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Contribution to the understanding effects of weak electrical phenomena

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ABSTRACT

Electronic emission spectra of N_2, $(N_2)_2$, $(N_2)_5$ O_2, $(O_2)_2$, $(O_2)_5$, H_2O, $(H_2O)_5$, CO_2, $(CO_2)_2$, $CO_2..H_2O$, NH_3 and $NH_3.H_2O$ situated in the electric field of 0.001, 0.005, 0.01 0.05 and 0.1 a.u. were simulated involving Monte Carlo optimization followed by the ZINDO/S approach. The simulated spectra showed irregular dependence on the energy of the electric field applied. Molecules without influence of the electric field emit in the vacuum ultraviolet region. Applied electric field only in case of $(O_2)_5$ generated transitions above 200 nm. The mapping of isosurface of the investigated molecules revealed that the electric field applied redistributed the charge densities in the molecules in the manner approximately parallel to the energy of the field. Applied electrical field resulted in an increase in the water acidity and ammonia basicity.

Keywords: Electronic Emission Spectra; Surface Effect; ZINDO/S Spectra Simulations

1. INTRODUCTION

There are numerous papers (see, for instance [1]) describing the effect of electromagnetic field upon biological systems. Particular attention has been paid to electrostimulation of the alcoholic fermentation [2,3]. Electric current changed the fermentation characteristics of yeast. Either the 10 mA direct current (DC) or 100 mA alternating current (AC) applied to the culture broth significantly increased the cell growth and alcohol production rate. Also accompanied formation of higher alcohols, esters and organic acids was influenced in such manner although some of them could result from the anodic oxidation of ethanol. Since the phenomena observed in the case of electrostimulation were observed in the wort likely the effect could not be assisted by the effect of the external field. Nechitailo and Gordeev [4] related observed effect of an artificial electric field upon growth of plants to perturbations occurred on the plant cell membranes.

Another electrical phenomenon known as corona discharges have found several practical applications [5,6]. Corona discharges (Saint Elmo's fire) have a straightforward physical background [5,7-14]. Recent studies on the effect of corona discharges on granular starch [15] showed that, in contrast to other solid material such as metals and plastics, it penetrated starch granules causing depolymerization of polysaccharides in the granule interior. Liu and Zou [16] presented hydrolysis of starch to mono- and di-saccharides with dielectric barrier discharge plasma. They showed that proton layer was formed within the steam layer. Recently, a series of papers on modification of carbon nanotubes with low-temperature glow plasma was published [17-20]. Electrical field could be used for regulation of viscosity of liquids and, hence, their flow (see, for instance [21]).

There are also weaker electric phenomena which, although common, did not find sufficient appreciation. They result from the effect of the surface. Atoms localized inside any solid and liquid structure are in different energetic situation than these situated on the surface of these structures *i.e.* on the phase borderlines. Atoms localized on the surface of the structures, particularly on sharp edges and tips of needles dispose with some excessive energy as their interactions with elements of another phase, especially gaseous, are weaker. Such circumstances are responsible for well known catalytic effects of the surface, effect of lightning rod and so on. The non-saturation of interactions of the peripheral atoms generate a gradient of potential and, in consequence, the electromagnetic field around the object. Molecules residing in this thin layer interact with the surface and with one another. Energy of such molecules is, additionally, influenced by external electric field to the extent which might be reflected in their electronic spectra.

Electromagnetic field is a volume of space around the object in which energy particles called photons can migrate either from that object into the space or from the space to that object causing a ionization. In such manner a cold plasma is formed. Properties of the molecules in such plasma remain unknown.

In this paper evaluation of differences between molecules outside and inside plasma surrounding the surface of inanimate objects is carried out involving electronic emission spectra of simple small molecules as nitrogen, oxygen, water, carbon dioxide and ammonia are simulated when placed in an electric field and without application of that field.

There are available in the literature electronic spectra of the same molecules covering the region from 200 to 20 nm and these spectra have been computed with more advanced methods [22-24] but the spectra of these molecules in the electric field are lacking. In this paper, for diagnostic purposes of the effect of the electric field upon the structure of the molecules spectra were calculated using less sophisticated ZINDO/S [25] method which was specially designed by its inventor for simulation of the spectra in the UVVIS region.

2. COMPUTATIONS

Applying the Monte Carlo method [26] single molecules of N_2, O_2 (considered as biradical), water, CO_2, CO_2 with water, ammonia and ammonia in water were brought to temperature of 300 K and with influence of electric field of 0.01 a.u (and electronic spectra were simulated with HyperChem 8.0 involving ZINDO/S semiempirical method. These computations were also performed for 2 and 5 molecules of N_2 and O_2, 2 molecules of CO_2 and 5 molecules of water and, additionally, for single molecules of N_2 and O_2 in the one-direction electric field varying between 0.005 and 0.1 a.u. (1 a.u. = $1.49x10^{-10}$ J = 931 MeV)

Visualization of the iusosurface was performed with HyperChem 8, Plot Molecular Graphs, 3D Mapped Isosurface.

3. RESULTS AND DISCUSSION

Because of the surface effect, the UV spectra of molecules present in aura surrounding surface of the matter should somehow differ from the spectra of the molecules over the region of aura. Changes in the molecular structure induced by external electric field could be available and visualized in form of electronic spectra simulated involving suitable software. This study should be understood as an approach to the recognition of the effect of electric field upon non-recordable plasma (aura) residing on the surface of inanimate objects.

Table 1 presents results of the computations carried out for nitrogen molecules.

Computations for small diatomic symmetric molecule

Table 1. Simulated electronic spectra of one, two and five nitrogen molecules without exposure and with exposure to external electric field.

Molecule (total number of transitions)	Transition energy (E) [nm] and its characteristics^{a}					
	Without electric field			With electric field		
	E	f^{b}	*Orbital → orbital* (HOMO → LUMO) and **total energy** [a.u]	E	f^{b}	*Orbital → orbital* (HOMO → LUMO) and total energy [a.u.]
N_2 (30)	100.2	0.2528	*1→15*, 2→6	100.0^{c}	0.2520	*1→15*; 2→6
	100.2	0.2528	*1→16*, 2→7	100.0	0.2520	*1→16*; 2→7
	90.8	0.8100	*1→17*, 4→7	90.0	0.8029	*1→17*; 4→6, 3→7
	56.9	1.2466	*1→23*, 5→8	57.0	1.2217	*1→23*; 5→8
	23.6	0.4178	*1→31*, 1→8	*51.7*	0.0001	*1→25*; 2→8
			–16.514669174	23.5	0.4003	*1→31*; 1→8
						–16.531251288
				175.0^{d}	0.0001	*1→9*, 5→7
				175.0	0.0001	*1→10*, 5→6
				174.7	0.0001	*1→11*, 5→7, 4→6, 3→7
				174.7	0.0001	1→12, 5→6, 4→7, 3→6
				100.2	0.2525	*1→15*, 2→6
				100.2	0.2525	*1→16*, 2→7
				90.6	0.8087	*1→17*, 4→6, 3→7
				56.9	1.2398	*1→23*, 5→8
				51.7	0.0028	*1→25*, 2→8
				23.6	0.4150	*1→31*, 1→8
						–16.517425927
				175.4^{e}	0.0003	*1→9*, 5→7, 4→6
				175.4	0.0003	*1→10*, 5→6, 4→7
				174.8	0.0003	*1→11*, 5→7, 4→6, 3→7
				174.8	0.0003	*1→12*, 5→6, 4→7, 3→6

