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QUANTUM CHEMICAL CALCULATION OF STRUCTURAL AND THERMODYNAMIC PROPERTIES OF ETHYL METHYL SULFONE IN THE GAS PHASE

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A detailed conformational analysis of ethyl methyl sulfone has been carried out using quantum chemical approaches, by revealing all stable conformers, their energy, structural parameters, relative population, and IR spectra at different levels of theory. Thermochemical parameters, such as energy, entropy and heat capacity of ethyl methyl sulfone stable conformers in the gas phase were calculated directly using the wB97XD/6-311++G(2df, 2pd) density functional theory method. Some correlation has been established between the structural characteristics of various conformers and their thermodynamic properties.

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Keywords**:** ethyl methyl sulfone, density functional theory, thermochemistry.

Introduction. Quantum chemical calculation of potential energy of the molecule results in the assessment of the stability of the system. The analysis of potential energy surfaces reveals different stable conformations corresponding to local minima. The main issue is then to relate the potential energy of a single molecule to the macroscopic properties that can be measured experimentally. The first-principles calculation of thermodynamic properties, such as the internal energy, the entropy, the enthalpy, the heat capacity etc., has shown dramatic progress over the past decades in the prediction and chemical accuracy of these parameters through the development of new theoretical methods and approaches [1]. The combination of the quantum chemical approaches with statistical thermodynamics makes it possible to relate the energy of a single molecule and an ensemble of particles [2]. The ideal-gas approximation allows one to simply use the molecular partition functions containing contributions from translational, rotational, vibrational, and electronic degrees of freedom, neglecting the intermolecular interactions. A number of theoretical studies carried out to evaluate the gas-phase thermochemical properties of various organic compounds at different temperatures have shown that the computational prediction has reached a level of accuracy compared to the experimental one [3–6].

Recently, using the methodology proposed for alkanes [7] the thermodynamic characteristics of dimethyl, ethyl methyl and diethyl sulfones have been reported,

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where only one stable conformer was considered [8]. The main goal of this work was to determine the structural and thermodynamic parameters of ethyl methyl sulfone (EMSO2), a widely used solvent in lithium batteries [9], as well as to establish some correlation between the structural characteristics of various conformers and their thermodynamic properties at wB97XD/6-311++G(2df, 2pd) levels of theory. The latest was shown to be the best method-basis set combination for processing sulfone molecules [10].

Computational Part. The quantum chemical calculations of ethyl methyl sulfone were performed using Gaussian 09 program package [11]. The coexistence of stable conformers has been elucidated from an analysis of the potential energy surface of EMSO2, which was done by Becke three-parameter hybrid functional with non-local Perdew-Wang 91 correlation B3PW91 at relatively large 6–311++G(d, p) basis set. The relaxed scan method was used to calculate the dependence of the potential energy of the system on one dihedral angle describing the rotation of the ethyl group around C-S bond. The appropriate dihedral angle value was changed in the range from 0 to 355° with a step of 5°. Further geometry optimization of the minimum energy structures found on the EMSO2 PES, as well as calculations of their IR frequencies verifying the real minima, were carried out using various theoretical methods and basis set combinations, such as restricted Hartree-Fock RHF, density functional theory hybrid functionals B3LYP and B3PW91, post-Hartree-Fock MP2 method with Pople 6–311++G(d, p) basis set and Dunning aug-cc-pVTZ correlation-consistent basis sets with diffuse part. In addition, dispersion corrected wB97XD functional combined with 6-311++g(2df, 2pd) basis set was used to perform high-quality thermochemical calculations (following the complete geometry optimization and frequency calculation at the same level of theory). This method/basis set combination proved to be the best method for dimethyl sulfone and its homologues in terms of structure and IR spectra prediction [10].

The thermodynamic properties of EMSO2, namely internal energy, entropy and heat capacity, were determined by connecting quantum chemical and statistical thermodynamics approaches. The latter is based on the calculation of the molecular partition function of isolated molecule in the gas phase at 1 *atm* using Boltzmann distribution. The molecular partition function containing contributions from translational, rotational and vibrational degrees of freedom of a molecule was taken into account to calculate aforementioned thermodynamic properties. The temperature dependence of internal energy, entropy and heat capacity was determined from 100 K to 1000 K. Electronic contributions were neglected, since electronic excitations require temperatures above 1000 K.

