WPŁYW STATYCZNEGO HIPER EKSTREMALNEGO POLA MAGNETYCZNEGO NA PROSTE STRUKTURY MOLEKULARNE WYSTĘPUJĄCE W BIOLOGICZNIE WAŻNYCH TYPACH ZWIĄZKÓW CHEMICZNYCH. CZĘŚĆ 1. DŁUGOŚCI WIĄZAŃ

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Influence of static hyper extremely magnetic field on simple molecular structures found in biologically important types of chemical compounds. Part 1. Bond lengths

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Streszczenie/Abstract

Wstęp. Pole magnetyczne otacza cały żyjący świat, zatem zbadanie jaki ono wywołuje wpływ na podstawowe procesy życiowe jest ważne. Długości wiązań w bioaktywnych związkach organicznych są decydujące o geometrii cząsteczek a zatem i o przebiegu procesów biochemicznych istotnych dla zdrowia.

Metody badawcze. Obiektami badań były niskocząsteczkowe związki modelowe zawierające ugrupowania występujące w aktywnych biochemicznie molekułach. Przeprowadzono obliczenia kwantowo-mechaniczne w nałożonym statycznym polu magnetycznym (SMF) których wynikiem były nowe długości wiązań.

Wnioski. Obserwowane zmiany długości wiązań, wywołane polem nawet o hiprekstermalnym natężeniu ponad 1000 T, są bardzo małe i rzadko przekraczają 1% pierwotnej długości, zatem SMF wydaje się nie stanowić zagrożenia, biorąc pod uwagę zmiany geometrii związków chemicznych oraz brak możliwości generowania w warunkach ziemskich pola o tak wysokim natężeniu.

Słowa kluczowe: **deformacje cząsteczki; długości wiązań; niskocząsteczkowe pochodne alkanów i alkenów; pole magnetyczne.**

Introduction. Magnetic fields surround the entire living world, so it is important to investigate how it affects basic life processes. Bond lengths in bioactive organic compounds are decisive for the geometry of molecules and thus for the course of biochemical processes important for health.

Research methods. The objects of the study were low-molecular model compounds containing moieties found in biochemically active molecules. Quantum-mechanical calculations were performed in an superimposed static magnetic field (SMF), resulting in new bond lengths.

Conclusions. The observed changes in bond length, caused by a field even with a hyper extremely intensity of over 1000 T, are very small and rarely exceed 1% of the original length, so SMF does not seem to pose a threat, given the changes in the geometry of the chemical compounds and the inability to generate such a high field intensity under earth conditions.

Key words: **bond lengths; deformations of the molecule; low-molecular derivatives of alkanes and alkenes; magnetic field.**

1. Introduction

Magnetic fields permeate the Universe, and it can be extremely strong in some areas of space. Their sources are stars, black holes, pulsars, as well as ionized atoms and molecules orbiting stars. In our immediate surroundings, it is produced in a natural way, by the spinning motion of the Earth's core, but also artificially, in specially created electromagnets or incidentally, e.g. in electrical systems for various purposes. The electric current flowing in them induces a significant static magnetic field (SMF) or alternating magnetic field, which sometimes escapes to the outside. Strong magnetic fields are also generated by some molecules, e.g. those with strong ring currents.

The magnetic field also plays a fundamental role in the existence of chemical compounds, because atoms form bonds with the help of valence electrons, and the movement of these electrons generates an intramolecular electric field interacting with the external magnetic field. However, the use of a very strong external field, difficult to produce or even impossible under terrestrial conditions, can cause completely different effects.

Magnetosensitive is an electron pair responsible for the durability of atomic bonds. The electrons in such paired electrons are maintained using the attractive magnetic forces of oppositely directed spins, which far exceed the electrostatic repulsion of the same charges, so a strong external magnetic field can compete with the field holding the electrons together, leading to a weakening of the mutual force binding the electrons and, at a sufficiently high intensity, lead to the complete disintegration of the bond. With an extremely high field strength, which is unattainable on Earth but occurs in the Universe (over 10^9 T, Pulsar Swift J0243.6+6124), Tsygankov [12], all molecular matter would be atomized.