				100.1	0.2521	*1→15*, 2→6
				100.1	0.2521	*1→16*, 2→7
				90.7	0.8085	*1→17*, 4→6, 3→7
				64.4	0.0001	*1→21*, 3→8
				64.4	0.0001	*1→22*, 4→8
				57.0	1.2325	*1→23*, 5→8
				51.6	0.0114	*1→25*, 2→8
				34.2	0.0001	*1→28*, 1→6
				34.2	0.0001	*1→29*, 1→7
				23.6	0.4164	*1→31*, 1→8
						–16.516281055
				202.2[f]	0.0001	*1→7*, 4→7, 3→7
				183.0	0.0096	*1→9*, 5→7
				182.9	0.0094	*1→10*, 5→7
				179.2	0.0015	*1→11*, 4→6, 3→7
				179.2	0.0015	*1→12*, 4→7, 3→6
				97.7	0.2411	*1→15*, 2→6
				97.7	0.2412	*1→16*, 2→7
				92.4	0.7927	*1→17*, 4→6, 3→7
				65.1	0.0031	*1→21*, 3→8
				65.1	0.0013	*1→22*, 4→8
				58.1	1.1208	*1→23*, 5→8
				50.6	0.1646	*1→25*, 2→8
				34.6	0.0026	*1→28*, 1→6
				34.6	0.0026	*1→29*, 1→7
				23.8	0.4392	*1→31*, 1→8
						–16.500365172
				206.7[g]	0.0217	*1→7*, 5→6
				204.7	0.0277	*1→8*, 5→7
				197.1	0.0055	*1→10*, 4→7, 3→6
				177.9	0.0003	*1→11*, 4→7, 3→6
				177.9	0.0003	*1→12*, 4→6, 3→7
				94.4	0.7174	*1→15*, 4→6, 3→7
				91.1	0.2196	*1→16*, 2→6
				91.1	0.2234	*1→17*, 2→7
				65.5	0.0219	*1→21*, 3→8
				65.4	0.0052	*1→22*, 4→8
				60.7	1.0227	*1→23*, 5→8
				48.5	0.2690	*1→25*, 2→8
				34.8	0.0104	*1→28*, 1→6
				34.8	0.0104	*1→29*, 1→7
				23.9	0.4354	*1→31*, 1→8
						–16.520177428
$(N_2)_2$ (120)	180.4	0.0001	*1→16*; 10→11,8→12	183.5[e]	0.0001	*1→14*; 10→11,6→12,5,→11
	169.6	0.0001	*1→23*; 6→13	177.1	0.0001	*1→16*; 10→13
	109.3	0.0011	*1→12*; 9→12	176.2	0.0015	*1→18*; 7→12
	109.2	0.0053	*1→29*; 9→11	175.6	0.0002	*1→19*; 7→11
	106.8	0.0744	*1→32*; 10→11,5→11	163.8	0.0012	*1→22*; 6→11,5→12
	106.7	0.0197	*1→33*; 5→12	121.0	0.0532	*1→28*; 10→12
	106.5	0.0424	*1→34*; 10→14	120.3	0.0024	*1→29,* 10→11,9→11
	106.3	0.0001	*1→36*; 6→12	117.5	0.0097	*1→36*; 9→12
	106.3	0.0010	*1→38*; 6→11	116.8	0.0010	1→37; 9→11
	106.3	0.0055	*1→39*; 10→13,7→13,5→13	102.9	0.1790	*1→40*; 5→13,4→13
	106.3	0.0005	*1→41;* 8→13	102.9	0.1941	*1→41*; 5→14,4→14
	105.1	0.0075	*1→48;* 7→14	98.9	0.2436	*1→42*; 3→11
	105.0	0.0025	*1→49*; 7→13,5→13	98.9	0.2411	*1→43*; 3→12
	100.1	0.2382	*1→52*; 4→11,3→11	97.3	0.0193	*1→46*; 7→13
	100.1	0.2310	*1→53*; 4→12,3→12	97.3	0.0208	*1→47*; 7→14
	99.5	0.2103	*1→54;* 4→14	92.8	0.0072	*1→48*; 6→13
	99.5	0.2436	*1→55*; 4→13, 3→13	90.8	0.3440	*1→54*; 9→14,4→14
	91.6	0.6090	*1→56*; 8→12	90.1	0.0520	*1→55*; 5→13.4→13
	89.4	09337	*1→57*; 6→13,5→14	89.5	0.4583	*1→56;* 5→14
	79.0	0.0001	*1→59*; 4→12,3→12	88.2	0.6163	*1→57*; 5→12
	79.0	0.0010	*1→61*; 4→11,3→11	84.6	0.0031	*1→60*; 4→11
	77.4	0.0001	*1→63*; 4→13,3→13	83.5	0.1413	*1→61*; 4→12
	77.4	0.0018	*1→65*; 3→14	72.2	0.0008	*1→64*; 3→13
	65.1	0.0001	*1→72;* 10→15,7→15	72.2	0.0009	*1→65*; 3→14
	57.1	0.6428	*1→76*; 9→16	63.5	0.0006	*1→72*; 9→16
	56.8	1.8393	*1→77*; 7→15	63.4	0.0074	*1→74*; 10→15,5→15

	52.8	0.0029	*1→80*; 9→15	57.6	1.0470	*1→76*; 10→16,7→15
	52.3	0.0056	*1→82*; 5→15,3→15	57.1	1.2236	*1→77*; 10→16,7→15
	52.2	0.0041	*1→83*; 10→16,5→16	55.3	0.0614	*1→79*; 19→15,9→15
	51.9	0.0007	*1→90*; 7→16	54.6	0.0176	*1→83*; 9→15
	51.4	0.0008	*1→92;* 4→16	52.2	0.0004	*1→86*; 5→16,4→16
	51.4	0.0036	*1→93*; 5→15,3→15	51.5	0.0038	*1→87*; 3→15
	44.5	0.0002	*1→95*; 4→15,3→15	49.9	0.0017	*1→89*; 7→16
	44.1	0.0002	*1→97*; 4→16,3→16	48.0	0.0033	*1→93*, 5→16,4→16
	24.0	0.0033	*1→116*; 2→16	46.4	0.0021	*1→95*; 4→15
	23.9	0.0315	*1→118*; 1→15	32.0	0.0010	*1→109*; 2→12
	23.8	0.3691	*1→120*; 2→15	24.4	0.0007	*1→116*; 2→15
	23.5	0.4317	*1→121*; 1→16	23.5	0.3704	*1→118*; 2→16
			–33.037415255	23.3	0.3637	*1→119*; 1→15
				23.0	0.0030	*1→121*; 1→16
						–33.125361948
$(N_2)_5$[h] (750)	107.8	0.0855	*1→122*; none	104.4[e]	0.1559	*1→187*; 11→28,11→29
	107.5	0.0755	*1→126*; 12→29	104.3	0.0878	*1→188*; 11→28,11→29
	105.8	0.1090	*1→157*; none	104.1	0.1225	*1→189*; none
	105.7	0.0561	*1→159*, none	104.0	0.0821	*1→190*; none
	100.2	0.0573	*1→232*; none	103.6	0.1348	*1→191*; 22→34,10→34
	99.7	0.0773	*1→238*; 13→32	103.5	0.1039	*1→192*; 22→35,10→35
	98.2	0.1304	*1→259*; 8→26	102.7	0.0575	*1→196*; 19→33
	98.2	0.1615	*1→261*; 8→27	102.0	0.0686	*1→200;* 13→28,8→31
	97.9	0.0550	*1→268*; 12→33	102.0	0.1344	*1→202*; 16→30,8→30
	97.7	0.0764	*1→270*; none	101.5	0.0704	*1→205*; 22→34
	97.6	0.0697	*1→273*; none	101.5	0.0817	*1→206*; 22→35
	97.5	0.0700	*1→276*; none	100.0	0.1319	*1→217*; 16→31
	97.0	0.1010	*1→279*; 13→31	99.9	0.2495	*1→219*; 6→27
	96.8	0.1767	*1→280*; none	99.9	0.1514	*1→220*; 6→26
	96.4	0.0520	*1→281*; 13→30	97.1	0.1524	*1→226*; 17→33,9→33
	96.3	0.0707	*1→282*; none	96.9	0.0574	*1→235*; none
	96.2	0.0575	*1→283*; 10→35	96.4	0.1476	*1→235*; 7→28,7→29
	96.1	0.1212	*1→284*; 10→33	96.2	0.1180	*1→237*; 7→28,7→29
	95.3	0.0629	*1→296*; none	95.9	0.0688	*1→241*; 20→35
	95.1	0.0534	*1→298*; none	95.1	0.0564	*1→244*; 14→31
	90.4	0.5087	*1→317*; none	94.6	0.0649	*1→247*; 19→35
	89.4	0.7134	*1→318*; none	91.6	0.7556	*1→261*; none
	88.7	0.5659	*1→319*; none	91.4	0.0562	*1→266*; 15→33,12→31
	88.1	0.8357	*1→320*; none	90.8	0.3470	*1→272*; none
	87.8	0.8161	*1→321*; none	90.6	0.2270	*1→273*; none
	57.7	0.2806	*1→427*; 24→37	90.4	0.0968	*1→275*; 14→32,14→33
	57.5	1.8171	*1→428*; 25→38	90.3	0.0718	*1→277*; none
	57.2	0.7356	*1→429*; none	89.9	0.7598	*1→279*; none
	57.2	1.4507	*1→430*; 21→39	89.6	0.0588	*1→282*; 11→30
	57.1	1.6333	*1→431*; 23→36	89.3	0.0992	*1→284*; 10→26
	23.6	0.2989	*1→731*; 5→36	89.2	0.3172	*1→286*; 10→26
	23.5	0.3817	*1→738*; 4→37	88.8	0.5672	*1→289*; none
	23.4	0.2869	*1→745*; 3→38	57.6	0.5401	*1→431*; 22→39,19→38
	23.3	0.3947	*1→748*; 2→39,1→39	57.4	0.0624	*1→432*; 25→37,22→37
	23.3	0.4136	*1→749*; 2→40,1→40	57.3	0.5997	*1→434*; 16→37
			–82.746665858	57.2	2.9915	*1→435*; none
				57.1	0.0504	*1→437*; 23→36
				57.0	1.1596	*1→438*; 25→40
				57.0	0.1159	*1→439*; 22→36
				56.9	0.2865	*1→441*; 22→36,13→36
				55.8	0.1408	*1→453*; 24→38,23→38
				23.7	0.4665	*1→727*; 5→40
				23.6	0.2956	*1→730*; 1→36
				23.5	0.2579	*1→733;* 3→38
				23.5	0.5530	*1→734*; 2→37
				23.4	0.3665	*1→735*; 4→39
						–82.654318825