Internal energy (U), entropy (S) and heat capacity (C_V) were determined as sums

$$U = E_{pot} + E_{ZPE} + U_{trans} + U_{rot} + U_{vibr}, \tag{1}$$

$$C_V = C_{V,trans} + C_{V,rot} + C_{V,vibr}, \tag{2}$$

$$S = S_{trans} + S_{rot} + S_{vibr}, \tag{3}$$

where E_{pot} is the potential energy of the molecule, E_{ZPE} is the zero point energy at 0 K, U_{trans} ($C_{V,trans}$, S_{trans}), U_{rot} ($C_{V,rot}$, S_{rot}), and U_{vibr} ($C_{V,vibr}$, S_{vibr}) are the translational, rotational, and vibrational part of the internal energy (constant-volume heat capacity, entropy) at non zero temperature, respectively.

The translational components of these quantities depend on the mass of molecule, the rotational components depend on the principal moments of inertia, and the vibrational contribution depends on the frequency. The vibrational contributions (the harmonic approximation was used to consider molecular vibrations) were calculated from the wavenumber of a single vibrational mode as follows:

$$U_{vibr} = R\sum_i \frac{\Theta_{v,i}}{T^2}\left(\frac{1}{2}+\frac{1}{e^{\Theta_{v,i}/T}-1}\right), \tag{4}$$

$$C_{V,vibr} = R\sum_i e^{\Theta_{v,i}/T}\left(\frac{\Theta_{v,i}/T}{e^{\Theta_{v,i}/T}-1}\right)^2, \tag{5}$$

$$S_{vibr} = R\sum_i \left[\frac{\Theta_{v,i}/T}{e^{\Theta_{v,i}/T}-1} - \ln\left(1-e^{-\Theta_{v,i}/T}\right)\right], \tag{6}$$

where R is the universal gas constant, $\Theta_{v,i}$ is the vibrational temperature ($\Theta_{v,i} = h\nu_i/k_B$, where h is the Planck's constant, k_B is the Boltzmann constant, and ν_i is the frequency of i-th vibration) [2].

Results and Discussion. A conformational analysis of an isolated EMSO2 molecule in vacuum was carried out to reveal the structures of stable conformers using the B3PW91/6-311++G(d, p) density functional theory method. The potential energy surface (PES) of EMSO2 was calculated by the method of relaxed PES scanning, in which for an arbitrarily chosen internal coordinate, in this case the dihedral angle D(C6C5S1C4), characterizing the rotation of the ethyl fragment around the C5-S1 bond, with a given range of values and a small step, the energy of the system was minimized for all other coordinates.

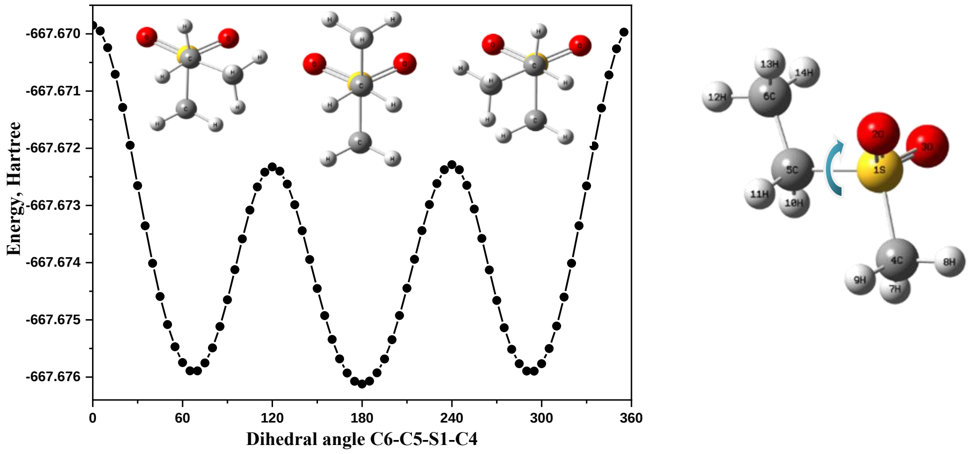

Fig. 1. Potential energy surface of ethyl methyl sulfone along the dihedral angle D(C6C5S1C4), calculated by B3PW91/6-311++G(d, p) method.

