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DETERMINATION OF THE ENTHALPY OF COMBUSTION OF DIMETHYL SULFOXID

Abstract. This study explores the physicochemical properties, synthesis, and applications of dimethyl sulfoxide (DMSO), a polar aprotic solvent with significant commercial and scientific relevance. The paper details its molecular structure, production methods – primarily the oxidation of dimethyl sulfide and diverse uses, including its role as a solvent, cryoprotectant, PCR inhibitor, and therapeutic agent. Experimental work focuses on thermochemical analysis using an IKA C 6000 calorimeter to determine the combustion enthalpy of substances. The calorimetric setup, calibration with benzoic acid, and measurement protocols are described, emphasizing the precision and automation of modern calorimetry. The study underscores DMSO's versatility in industrial, medical, and laboratory contexts, supported by its unique properties such as high boiling point, dipole moment, and ability to penetrate biological membranes.

Keywords: dimethyl sulfoxide (DMSO), polar aprotic solvent, thermochemical analysis, enthalpy of combustion, calorimetry (IKA C 6000).



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Introduction. Dimethyl sulfoxide (DMSO) is an organosulfur compound with the formula (CH₃)₂SO. This colorless liquid is a sulfoxide and is the most widely used commercially. It is an important polar aprotic solvent that dissolves both polar and nonpolar compounds and is miscible with a wide range of organic solvents as well as water. It has a relatively high boiling point. DMSO is metabolized into compounds that leave a garlic-like taste in the mouth after being absorbed through the skin [1,5].

From a chemical structure perspective, the molecule has an idealized rotational symmetry. It exhibits a trigonal pyramidal molecular geometry, characteristic of other three-coordinate S(IV) compounds, with a lone electron pair on the approximately tetrahedral sulfur atom.

Dimethyl sulfoxide was first synthesized in 1866 by the Russian scientist Alexander Zaitsev, who reported his findings in 1867 [3]. Its modern use as an industrial solvent began with the efforts of Thor Smedslund from the Stepan Chemical Company. Dimethyl sulfoxide is produced on an industrial scale from dimethyl sulfide, a byproduct of the kraft process, through oxidation with oxygen or nitrogen dioxide. The primary method for obtaining DMSO is the oxidation of dimethyl sulfide (C_2H_6S). In industry, this process is carried out using nitric acid, oxygen, or nitrogen dioxide [4].

DMSO is also a byproduct of paper production. In laboratory conditions, potassium periodate in an organic solvent–water mixture can be used for the mild and selective oxidation of dimethyl sulfide. However, laboratory methods for DMSO synthesis have no practical significance, as dimethyl sulfide is inconvenient to handle, and industrially produced DMSO is readily available. The annual production of DMSO is measured in tens of thousands of tons.

Materials and methods. In this work, three thermochemical experiments were carried out on the combustion of various samples of dimethyl sulfoxide in polyethylene ampoules. To determine the heat capacity of the calorimetric system in the IKA C 6000, a specific amount of a reference substance benzoic acid is burned. Calibration with benzoic acid is performed in isoperibolic mode at a temperature of 25°C. The value is displayed on the instrument screen during measurement.

Solid samples can be burned directly in the decomposition vessel in the form of powders or tablets. When working with unknown substances, the sample mass for preliminary testing should not exceed 0.25 g. As part of educational tasks, the heat of combustion of activated carbon, glucose, succinic and acetylsalicylic acids, sugar, flammable polar solvents, and other substances is determined.

1. System Startup By turning the oxygen cylinder valve counterclockwise, oxygen is supplied to the calorimeter, and the O_2 pressure is checked – it should be 30 bar. The switch for the calorimeter (1) is turned on on the right wall, while on the upper left side of the back wall, the switch for the cooling liquid supply system RC 2 basic (cryothermostat) (3) is turned on (Fig. 1).

To start the cryothermostat, press and hold the “Temp” button. When the “Set” indicator light is on, the set temperature is displayed. This temperature alternates with the current temperature of the cryothermostat (when the “Set” light is off). The right side of the display also shows the pump speed (2000 or 2500).

After switching on the instrument, an initial system check is performed (Fig. 3a), during which the required temperature is set (for operation at 25°C, the coolant temperature is maintained within $20.5 < t < 23.0^\circ C$). Once the initial system check is completed, the calorimeter is ready for use, indicated by green check marks in the “External circuit flow check” and “Internal circuit flow check” lines (Fig. 1a).

2. Preparing the Calorimetric Vessel. During the system’s preliminary check, the calorimetric vessel is disassembled (Fig. 3b). The lid is removed and placed on a stand (Fig. 1c).