Advanced instrumental research methods - NMR and ESR spectrometry - are based on the subtle effects of intramolecular magnetism with medium-strong external magnetic field (up to approx. 20 T), using magnetic nuclei of elements or unpaired electrons.

In our previous works, we presented the calculated effects of extremely high magnetic fields (up to over 10^5 T) on selected types of molecules, from very simple to complex and playing key roles in biochemistry, Ciesielski [3–7].

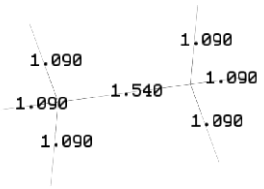
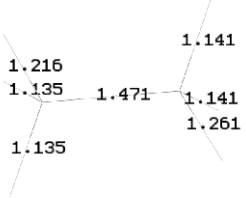
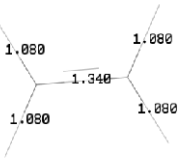
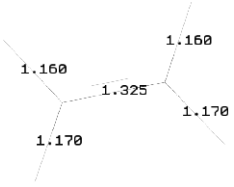
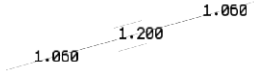
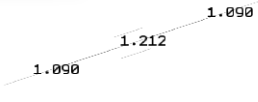
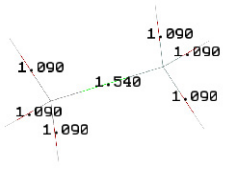
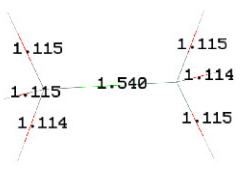
In this paper, we present the effect of changes in the geometry of selected relatively simple model molecules, the fragments of which make up large objects, including those that determine the biochemistry of organisms, and thus their life. We will present a comparison of bond lengths in a zero magnetic field with lengths in a field with an intensity of over 10^4 T, i.e. from 0 to 10 AMFU (arbitrary magnetic field unit, 1 AMFU ≥ 1000 T), Ciesielski [6]. In the calculations carried out *in silico and in computer vacuum*, the field lines were parallel to the long axis of the molecule.

In the next paper, we plan to analyze changes in charge distribution under the influence of SMF, Ciesielski [8].

2. Numerical calculations

Using the Gaussian 0.9 software equipped with a 6-31G database**, Frisch [10], selected molecules were optimized and all bond length values were calculated. In the next step, the effect of SMF acting along the long optimized molecules was calculated using the advanced Amsterdam Modelling Suite software, Charistov [2], Farberovich [9], containing the NR_LDOTB method (non-relati-

Tab. 1. Non-polar linear compounds

No & Compound	Bond Lengths, Å	
	Magnetic Field, 0 AMFU	Magnetic Field, 10 AMFU
1 **CH_3-CH_3**		
2 **CH_2=CH_2**		
3 **CH≡CH**		
4 **CH_3-SiH_3**		

vistically orbital L-dot-B momentum), Carpenter [1], Glendening [11]. The bond lengths and charge distribution were then recalculated using Gaussian 0.9 software equipped with a 6-31G base**, Frisch[10].

3. Calculation results

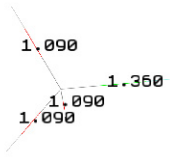
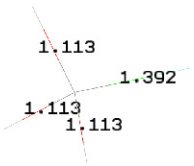
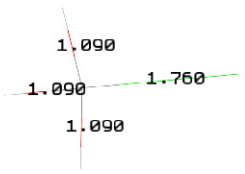
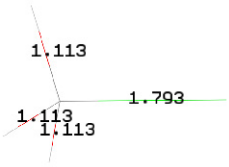
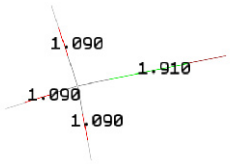
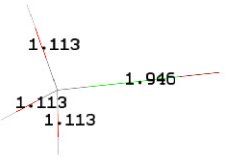
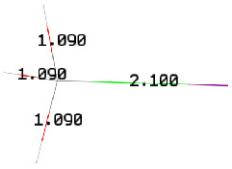
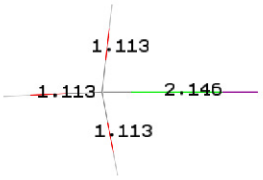
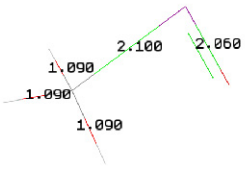
Tables 1–6 present the results of the calculations in the form of a schematic structure of the compound on which the calculated bond lengths are given for the compound located in the zero SMF and in the field parallel to the longer axis of the molecule with an induction of 10 AMFU (1 AMFU is at least 1000 T, i.e. 10^7 Gs). The first column in these tables contains the sequential number of the compound and its chemical formula. In order to compare the observed changes, the results were converted to %/AMFU specifying the percentage change in bond length with respect to the length without the action of a static magnetic field (SMF) caused by the action of a field of 1 AMFU intensity.

