

# WPŁYW STATYCZNEGO HIPEREKSTREMALNEGO POLA MAGNETYCZNEGO NA PROSTE STRUKTURY MOLEKULARNE WYSTĘPUJĄCE W BIOLOGICZNIE WAŻNYCH TYPACH ZWIĄZKÓW CHEMICZNYCH. CZĘŚĆ 2\*. ROZKŁAD ŁADUNKÓW

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## Influence of static hyper extremely magnetic field on simple molecular structures found in biologically important types of chemical compounds. Part 2\*. Charge distribution

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### Streszczenie/Abstract

**Wstęp:** Wpływ pól elektrycznych, elektromagnetycznych i magnetycznych na organizmy żywe jest ważny dla zdrowia. Stosunkowo niewiele wiadomo o skutkach działania statycznego pola magnetycznego SMF, zatem przewidywanie jego wpływów na wybrane a ważne pod względem biochemii obiekty molekularne jest celowe. Przedmiotem symulacji komputerowej stały się 34 proste organiczne molekuły należące do 6 klas, których elementy odgrywają kluczowe role w biochemii.

**Metody badawcze:** Kwantowo-mechaniczne symulacje komputerowe skutków działania pola magnetycznego na związki modelowe dały wgląd w zmiany rozkładu gęstości elektronicznej, zmiany elektrycznego momentu dipolowego oraz energii tworzenia, będącej miarą trwałości molekuly.

**Wnioski:** Wpływ bardzo silnego statycznego pola magnetycznego, rzędu 10<sup>4</sup>T, jest niewielki. Zmienia się znacząco rozkład ładunków jedynie w sulfonach, sulfotlenkach, grupach nitrowej, estrowej, cjanianowej i tiocjanianowej. Wzrost zewnętrznego statycznego pola magnetycznego powoduje zmniejszenie trwałości cząsteczek oraz wzrost ich elektrycznych momentów dipolowych, będące skutkiem polaryzacji cząsteczek i wydłużenia ich wiązań. Symulowane zmiany nie wydają się być groźne dla zdrowia.

*Słowa kluczowe:* statyczne pole magnetyczne, rozkład ładunków elektrycznych, elektryczne momenty dipolowe, energie tworzenia, symulacje komputerowe.

**Introduction:** The effects of electric, electromagnetic and magnetic fields on living organisms are important for health. Relatively little is known about the effects of the static magnetic field (SMF), so predicting its effects on selected biochemically important molecular objects is expedient. The computer simulation were performed for 34 simple organic molecules belonging to 6 classes, the elements of which play key roles in biochemistry.

**Research methods:** Quantum-mechanical computer simulations of the effects of magnetic fields on model compounds provided insight into changes in electron density distribution, changes in electric dipole moment and formation energy, which is a measure of the stability of a molecule.

**Conclusions:** The influence of a very strong static magnetic field, on the order of 10<sup>4</sup>T, is fairly weak. The charge distribution changes significantly only in sulfones, sulfoxides, nitro, ester, cyanate and thiocyanate groups. An increase in the external static magnetic field causes a decrease in the durability of molecules and an increase in their electrical dipole moments, resulting from the polarization of molecules and the elongation of their bonds. The simulated changes suggest that applied SMF do not seem to be dangerous for health.

*Key words:* static magnetic field, distribution of electric charges, electric dipole moments, formation energies, computer simulations.

## Introduction

The surrounding us magnetic field provides a natural shield protecting life on the Earth from cosmic radiation. In contrast to static electric or alternating electromagnetic fields whose influence on living organisms is relatively well understood, Mazurkiewicz [12, 13], the influence of magnetic field still takes additional studies.

The influence of the magnetic field on life processes is an important issue, therefore other numerous research centers around the world are engaged in research on the mechanisms of influence and its effects [14, 16].

The previous paper, Ciesielski [7], presents the results of simulation studies of changes in bond length of selected 34 model compounds grouped into six classes. This report presents the results of calculations of changes in charge distributions, electric dipole moments and formation energy of the previously presented model compounds, induced by the static magnetic field (SMF).