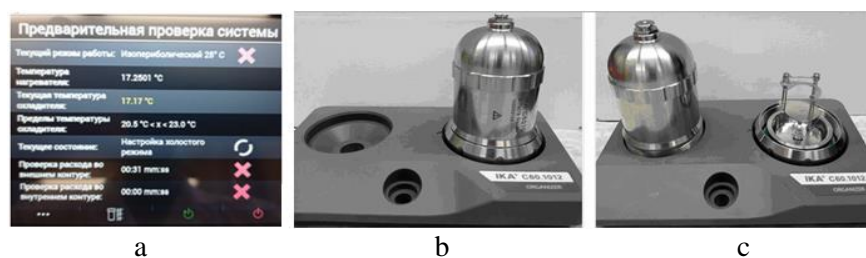


Fig. 1. Indication on the display of the system preliminary check mode (a), calorimetric vessel on a stand (b) and disassembled (c)

3. 1.0 ml of distilled water is poured into the lower lid of the calorimeter vessel using a measuring pipette (Fig. 2a), and the test substance (liquid or tablets), pre-weighed to an accuracy of 0.1 mg, is placed in the crucible (Fig. 2b).

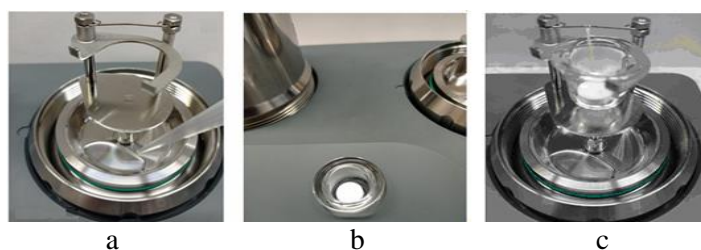


Fig. 2. The lower lid of the calorimetric vessel (a), the crucible with tablets of benzoic acid (b) and the lower lid assembly (c)

4. Placing the Crucible. The crucible is placed into the socket of the lower lid of the calorimetric vessel (Fig. 4c), and the position of the cotton ignition thread is fixed in the ignition device using tweezers. The decomposition vessel is then sealed (2).

5. Switching to Measurement Mode. To switch to operation mode, tap on the graph icon (Fig. 3a) and select the “Measurement” mode (Fig. 5a). Then, press the “+” button (add measurement) at the bottom of the display (Fig. 5b). A “New Measurement” window will open on the display (Fig. 5b). In this window, enter the sample name, sample mass, and experiment type (Measurement). The entered data is saved and displayed on the instrument screen (Fig. 5c).



Fig. 3. The sequence of operating modes during calibration of the calorimeter: a – switching to the “Measurement” mode, b – entering the mass of tablets and selecting the operating mode, c – saving the entered data

6. The decomposition vessel (2) is scanned by the calorimeter reader. If the device is ready for operation and the calorimeter recognizes its decomposition vessel, then after an audible signal, the vessel (2) is inserted into the lid of the calorimeter (1), (Fig. 1). After fixing the vessel in the lid of the calorimeter, a window appears on the display with the inscription “Do you want to start measuring?” (Fig. 6a).

7. Starting the Measurement. Press the “Start Measurement” (✓) button or “Cancel Measurement” (X). After confirming the start of the measurement, the decomposition vessel is lowered into the calorimeter. The measurement process is then indicated on the display (Fig. 6b and 6c).

8. Automatic Experiment Execution. The experiment runs automatically. Over 15-20 minutes, the external and internal chambers are filled with water, and their temperatures are equalized. The benzoic acid tablet is ignited, and the temperature is recorded during combustion (Fig. 4 b and c).

The combustion results of 0.48663 g of DMSO are presented in Table 1.

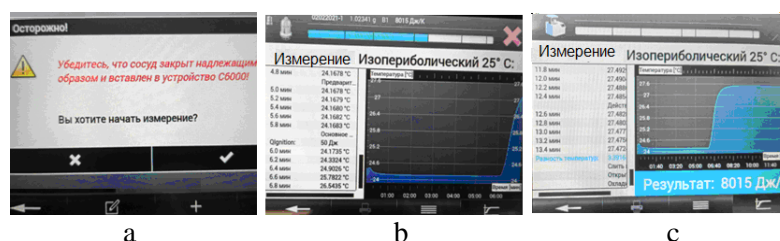


Fig. 4. Transition to the beginning of measurements (a) and indication of the measurement stages: filling the boiler with water and igniting the tablet (b), measurement results with a graph of temperature versus time (c)