The non-polar compounds are shown below (Table 1). Ethane 1, ethylene 2, acetylene 3 and methylsilane 4 show different susceptibility of the methyl and silane groups to SMF. As the unsaturation increases, the elongation of the bond decreases. For ethane, ethylene and acetylene, it is 0.133, 0.085 and 0.030 Å, respectively, while for methylsilane, both the C-H and Si-H bond length increases by 0.025 Å. Considering the elongation is 1.22 to 0.23 %/AMFU. At the same time, the C-C distances were shortened by 0.069, 0.015, 0.012 Å, i.e. 0.45, 0.11 and 0.1%/AMFU. The length of the C-Si bond did not change.

The changes are insignificant, the most surprising is the very high sensitivity of the ethane molecule.

The next group are halogen methane derivatives (Table 2). The length of the CH bonds of all methyl halides increases

Tab. 2. Methyl halides

No & Compound	Bond Lengths, Å	
	Magnetic Field, 0 AMFU	Magnetic Field, 10 AMFU
5 **CH_3F**		
6 **CH_3Cl**		
7 **CH_3Br**		
8 **CH_3I**		
9 **CH_3IO**		

the same, i.e., 0.023 Å, which is 0.21%/AMFU. This is a negligible value that cannot significantly change the geometry of the molecule. The length of the halogen-carbon bond increased slowly from fluoromethane 5 to iodomethane 8 with increments of 0.032, 0.033, 0.036 and 0.045 Å, respectively, which is 0.22± 0.02 %/AMFU.

Different data were obtained for iodozomethane 9. The lengths of the C-H bonds increased by 0.064 Å, the length of the C-I bond by 0.014 Å, and the I=O bonds decreased by as much as 0.202 Å, which is 0.58, 0.007 and 0.98 %/AMFU, respectively. This extremely high susceptibility of the iodozo group to SMF can noticeably change geometries, fortunately such a group is extremely rarely present in nature.

Sulphur derivatives are one of the most common objects in biochemistry (methionine, thionine, cystine and cysteine and many others). Biologically active selenium derivatives are also important, as they often disrupt the homeostasis of organisms by "impersonating" sulfur. Data on the predicted behaviour of compounds containing these elements in SMF are presented in Table 3 below. The length of the C-H bonds in the methyl groups of compounds 10, 12, 13, 14