Fig. 1 shows the dependence of the potential energy of EMSO2 on the dihedral angle D(C6C5S1C4), as well as the structures of stable conformers corresponding to minima on the PES. PES of EMSO2 is characterized by three minima with dihedral angles of 65°, 180°, and 295°, respectively. Two gauche conformers (conformer I) (with dihedral angles of 65° and 295°) corresponding to local minima are symmetrical in structures and are therefore doubly degenerate. The structure of the third trans conformer (conformer II) (with a dihedral angle of 180°) corresponds to the global minimum and is singly degenerate.

The energies of gauche and trans conformers calculated by full optimization of the geometry of their structures using B3PW91/6-311++G(d, p) method differ insignificantly, by only 0.53 *kJ*/*mol*. For comparison, the energy of thermal motion at standard temperature is about 2.48 *kJ*/*mol*. The energy barrier of internal rotation from the trans- to gauche conformer is 9.96 *kJ*/*mol*, and of the mutual gauche-gauche transition is 15.86 *kJ*/*mol*.

The relative population of equilibrium conformers (P_i) was calculated using Boltzmann distribution formula:

$$P_i = \frac{g_i e^{\frac{-\varepsilon_i}{k_B T}}}{\sum_i g_i e^{\frac{-\varepsilon_i}{k_B T}}}, \tag{7}$$

where ε_i is the potential energy of i-th conformer, and g is the degeneracy of i-th conformer.

Table 1

Main structural parameters for two stable EMSO2 conformers optimized at different levels of theory

Conformer I						
Method	RHF	B3LYP	B3PW91	MP2	MP2	wB97XD
Basis set	6–311++G(d, p)				aug–cc–pvtz	6–311++G(2df, 2pd)
Bond length, Å						
S(1)-O(2)	1.43267	1.46815	1.46276	1.46091	1.45853	1.44156
S(1)-O(3)	1.43302	1.46885	1.46347	1.46174	1.45946	1.44231
C(4)-S(1)	1.77538	1.81037	1.79754	1.78611	1.78005	1.78080
C(5)-S(1)	1.78476	1.82383	1.80996	1.79341	1.78827	1.79109
C(6)-C(5)	1.52412	1.52360	1.51803	1.52370	1.51868	1.51821
C(5)-H(11)	1.08435	1.09275	1.09388	1.09457	1.09137	1.09077
Angle						
O(2)-S(1)-O(3)	119.5673	120.3901	120.3957	120.8808	120.3150	120.0836
C(5)-S(1)-C(4)	105.8508	104.9929	104.9499	104.3469	104.2986	104.6101
S(1)-C(5)-C(6)	114.7988	114.381	114.3547	113.7827	113.1892	114.2033
Dihedral angle						
C(6)-C(5)-S(1)-C(4)	–66.72344	–67.8728	–67.6893	–66.6466	–65.8925	–65.0490
O(2)-S(1)-C(5)-C(6)	178.8305	178.0199	178.1727	179.4462	179.9513	179.3249
Dipole moment, *D*	5.5294	5.0873	5.0226	5.6553	5.3775	4.83745
Energy, *Hartree*	–665.5233029	–667.8281933	–667.6759249	–666.5359768	–666.8194638	–667.781369008
Conformer II						
Method	RHF	B3LYP	B3PW91	MP2	MP2	wB97XD
Basis set	6–311++G(d, p)				aug–cc–pvtz	6–311++G(2df, 2pd)
Bond length, Å						
S(1)-O(2)	1.43323	1.46895	1.46353	1.46182	1.45953	1.44233
S(1)-O(3)	1.43323	1.46895	1.46353	1.46182	1.45953	1.44233
C(4)-S(1)	1.77439	1.80929	1.79667	1.78469	1.77861	1.77978
C(5)-S(1)	1.78508	1.82517	1.81144	1.79444	1.78921	1.79242
C(6)-C(5)	1.52714	1.5259	1.52051	1.52634	1.52150	1.52056
C(5)-H(11)	1.08367	1.09206	1.09300	1.09357	1.08994	1.08978
Angle						
O(2)-S(1)-O(3)	119.3562	120.0896	120.0867	120.5312	119.9974	119.8142
C(5)-S(1)-C(4)	104.3685	103.7540	103.7403	103.5043	103.7051	103.5359
S(1)-C(5)-C(6)	110.9399	110.5031	110.2702	109.6382	109.0257	110.2351
Dihedral angle						
C(6)-C(5)-S(1)-C(4)	180	180	179.9996	180	180	180
O(2)-S(1)-C(5)-C(6)	65.3383	65.7263	65.7071	65.8485	65.6415	65.6297
Dipole moment, *D*	5.2842	4.8507	4.7879	5.4029	5.1089	4.59227
Energy, *Hartree*	–665.5239288	–667.8284525	–667.6761276	–666.5360445	–666.8197256	–667.781311953