Under terrestrial conditions, it is almost impossible to achieve extremely high magnetic field strengths in excess of 2000 T, but there are gigantic fields (over  $10^9$  T) in space, Tsygankov [15]. However, it cannot be ruled out that fields of up to  $10^4$  T could be formed in our surroundings as a result of power plant accidents or during high-energy experiments, so it is important to understand the potential health effects of these fields.

In current calculations, the influence of a field with an intensity of 10 AMFU (an arbitrary unit of magnetic field) equal to approximately  $10^3$  T = 107 G, Ciesielski [5] is accepted.

In the latest papers, Ciesielski [2, 4, 5, 6], the calculated effect of extremely strong magnetic fields (up to over 105 T) on selected types of molecules, from very simple to complex and playing a key role in biochemistry, is presented. In

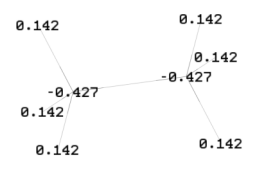
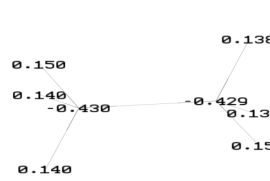
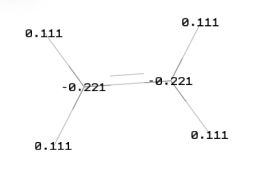
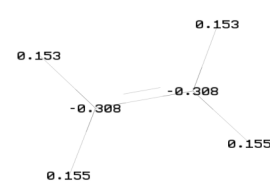
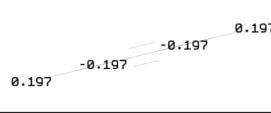
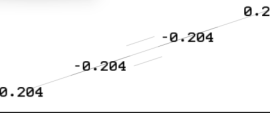

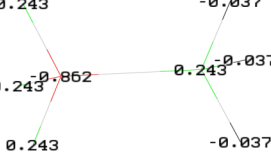
calculations currently carried out *in silico* and in a *computer vacuum*, field lines parallel to the long axis of the molecule were assumed.

Recently, the effect of strong magnetic fields has become a subject of interest for the Nottingham team, Irons T.J.P. et al. [10, 11]. They undertook a modification of the structural optimization calculations at the Hartree-Fock level and the current density functional theory, taking into account the motion of high-angular momentum electrons.

of the electron density distribution were calculated, then the effect of SMF along the optimized molecules was calculated using advanced Amsterdam Modelling Suite software containing the NR\_LDOTB method (non-relativistic orbital L-dot-B momentum), Carpenter [1] and Glendening [9].

The charge distribution and the electric dipole moments and formation energies were then recalculated using the previously used Gaussian 0.9 software with a 6-31G base\*\*.

Tab. 1. Non-polar linear compounds

No & Compound	Charge Distribution, a.u.	
	Magnetic Field, 0 AMFU	Magnetic Field, 10 AMFU
1 CH <sub>3</sub> -CH <sub>3</sub>		
2 CH <sub>2</sub> =CH <sub>2</sub>		
3 CH=CH		
4 CH <sub>3</sub> -SiH <sub>3</sub>		

They demonstrated the usefulness of the new approach only for optimizing the geometry of simple atomic systems (OH group) and the more complex, but highly symmetric, benzene [10].

## Numerical calculations

The calculations involved Gaussian 0.9 software equipped with a 6-31G\*\* database, Frisch [8], in which selected molecules were optimized and all values

## Results of calculations

Tables 1-6 and 1a-6a collect results of calculations in the form of a schematic structure of the compound on which the calculated bond lengths are given for the compound located in the zero SMF and in the field parallel to the longer axis of the molecule with an induction of 10 AMFU (1 AMFU is at least 1000 T, i.e.  $10^7$  G).

The first column in these tables contains the sequential number of the compound and its chemical formula.

