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Theoretical study of structures and stability of hydrogen-bonded systems between pyridine-3-carboxamide (nicotinamide) and DMSO

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Dedicated to Academician Ivan Juchnovski on the occasion of his 70th birthday

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The structures and stability of hydrogen-bonded complexes between nicotinamide and DMSO are studied by *ab initio* and DFT calculations at various basis sets. Full geometry optimization was made of the complexes studied. According to the energy analysis, the complex between (Z)-nicotinamide and two molecules DMSO is more stable by 1.91–2.68 kcal·mol^{-1} than the complex, formed between (E)-nicotinamide and two molecules DMSO. This result is in agreement with their coexistence, found experimentally. The changes in the geometrical parameters and charge distribution of the monomers upon hydrogen bonding have been studied.

Key words: hydrogen-bonded nicotinamide-DMSO complexes, *ab initio*, DFT.

INTRODUCTION

Hydrogen bonds constitute an area of research that is a typical interdisciplinary field concerning physicist as well as chemists and biologists. The structure and dynamics of the hydrogen-bonded complexes has become of greater and greater interest to chemists in a variety of fields. The elucidation of the structure and energetics of the hydrogen-bonded complexes pertains to the understanding of intermolecular interactions and a concerted application of experimental and theoretical methods can be used to obtain a clear picture of hydrogen-bonded structures [1–5].

Pyridine-3-carboxamide (nicotinamide) is known as a component of the vitamin B complex as well as a component of a coenzyme, nicotinamide adenine dinucleotide. Vitamin B_3 plays a crucial role in biological oxidative chemistry. Therefore, the structure of nicotinamide has been the subject of many experimental [6–8] and theoretical studies [7–11]. The amide group in nicotinamide can adopt a variety of tautomeric and rotameric structures in addition to forming interesting molecular associations *via* hydrogen bonding [12].

In a recent study [10] the solvent effects of DMSO on the vibrational spectrum of nicotinamide have been estimated on the basis of spectroscopic measurements. The authors [10] suppose the formation of hydrogen bonds between nicotinamide and DMSO. In this connection, the objects of the present study are the hydrogen-bonded complexes formed between nicotinamide and DMSO. The aim of the study is to establish the most stable structures of the hydrogen-bonded complexes and to estimate the influence of the hydrogen bonding on the structural parameters and charge distribution in the monomers using *ab initio* and DFT calculations at various basis sets.

METHODS

The structural and geometrical features of the hydrogen-bonded complexes of nicotinamide with DMSO were studied by *ab initio* and DFT calculations with various basis sets: 6-31G(d,p), 6-31+G(d,p), 6-311++G(d,p) using GAMMESS software [13] and CAUSSIAN 98 series of programs [14]. The density functional calculations were carried out in the framework of the Kohn-Sham density functional theory [15] with Becke exchange functional coupled with the Lee-Yang-Parr correlation [16].

RESULTS AND DISCUSSION

Dissociation energy

As is noted in previous studies [7–10], the nicotinamide molecule can exist in two conformers: NA(Z) and NA(E) (See Fig. 1). The conformational population in nicotinic acid derivatives was studied by Kuthan *et al*. [9] *via* dipole moment measurements in benzene solution together with theoretical moments of their CNDO/2 models, following earlier measurements of Purcell and co-workers [17, 18].

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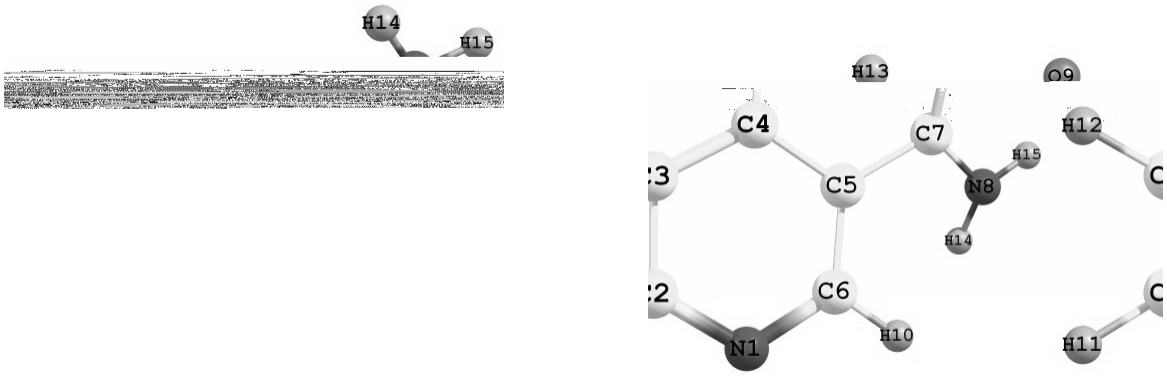
By means of microwave spectroscopy Vogelsanger *et al*. [7] detected both the NA(E) and NA(Z) conformer of nicotinamide in the gas-phase and found that (E)-conformer is more stable than (Z)-conformer. The calculated *ab initio* and DFT energy difference between the molecular conformers NA(E) and NA(Z) of 2.92–4.14 kJ·mol^{-1} is low and this results is in agreement with their coexistence, found experimentally [10]. NA(E) was found to be prevalent in solutions [9, 17], in the gas-phase [7], and the conformation in the monocrystal is firmly NA(E) [6].