The estimated relative population of gauche conformer at a standard temperature (298 *K*) was 61.7%, taking into account the doubly degeneration of this conformer, and of trans conformer was 38.3%, i.e. despite the fact that the trans conformer corresponds to the global minimum on PES the equilibrium is shifted towards the gauche conformer.

Table 2

Internal energy (U), entropy (S) and heat capacity (C_V) of two stable conformers of EMSO2 at different temperatures, calculated with B3PW91/6-311++G(d,p) and wB97XD/6-311++G(2df,2pd) methods, as well as their average value

	Conformer I			**Conformer II**		
T, K	*U*, $kcal\cdot mol^{-1}$	C_V, $cal\cdot mol^{-1}\cdot K^{-1}$	*S*, $cal\cdot mol^{-1}\cdot K^{-1}$	*U*, $kcal\cdot mol^{-1}$	C_V, $cal\cdot mol^{-1}\cdot K^{-1}$	*S*, $cal\cdot mol^{-1}\cdot K^{-1}$
	B3PW91/6-311++G(d,p)					
100	72.046	12.336	61.817	72.029	12.698	62.288
200	73.675	19.892	74.187	73.680	19.989	74.819
298.15	75.955	26.566	84.164	75.964	26.582	84.816
300	76.004	26.692	84.341	76.013	26.707	84.993
400	79.009	33.317	93.512	79.019	33.320	94.166
500	82.640	39.141	102.033	82.650	39.145	102.688
600	86.805	44.012	109.976	86.815	44.016	110.631
700	91.415	48.078	117.381	91.426	48.081	118.037
800	96.400	51.518	124.297	96.411	51.520	124.954
900	101.702	54.464	130.774	101.714	54.465	131.430
1000	107.279	57.007	136.856	107.290	57.006	137.513
	wB97XD/6-311++G(2df,2pd)					
100	72.842	12.148	61.537	72.700	12.506	62.160
200	74.440	19.520	73.703	74.323	19.661	74.504
298.15	76.680	26.131	83.519	76.572	26.208	84.360
300	76.728	26.257	83.693	76.621	26.333	84.535
400	79.688	32.858	92.734	79.588	32.927	93.597
500	83.274	38.698	101.155	83.180	38.765	102.032
600	87.396	43.603	109.020	87.309	43.667	109.909
700	91.968	47.707	116.365	91.887	47.765	117.264
800	96.917	51.183	123.234	96.842	51.235	124.140
900	102.188	54.161	129.672	102.117	54.208	130.585
1000	107.735	56.732	135.725	107.670	56.774	136.642
	B3PW91/6-311++G(d,p) average value			wB97XD/6-311++G(2df,2pd) average value		
T, K	*U*, $kcal\cdot mol^{-1}$	C_V, $cal\cdot mol^{-1}\cdot K^{-1}$	*S*, $cal\cdot mol^{-1}\cdot K^{-1}$	*U*, $kcal\cdot mol^{-1}$	C_V, $cal\cdot mol^{-1}\cdot K^{-1}$	*S*, $cal\cdot mol^{-1}\cdot K^{-1}$
100	72.039	12.475	61.997	72.788	12.285	61.776
200	73.677	19.929	74.429	74.395	19.574	74.010
298.15	75.958	26.572	84.414	76.639	26.160	83.841
300	76.007	26.698	84.591	76.687	26.286	84.015
400	79.013	33.318	93.762	79.650	32.884	93.065
500	82.644	39.143	102.284	83.238	38.724	101.491
600	86.809	44.014	110.227	87.363	43.628	109.360
700	91.419	48.079	117.632	91.937	47.729	116.709
800	96.404	51.519	124.549	96.888	51.203	123.581
900	101.707	54.464	131.025	102.161	54.179	130.022
1000	107.283	57.007	137.108	107.710	56.748	136.076