[a] Values of E [nm] given in italics denote novel transitions generated on the application of electric field. Values in bold italics denote transitions which will cease on application of more intensive electric field; [b] The oscillator strength; [c] In the field of 0.001 a.u; [d] In the field of 0.005 a.u; [e] In the field of 0.01 a.u; [f] In the field of 0.05 a.u; [g] In the field of 0.10 a.u; [h] There were 285 and 291 active transitions in the spectra without and with the 0.01 a.u. electric field, respectively. In this Table only transitions with *f* >0.0500 are quoted.

of nitrogen provided UV spectrum composed of 5 bands in the range of 100.2 to 23.6 nm, although the computations considered totally 30 transitions. Majority of those transitions appeared inactive *i.e.* their oscillator strength,

f = 0.0000. The most intensive transition was located at 56.9 nm. Application of the electric field of 0.001 a.u. only slightly modifies the original spectrum. There is an increase in the number of active transitions by one extremely weak transition at 51.7 nm and the 1→17 transition at 57.0 nm changed its HOMO →LUMO characteristics. Application of the electric field of such energy stabilizes the molecule by 0.016582114 a.u. The 0.005 a.u. electric field increases the number of the active transitions to 10. All four extremely weak transitions appear on the red side of the spectrum around 175 nm. The bands shifts are almost negligible. The longwavelength transitions move slightly red whereas the shortwavelength transitions slightly migrate towards blue. Intensities of the transitions increase. The field of such energy destabilizes the molecule in respect to that under the influence of the weaker field. The destabilization energy is only 0.013825361 a.u but nevertheless this system is still more stable than that without the influence of the electric field. Further increase in the energy of applied electric field to 0.01 a.u. produces this time additional transitions in the central (transitions 1→21 and 1→22 at 64.4 nm) and in shortwavelength region of the spectrum (1→28 and 1→29 transitions at 34.2 nm). Thus, the total number of active transitions rises to 14. Additionally, two the longest wavelength transitions changed their HOMO→LUMO structure. The electric field of such energy consequently produces further destabilization of the nitrogen molecule by 0.014970233 a.u but even now the molecule still remains more stable than without the influence of the field. Just the application of the 0.05 a.u. field which destabilizes the molecule by 0.0308861116 a.u. reduces the stability of that molecule below that it had without the influence of the electric field. That field adds further longest wavelength transition at 202.2 nm causing additionally slight bathochromic shifts of the transitions on both red and blue sides of the spectrum and some bands in the central region of the spectrum move slightly hypsochromically. The electric field of 0.1 a.u. introduces more pronounced changes in the spectrum. The 1→9 transition ceases and the 1→8 transition appears instead. Some transitions change their HOMO-LUMO structure. The 0.1 a.u. electric field increases the molecule stability over that noted without field by 0.011073860 a.u. Thus, the stabilization of the molecule by electric field is non-linear in the energy of that field.

The simulations of the spectrum for the system of two nitrogen molecules provides the spectrum considerably enriched in the transitions. In the spectrum for the system without any influence of the external electric field the number of transitions increases from totally 30 and 5 among them active for single nitrogen molecule to totally 120 and 38 active, respectively. In this spectrum, all excitations specific for the spectrum of the single nitrogen molecule cannot be recognized. The 1→52, 1→53, 1→57, 1→77 and 1→121 transitions resembling these in the spectrum of the single nitrogen molecule in their position and intensity have more complex structure. In this spectrum, two longest wavelength transitions are less intensive than relevant transitions in the spectrum of the single molecule but three shorter wavelength transitions are more intensive than the corresponding transitions in the spectrum of the single molecule. In the system of two nitrogen molecules the total energy of the system is lower than doubled energy of the single nitrogen molecule. The energy of stabilization due to intermolecular interactions of two nitrogen molecules is 0.008076807 a.u. The system of five nitrogen molecules provides stabilization energy of 0.173319988 a.u. Thus, the electric field providing stabilization of the system increases with the number of interacting molecules.

In the bimolecular nitrogen system under the influence of the 0.01 a.u. electric field also the stabilization resulting from the intermolecular interactions is noted. This stabilization by 0.082799838 a.u. is stronger than in corresponding monomolecular system However, in the pentamolecular nitrogen system under the influence of the same electric field the stabilization energy is lower and reaches 0.072913550 a.u. Thus, in contrast to electric field non-perturbed systems an increase in the number of interacting molecules of nitrogen decreases the energy of stabilization.

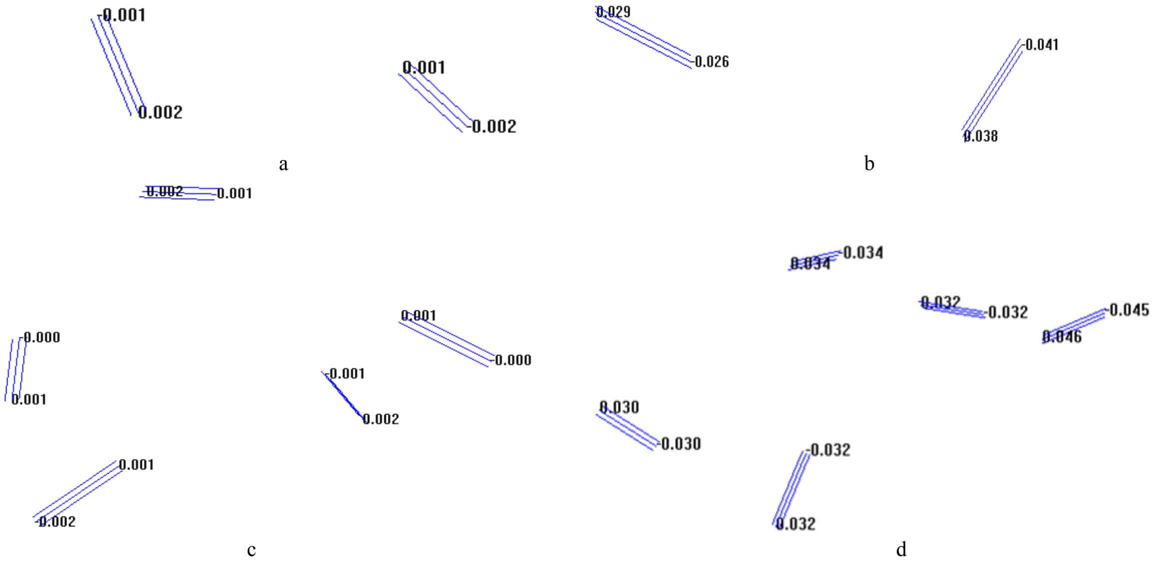
Figure 1 presents mapping of isosurface of the nitrogen molecule prior (left) and after (right) exposure to the electric field of 0.01 a.u. In electric field perturbed molecule a negative charge concentrates on both nitrogen atom increasing from 0.000 in non-perturbed molecule to -0.048 in the molecule in the electric field.

Figure 2 presents optimized natural and 0.01 a.u. electric field induced orientation of two and five nitrogen molecules.

Two nitrogen molecules without any influence of the electric field remain practically nonpolarized and are fairly arbitrarily mutually oriented. Under the influence of the electric field they turn polarized and their bipolar character induces certain charge density dependent mutual orientation. Under the absence of the external electric field, very slightly polarized five nitrogen molecules form practically disordered system whereas the electric field polarized the molecules and the polarization for particular molecules is different from one another as the effect of their own field. Mutual orientation of these molecules is clearly controlled by charge density interactions.

The oxygen molecule considered as biradical provides

Figure 1. Mapping of isosurface of the nitrogen molecule prior (left) and after (right) exposure to the electric field of 0.01 a.u.



a b c d

Figure 2. Optimized mutual orientation of two and five nitrogen molecules without field (a and c) and under the influence of the 0.01 au. electric field (b and d).

the spectrum composed of 8 transitions residing between 131.1 and 20.1 nm although there were considered 22 transitions (**Table 2**).