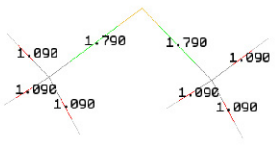
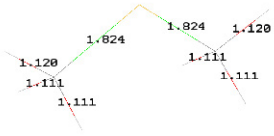
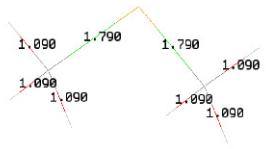
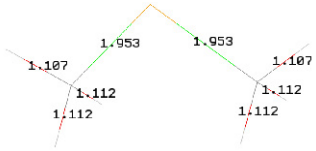
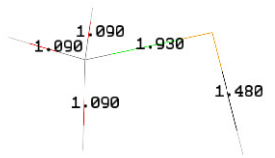
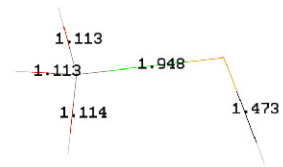
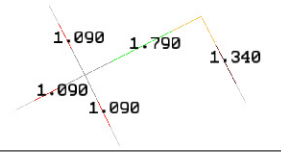
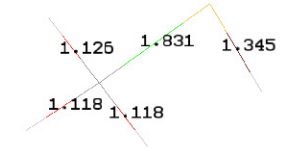
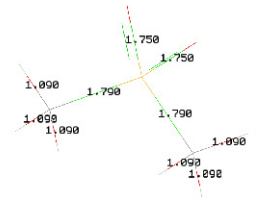
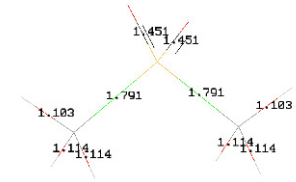
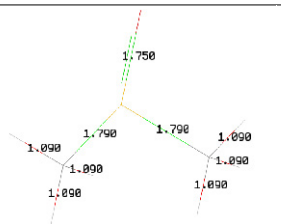
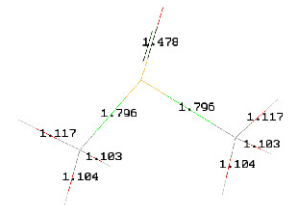
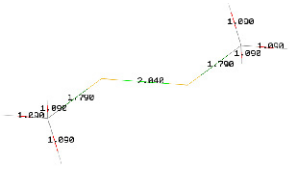
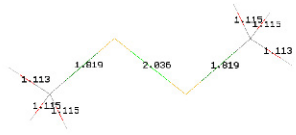
and 16 increased by 0.024 Å, slightly less by 15 (0.018 Å) and twice as much by dimethyl selenide 11 (0.011 Å), which on the susceptibility scale is 0.22, 0.16 and 0.1 %/AMFU, respectively.

The C-S bond lengths increased by 0.034 (10), 0.163 (11), 0.048 (12), 0.041 (13), 0.001 (14), 0.006 (15), 0.029 Å (16). Of note are the practically SMF--resistant sulfone (14) and dimethyl sulfoxide (15), while dimethyl selenide (11) has the predicted extremely high susceptibility. Very large changes can be seen in the case of S=O groups, which are shortened by 0.299 (14) and 0.272 Å (15). The observed bond elongations in the entire group therefore range from 0 to 1.38 %/AMFU and, with the exception of selenide (11), should not affect geometry changes.

The intensity of the contractions is very high and amounts to 0.299 (14) and 0.277 Å (15), which corresponds to 1.71 and 1.85 %/AMFU. Since sulfones and sulfoxides are found in living organisms, their changes can translate into altered behavior of these organisms.