The main structural parameters, such as bond lengths, angles, dihedral angles, dipole moment and total energy for two stable conformers of EMSO2, as calculated by various methods and basis sets, are given in Tab. 1. The difference in the predicted bond lengths varies between 0.01–0.03 Å depending on the method used. The comparison with available data for dimethyl sulfone [12] shows that the structural parameters are best described by the RHF and wB97XD methods. One of the interesting features of conformer II is that both S=O bonds are equal regardless of the method used, and it has a smaller dipole moment than conformer I.

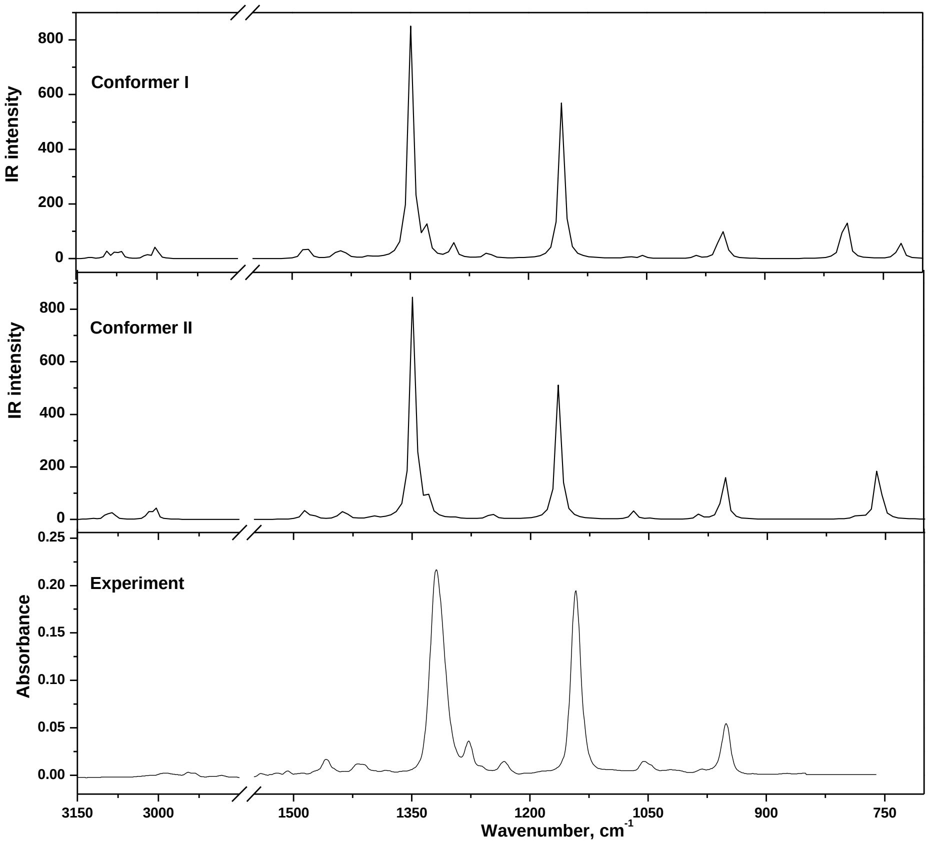

Fig. 2. Calculated IR spectra of two stable conformers with wB97XD/6-311++G(2df, 2pd) method corrected in frequencies with a linear scaling equation (k = 0.97668, b = 9.47251 [10]), as well as experimental FTIR ATR spectra of ethyl methyl sulfone solution in CCl_4 (0.1 *mol*/*L*).