Its total energy is almost twice as low as that of the nitrogen molecule. Exposure of the molecule to the electric field influences the total energy of the molecule in an alternant way. A weak 0.001 a.u. electric field increases the total energy of the molecule by 0.018720379 a.u. what means that the molecule becomes more oxidative. Increase in the energy of the applied electric field to 0.005 a.u. stabilizes the former system by 0.025063273 a.u. in respect to the total energy of the initial and exposed to the 0.001 a.u. energy molecules. The exposure of the molecule to 0.01, 0.05 and 0.1 a.u. electric field accordingly increases the total energy of the molecule by 0.046010234, decreases it by 0.047923038 and increases again by 0.012487111 a.u., respectively. On exposure to the 0.001 a.u. field, the number of the transitions increases by one (1→5) appearing on the red side of the spectrum at 136.6 nm. A slight bathochromic shift of the other bands is observed with the decrease in the intensity of the longwavelength and increase in the intensity of the shortwavelength transitions. At the 0.005 a.u. field two additional bands on the shortwavelength side of the spectrum (1→18 and 1→19) are added. Simultaneously, the 1→23 transition vanishes. This time, a slight hypsochromic shift of all the bands takes place and their intensities increase and decrease in the longwavelenght and short wavelength regions, respectively. Further increase in the energy of the applied electric field to 0.01 a.u. produces two additional transitions appearing in the longwavelength (1→6) and central (1→14) region of the spectrum. The “native” transitions practically stay in place and their intensities change subtly. The increase in the energy of applied field to 0.05 a.u. generates four novel transitions in the central region (1→12, 1→13, 1→15 and 1→16) and, additionally, two transitions in the shortwavelength region (1→20 and 1→21) of the

Table 2. Simulated electronic spectra of one, two and five oxygen molecules without exposure and with exposure to external electric field.

Molecule (total number of transitions)	Transition energy (E) [nm] and its characteristics[a]					
	Without electric field			With electric field		
	E	f^{b}	Orbital → orbital; HOMO → LUMO and **total energy** [a.u.]	E	f^{b}	Orbital → orbital; HOMO → LUMO and **total energy** [a.u.]
O_2 (22)	131.1	0.3559	1→7	*136.6*^{c}	0.0010	1→5
	88.0	0.0504	1→8	135.4	0.3525	1→7
	88.0	0.0504	1→9	88.2	0.0490	1→8
	80.3	0.0926	1→10	88.2	0.0490	1→9
	80.3	0.0926	1→11	80.7	0.0936	1→10
	46.1	0.8969	1→17	80.7	0.0936	1→11
	23.3	0.0057	1→22	46.2	0.9227	1→17
	20.1	0.2837	1→23	23.5	0.0060	1→22
			–23.930508098	20.3	0.2925	1→23
						–23.911787719
				136.0^{d}	0.0031	1→5
				132.40	0.3535	1→7
				87.9	0.0507	1→8
				87.9	0.0507	1→9
				80.2	0.0924	1→10
				80.2	0.0924	1→11
				46.1	0.8888	1→17
				43.0	0.0001	1→18
				39.1	0.0001	1→19
				23.2	0.0056	1→22
				20.1	0.2810	1→23
						–23.936250992
				136.1^{e}	0.0068	1→5
				136.0	0.0002	1→6
				132.1	0.3499	1→7
				87.9	0.0502	1→8
				87.9	0.0501	1→9
				80.2	0.0927	1→10
				80.2	0.0927	1→11
				53.5	0.0001	1→14
				46.1	0.8839	1→17
				42.9	0.0018	1→18
				39.1	0.0007	1→19
				23.2	0.0056	1→22
				20.1	0.2801	1→23
						–23.890240758
				141.1^{f}	0.0088	1→5
				141.1	0.0079	1→6
				126.8	0.3445	1→7
				85.0	0.0213	1→8
				85.0	0.0212	1→9
				78.9	0.1124	1→10
				78.9	0.1123	1→11
				59.7	0.0005	1→12
				59.7	0.0004	1→13
				52.8	0.0006	1→14
				52.7	0.0005	1→15
				52.7	0.0012	1→16
				46.5	0.7697	1→17
				42.0	0.0411	1→18
				38.7	0.0341	1→19
				29.8	0.0023	1→20
				29.8	0.0023	1→21
				23.0	0.0051	1→22
						–23.938163796
				157.2^{g}	0.0196	1→5
				157.0	0.0191	1→6
				127.8	0.2882	1→7
				83.7	0.0036	1→8
				83.7	0.0036	1→9
				74.4	0.1116	1→10

				74.4	0.0015	1→11
				61.9	0.0019	1→12
				61.9	0.00100.	1→13
				56.0	0086	1→14
				54.8	0.0026	1→15
				54.8	0.0022	1→16
				48.3	0.7561	1→17
				41.2	0.0565	1→18
				38.1	0.1100	1→19
				30.7	0.0096	1→20
				30.7	0.0096	1→21
				23.8	0.0064	1→22
				20.5	0.2826	1→23
						−23.925676685
$(O_2)_2$ (94)	147.1	0.2070	1→12	151.3^{g}	0.2056	1→10
	85.6	0.1178	1→22	135.5	0.0001	1→12
	81.0	0.0264	1→25	85.8	0.1182	1→24
			−47.926248950	81.4	0.0255	1→27
						−47.906263740
$(O_2)_5$ (598)				286.9^{g}	0.0088	1→2
				286.8	0.0089	1→3
	203.8	0.0001	1→27	286.1	0.0004	1→4
	179.5	0.0007	1→38	241.6	0.0002	1→6
	169.6	0.0012	1→40	165.2	0.0018	1→11
	161.8	0.0003	1→43	161.9	0.0008	1→13
	157.5	0.0354	1→49	156.4	0.0023	1→16
	153.6	0.0006	1→50	142.1	0.0005	1→20
	152.5	0.1145	1→52	131.5	0.0005	1→21
	147.4	0.0501	1→59	104.9	0.0026	1→27
	137.9	0.0001	1→67	101.3	0.0005	1→32
	135.5	0.0008	1→70	97.4	0.0022	1→38
	134 2	0.0013	1→72	97.3	0.0021	1→39
	129.9	0.0001	1→77	46.1	0.0001	1→83
	88.1	0.0004	1→122	45.2	0.0694	1→84
	87.7	0.0003	1→125	41.5	0.00010.	1→96
	85.8	0.0005	1→132	41.5	0009	1→97
	85.7	0.0005	1→133	40.8	0.4430	1→99
	85.6	0.1161	1→134	38.9	0.0017	1→107
	81.6	0.0251	1→152	37.6	0.0002	1→120
	71.6	0.0002	1→193	37.5	0.0001	1→121
	59.2	0.0004	1→240	37.3	0.0005	1→122
	56.8	0.0003	1→255	32.4	0.0004	1→145
	47.6	0.0001	1→350	32.4	0.00040.	1→146
	29.9	0.0007	1→491	32.0	0055	1→148
			−119.316786473	31.3	0.0001	1→149
				29.6	0.0002	1→161
				23.4	0.0001	1→247
						−102.846760782

[a]The data in the Table presented in italics relate to the novel transitions generated by the application of an electric field of a given energy. Such values in bold italics denote transitions which cease on application of the electric field of the next higher energy; [b]The oscillator strength; [c]In the field of 0.001 a.u.; [d]In the field of 0.005 a.u; [e]In the field of 0.01 a.u.[f]In the field of 0.05 a.u; [g]In the field of 0.10 a.u.

spectrum. The longest wavelength transitions shift bathochromically whereas the other transitions move op--posite direction. At the 0.1 a.u. field only one novel band appears as the shortest wavelength 1→23 transition. All transitions except 1→18 and 1→19 move bathochromically. Simultaneously, longwavelength bands decrease their intensities whereas the transitions in the shortwavelength and central regions increase their intensities. Except the 1→18 transition, the other transitions increase their intensities.

Such lack of relationships between applied electric field and changes in the spectra pattern could result from a complex response from lone electron pairs and unpaired spins of both oxygen atoms to the varying dipole moment forced by applied electric field.

Figure 3 presents mapping of isosurface of the oxygen molecule without and with electric field of 0.01 a.u.

In the system of two oxygen molecules there is a stabilization due to the intermolecular interactions. The total energy of the system is lower by 0.063232754 a.u. than doubled total energy of the single molecule. The 0.01 a.u. field cooperates with these interactions and the stabilization of the system reaches 0.125782224 a.u. In the system of five oxygen molecules intermolecular interactions are less efficient. The total energy of the system is higher by 0.336754017 a.u. than five-fold energy

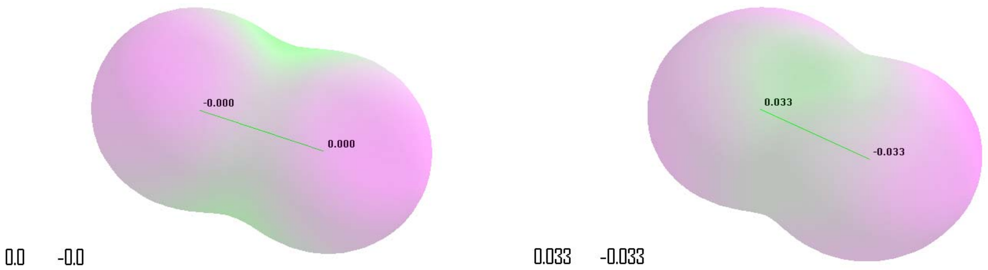


Figure 3. Mapping of isosurface of the oxygen molecule without electric field (left) and at 0.01 a.u. electric field (right).

of the single molecule. The 0.1 a.u. electric field introduces dramatic destabilization of the system. The cor-res-ponding energy of destabilization is -16.604443008 a.u pointing to a highly oxidative ability of such system.