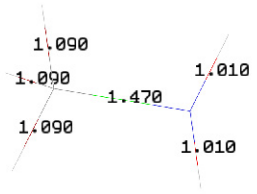
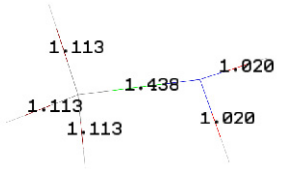
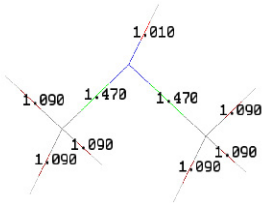
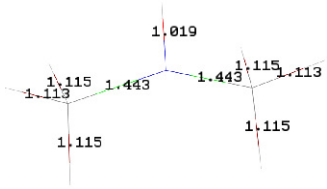
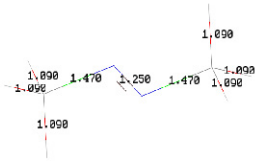
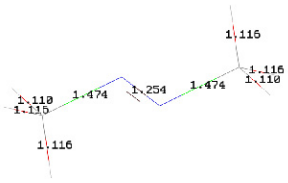
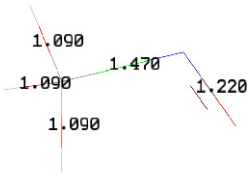
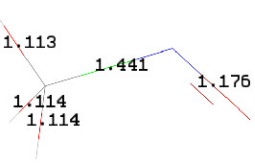
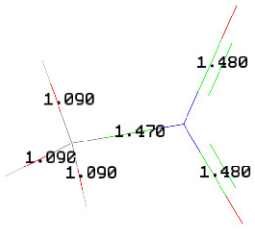
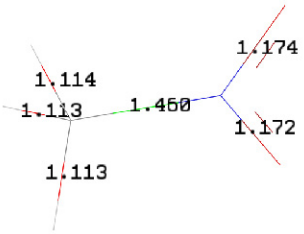
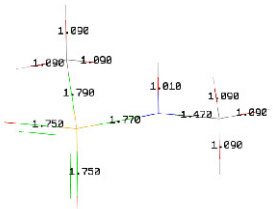
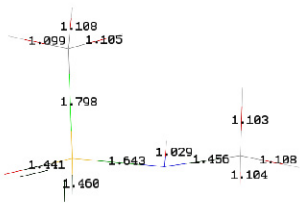
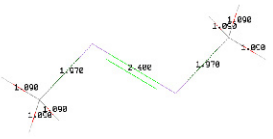
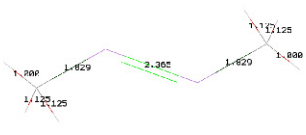
Nitrogen, along with carbon, hydrogen, oxygen, sulfur, phosphorus, sodium, potassium, calcium, magnesium, iron and others in trace amounts, is one of the basic elements of the living world. The behavior of compounds containing basic nitrogen moieties, but also arsenic, is shown in Table 4 below. The elongation of the CH bond is almost constant and for compounds 17-21 it is 0.023±0.001 Å. However, this is not the case with sulfonamide (22), in which it hardly changes, and the arsenic derivative (23), in which it increases slightly more by 0.035 Å. The relative sensitivity to SMF therefore ranges from 0.07 (22) through 0.21 (17-21) to 0.32 (23) %/AMFU. The length of the C-N bond in most cases decreases or almost remains constant being positive: +0.004 (19) and + 0.008 (22) Å.

Tab. 3. Sulfur and selenium contained compounds

No & Compound	Bond Lengths, Å	
	Magnetic Field, 0 AMFU	Magnetic Field, 10 AMFU
10 **CH_3SCH_3**		
11 **CH_3SeCH_3**		
12 **CH_3SeH**		
13 **CH_3SH**		
14 **$CH_3SO_2CH_3$**		
15 **CH_3SOCH_3**		
16 **CH_3SSCH_3**		

The least shortened is in the case of nitromethane (21) -0.010 Å, the most in the case of diarsenedimethane (23) -0.141 Å. The relative sensitivity calculated for the compounds in Table 4 is as follows: -0.21 (17), -0.18 (18), +0.03 (19), -0.20 (20), -0.07 (21), +005 (22) and 0.96 (23) %/AMFU. The NH bond length increased by 0.01 (17), 0.009 (18), and 0.019 Å (22), corresponding to the relative sensitivity to SMF of 0.099, 0.089, and 0.188 %/AMFU, respectively.

Tab. 4. Containing nitrogen or arsenic compounds

No & Compound	Bond Lengths, Å	
	Magnetic Field, 0 AMFU	Magnetic Field, 10 AMFU
17 **CH_3NH_2**		
18 **CH_3NHCH_3**		
19 **CH_3NNCH_3**		
20 **CH_3NO**		
21 **CH_3NO_2**		
22 **$CH_3NHSO_2CH_3$**		
23 **$CH_3AsAsCH_3$**		

The NO bond was slightly shortened by 0.029 Å in nitrosomethane (20) and by a greater 0.306Å in nitromethane (21), corresponding to the relative susceptibility of the bonds to SMF of -0.23 and -2.07 %/AMFU, respectively.