The relative population values have been used to predict average thermochemical properties of EMSO2 in the large temperature range between 100 *K* and 1000 *K*, such as entropy, heat capacity and free energy given by Eqs. (1)–(6), which are summarized in Tab. 2. A certain difference (up to 4.184 $J{\cdot}K^{-1}{\cdot}mol^{-1}$) in thermochemical values such as entropy and heat capacity calculated by different method/basis set for the same conformer is due to the vibrational contribution, which is directly related to the vibrational frequency calculations. In this case, the use of wB97XD/6-311++G(2df, 2pd) is justified, as have recently been shown for processing sulfone molecules [10]. One confirmation of this is the good agreement between the calculated IR spectra (frequency-corrected using the linear scaling equation with $k = 0.97668$ and $b = 9.47251$ [10]) of two stable conformers with wB97XD/6-311++G(2df, 2pd) method, as well as experimental FTIR ATR spectra of ethyl methyl sulfone solution in CCl_4 (0.1 mol/L) presented in Fig. 2. The most active vibrational bands between 1400 cm^{-1} and 1100 cm^{-1} wavenumbers are antisymmetric and symmetric stretching vibrations of the SO_2 group, respectively. Their frequencies and relative intensities are comparable with experimental one.

Conclusion. Thus, the analysis of PES of isolated ethyl methyl sulfone molecule in the gas phase has revealed two stable conformers. Their structural and thermochemical parameters, such as bond lengths, bond angles, dihedral angles, absolute energies, dipole moment and IR spectra, entropy and heat capacity, calculated by various quantum chemical methods are presented. The results obtained can be useful in predicting the thermochemistry of reactions involving ethyl methyl sulfone.

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ԳԱԶ ՓԱԶՈՒՄ ԷԹԻԼՄԵԹԻԼՍՈՒԼՖՈՆԻ ԿԱՌՈՒՑՎԱԾՔԱՅԻՆ ԵՎ ԹԵՐՄՈԴԻՆԱՄԻԿԱԿԱՆ ՀԱՏԿՈՒԹՅՈՒՆՆԵՐԻ ՔՎԱՆՏԱՔԻՄԻԱԿԱՆ ՀԱՇՎԱՐԿԸ

Քվանտաքիմիական մոտեցումների շրջանակում իրականացվել է էթիլմեթիլսուլֆոնի կոնֆորմացիոն վերլուծություն՝ բոլոր կայուն կոնֆորմերների, դրանց էներգիայի, կառուցվածքային պարամետրերի, հարաբերական բնակեցվածության և ԻԿ սպեկտրների որոշմամբ: Օգտագործելով wB97XD/6-311++G(2df, 2pd) խտության ֆունկցիոնալի տեսության մեթոդը՝ հաշվարկվել են գազ փազում էթիլմեթիլսուլֆոնի կայուն կոնֆորմերների ջերմաքիմիական պարամետրերը, ինչպիսիք են էներգիան, էնտրոպիան և ջերմունակությունը: Հաստատվել է որոշ կորելյացիա տարբեր կոնֆորմերների կառուցվածքային բնութագրերի և դրանց թերմոդինամիկական հատկությունների միջև:

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КВАНТОВО-ХИМИЧЕСКИЙ РАСЧЕТ СТРУКТУРНЫХ И ТЕРМОДИНАМИЧЕСКИХ СВОЙСТВ ЭТИЛМЕТИЛСУЛЬФОНА В ГАЗОВОЙ ФАЗЕ

Проведен детальный конформационный анализ этилметилсульфона с использованием квантово-химических подходов с выявлением всех стабильных конформеров, их энергии, структурных параметров, относительной заселенности и ИК-спектров. С использованием метода теории функционала плотности wB97XD/6-311++G(2df, 2pd) рассчитаны термохимические параметры, такие как энергия, энтропия и теплоемкость стабильных конформеров этилметилсульфона в газовой фазе. Установлена некоторая корреляция между структурными характеристиками различных конформеров и их термодинамическими свойствами.