053	.053	.098						
	0.001	-.330	-.074				.196	.056	.056	.096						
	0.01	-.363	-.077				.250	.078	.078	.078						
	0.05	-.508	-.091				.341	.178	.178	-.006						
Ethanol	0.000	-.330	-.019	-.215			.197	.058	.058	.087	.087	.077				
	0.001	-.333	-.020	-.215			.197	.060	.060	.085	.085	.080				
	0.01	-.364	-.027	-.211			.143	-.025	-.025	.054	.064	.101				
	0.05	-.505	-.063	-.190			.232	.191	.190	.211	-.033	.033				
Propanol	0.000	-.330	-.019	-.164	-.212		.197	.059	.059	.094	.094	.078	.072	.072		
	0.001	-.333	-.020	-.163	-.212		.198	.061	.061	.091	.091	.076	.075	.075		
	0.01	-.364	-.027	-.154	-.220		.204	.085	.085	.067	.067	.096	.096	.065		
	0.05	-.503	-.065	-.093	-.267		.226	.184	.184	-.052	-.052	.201	.201	.036		
Butanol	0.000	-.329	-.158	-.163	-.019	-.329	.197	.059	.059	.095	.095	.077	.077	.074	.074	.073
	0.001	-.333	-.020	-.162	-.159	-.209	.198	.061	.061	.092	.092	.080	.080	.075	.072	.072
	0.01	-.363	-.027	-.154	-.169	-.205	.203	.084	.084	.069	.069	.103	.103	.098	.052	.052
	0.05	-.502	-.064	-.099	-.219	-.102	.218	.179	.179	-.042	-.043	.209	.209	.223	-.033	-.033

Note: [a]In the methanol ethanol and 1-propanol molecules H4, H5 and H8 atoms take positions of C2, C3 and C4, respectively.

Computations performed indicated that in every alcohol the negative charges were invariantly localized at oxygen and carbon atoms. The charge at the oxygen atom always prevailed over these at the carbon atoms. The increase in the strength of the electric field always resulted in a concentration of the negative charge at the oxygen, C1 and C3 atoms. A decrease of that charge at C2 and C4 atoms could be simultaneously noted. Among the hydrogen atoms always that of the OH group (H1) carried the lowest electron density. Except the ethanol molecule at the 0.01 a.u. field the increase in the strength of electric field provided increase in the positive charge at that atom, that is, the increase in the strength of the electric field applied increased the acidity of the alkanols. The charge density at remaining hydrogen atoms behaved more chimerically. Mostly it turned more positive with the increase of the field strength producing more remarkable polarization of the C-H bonds. Reversed trend could be noted for the H4 atom in the methanol molecule at the 0.05 a.u. field. The charge density at this atom decreased and reached a slightly negative value. It could suggest that under such circumstances combustion of methanol could be facilitated as the first step of that process, i. e. the free radical insertion of the oxygen molecule is favored by increasing localization of the electrons at this reaction place (Figure 3).

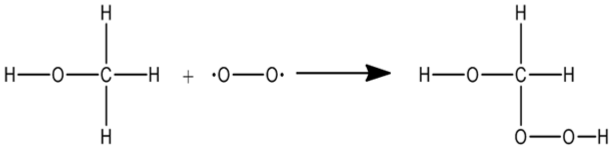


Figure 3
The First Step of Combustion of Methanol

Similarly, the negative charge was found at H2 and H3 atoms in the ethanol molecule placed in the 0.01 a.u. field and H5 and H6 atoms of that molecules in the 0.05 a.u. field. The latter field could generate negative charge also at the H4 and H5 atoms of 1-propanol and all H4, H5, H9 and H10 atoms of the 1-butanol molecules.

Polarizability is a tensor with nine values related to three axes of the Cartesian system. They compose the average values reported in Table 3. The total polarizability is a sum of polarizability of electrons, atoms and dipoles, the latter resulting in eventual reorientation of the molecules along the applied field. The latter is available from the computations.