In the case of ethane **1**, an alternating (*s-trans*) increase or decrease in electron density under the influence is observed (in the figures in Tab. 1-6, a positive number – electron deficit, a negative number – an excess of electrons). In the case of ethylene **2**, the electron acceptor effect of carbon atoms is increased under the influence of SMF, similarly in the case of acetylene **3**, but to a lesser extent. Methylsilane **4** is only subtly susceptible to SMF.

The largest and the weakest increase in the electric dipole moment is met in acetylene **3**, and ethylene **2**, respectively. The most and least remarkable weakening of bonds, visible in the formation energy, is observed in the case of methylsilane **4** and ethylene **2**, respectively. It can be rationalized in terms of the non-stress structure of  $sp^2$  of ethylene **2** and the heteroatomic nature of the elongated C-Si bond of methylsilane **4**.

In fluoromethane **5**, SMF subtly interferes with charge distribution, but in other halides **6-9**, the halogen becomes a stronger electron acceptor under the influence of SMF. In iodosomethane **9**, under the influence of SMF, the electro-acceptor character of the oxygen atom of the iodozo group increases the most, and there is also the highest increase in the electrical dipole moment and the largest decrease in bond stability measured by the formation energy.

The least change in this moment forced by SMF is observed in the case of fluoromethane **5**.

In dimethyl sulfide **10**, the sulfur atom became a weak electron acceptor, and hydrogen atoms turned into donors, similarly as in dimethyl selenide **11**. In methyl selenide **12** subjected to SMF, the observed changes are very subtle, this compound turned out to be very resistant, and the same deals with methyl mercaptan **13**.

Tab. 1a. Changes in macroscopic parameters of non-polar linear compounds.

No & Compound	Dipole Moment $\mu$ [D]		$\Delta\mu$ [D/AMFU]	Energy of creation [kJ/mol]		$\Delta E$ [J/(mol·AMFU)]
	0 AMFU	10 AMFU		0 AMFU	10 AMFU	
<b>1</b> CH <sub>3</sub> -CH <sub>3</sub>	0	0.6	0.060	-86	-53	33
<b>2</b> CH <sub>2</sub> =CH <sub>2</sub>	0	0.5	0.050	-54	-33	21
<b>3</b> CH≡CH	0	0.8	0.080	216	239	23
<b>4</b> CH <sub>3</sub> -SiH <sub>3</sub>	4,31	4.89	0.058	-384	-331	53

Tab. 2. Methyl halides

No & Compound	Charge Distribution, a.u.	
	Magnetic Field, 0 AMFU	Magnetic Field, 10 AMFU
<b>5</b> CH <sub>3</sub> F		
<b>6</b> CH <sub>3</sub> Cl		
<b>7</b> CH <sub>3</sub> Br		
<b>8</b> CH <sub>3</sub> I		
<b>9</b> CH <sub>3</sub> IO		

Tab. 2a. Changes in macroscopic parameters of methyl halides.

No & Compound	Dipole Moment [D]		$\Delta\mu$ [D/AMFU]	Energy of creation [kJ/mol]		$\Delta E$ [J/(mol·AMFU)]
	0 AMFU	10 AMFU		0 AMFU	10 AMFU	
<b>5</b> CH <sub>3</sub> F	1.87	1.93	0.006	-73	-52	21
<b>6</b> CH <sub>3</sub> Cl	1.49	1.69	0.020	-39	-21	18
<b>7</b> CH <sub>3</sub> Br	1.78	1.93	0.015	-32	-19	13
<b>8</b> CH <sub>3</sub> I	1.63	1.87	0.024	-26	-11	15
<b>9</b> CH <sub>3</sub> IO	6.54	6.94	0.040	-218	-182	36

Tab. 3. Either sulfur or selenium containing compounds.

No & Compound	Charge Distribution, a.u.	
	Magnetic Field, 0 AMFU	Magnetic Field, 10 AMFU
<b>10</b> <chem>CH3SCH3</chem>		
<b>11</b> <chem>CH3SeCH3</chem>		
<b>12</b> <chem>CH3SeH</chem>		
<b>13</b> <chem>CH3SH</chem>		
<b>14</b> <chem>CH3SO2CH3</chem>		
<b>15</b> <chem>CH3SOCH3</chem>		
<b>16</b> <chem>CH3SSCH3</chem>		

Tab. 3a. Changes in macroscopic parameters of either sulfur or selenium containing compounds.