The field-perturbed oxygen molecules are clearly polar and, therefore, they form the charge density regulated system. In the system of five molecules their polarization entirely ceases and their orientation is rather arbitrary. The application of the electric field recovers the polarization of the molecules which influences certain mutual orientation of those molecules.

Figure 4. presents optimized orientation of two and five oxygen molecules without intervention of electric field and in the 0.01 a.u. electric field.

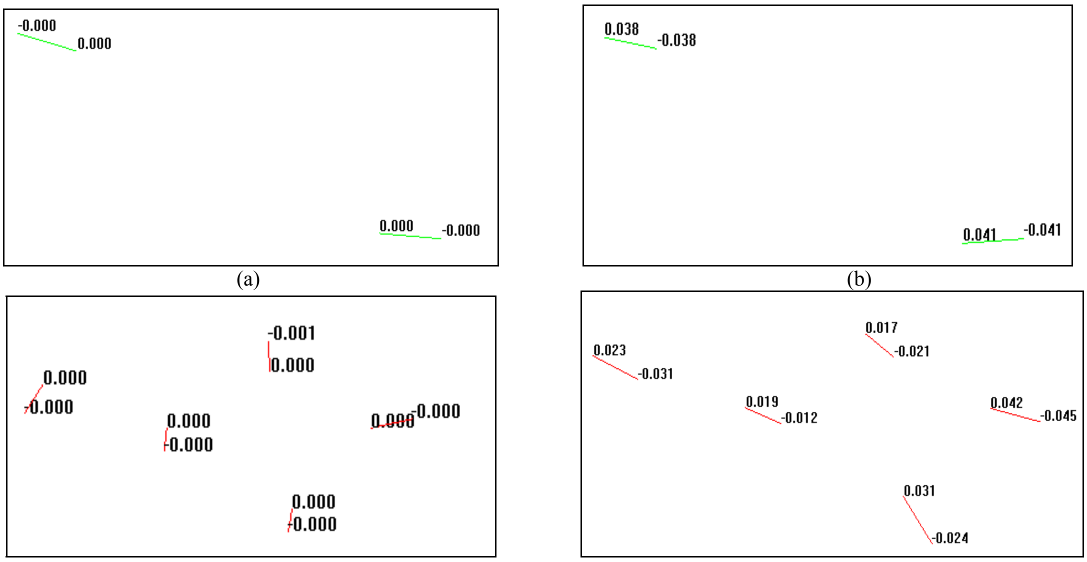
The simulation provided the UV spectrum of a single water molecule consisting of 7 transitions, all with $f >> 0.0000$ (**Table 3**). Nine other transitions are inactive ($f = 0.0000$).

Application of the electric field of 0.01 a.u. modifies the spectral pattern of unperturbed molecule on the red side. Novel transitions appear at 100.1 and 91.8 nm and one transition in original, unperturbed spectrum located at 90.9 nm ceases. The transitions shift slightly towards blue and their intensities vary irregularly.

Figure 5 presents the mapping of the isosurface of individual water molecules without and with the influence of electric field of 0.01 a.u.

The electric field concentrates the negative charge on the oxygen atom. The negative charge declines from -0.383 to -0.414 and, in the same time, the positive charge increased from 0.191 to 0.207. Thus, water molecule becomes more acidic and more prone to form dimers, trimers and so on. Such behavior can be responsible for several peculiar, poorly understood properties of water [27]. This result can be responsible for stabilization of the molecule in the 0.01 a.u. field by 0.019448846 a.u.

In the spectrum of the system of 5 water molecules totally 400 transitions in the UV region are considered and among them only 199 transitions are characterized by f > 0.0000. (**Table 3**). The transitions are situated in the region from 111.3 to 27 nm. The five fold increase of



(a) (b)

(c) (d)

Figure 4. Optimized orientation of two and five oxygen molecules without intervention of electric field (a and c) and in the 0.01 a.u. electric field (b and d).

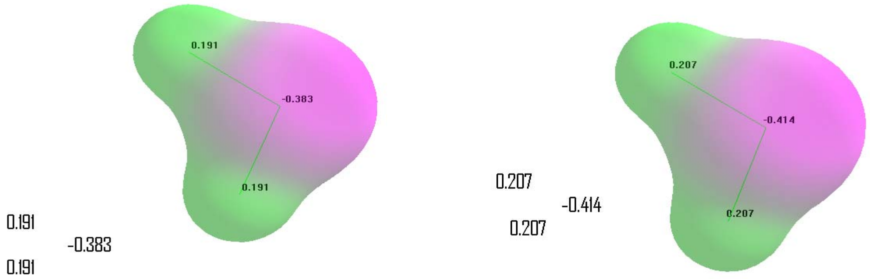


Figure 5. Mapping of isosurface of the water molecule prior (left) and after (right) exposure to the electric field of 0.01 a.u.

Table 3. Simulated electronic spectra of one and five water molecules without exposure and with exposure to 0.01 a.u. external electric field.

Molecule (total number of transitions)	Transition energy (E) [nm] and its characteristics[a]					
	Without electric field			With electric field		
	E	f^b	*Orbital → orbital* HOMO → LUMO and **total energy** [a.u.]	E	f^b	*Orbital → orbital* HOMO → LUMO and **total energy** [a.u.]
H_2O (16)	111.3	0.0329	*1→3;* 4→5	110.9	0.0317	*1→3;* 4→5
	90.9	0.0106	*1→8*; 3→5	*100.1*	0.0034	*1→6*; 4→6
	84.3	0.1866	*1→9;* 3→6	*91.8*	0.0140	*1→7;* 3→5
	64.5	0.2536	*1→12*; 2→5	83.0	0.1729	*1→9*; 3→6
	56.1	0.3382	*1→13*; 2→6	62.9	0.2860	*1→12*; 2→5
	29.6	0.0909	*1→16*; 1→5	54.4	0.2969	*1→13*; 2→6
	29.0	0.1760	*1→17;* 1→6	29.8	0.0787	*1→16*; 1→5
				28.7	0.1817	*1→17*; 1→6
			–13.581465020			**–13.600913866**
$(H_2O)_5$[c] (400)	91.3	0.0574	*1→*33; none	110.6	0.0510	*1→9;* none
	85.7	0.1692	*1→37;* 13→26,11→26	94.5	0.0800	*1→29*; none
	84.9	0.1205	*1→40*; 15→30	87.4	0.1169	*1→43*; 20→28
	84.4	0.2383	*1→43*; 13→27,11→27	86.8	0.0950	*1→46;* 18→21
	84.1	0.0951	*1→45*; 19→21	86.6	0.0765	*1→47*; 17→29
	83.9	0.1172	*1→46*; 12→28	85.6	0.1341	*1→50;* 14→26,13→26
	83.1	0.0607	*1→50*; none	84.7	0.1493	*1→52;* 17→30
	83.1	0.1003	*1→51*; 16→21	81.8	0.0939	*1→59;* 11→27
	66.2	0.1030	*1→181*; 10→21	68.3	0.0540	*1→156*; 12→25
	65.1	0.2198	*1→191*; 9→22	65.8	0.0775	*1→172*; none
	63.8	0.0922	*1→199;* none	64.6	0.0545	1→179; none
	63.4	0.1638	*1→204*; 13→29	62.3	0.1045	*1→198*; 11→22,11→23
	62.8	0.2308	*1→208;* 8→23	62.1	0.5283	*1→199;* 6→21
	58.4	0.0934	*1→219;* 10→22,10→26	61.8	0.2575	*1→202*; 7→23,7→24
	58.1	0.1485	*1→221;* 10→22,10→26	55.8	0.5738	*1→231*, 7→27
	57.3	0.1396	*1→226;* 9→27,7→21	55.7	0.0652	*1→233*; 10→29
	57.1	0.0900	*1→228*; 7→21	55.7	0.0967	*1→234*; 8→24
	56.3	0.4467	*1→233*; 10→28	55.4	0.0909	*1→234*; 10→26
	55.8	0.0622	*1→238*; 10→29	55.2	0.0635	*1→239*; 10→28
	54.9	0.0796	*1→247*; 8→25	54.6	0.0721	*1→246*; 11→30,10→30
	54.6	0.0880	*1→250*; none	54.2	0.0558	*1→252*; none
	54.3	0.0519	*1→255*; 6→24	53.8	0.1820	*1→254*; 6→26
	30.1	0.0936	*1→313*; 4→21, 4→23	30.3	0.0584	*1→319*; 4→21,4→22
	30.0	0.1125	*1→314;* 5→22	29.9	0.0767	*1→323*; 5→29
	29.7	0.1123	*1→316*; 5→26	29.6	0.1206	*1→327*; 5→26
	29.6	0.0685	*1→317;* none	29.6	0.0849	*1→328*; 4→24,4→25
	29.5	0.1576	*1→319;* 5→27	29.6	0.1848	*1→329*; 5→30
	29.0	0.1042	*1→329*; 3→28	28.4	0.0722	*1→350*; 5→26,3→26
	29.0	0.1683	*1→331*; 4→24	27.8	0.0681	*1→358*; 3→27,2→27
	28.8	0.0947	*1→336*; none	27.3	0.0518	*1→368*; 3→27,2→27
			–67.963599996			**–68.055033213**