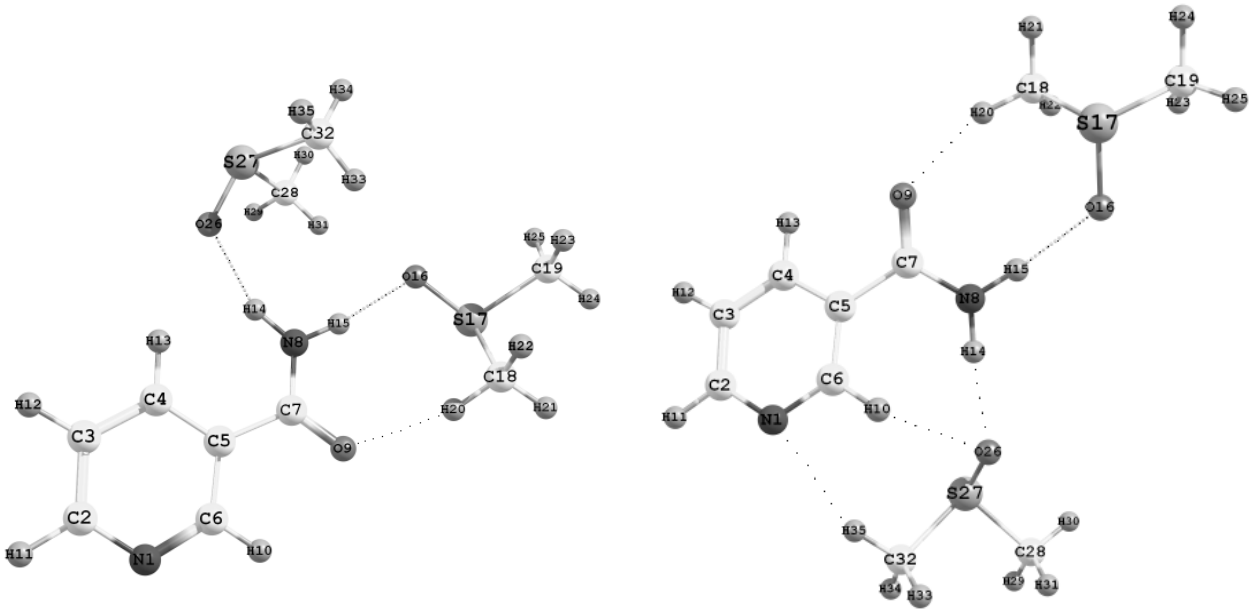
The complexation between NA(Z) nicotinamide and two molecules DMSO leads to the formation of complex **1**, and the hydrogen bonded systems between NA(E) nicotinamide and two molecules DMSO is marked as complex **2** (see Fig. 2).

Full geometry optimization has been performed for the complexes studied by *ab initio* and DFT (BLYP) calculations with various basis sets: 6-31G(d,p), 6-31+G(d,p) and 6-311++G(d,p) using the GAUSSIAN 98 series of programs [14]. In Fig. 2 are shown the optimized structures of complexes **1** and **2** with BLYP/6-311++G(d,p) calculations. As can be seen, the hydrogen bonding between (E)-nicotinamide and two DMSO molecules leads to the formation of a fully cyclic structure (complex **2**), while the hydrogen-bonded system between (Z)-nicotinamide and two DMSO molecules (complex **1**) is open with one DMSO molecule.