No & Compound	Dipole Moment [D]		$\Delta\mu$ [D/AMFU]	Energy of creation [kJ/mol]		$\Delta E$ [J/(mol·AMFU)]
	0 AMFU	10 AMFU		0 AMFU	10 AMFU	
<b>10</b> <chem>CH3SCH3</chem>	4.30	4.82	0.052	-152	-81	71
<b>11</b> <chem>CH3SeCH3</chem>	1.02	1.63	0.061	-268	-211	57
<b>12</b> <chem>CH3SeH</chem>	1.32	1.65	0.033	-125	-98	27
<b>13</b> <chem>CH3SH</chem>	3.51	3.86	0.035	-42	-31	11
<b>14</b> <chem>CH3SO2CH3</chem>	4.85	5.06	0.021	-101	-79	22
<b>15</b> <chem>CH3SOCH3</chem>	5.49	6.01	0.052	-57	-36	21
<b>16</b> <chem>CH3SSCH3</chem>	0.00	0.70	0.070	-178	-142	36

The most magnetopolarizable (sensitive  $\mu$  to SMF) was dimethyl **16** disulfide, while dimethylsulfone **14** was the least magnetopolarizable. Under the influence of SMF, the bonds in dimethyl **10** sulfide and methyl **13** mercaptan weaken the most and least, respectively.

In methylamine **17**, an increase in SMF decreases the alkalinity of the nitrogen atom at the expense of both hydrogen atoms associated with it. Dimethylamine **18** is very susceptible to the effects of SMF. In azomethane **19**, SMF reduces the basicity of the atoms of the azo group, while the hydrogen atoms of the methyl groups become stronger electron donors.

In nitrosomethane **20**, the electron density of atoms of both atoms of the nitroso group decreases to a small extent in favour of an increase in density on the carbon atom. In turn, in nitromethane **21**, the nitro group turned out to be the most magnetosensitive.

SMF causes the electron shift from the nitrogen atom to both the oxygen atoms. This causes an increase in the electron density of the carbon atom at the expense of the hydrogen atoms of the methyl group. In methylsulfonylamide **22**, an increase in the dipolarity of the sulfone group is observed due to the increased acceptance of electrons of both oxygen atoms of this group. The carbon atom of the methylsulfone part becomes more basic at the expense of the hydrogen atoms associated with it. This effect is more intense than in the methylamine part.

In arsenometan **23**, SMF increases the electron donor effect of both arsenic atoms by more effectively transferring electrons to methyl groups, in which the electron density of hydrogen atoms also decreases. The highest and the lowest magnetopolarizability, manifested as a change in the dipole moment under the influence of SMF, is presented by dimethylsulfonamide **22**, and nitrosomethane **20**, respectively. SMF loosens bonds the most efficiently in nitromethane **21**, and the

Tab. 4. Either nitrogen or arsenic containing compounds.

No & Compound	Charge Distribution, a.u.	
	Magnetic Field, 0 AMFU	Magnetic Field, 10 AMFU
17 CH <sub>3</sub> NH <sub>2</sub>		
18 CH <sub>3</sub> NHCH <sub>3</sub>		
19 CH <sub>3</sub> NNCH <sub>3</sub>		
20 CH <sub>3</sub> NO		
21 CH <sub>3</sub> NO <sub>2</sub>		
22 CH <sub>3</sub> NHSO <sub>2</sub> CH <sub>3</sub>		
23 CH <sub>3</sub> AsAsCH <sub>3</sub>		

least efficiently in methylamine **17**, nitrosomethane **20** and dimethylamine **18**.