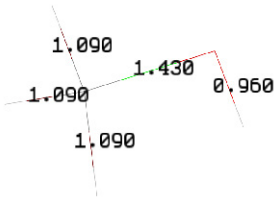
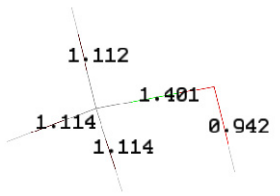
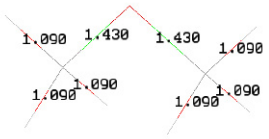
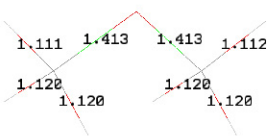
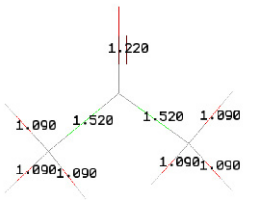
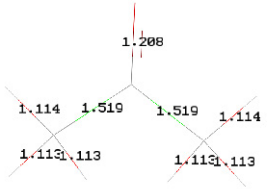
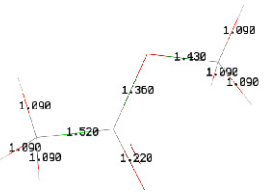
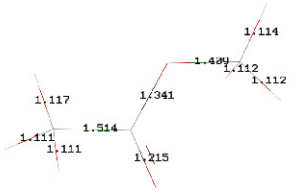
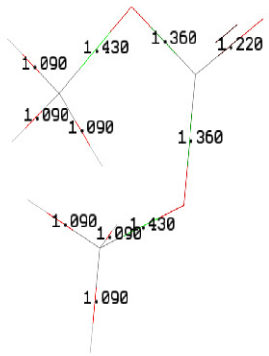
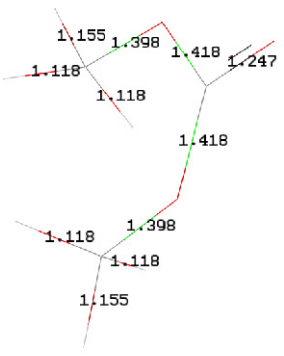
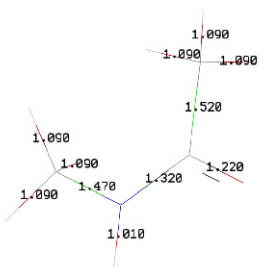
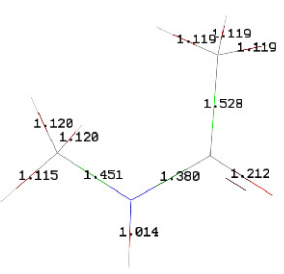
The C-As bond was shortened by 0.141 Å in 23, the S=O bond shortened by 0.309 Å in (22) and the C-S bond was shortened in 22 by 0.008 Å, corresponding to a relative SMF susceptibility of -0.71, -1.77 and +0.004 %/AMFU, respectively. The data in Table 4 show that significant changes are less than 1%/AMFU except for the shortened bonds of NO in the nitro group and SO in the sulfonamide group. The magnetic field can therefore cause a slight modification of the geometry of compounds containing these two moieties, potentially altering their biological activity.

Table 5 below presents the results of calculations performed for model compounds containing oxygen. The length of the C-H bond in the methyl group increased little and very similarly by 0.020 (29), 0.023 (24, 26, 27, 28), 0.028 (25, 29) Å, which corresponded to a relative susceptibility to SMF of 0.18, 0.21, 0.25 and 0.26 %/AMFU, respectively. The values are very small and do not cause a significant change in the geometry of the compound.

The length of the CO bond in the carbonyl group varies little and depending on the compound in which it is. This length decreases but also increases. Thus, the change is -0.012 (26), -0.005 (27), +0.027 (28), -0.008 (29) Å, which corresponds to a relative susceptibility to SMF equivalent to -0.098, -0.040, +0.221,and -0.066 %/AMFU.

The length of the C-O bond varies from -0.029 (24), -0.002 (29) to +0.009 Å (27), corresponding to a relative susceptibility to SMF of -0.202, -0.018 and +0.06 %/AMFU, respectively. The

Tab. 5. Containing oxygen compounds

No & Compound	Bond Lengths, Å	
	Magnetic Field, 0 AMFU	Magnetic Field, 10 AMFU
24 **CH_3OH**		
25 **CH_3OCH_3**		
26 **CH_3COCH_3**		
27 **CH_3COOCH_3**		
28 **$CH_3OCOOCH_3$**		
29 **$CH_3CONHCH_3$**		

changes in the length of the remaining bonds are very small, their relative susceptibility to SMF is CN-R: 0.052 (29), N-CO: +0.50 (29), NH:+0.039 (29), OH: -0.187 (24) %/AMFU. The changes predicted on the basis of calculations are negligible.