NA(Z) NA(E)

Fig. 1. Optimized by BLYP/6-311++G(d,p) calculations structures of the conformers of nicotinamide molecule.



Complex **1** Complex **2**

Fig. 2. Optimized structures by BLYP/6-311++G(d,p) calculations for the hydrogen-bonded: (Z)-nicotinamide with two molecules DMSO (complex **1**); (E)-nicotinamide with two molecules DMSO (complex **2**).

The dissociation energy is used for estimation of the stability of hydrogen-bonded systems between two and more partners. The supramolecular variation method determines dissociation energy (ΔE) as a difference between the energy of the complex and the energies of the isolated molecules.

$$\Delta E = E_{\text{com.}} - (E_1 + E_2 + E_3\ldots) \quad (1)$$

where E_1, E_2, $E_3\ldots$ are the energies of the isolated monomers in their own basis set and $E_{\text{com.}}$ is the energy of the complex.

The supramolecular approach is theoretically able to provide dissociation energy at any accuracy, however, only if a sufficiently large basis set and a sufficiently high level of correlation are used. For the exact determination of the interaction energy in the supramolecular approach the consideration of zero-point energies is very important.

The zero-point vibrational energy correction for the studied complexes can be defined as a difference between the calculated zero-point vibrational energy of the complex and the zero-point energies of the monomers:

$$\Delta E_{\text{zp vib}} = E_{\text{zp vib.}}(\text{com.}) - (E_{\text{zp vib}}(1) + E_{\text{zp vib}}(2) + E_{\text{zp vib}}(3)\ldots) \quad (2)$$

The dissociation energies, uncorrected and corrected with zero-point energy differences are calculated by *ab initio* and DFT calculations with different basis sets. The results from the calculations are presented in Table 1.

As can be seen from the data of ΔE (uncorrected and corrected with ΔE(zp vib), the calculated values of the dissociation energy with *ab initio* SCF and DFT (BLYP) calculations at 6-31G(d,p) basis set are very close, while the calculated values with BLYP calculations with larger basis sets, including s and p diffuse functions (6-31+G(d,p) and 6-311++G(d,p)), are smaller by about 20%.

The following comments can be made on the basis of the corresponding energy values:

a). According to all calculation performed, complex **1** is by 1.91–2.68 kcal·mol^{-1} more stable than complex **2**.

b). The calculated energy difference between the complexes is very small. This result is in agreement with their coexistence, found experimentally.

In Table 1 are presented also the optimised values of the hydrogen bonds formed between (Z)-nicotinamide and two molecules DMSO (complex **1**) and (E)-nicotinamide and two DMSO molecules (complex **2**). For complex **1** the calculated values of the $O_{16}\ldots H_{15}$ is much longer than for complex **2**. On the contrary, the hydrogen bond $O_{26}\ldots H_{14}$ for complex **1** is shorter than in complex **2**. In complex **2** this hydrogen bond is bifurcated and involves also H_{10}. Bearing in mind the optimized values of the hydrogen bonds of the complexes, it could be concluded that the hydrogen bond $O_{26}\ldots H_{14}$ in complex **1** is the strongest. The optimized values of the hydrogen bonds show that complex **1**, with stronger hydrogen bonds, is more stable than complex **2**.

Changes in geometrical parameters upon hydrogen bonding

The optimized geometrical parameters by BLYP/6-311++G(d,p) calculations for the both complexes, as well as for the monomers are presented in Tables 2 and 3. In order to estimate the accuracy of the calculations, the optimized geometrical parameters of the monomers are compared with the available experimental data [6–8]. In this case, as well as in the previous studies [5, 20–23] is observed a good agreement between experimental and DFT calculated geometrical parameters. The crystal structure determined by X-ray and neutron diffraction [6] shows that nicotinamide takes a non-planar (E)-form, in which the dihedral angle $C_6C_5C_7N_8$ is 22º. In the crystal of nicotinamide adenine dinucleotide (NAD) the conformation of the nicotinamide is similar to that of (E)-nicotinamide [24, 25]. In the study of Vogelsanger *at al.* [7] the dihedral angle $C_6C_5C_7N_8$ of the (E) and (Z) conformers was estimated to be 14(2)º and 158(2)º, respectively. Our calculations at BLYP/6-311++G(d,p) gave essentially the same values: 21º (E-form) and 156º (Z-form). By complexation the non planar (Z)-nicotinamide converts into a planar complex **1**: the dihedral angle $C_6C_5C_7N_8$ is 173º. For complex **2** this angle takes nearly the same value *via* non bonded nicotinamide: 24º (Tables 2 and 3).