In methanol **24**, SMF increased electron density of the carbon atom and decreased electron density of the accompanying hydrogen atoms. The hydroxyl group is almost unchanged. In dimethyl ether **25**, a slight influence of SMF can

be seen in the shift of electrons from hydrogen atoms, through the carbon atom to the oxygen atom. Dimethyl ether was found to be very insensitive to SMF.

In acetone **26**, SMF causes an increase in the electron density of the carbon atoms of the methyl groups at the expense of the carbonyl carbon atom.

In methyl **27** acetate, visible changes are visible in both carbon atoms of the acetate part, especially the methyl group, causing a stronger polarization of the C-C bond.

In methyl carbonate **28**, an increased transfer of electrons in the H→C→O sequence is observed, which results in a marked increase in the electron density of both oxygen atoms associated with the carbonyl group.

In N-methylacetamide **29**, SMF causes an increase in the alkalinity of the nitrogen atom, the electron density in the other components of the molecule changes very little. The largest changes in the electric dipole moment are seen in the case of esters **27** and **28**, the smallest in the case of methanol **24**.

The bonds in dimethyl carbonate **28** are weakened the most, and they are the weakest in the case of acetone **26**.

In acetonitrile **30**, the changes in electron density caused by SMF are almost invisible. In methyl cyanate **31**, SMF causes very large changes. The displacement of electrons can be visualized by the sequence H←C→C←N→O. In methyl thiocyanate **32**, the sequence of SMF-induced electron displacement starting from the hydrogen atoms of the methyl group looks analogous: H←C→C←N→S and is equally intense.

In the case of methyl isonitrile **33**, the sequence of SMF-induced electron displacement is different: H→C←N→C. In acetaldehyde **34**, SMF practically does not induce changes, this compound is highly stable.

The largest increase in the electric dipole moment is observed when SMF affects methyl isonitrile **33** and the smallest when acetaldehyde **34** is affected. Extreme examples of changes in the energy of creation involve the same compounds, except that the order is reversed. The structure of acetaldehyde **34** is weakened the most, while the structure of isonitrile **33** is the weakest.

Tab. 4a. Changes in macroscopic parameters of either nitrogen or arsenic containing compounds.

No & Compound	Dipole Moment [D]		$\Delta\mu$ [D/AMFU] (x1000)	Energy of creation [kJ/mol]		$\Delta E$ [J/(mol·AMFU)]
	0 AMFU	10 AMFU		0 AMFU	10 AMFU	
17 <chem>CH3NH2</chem>	1.68	1.88	0.020	-23	-8	15
18 <chem>CH3NHCH3</chem>	1.92	2.06	0.014	-88	-72	16
19 <chem>CH3NNCH3</chem>	0.00	0.38	0.038	-33	-11	22
20 <chem>CH3NO</chem>	2.52	2.63	0.011	-36	-21	15
21 <chem>CH3NO2</chem>	5.22	5.69	0.047	-123	-82	41
22 <chem>CH3NHSO2CH3</chem>	8.63	9.67	0.104	-225	-189	36
23 <chem>CH3AsAsCH3</chem>	0.00	0.21	0.021	-154	-131	23

Tab. 5. Oxygen containing compounds

No & Compound	Charge Distribution, a.u.	
	Magnetic Field, 0 AMFU	Magnetic Field, 10 AMFU
24 <chem>CH3OH</chem>		
25 <chem>CH3OCH3</chem>		
26 <chem>CH3COCH3</chem>		
27 <chem>CH3COOCH3</chem>		
28 <chem>CH3OCOOCH3</chem>		
29 <chem>CH3CONHCH3</chem>		