Table 1

Temperature in Various Calorimeter Modes During the Combustion of 0.48663 g of DMSO and 0.17477 g of Polyethylene

Mode “Align”		“Basic” mode		“Basic” mode	
τ , min	t , °C	t , min	t , °C	τ , min	t , °C
1	2	3	4	5	6
0.0	25.0394	4.4	25.0283	9.2	28.1306
0.2	25.0383	4.6	25.269	9.4	28.1283
0.4	25.0351	4.8	26.0576	9.6	28.126
0.6	25.0319	5.0	26.9796	9.8	28.1237
0.8	25.0298	5.2	27.5352	10.0	28.1213
1.0	25.0283	5.4	27.8127	10.2	28.1189
1.2	25.0271	5.6	27.954	10.4	28.1164
1.4	25.0262	5.8	28.0306	10.6	28.1138
1.6	25.0256	6.0	28.0744	10.8	28.1113
1.8	25.0252	6.2	28.1001	11.0	28.1087
2.0	25.0248	6.4	28.1167	11.2	28.1061
2.2	25.0245	6.6	28.1263	“Action” mode	
2.4	25.0244	6.8	28.133		
2.6	25.0243	7.0	28.1372	τ , min	t , °C
2.8	25.0242	7.2	28.1397	11.4	28.7035
3.0	25.0242	7.4	28.1411	11.6	28.1009
				11.8	28.0982

Table 1 (continued)

1	2	3	4	5	6
3.2	25.0242	7.6	28.1416	12.0	28.0956
Mode "Preliminary"		7.8	28.1413	12.2	28.0930
τ , min	t , °C	8.0	28.1405		
3.4	25.0243	8.2	28.1394		
3.6	25.0243	8.4	28.1381		
3.8	25.0243	8.6	28.1366		
4.0	25.0244	8.8	28.1347		
4.2	25.0246	9.0	28.1327		

Throughout the experiment, the display on the left shows status indicators such as "Close...", "Fill...", "Stabilization...", etc. The "Fill..." mode is accompanied by temperature recordings at intervals of 0.2 minutes: "Equalization..." (00.0-04.4 min)

Research results and discussion. Comparison of graphical and measured values of temperature rise and amount of heat.

Experiment №1. The dependence of temperature on time during the combustion of 0.48663 g of DMSO and 0.17477 g of polyethylene is shown in Figure 5.

The inflection point of the main period of experience (Fig. 3) is equal to 5 minutes. For a time of 5 minutes, we get:

$$\begin{aligned} t_{\text{finite}} &= 28,25341 - (0,01315 \cdot 5) = 28,18766^{\circ}\text{C}. \\ t_{\text{Start}} &= 25,0512891 + (0,00035 \cdot 5) = 25,0248^{\circ}\text{C}. \\ \Delta t_{\text{graph}} &= 28.18766 - 25.0248 = 3.16286^{\circ}\text{C}. \end{aligned} \quad (1)$$

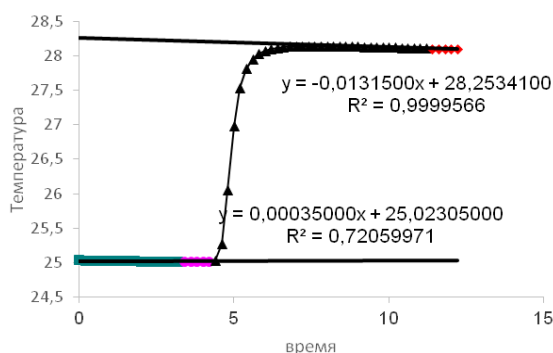


Fig. 5. Temperature versus time dependence during combustion of 0.48663 g of DMSO and 0.17477 g of polyethylene

Using the formula, we calculate the heat of combustion of DMSO:

$$Q_{\text{graph}} = W \Delta t = 8036 \cdot 3.16286 = 25416 \text{ J/g} = 25.416 \text{ kJ/g} \quad (2)$$

The heat of combustion measured by the device was 30.331 kJ/g.

The molar mass of DMSO is 78.13 g/mol. We calculate the experimentally obtained enthalpies of combustion of DMSO:

$$\begin{aligned} \Delta H^{\circ}_{\text{c, graph}} &= 25.416 \cdot 78.13 = 1985.75 \text{ kJ/mol}. \\ \Delta H^{\circ}_{\text{c, device}} &= 30.311 \cdot 78.13 = 2368.19 \text{ kJ/mol}. \end{aligned} \quad (3)$$

During the combustion of a substance, water is formed, therefore, it is necessary to subtract the heat of its condensation from the value obtained.