Our aim is to estimate the influence of hydrogen bonding on the structural parameters of nicotinamide (Z and E) and DMSO. For this aim, the changes in the geometrical parameters from monomers to a complex are defined. It is seen from the results in Tables 2 and 3 that the optimized values of the bond lengths and angles for complex **1** and complex **2** are slightly perturbed from their values in the monomers. The calculated changes (Δ) in the structural parameters show that the formation of the hydrogen-bonded systems results in changes in the bond lengths and angles. These changes concern the atomic groups taking part directly in the formation of hydrogen bonds or situated in immediate vicinity to them. Upon formation of hydrogen bonds, the bonds: N_8H_{14}, N_8H_{15} and $O_{26}S_{27}$ are lengthened in the complexes. The bond lengths of the adjacent atomic groups are shortened.

Table 1. Dissociation energies ΔE (uncorrected and corrected), zero-point vibrational energy differences ΔE_{zpve} in kcal/mol and intermolecular distances in Å for the hydrogen-bonded complexes between DMSO and nicotinamide.

Complex [a]	Basis set	$\Delta E_{uncorr.}$	ΔE_{zpve}	ΔE_{corr}	R $O_{16}…H_{15}$	R $O_{26}…H_{14}$	R $O_{26}…H_{10}$	R $O_{9}…H_{20}$	R $N_{1}…H_{35}$
Complex **1**	HF/6-31G(d,p)	–22.32	2.27	–20.05	2.035	1.998	-	2.328	-
	BLYP/6-31G(d,p)	–23.66	2.40	–21.25	1.985	1.924	-	2.184	-
	BLYP/6-31+G(d,p)	–17.12	2.05	–15.06	2.001	1.953	-	2.242	-
	BLYP/6-311++G(d,p)	–18.09	2.09	–16.00	1.982	1.943	-	2.240	-
Complex **2**	HF/6-31G(d,p)	–19.46	2.09	–17.37	2.015	2.071	2.464	2.378	2.817
	BLYP/6-31G(d,p)	–20.87	2.28	–18.59	1.932	2.020	2.414	2.287	2.534
	BLYP/6-31+G(d,p)	–15.38	2.14	–13.24	1.968	2.025	2.527	2.309	2.657
	BLYP/6-311++G(d,p)	–16.36	2.27	–14.09	1.945	1.998	2.461	2.293	2.693

a - For the structures see Fig. 2.

Table 2. Calculated geometries for free and complexed nicotinamide NA(Z) and DMSO (1:2) by DFT (BLYP/6-311++G(d,p)) calculations.

Parameter [a]	Monomers		Complex **1**	Δ^h Change of the parameters
	Experiment	BLYP/6-311++G(d,p)	BLYP/6-311++G(d,p)	BLYP/6-311++G(d,p)
Bond lengths [b]				
N_1C_2	1.330 [d]	1.351	1.350	0.001
N_1C_6	1.328 [d]	1.346	1.348	0.002
C_2C_3	1.402 [d]	1.403	1.401	–0.002
C_3C_4	1.400 [d]	1.401	1.403	0.002
C_4C_5	1.404 [d]	1.408	1.409	0.001
C_5C_6	1.407 [d]	1.412	1.412	0.000
C_5C_7	1.497 [d]	1.511	1.517	0.006
C_7O_9	1.216 [d]	1.233	1.249	0.016
C_7N_8	1.366 [d]	1.387	1.359	–0.028
N_8H_{14}	1.022 [d]	1.015	1.025	0.010
N_8H_{15}	1.022 [d]	1.017	1.025	0.008
$O_{16}S_{17}$	1.531(5) [e]	1.534	1.555	0.021
$S_{17}C_{18}$	1.775(8) [e]	1.872	1.856	–0.016
$S_{17}C_{19}$	1.821(11) [e]	1.872	1.861	–0.011
$C_{18}H_{20}$	1.531(5) [e]	1.096	1.100	0.004
$O_{26}S_{27}$	1.775(8) [e]	1.534	1.547	0.013
$S_{27}C_{28}$	1.821(11) [e]	1.872	1.866	–0.006
$S_{27}C_{32}$	1.531(5) [e]	1.872	1.866	–0.004
Angle [c]				
$H_{14}N_8H_{15}$	-	116.97	116.06	–0.91
$H_{14}N_8C_7$	121.3(21) [d]	121.14	125.48	4.34
$H_{15}N_8C_7$	118.5(21) [d]	116.08	118.31	2.23
$N_8C_7O_9$	123.1 [d]	121.94	122.33	0.39
$C_7C_5C_4$	117.1 [d]	124.04	124.47	0.43
D $C_6C_5C_7N_8$	**158.0** [g]	**156.14**	**172.58**	**16.44**
$O_{26}S_{27}C_{28}$	106.7(40) [e]	107.10	107.24	0.14
$C_{28}S_{27}C_{32}$	97.4(40) [e]	96.02	96.39	0.37
$O_{16}S_{17}C_{18}$	106.7(40) [e]	107.10	106.70	–0.40
$C_{18}S_{17}C_{19}$	97.4(40) [e]	96.02	97.58	1.56