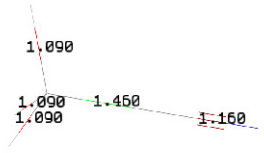
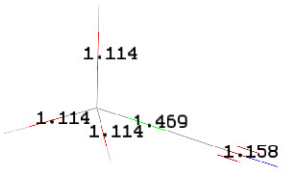
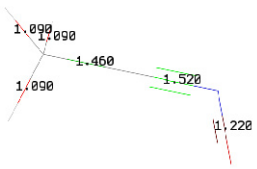
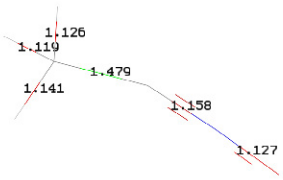
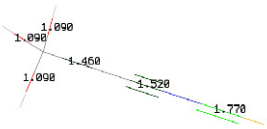
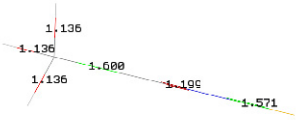
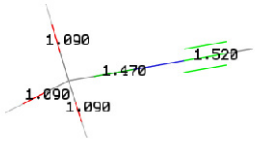
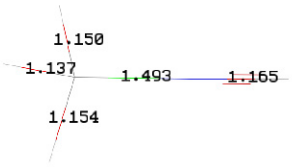
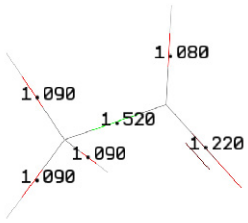
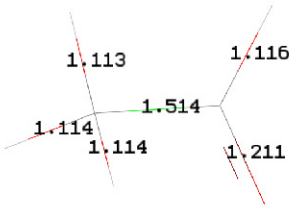
Calculations for monosubstituted methane with unsaturated groups are presented in Table 6. The length of the CH bond increases slightly: 0.024 (30, 34), 0.029 (31), 0.046 (32) and 0.057 (33) which corresponds to the following sequence of relative susceptibility to SMF: 0.22, 0.27, 0.42 and 0.52 %/AMFU. Larger changes are seen in the NC bond length in isonitrile 33 (-0.355 Å, or -2.33%/AMFU) and thiocyanate 32 (CN-S, -0.199 Å, or -1.12%/AMFU). They are noticeable for cyanate 31 (CN-O, -0.093 Å, or -0.76 %/AMFU) and isonitrile 33 (C-NC, 0.023 Å, or 0.16 %/AMFU).

The length of the C-CN bond increases from 0.009 (30) through 0.029 (31) to 0.040 (32) Å corresponding to a relative SMF susceptibility of 0.06, 0.20, 0.27 %/AMFU respectively. Changes in the length of the remaining bonds (C-CN- and C-CHO) are well below 0.1 %/AMFU and cannot affect the geometry of the molecule.

4. Conclusions

The calculations show that the action of the static magnetic field (SMF) on selected model compounds causes little effect considering the bond lengths. In the methyl group, an extremely high elongation of 1.22%/AMFU is observed only in the case of ethane, in other cases below 0.05%/AMFU. Strong effects occur in groups containing double bonds between non-carbon atoms. Thus, the IO bond in iodosomethane is shortened by 0.98%/AMFU, SO in dimethylsulfone, dimethylsulfoxide and in sulfonamide by

Tab. 6. Methane substituted by unsaturated radicals

No & Compound	Bond Lengths, Å	
	Magnetic Field, 0 AMFU	Magnetic Field, 10 AMFU
30 **CH_3CN**		
31 **CH_3CNO**		
32 **CH_3CNS**		
33 **CH_3NC**		
34 **CH_3CHO**		

approx. 1.8%/AMFU. A large shortening of the NC bond is observed in the isonitrile group (-2.33 %/AMFU) as well as in the cyanate and thiocyanate groups (approx. 1%/AMFU).

The numerical calculations show that the magnetic field does not cause significant changes in the bond length of model compounds, such as could change their biological functions, regardless of the changes that would undergo other biological objects cooperating with them. The exceptions are the sulfoxide and sulfone groups, as well as the iodine group, in which the SO or IO distance is shortened by approx. 1-2%/AMFU.

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