the water molecules makes the system more stable by 0.056274896 a.u. The electric field of. 0.01 a.u. reduces the number of active transitions with $f > 0.0000$ from 217 to 214. Applied field makes the structure of particular transitions entirely different from these in the field-unperturbed spectrum. Application of the 0.01 a,.u. field stabilizes the system of five water molecules in respect to that without influence of the field. The stabilization energy reaches relatively high value of 1.091433217 a.u. The stabilization can result from the facilitation of the formation of intermolecular hydrogen bonds.

The simulated UV spectrum of carbon dioxide consists of totally 64 transitions among whose 26 are active ($f > 0.0000$) (**Table 4**).

Based on the comparison of the wavelengths and intensities of computed transitions, the application of the 0.01 a.u. field eliminates from the spectrum of unperturbed molecule weak transition at 222.1, changes the structure of the 1→14 transition and adds another weak transitions 1→17, 1→20, 1→44 and 1→55. Comparable transitions in unperturbed and field-perturbed spectra shift irregularly towards blue and red and also their intensities vary irregularly. Applied 0.01 a.u. field destabilized the molecule by 0.018192592 a.u.

Figure 6 presents changes of the electron density in the carbon dioxide molecule prior to and after application of the field of 0.01 a.u.

That Figure shows that after application of the electric field of 0.01 a.u. negative charge non-equivalently concentrates on the oxygen atoms whereas positive charge on the carbon atom changes negligibly. The destabilization can result from the effect of the field upon interactions with involvement of induced dipoles. Simulation of the system of two CO_2 molecules analyzed totally 256 transitions among which 86 are active with $f > 0.0000$. The bimolecular system of CO_2 is less stable by 0.007099722 a.u. Likely this destabilization results from repulsion of the molecules. The 0.01 a.u. field increases the repulsion.

The spectrum of the $CO_2 – H_2O$ system illustrates the state of the well known equilibrium between carbonic acid and its components. As indicated by the total energy of the systems, the 0.01 a.u. field causes destabilization increasing total energy by 0.015102407 a.u. That field entirely changes the spectrum. Except the shortest wavelength 1→145 transition, corresponding transitions which can be recognized in both spectra have different HOMO-LUMO characteristics (**Table 4**).

The simulation of the UVVIS spectrum of the unperturbed and field perturbed ammonia molecule provids totally 24 transitions among whose only 12 transitions in both cases are active (**Table 5**).

This difference appears in the structure of the transi-

Table 4. Simulated electronic spectra of one and two carbon dioxide molecules as well as carbon dioxide – water 1:1 system without exposure and with exposure to 0.01 a.u. external electric field.

Molecule (total number of transitions)	Transition energy (E) [nm] and its characteristics^a					
	Without electric field			With electric field		
	E	f^b	*Orbital → orbital* HOMO → LUMO and **total energy** [a.u.]	E	f^b	*Orbital → orbital* HOMO → LUMO and **total energy** [a.u.]
	222.1	0.0004	*1→7*; 8→9,7→10	140.8	0.1730	*1→14*; 8→11
	142.2	0.3564	*1→14*; 8→9,8→11,7→10	*138.8*	0.0001	*1→17*; 7→11
	138.3	0.0001	*1→15*; 6→9,5→10	133.1	0.6290	*1→18*; 8→9, 8→11,7→10
	131.8	0.0014	*1→18*; 6→10,5→9	132.7	0.0059	*1→19*; 6→10,5→9
	131.6	0.0013	*1→19*; 6→9,5→10	*132.7*	0.0091	*1→20*; 6→9
	130.8	0.2958	*1→21*; 8→11,4→9	*122.3*	0.0032	*1→23*; 4→10
	120.3	0.2605	*1→24;* 4→9	121.9	0.0705	*1→24*; 4→9
	101.3	0.0362	*1→29*; 3→9	99.7	0.0325	*1→29*; 3→9
	97.7	0.1308	*1→30;* 3→10	97.9	0.1030	*1→30*; 3→10
	94.9	0.1582	*1→31*; 3→9	96.3	0.0906	*1→31*; 3→9
	91.8	0.0609	*1→33*; 6→11	93.4	0.0743	*1→33*; 6→11
	91.5	0.0110	*1→34*; 5→11	93.4	0.0858	*1→34*; 5→11
CO_2 (64)	77.2	1.3488	*1→36*; 4→11	77.5	1.3979	*1→36*; 4→11
	69.5	0.0012	*1→37*; 3→11	69.8	0.0092	*1→37*; 3→11
	61.8	0.0610	*1→40*; 8→12	61.9	0.0605	*1→40*; 8→12
	61.7	0.0618	*1→41*; 7→12	61.8	0.0606	*1→41*; 7→12
	52.2	0.0008	*1→45*; 5→12	*52.5*	0.0002	*1→44*; 6→12
	48.4	0.0062	*1→47*; 4→12	52.4	0.0003	*1→45*; 5→12
	45.6	0.1242	*1→49;* 3→12	48.4	0.0085	*1→47;* 4→12
	35.2	0.0021	*1→52*; 2→9	45.6	0.1209	*1→49*; 3→12
	33.3	0.0368	*1→57*; 1→9	*35.2*	0.0007	*1→53*; 2→9
	33.2	0.0406	*1→58*; 1→10	*35.2*	0.0002	*1→55*; 2→10
	30.3	0.2102	*1→60*; 2→11	33.4	0.0397	*1→57*; 1→9
	29.2	0.0022	*1→61*; 1→11	33.4	0.0406	*1→58*; 1→10
	23.8	0.0060	*1→64*; 2→12	30.4	0.2180	*1→60*; 2→11
	23.3	0.3157	*1→65*; 1→12	29.5	0.0030	*1→61*; 1→11