a - See Figs. 1 and 2, for numbering of atoms; b - In Å; c - In degree; d - Ref. [8]; e - Ref. [19]; f - Ref. [6]; g - Ref. [7];
Δ^h = parameter^{complex} – parameter^{monomer}

The changes in the angles from monomers to a complex are also estimated. The data in Tables 2 and 3 show that in complexes **1** and **2** the angles taking part in the hydrogen bonding are the most sensitive to complexation. The angles $H_{14}N_8C_7$, $H_{15}N_8C_7$, $N_8C_7O_9$ and $C_7C_5C_4$ from nicotinamide in complexes **1** and **2** become larger in comparison with their values in the monomer. The angles $C_{28}S_{27}C_{32}$ and $C_{18}S_{17}C_{19}$ from DMSO are also sensitive to complexation. Their values in the complexes are also larger in comparison with the monomer values. The dihedral angle $C_6C_5C_7N_8$ is the most sensitive to complexation. Its value in complex **1** changes by 16.4º and in the complex **2** by 3.2º. The remaining geometrical parameters of the monomers (nicotinamide and DMSO) in complexes **1** and **2** are either unchanged or changed slightly upon formation of hydrogen bonds. The results from the calculations show that the changes in the angles for complex **1** are more substantial than for the complex **2** (See Tables 2 and 3).

Table 3. Calculated and experimental geometries for free and complexed nicotinamide NA(E) and DMSO (1:2) by DFT (BLYP/6-311++G(d,p)) calculations.

Parameter [a]	Monomers		Complex **2**	Δ^h Change of the parameters
	Experiment	BLYP/6-311++G(d,p)	BLYP/6-311++G(d,p)	BLYP/6-311++G(d,p)
Bond lengths [b]				
N_1C_2	1.328 [d]	1.349	1.350	0.001
N_1C_6	1.328(6) [d]	1.348	1.351	0.004
C_2C_3	1.404 [d]	1.405	1.404	–0.001
C_3C_4	1.397 [d]	1.398	1.399	0.002
C_4C_5	1.404 [d]	1.408	1.406	–0.001
C_5C_6	1.406(4) [d]	1.410	1.409	–0.002
C_5C_7	1.498(8) [d]	1.513	1.520	0.007
C_6H_{10}	1.074 [f]	1.094	1.090	–0.004
C_7O_9	1.216(5) [d]	1.234	1.248	0.015
C_7N_8	1.362(12) [d]	1.383	1.359	–0.024
N_8H_{14}	1.022 [d]	1.015	1.024	0.010
N_8H_{15}	1.022 [d]	1.017	1.030	0.013
$O_{16}S_{17}$	1.531(5) [e]	1.534	1.547	0.013
$S_{17}C_{18}$	1.775(8) [e]	1.872	1.859	–0.013
$S_{17}C_{19}$	1.821(11) [e]	1.872	1.864	–0.008
$C_{18}H_{20}$	1.09 [e]	1.096	1.097	0.001
$O_{26}S_{27}$	1.531(5) [e]	1.534	1.546	0.012
$S_{27}C_{28}$	1.775(8) [e]	1.872	1.863	–0.009
$S_{27}C_{32}$	1.821(11) [e]	1.872	1.863	–0.009
Angle [c]				
$H_{14}N_8H_{15}$	-	117.55	118.36	0.81
$H_{14}N_8C_7$	121.3(21) [f]	121.85	123.25	1.40
$H_{15}N_8C_7$	118.5(21) [f]	116.59	118.13	1.54
$N_8C_7O_9$	123.1 [d]	121.91	123.51	1.60
$C_7C_5C_4$	117.0 [d]	118.36	118.97	0.62
D $C_6C_5C_7N_8$	**14.0 [g]**	**20.64**	**23.79**	**3.15**
$O_{26}S_{27}C_{28}$	106.7(40) [e]	107.10	105.78	–1.32
$C_{28}S_{27}C_{32}$	97.4(40) [e]	96.02	97.13	1.11
$O_{16}S_{17}C_{18}$	106.7(40) [e]	107.10	106.87	–0.23
$C_{18}S_{17}C_{19}$	97.4(40) [e]	96.02	97.36	1.34