## Conclusions

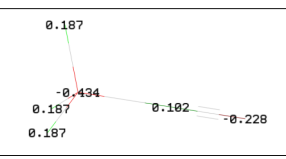
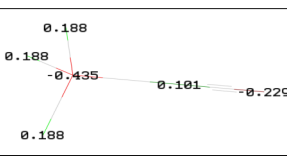
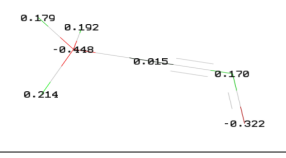
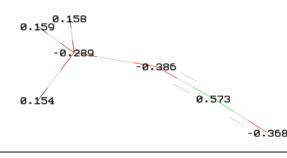
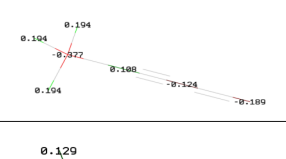
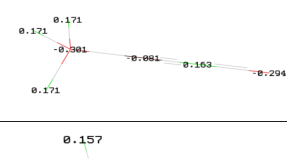
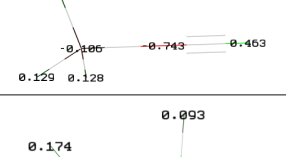

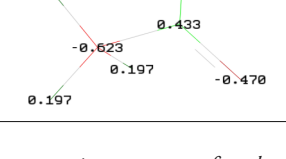
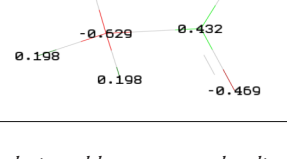
The effect of the static magnetic field of SMF on selected model compounds grouped into six classes is varied. As the energy of their formation increases, their stability decreases and the bonds become weaker. The values of the electric dipole moment also increase. This is the result of an increase in bond length and polarization of molecules due to the displacement of electrons. The latter effect can alter the durability and selectivity of binding to enzymes, which will undoubtedly affect the body's homeostasis and lead to its dysfunction.

A large change in polarity is observed in sulfone, sulfoxide, nitro, ester, cyanate and thiocyanate groups. Visible but less intense changes occur in methyl groups. In general, the intensity of changes in charge distribution caused by SMF is insignificant and the influence of magnetic fields achieved under terrestrial conditions seems harmless.

Tab. 5a. Changes in macroscopic parameters of oxygen containing compounds.

No & Compound	Dipole Moment [D]		$\Delta\mu$ [D/AMFU] (x1000)	Energy of creation [kJ/mol]		$\Delta E$ [J/(mol·AMFU)]
	0 AMFU	10 AMFU		0 AMFU	10 AMFU	
24 CH <sub>3</sub> OH	1.57	1.72	0.015	-235	-211	24
25 CH <sub>3</sub> OCH <sub>3</sub>	2.05	2.36	0.031	-94	-62	32
26 CH <sub>3</sub> COCH <sub>3</sub>	3.44	3.68	0.024	-75	-62	13
27 CH <sub>3</sub> COOCH <sub>3</sub>	6.32	6.86	0.054	-49	-31	18
28 CH <sub>3</sub> OCOOCH <sub>3</sub>	7.63	8.11	0.048	-268	-211	58
29 CH <sub>3</sub> CONHCH <sub>3</sub>	4.97	5.38	0.041	-133	-109	24

Tab. 6. Methane substituted by unsaturated radicals.

No & Compound	Charge Distribution, a.u.	
	Magnetic Field, 0 AMFU	Magnetic Field, 10 AMFU
30 CH <sub>3</sub> CN		
31 CH <sub>3</sub> CNO		
32 CH <sub>3</sub> CNS		
33 CH <sub>3</sub> NC		
34 CH <sub>3</sub> CHO		

Tab. 6a. Changes in macroscopic parameters of methane substituted by unsaturated radicals.

No & Compound	Dipole Moment [D]		$\Delta\mu$ [D/AMFU]	Energy of creation [kJ/mol]		$\Delta E$ [J/(mol·AMFU)]
	0 AMFU	10 AMFU		0 AMFU	10 AMFU	
30 CH <sub>3</sub> CN	3.69	3.99	0.030	-94	-61	33
31 CH <sub>3</sub> CNO	3.64	3.82	0.018	-158	-128	30
32 CH <sub>3</sub> CNS	5.78	6.25	0.047	-227	-201	26
33 CH <sub>3</sub> NC	0.53	1.06	0.053	-105	-92	13
34 CH <sub>3</sub> CHO	2.76	2.99	0.023	-166	-137	29

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