In methanol polarizability regularly decreased with an increase in the strength of the field and in 1-butanol it regularly increased under such circumstances. In ethanol it initially increased, then slightly decreased in the 0.01 a.u. field in order to raise again at the 0.05 a.u. field. The polarizability of 1-propanol initially decreased in order to considerably increase at the 0.05 a.u. field (Table 3).

Table 3
Average Field Strength Dependent Polarizability of Alkanols

Alkanol	Polarizability at a.u.			
	0.0	**0.001**	**0.01**	**0.05**
Methanol	12.57	12.29	12.12	11.63
Ethanol	20.40	20.53	20.38	20.62
1-Propanol	28.79	28.60	28.50	30.11
1-Butanol	36.55	36.66	37.57	40.77

Table 4 collects changes of the energy of molecules with the strength of the field applied and accompanying changes of dipole moments. Based on energies given in that table one can see that increasing strength of the field made particular molecules more stable.

Table 4
Energy and Dipole Moments of Alkanols Oriented Along *X*, *Y* and *Z* Axes of the Cartesian System

Alkanol	Field strength [a.u.]	Energy [kcal/mole]	Dipole moment [D] total and along axes of the Cartesian system			
			Total	DM_x	DM_y	DM_z
Methanol	0.000	-495.95	1.621	1.385	-0.043	0.000
	0.001	-496.36	1.653	-1.653	-0.006	0.000
	0.01	-500.35	1.939	-1.939	0.000	0.000
	0.05	-525.88	3.265	-3.265	0.000	0.000
Ethanol	0.000	-776.72	1.550	1.120	1.072	0.000
	0.001	-776.87	1.604	-1.604	0.009	-0.000
	0.01	-781.20	2.084	-2.084	0.001	-0.000
	0.05	-812.63	4.340	-4.340	-0.000	0.000
1-Propanol	0.000	-1058.73	1.537	0.207	1.523	0.000
	0.001	-1059.11	1.610	-1.610	0.036	-0.000
	0.01	-1063.42	2.265	-2.265	-0.001	0.000
	0.05	-1100.80	5.426	-5.426	-0.000	0.000
1-Butanol	0.000	-1340.65	1.521	1.369	0.664	-0.000
	0.001	-1341.04	1.614	-1.614	0.013	-0.000
	0.01	-1345.55	2.451	-2.451	0.001	-0.000
	0.05	-1388.95	6.470	-6.470	0.000	0.000

Total dipole moment (DM) for particular alkanols increased with the strength of the field applied. There was particularly sharp increase in DM at 0.05 a.u. field. One could also see that application even of the weakest field almost completely immobilized the molecules of alkanols along the x coordinate axis as seen on inspection of DM values along all three axes of the Cartesian system. Thus, external electric field affects charge distribution to the extent depending on the strength of the field applied and, therefore, in such manner the reactivity of the molecule to ionic and free radical reactions can be controlled.

Performed computations showed that except particular cases occurring at the extremely strong 0.05 a.u. electric field the external electric field does not promote combustion of alkanols. Metabolism of ethanol in the human organism involves enzymatic oxidation (see, for instance Crabb *et al.*, 1987; Ambroziak & Pietruszko, 1993). Because the effect of the external electric field upon oxidizes metabolizing alcohol in the organism remains unknown nothing can be said about the role of exposure of the organism to such field in the metabolism of alcohol. An interesting hypothesis in this respect (Berry *et al.*, 1993) should be, however, mentioned. It is presented based on the observation of the electrochemical regulation of metabolism.

CONCLUSIONS

External electric field of the strength of up to 0.01 a.u. induces only slight changes in the charge distribution at particular atoms of alkanols, polarizability of the molecules, their energy and dipole moments, however, it can have an influence upon their combustion and in case of ethanol also on its metabolism.

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