a - See Figs. 1 and 2, for numbering of atoms; b - In angstroms; c - In degree; d - Ref. [8]; e - Ref. [19]; f - Ref. [6]; g - Ref. [7];
Δ^h = parameter^{complex} – parameter^{monomer}.

Charge distribution

It is known from our previous studies [20–23] that the hydrogen bonding leads to charge rearrangement in the monomers forming a complex. Our aim was to determine the influence of hydrogen bonding on charge distribution in the studied hydrogen-bonded complexes between nicotinamide and DMSO, shown in Figure 2 (complex **1** and complex **2)**. In this connection, the atomic charges (q_i) for the monomers (nicotinamide and DMSO) and for the both complexes have been calculated by BLYP/6-311++G(d,p) calculations, using the Mulliken population analyses. The data are shown in Tables 4 and 5. In these tables are also included the changes of the atomic charges (Δq_i) upon hydrogen bonding: $\Delta q_i = q_i^{complex} - q_i^{monomer}$.

It was established that the most sensitive to complexation are the atoms, taking part in hydrogen bonding. In the complexes studied the atoms S_{17}, S_{27}, C_6, C_7 and N_8 act as acceptors of electric charge. The negativity of these atoms increases significantly in the complexes in comparison with the corresponding negativity in the monomers. At the same time, the carbon atoms C_4 and C_5 and the hydrogen atoms H_{14} and H_{15} become more positive in the complexes. The results from the calculations show that the changes in the charges (Δq_i) of the atoms taking part in hydrogen bonding depend on the strength of the hydrogen bonds. As can be seen from the results for Δq_i in Tables 4 and 5, the hydrogen bond formation between nicotinamide and DMSO lead to charge rearrangements of the monomers.

Table 4. Mulliken charges (q_i)) for free and complexed nicotinamide NA(Z) and DMSO (1:2) obtained by BLYP/6-31++G(d,p) calculations.

No	Atom [a]	Monomers	Complex **1**	Δq_i [b]
1	N	–0.018	–0.021	–0.003
2	C	–0.349	–0.326	0.022
3	C	–0.016	–0.208	–0.192
4	C	–0.163	–0.018	0.145
5	C	0.842	1.493	0.651
6	C	–0.497	–0.509	–0.012
7	C	–0.409	–1.218	–0.810
8	N	–0.303	–0.417	–0.113
9	O	–0.293	–0.327	–0.033
10	H	0.211	0.206	–0.005
11	H	0.166	0.165	–0.001
12	H	0.163	0.172	0.009
13	H	0.155	0.207	0.052
14	H	0.212	0.340	0.129
15	H	0.299	0.336	0.038
16	O	–0.446	–0.405	0.041
17	S	0.531	0.408	–0.123
18	C	–0.535	–0.522	0.013
19	C	–0.535	–0.425	0.109
20	H	0.178	0.216	0.038
21	H	0.130	0.143	0.014
22	H	0.184	0.175	–0.010
23	H	0.184	0.173	–0.011
24	H	0.130	0.144	0.015
25	H	0.178	0.174	–0.004
26	O	–0.446	–0.393	0.053
27	S	0.531	0.366	–0.165
28	C	–0.535	–0.512	0.023
29	H	0.178	0.182	0.004
30	H	0.130	0.141	0.011
31	H	0.184	0.224	0.040
32	C	–0.535	–0.541	–0.006
33	H	0.183	0.264	0.081
34	H	0.130	0.140	0.010
35	H	0.178	0.174	–0.004

a - See Figs. 1 and 2, for numbering of atoms;
b - $\Delta q_i = q_i^{complex} - q_i^{monomer}$.