			–29.238512694	23.8	0.0006	*1→64*; 2→12
				23.4	0.3206	*1→65*; 1→12
						–29.220320102
$(CO_2)_2$[c] (256)	134.6	0.0688	*1→34*; 16→17	140.9	0.2113	*1→34*; 14→21
	133.9	0.6023	*1→35*; 16→20	140.6	0.0587	*1→35*; 16→22
	132.9	0.9910	*1→38*; 13→17	134.1	0.8054	*1→42*; 16→19,15→20
	98.5	0.0585	*1→72*; 6→20	132.6	0.5640	*1→45*; 14→17,14→21,13→18
	98.3	0.0924	*1→73*; 5→17	121.9	0.0994	*1→55*; 7→17
	98.0	0.1127	*1→74*; 5→18	98.1	0.0870	*1→86*; 6→20
	98.0	0.1165	*1→75*; 6→19	97.6	0.1054	*1→87*; 5→18
	96.4	0.0520	*1→82*; 16→22,13→22	95.8	0.1055	*1→93*; 3→17
	93.0	0.0723	*1→88*; 10→21	94.0	0.1002	*1→96*; 12→22;11→22,6→19
	92.9	0.0772	*1→89*; 11→22	93.9	0.1033	*1→97*; 12→22,11→22,6→20
	92.8	0.0611	*1→90*; 12→21,9→21	93.0	0.0832	*1→99*; 9→21
	92.6	0.0659	*1→91*; 12→22,9→22	77.6	1.6660	*1→126*; 10→22
	77.6	2.5980	*1→118*; 8→22,7→21	77.5	1.1105	*1→127*; 7→21
	77.5	0.1587	*1→119*; 8→22	61.9	0.0603	*1→148*; 16→24
	61.7	0.1185	*1→150*; 16→23,13→24	61.9	0.0610	*1→149*; 15→24
	61.7	0.0574	*1→152*; 15→24	61.8	0.06910	*1→150*; 14→23
	61.7	0.0661	*1→153*; 14→23	61.8	.0603	*1→151*; 13→23
	45.6	0.1312	*1→176*; 5→23	45.5	0.1249	*1→182*; 6→24
	45.6	0.1142	*1→177*; 6→24	45.5	0.1115	*1→183*; 5→23
	33.3	0.0772	*1→209*; 2→18,1→18	30.5	0.2172	*1→226*; 4→22
	33.3	0.0755	*1→211*; 2→20,1→17	30.4	0.2118	*1→227*; 2→21
	30.4	0.4096	*1→230*; 4→21,3→22	23.5	0.3406	*1→250*; 3→24
	23.4	0,5414	*1→248*; 2→23,1→24	23.4	0.2747	*1→251*; 1→23
			–58.470925666			**–58.434944686**
CO_2+H_2O (144)	138.8	0.0772	*1→14*; 12→13,10→15	138.6	0.3129	*1→14*; 12→15,11→14
	132.9	0.7053	*1→24*; 11→14,10→13	129.9	0.0001	*1→21*; 12→15
	96.4	0.0840	*1→46*; 4→14	121.5	0.2548	*1→25*; 6→13
	95.8	0.0772	*1→47*; 4→13	100.7	0.0623	*1→36*; 9→13,5→13
	92.6	0.1133	*1→49*; 8→15,7→15	99.1	0.0971	*1→50*; 9→14,5→14
	92.4	0.0866	*1→50*; 8→15,7→15	89.8	0.0798	*1→53*; 8→15,7→15,5→14
	91.0	0.0901	*1→51*; 9→15,9→16	84.2	0.1528	*1→55*; 9→17
	86.6	0.1552	*1→53*; 9→15,9→16	78.4	1.1594	*1→62*; 9→15,6→15
	84.3	0.1701	*1→54*; 9→17	74.0	0.1325	*1→64*; 9→15,6→15
	76.7	1.1481	*1→64*; 6→15	65.4	0.2515	*1→78*; 4→16
	65.6	0.0577	*1→72*; 5→15	61.3	0.0632	*1→87*; 12→18
	63.1	01478	*1→76*; 5→15,5→16	61.3	0.0629	*1→88*; 11→18
	61.7	0.0511	*1→77*; 11→18,10→18	56.8	0.3200	*1→93*; 4→17
	61.7	0.0858	*1→78*; 11→18,10→18	46.1	0.0782	*1→105*; 9→18,5→18
	56.9	0.0663	*1→85*; 8→17	30.1	0.2431	*1→127*; 3→16,2→15
	55.5	0.2342	*1→91*; 5→17	29.5	0.0606	*1→128*; 3→15,3→17,2→15
	45.2	0.0938	*1→107*; 4→18	29.4	0.0950	*1→129*; 3→17
	30.1	0.1839	*1→128*; 2→15	23.1	0.2562	*1→145*; 1→18
	29.3	0.0502	*1→129*; 3→16			**–42.836673450**
	28.8	0.1674	*1→131*; 3→17			
	23.3	0.3009	*1→145*; 1→18			
			–42.851775857			

[a]The data in the Table presented in italics relate to the novel transitions generated by the application of an electric field of a given energy. Such values in bold italics denote transitions which cease on application of the electric field of the next higher energy; [b]The oscillator strength; [c]In this Table only transitions of *f* ≥0.0500 are given. The total number of the transitions with; *f* > 0.0000 is 86 and 82 in the spectra of one and two carbon dioxide without and with electric field, respectively. In the carbon dioxide – water system the relevant numbers are 67 and 68, respectively. Values of E [nm] given in italics denote novel transitions generated on the application of electric field. Values in bold italics denote transitions which will cease on application of more intensive electric field.

Table 5. Simulated electronic spectra of single molecule of ammonia without exposure and with exposure to 0.01 a.u. external electric field and analogous computations for the ammonia-water system.

Molecule (total number of transitions)	Transition energy (E) [nm] and its characteristics Without electric field				With electric field	
	E	*f*[a]	*Orbital → orbital* HOMO → LUMO and **total energy** [a.u.]	E	*f*[a]	*Orbital → orbital* HOMO → LUMO and **total energy** [a.u.]
NH_3 (24)	123.3	0.0270	*1→3*; 4→5	120.9	0.0191	*1→3*; 4→5
	111.7	0.0532	*1→6*; 4→6	109.9	0.0682	*1→6*; 4→6
	106.0	0.0643	*1→7*; 4→7	105.9	0.0738	*1→7*; 4→7
	71.2	0.0112	*1→11*; 3→5	71.2	0.0189	*1→11*; 3→5

	67.6	0.0050	*1→14*; 2→5	69.7	0.0030	*1→14*; 2→5
	65.9	0.0107	*1→15*; 3→7,2→6	67.5	0.0012	*1→15*; 3→7,2→6
	62.9	0.4495	*1→17*; 3→6,2→7	63.9	0.4548	*1→17*, 3→6,3→7,2→6
	62.0	0.4795	*1→18*; 3→7,2→6	63.5	0.4811	*1→18*; 3→6,2→6
	54.5	0.1984	1→19; 3→6,2→7	55.7	0.2366	*1→19;* 3→2,2→7
	32.5	0.0196	*1→23*; 1→5	32.8	0.0278	*1→23*; 1→5
	31.6	0.1124	*1→24*; 1→6	32.1	0.1187	*1→24*; 1→6
	31.1	0.1380	*1→25*; 1→7	31.7	0.1347	*1→25*; 1→7
			–10.944414844			**–10.905433106**
$NH_3 + H_2O$ (80)	128.3	0.0520	*1→3*; 8→9	115.7	0.0063	*1→5;* 8→10
	110.8	0.0300	*1→7;* 8→12	108.9	0.0679	*1→7*; 8→12
	109.6	0.0300	*1→8*; 7→10	107.4	0.0316	*1→9;* 7→9
	109.3	0.0342	*1→9*; 8→13	102.4	0.0362	*1→10*; 8→13,7→11
	103.1	0.0019	*1→11*; 7→11	102.4	0.0588	*1→11;* 8→13,7→11
	89.6	0.0149	*1→14*; 8→10,6→10	95.4	0.0649	*1→13*; 8→9
	88.8	0.0026	*1→16*; 8→10,6→10	89.0	0.0593	*1→15*; 8→11,6→11
	83.5	0.1751	*1→18*; 6→11	84.8	0.0040	*1→17*; 6→9
	83.3	0.0094	*1→19*; 7→9	78.5	0.1286	*1→21*; 8→11,6→11
	80.3	0.0034	*1→21;* 8→11	75.6	0.0013	1→23; 7→23
	73.7	0.0061	*1→25;* 6→9	73.6	0.0027	*1→25;* 5→10
	71.7	0.0082	*1→28*; 7→12	70.9	0.0006	*1→28*; 7→12
	69.5	0.0025	*1→31*; 7→13	69.2	0.0197	*1→30*; 5→13
	69.0	0.0108	*1→33*; 5→9	68.3	0.0387	*1→33;* 5→12. 4→10
	66.9	0.0268	1→34; 4→9	67.8	0.0005	*1→35*; 7→13
	64.4	0.1634	*1→37*; 6→12,3→10	66.8	0.0119	*1→38*; 6→10
	64.3	0.0589	*1→38*; 6→12,3→10	66.2	0.0073	*1→39*; 5→9
	63.7	0.0410	*1→40*; 6→13,5→13,4→12	65.0	0.3505	*1→41*; 5→12,4→10
	62.0	0.0178	*1→42*; 6→13,4→12	64.2	0.3906	*1→42*; 4→12
	60.1	0.4280	*1→44*; 5→12,4→13	63.4	0.2631	*1→43;* 3→9
	59.9	0.5103	*1→45*; 5→13,4→12	63.2	0.0268	*1→45*; 6→12
	58.2	0.0107	*1→47*; 5→10	61.5	0.0298	*1→46*; 3→11
	57.4	0.0024	*1→49;* 3→9	61.0	1.0054	*1→49*; 4→9
	56.3	0.3176	*1→50*; 5→11,3→11	60.7	0.0076	*1→51*; 6→13
	56.1	0.0012	*1→52*; 4→10	57.3	0.0394	*1→52*; 4→11
	54.3	0.0241	*1→54*; 5→11,3→11	55.9	0.4434	*1→54;* 3→11
	53.5	0.1057	*1→55*; 5→12,4→13	55.6	0.1134	*1→55*; 4→13
	52.5	0.0002	*1→57*; 4→11	54.0	0.0016	*1→57*; 3→10
	51.6	0.0044	*1→59*; 3→12	51.6	0.0042	*1→59*; 3→12
	50.4	0.0011	*1→61*; 3→13	49.9	0.0008	*1→61;* 3→13
	33.1	0.0069	*1→65*; 2→9	32.2	0.0137	*1→66*; 2→9,2→10
	31.4	0.1313	*1→67*; 2→12	31.8	0.0975	*1→67*; 2→12
	31.2	0.1521	*1→69*; 2→13	31.7	0.0475	*1→68*; 2→9,2→10
	31.0	0.0003	*1→70;* 2→10	31.2	0.1456	*1→71*; 2→13
	30.0	0.0150	*1→72;* 2→11	30.8	0.0080	*1→72*; 2→11
	29.2	0.0866	*1→74*; 1→10	29.1	0.0745	*1→74;* 1→9
	28.6	0.0164	*1→76*; 1→9	28.6	0.1713	*1→75*; 1→11
	28.6	0.1480	*1→77;* 1→11	27.8	0.0050	*1→77*; 1→10
	27.1	0.0019	*1→79*; 1→12	27.1	0.0034	*1→79*; 1→12
	26.8	0.0003	*1→81*; 1→13	26.7	0.0022	*1→81*; 1→13
			–24.567018796			**–24.547055634**