The error in determining Q is equal to $\delta = (20048 - 25416) / 20048 \cdot 100 = 26,8\%$

The error in determining $\Delta t = (3,77439 - 3,16286) / 3,77439 \cdot 100 = 16,2\%$

Conclusion. As a result of experimental studies in the scientific laboratory of the Department of General and Inorganic Chemistry, we got acquainted with the operation of the IKA C 6000 global standard/isoperibol calorimeter. This calorimeter was used to conduct experiments on the combustion of three samples of acetonitrile (AN) and dimethyl sulfoxide (DMSO). As a result of processing the obtained experimental data, the experimental value of the enthalpy of combustion of AN $\Delta H_{\text{co}}(\text{AN}_{\text{exp}})$ was calculated, which was -1197.4 kJ/mol . And also the value of the temperature change (Δt_{graph}) was determined graphically and the heat of combustion of DMSO Q_{graph} was calculated. A comparison of Δt_{graph} and Δt_{device} , as well as Q_{graph} and Q_{device} was made. The obtained value was compared with the theoretically calculated $\Delta H_{\text{co}}(\text{AH-theor.})$ using the equation of the AN combustion reaction and reference values of the enthalpies of formation of substances (-1175.2 kJ/mol). Comparison of these values gives an error in determining $\Delta c_{\text{He}}(\text{AH-exp.})$ equal to 1.9% .

A comparison was made between Δt_{graph} and Δt_{device} , as well as Q_{graph} and Q_{device} .

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ДИМЕТИЛ СУЛЬФОКСИДИНІҢ ЖАНУ ЭНТАЛПИЯСЫН АНЫҚТАУ

Аңдатпа. Бұл зерттеу маңызды коммерциялық және ғылыми маңызы бар полярлы апротикалық еріткіш диметилсульфоксидтің (DMSO) физика-химиялық қасиеттерін, синтезін және қолданылуын зерттейді. Қағаз оның молекулалық құрылымын, өндіру әдістерін - ең алдымен диметил сульфидінің тотығуын және оның еріткіш, криопротектор, ПТР ингибиторы және терапевтік агент ретіндегі рөлін қоса алғанда, әртүрлі қолдануларды егжей-тегжейлі сипаттайды. Эксперименттік жұмыс заттардың жану энтальпиясын анықтау үшін IKA C 6000 калориметрін пайдаланып термохимиялық талдауға бағытталған. Калориметриялық орнату, бензой қышқылымен калибрлеу және өлшеу протоколдары сипатталған, қазіргі заманғы калориметрияның дәлдігі мен автоматтандырылуына баса назар аударылады. Зерттеу DMSO-ның жоғары қайнау температурасы, дипольдік моменті және биологиялық мембраналарға ену қабілеті сияқты бірегей қасиеттерімен расталған өнеркәсіптік, медициналық және зертханалық контексттегі әмбебаптығын көрсетеді.

Тірек сөздер: диметил сульфоксиді (DMSO), полярлық апротикалық еріткіш, термохимиялық талдау, жану энтальпиясы, калориметрия (IKA C 6000).

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ОПРЕДЕЛЕНИЕ ЭНТАЛЬПИИ СГОРАНИЯ ДИМЕТИЛСУЛЬФОКСИДА

Аннотация. В данном исследовании изучаются физико-химические свойства, синтез и применение диметилсульфоксида (ДМСО), полярного апротонного растворителя, имеющего важное коммерческое и научное значение. В статье подробно описывается его молекулярная структура, методы производства (в первую очередь окисление диметилсульфида) и различные варианты его применения, включая его роль в качестве растворителя, криопротектора, ингибитора ПЦР и терапевтического агента. Экспериментальная работа была сосредоточена на термохимическом анализе с использованием калориметра IKA C 6000 для определения энтальпии сгорания веществ. Описаны калориметрическая установка, калибровка с использованием бензойной кислоты и протоколы измерений с упором на точность и автоматизацию современной калориметрии. Исследование подчеркивает универсальность ДМСО в промышленных, медицинских и лабораторных условиях, о чем свидетельствуют его уникальные свойства, такие как высокая температура кипения, дипольный момент и способность проникать через биологические мембраны.

Ключевые слова: диметилсульфоксид (ДМСО), полярный апротонный растворитель, термохимический анализ, энтальпия сгорания, калориметрия (IKA C 6000).