Table 5. Mulliken charges (q_i) for free and complexed nicotinamide NA(E) and DMSO (1:2) obtained by BLYP/6-31++G(d,p) calculations

No	Atom [a]	Monomers	Complex **2**	Δq_i [b]
1	N	–0.017	0.051	0.067
2	C	–0.339	–0.147	0.192
3	C	–0.057	–0.171	–0.114
4	C	–0.015	0.136	0.151
5	C	0.839	1.625	0.786
6	C	–0.654	–1.556	–0.902
7	C	–0.356	–0.683	–0.326
8	N	–0.298	–0.491	–0.193
9	O	–0.304	–0.350	–0.046
10	H	0.152	0.166	0.014
11	H	0.169	0.168	–0.001
12	H	0.167	0.180	0.013
13	H	0.201	0.214	0.014
14	H	0.220	0.337	0.117
15	H	0.295	0.473	0.178
16	O	–0.446	–0.454	–0.008
17	S	0.531	0.492	–0.039
18	C	–0.535	–0.574	–0.039
19	C	–0.535	–0.453	0.081
20	H	0.178	0.228	0.050
21	H	0.130	0.134	0.004
22	H	0.184	0.181	–0.004
23	H	0.178	0.168	–0.010
24	H	0.130	0.134	0.005
25	H	0.184	0.181	–0.003
26	O	–0.446	–0.477	–0.031
27	S	0.531	0.509	–0.022
28	C	–0.535	–0.482	0.053
29	H	0.178	0.177	–0.001
30	H	0.130	0.141	0.011
31	H	0.184	0.183	–0.001
32	C	–0.535	–0.533	0.002
33	H	0.184	0.182	–0.002
34	H	0.130	0.133	0.003
35	H	0.178	0.180	0.002

a - See Figs. 1 and 2, for numbering of atoms;
b - $\Delta q_i = q_i^{complex} - q_i^{monomer}$.

CONCLUSION

In the present study the structures and stability of the hydrogen-bonded complexes between nicotinamide and DMSO have been investigated using *ab initio* and DFT calculations. The main results of the study are:

1. The hydrogen bonding between (E)-nicotinamide and two DMSO molecules leads to the formation of a cyclic structure (complex **2**), while the hydrogen-bonded system between (Z)-nicotinamide and two DMSO molecules (complex **1**) is open with one DMSO molecule.

2. According to the calculated values of the dissociation energy, complex **1** is more stable than complex **2** by 1.91–2.68 kcal·mol^{-1}

3. The calculated changes (Δ) in the structural parameters show that the formation of the hydrogen-bonded systems results in changes in the bond lengths and angles. These changes concern the atomic groups taking part directly in the formation of the hydrogen bonds or situated in immediate vicinity to them. The most sensitive to complexation is the dihedral angle $C_6C_5C_7N_8$. Its value in complex **1** changes by 16.4º and in complex **2** by 3.2º.

4. In the studied complexes, the atoms S_{17}, S_{27}, C_6, C_7 and N_8 act as acceptors of electric charge. The negativity of these atoms increases significantly in the complexes in comparison with the corresponding negativity in the monomers. At the same time, the carbon atoms C_4 and C_5 and the hydrogen atoms H_{14} and H_{15} become more positive in the complexes.

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ТЕОРЕТИЧНО ИЗСЛЕДВАНЕ НА СТРУКТУРИ И СТАБИЛНОСТ НА ВОДОРОДНО-СВЪРЗАНИ СИСТЕМИ МЕЖДУ ПИРИДИН-3-КАРБОКСАМИД (НИКОТИНАМИД) И ДМСО

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(Резюме)

Структурата и стабилността на водородно-свързаните комплекси между никотинамида и ДМСО са изследвани посредством *ab initio* и ТФП пресмятания с различни базисни набори. Съгласно анализа на енергиите на свързване комплексът между (Z)-никотинамида и две молекули ДМСО е по-стабилен с 1.91–2.68 $kcal \cdot mol^{-1}$ от комплекса, образуван между (E)-никотинамида и ДМСО. Този резултат е в съгласие с експериментално установеното съществуване на двете форми в разтвор. Изследвани са промените в геометричните параметри и разпределението на зарядите при мономерите под действие на водородното свързване.