[a] The oscillator strength

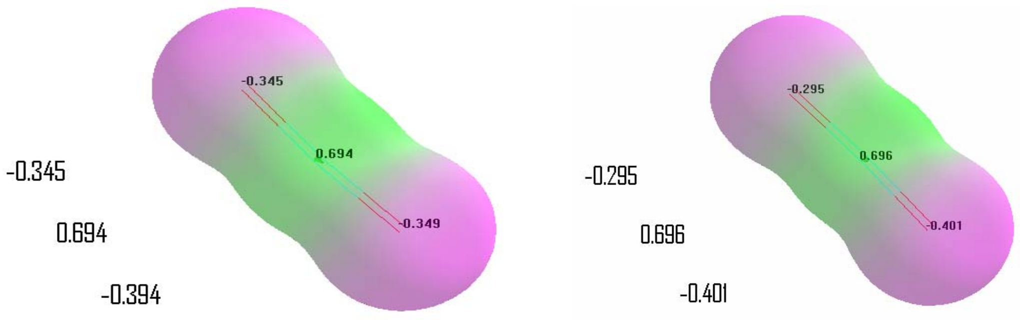


Figure 6. Changes of the electron density in the carbon dioxide molecule prior to (left) and after application (right) of the field of 0.01 a.u.

tions in the central part of the spectrum (transitions 1→17, 1→18 and 1→19). Applied electric field destabilizes the system. Energy of destabilization is 0.038981738 a.u. *i.e.* the total energy of the molecule in the field is higher than the total energy of field-unperturbed molecule.

Figure 7 presents mapping of isosurface of the ammonia molecule in unperturbed state and after its exposure to the 0.01 a.u. electric field.

Applied electric field concentrates the charge on the lone electron pair orbital of the nitrogen atom making ammonia a stronger base. Corresponding data showed that the negative charge on the nitrogen atom declined from –0.415 into -0.420.

Totally 80 transitions were analyzed on simulation of the UVVIS spectrum of the ammonia-water system (**Table 5**). Forty of them appears active in the spectra without and with the field of 0.01 a.u. Because in the electric field water and ammonia turn into stronger acid and base, respectively, their mutual interactions introduce a complex spectral changes. Only in the most blue part of the spectrum these changes appear minute.

The electric field of 0.01 a.u. destabilized also this system. The energy of destabilization reaching 0.019963162 a.u. is lower than that in single ammonia molecule placed in this field.

Figure 8 presents mapping of isosurface of the ammonia – water system

One can see that in that system out of the electric field the negative charge (–0.432) is more pronounced at the nitrogen atom of ammonia than at the oxygen atom of the partnering water molecule (–0.428). After the application of the 0.01 a.u. electric field, the negative charge is more concentrated at the water oxygen atom (–0.452) than at the ammonia nitrogen atom (-0.420). It provides an evidence that in the electric field enhanced acidic and basic properties of water and ammonia molecules, respectively, result in the acid-base interactions in which water is hydrogen donor and ammonia its acceptor.

Thus, except CO_2, all investigated single small molecules out of aura emit UV light in the area of the vacuum ultraviolet. In the spectrum of CO_2 one weak transition appears at 221.1 in order to cease after application of the 0.01 a.u. electric field. In the system of two molecules checked for nitrogen the first transitions appear at 180.4 and 169.6 nm, however, they are very weak. The transi-

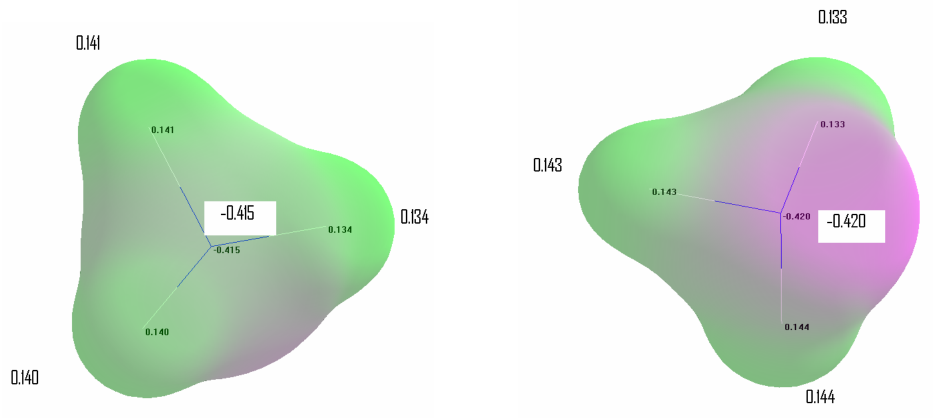


Figure 7. Mapping of isosurface of the ammonia molecule in unperturbed state and after its exposure to the 0.01 a.u. electric field.

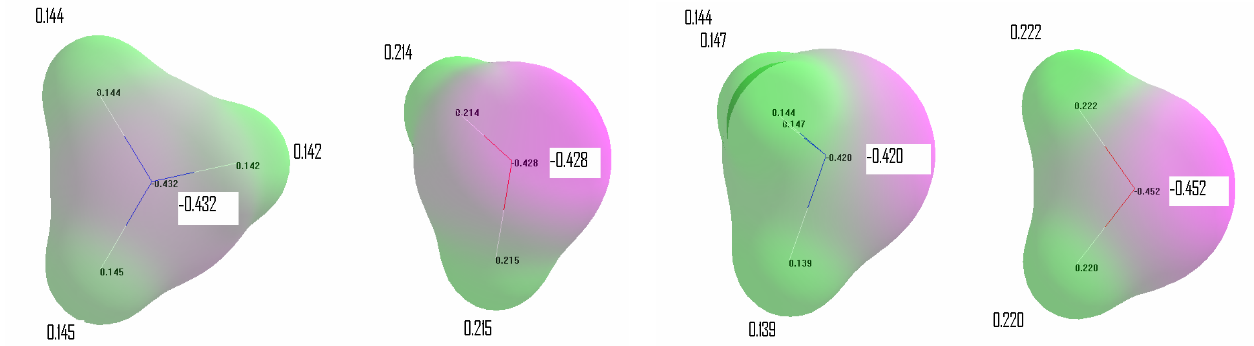


Figure 8. Mapping of isosurface of the ammonia water molecules system in unperturbed state (two left images) and after its exposure (two right images) to the 0.01 a.u. electric field.

tions of the intensity comparable to these in the spectrum of the single nitrogen molecule are met also at 100 nm. In the spectrum of two oxygen molecules the first intensive transition resides at the wavelength by 16 nm higher than in the spectrum of the single molecule. However, majority of the shorter wavelength transitions completely ceases. The spectrum of two CO_2 entirely differ from the spectrum of the single molecule. Anyway, the longest wavelength transitions disappears. Further increase in the number of molecules in the systems checked for N_2, O_2 and H_2O provides diverse results. In the spectra of five nitrogen and five water molecules the longest wavelength transitions seen in their spectrum of two molecules are now absent. In contrast to them in the spectrum of five O_2 molecules longwavelength transitions are added.

The effect of the electric field and on a given molecule and their sets depends on the energy of the field and it is not linear in that energy. Moreover, that effect is specific for particular molecules. Only in the spectrum of $(O_2)_5$ the electric field of 0.01 a.u. can generate long-wavelength transitions beyond the vacuum ultraviolet region. Also in the spectrum of N_2 in the field of 0.05 a.u. a weak transition at 202.2 nm can be seen. In no case emission in the visible region can be found.

Since all transitions of the molecules under considerations situated in the electric field are observed in the vacuum ultraviolet region only spectrum of oxygen would be observed for genuine plasma containing all the molecules considered in this project.

4. CONCLUSIONS

Electric field over surfaces of inanimate objects rather insignificantly change the electronic transitions in the molecules constituting aura (N_2, O_2, H_2O, CO_2 and NH_3). All these molecules emit in the region of vacuum ultraviolet. Only a system of 5 oxygen molecules in the field of 0.01 a.u. exhibits weak transitions above 200 nm.

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