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Equilibrium and thermodynamics for 2-methyl-2-methoxybutane liquid-phase decomposition [☆]

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Abstract

The chemical equilibrium for the liquid-phase decomposition of 2-methyl-2-methoxybutane (*tert*-amyl methyl ether) was studied experimentally in the temperature range 313–353 K and at 700 kPa. To reach decomposition equilibrium, the macroporous acid resin K-2631 (Bayer) was used as the catalyst. Equilibrium constants and standard enthalpies, free energies, and entropies for addition of methanol to 2-methyl-1-butene and 2-methyl-2-butene (forward reactions) were determined as a temperature function and compared with literature data. The UNIFAC estimates of activity coefficients were used to describe the liquid-phase non-ideality.

Keywords: Amylenes; 2-Methylbutene; 2-Methyl-2-butene; 2-Methyl-2-methoxybutane

List of symbols

a, b, c, d	changes in molar heat capacity coefficients with chemical reaction
a_j, b_j, c_j, d_j	coefficients in the equation for molar heat capacity of component j
a'_j	activity of component j (dimensionless)
C_P	molar heat capacity/(J mol^{-1} K^{-1})
$f(T)$	function of a, b, c, d and T defined in Eq. (7)
I_H	integration constant in van't Hoff equation (dimensionless)
I_K	integration constant in Kirchoff's equation/(J mol^{-1})
K_i	thermodynamic equilibrium constant of reaction i

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K_γ	ratio of activity coefficients
K_x	experimental equilibrium constant based on molar fractions
R	gas constant/(J mol^{-1} K^{-1})
T	temperature/K
$\Delta_r G^\ominus$	standard molar free energy change of reaction/(kJ mol^{-1})
$\Delta_r H^\ominus$	standard molar enthalpy change of reaction/(kJ mol^{-1})
$\Delta_r S^\ominus$	standard molar entropy change of reaction/(J mol^{-1} K^{-1})

Greek Symbols

γ_j	activity coefficient of component j
ν_j	stoichiometric coefficient of component j

Subscripts

2M1B	2-methyl-1-butene
2M2B	2-methyl-2-butene
M	methanol
TAME	2-methyl-2-metoxybutane, *tert*-amyl methyl ether

1. Introduction

The addition of fuel-oxygenated organic compounds to gasoline has allowed lead additives to be phased out and, at the same time, has raised combustion temperatures and improved engine efficiencies, which results in lower levels of carbon monoxide and unburned hydrocarbons in auto exhaust. Emissions standards imposed by governments require the presence of oxygenates in gasolines. To be effective, oxygenated gasolines require a minimum oxygen content of 2 wt%. The petroleum refining industry is focused on the question of which oxygenated organic compounds are more desirable. Refiners prefer tertiary ethers to lighter alcohols as blending components of gasoline because they behave more like conventional hydrocarbon components in their physical properties such as vapour pressure and phase separation.

To date, almost all the ether that has been blended to gasoline has been methyl *tert*-butyl ether (MTBE) produced by adding methanol to isobutene, but the insufficient supply of isobutene feedstock has increased interest in the use of higher tertiary ethers. One of these is TAME (2-methyl-2-methoxybutane, *tert*-amyl methyl ether), which is formed in the catalysed reaction of the isoamylenes 2-methyl-1-butene (2M1B) and 2-methyl-2-butene (2M2B) and methanol. However, olefins have been shown to promote the formation of ozone in the atmosphere, particularly isoamylenes existing in the olefinic C_5 cut used in gasoline blending [1]. Therefore, the production of TAME can not only add oxygen to gasoline but also reduce isoamylene content.

TAME synthesis reactions are reversible and moderately exothermic. Usually, the reactions are performed under pressure (700–900 kPa) and temperatures in the range 313–373 K. Of amylenes, in the etherification conditions indicated, only 2M1B and

2M2B are reactive because they have a double bond attached to a tertiary carbon atom. Besides etherification reactions, the isomerization reaction between the two reactive amylenes also has to be considered because fast-reacting 2M1B is replaced with slow-reacting 2M2B. Other side reactions such as dimerization of amylenes, dimerization of methanol and the formation of *tert*-amyl alcohol (TAA) are of little importance in normal operation conditions. Thus, the three following reactions are the most important to be considered in TAME production from a C_5 olefinic fraction

$$\mathrm{2M1B + MeOH \rightleftharpoons TAME} \quad (1)$$

$$\mathrm{2M2B + MeOH \rightleftharpoons TAME} \quad (2)$$

$$\mathrm{2M1B \rightleftharpoons 2M2B} \quad (3)$$

As discussed later in the paper, literature on the thermodynamic properties of such reactions is rather scarce and present significant dispersion. The aim of the present work was to report an experimental study of the splitting reaction, i.e. the backward reaction of ether to isoamylenes and methanol. The experimental equilibrium constant was used to obtain the thermodynamic properties of the reactions, which were compared with literature data in order to have more reliable data.

2. Experimental

2.1. Materials

Methanol HPLC (ROMIL Chemicals Ltd, Shepshed, England), with a minimum purity of 99.9%, and TAME (Fluka Chemie AG, Buchs, Switzerland), with a purity > 98 wt% (GC), were used in the experiments for investigation of the equilibrium of the reactions. Methanol was dried over 3 Å molecular sieve before use. TAME was used without further purification because all its impurities (2M2B, 2M1B and TAA) were present in the reacting system. TAA is produced by reacting water, which was present in the catalyst, with 2M2B and/or 2M1B. The pure compounds (GC) were used for analytical calibrations. Nitrogen supplied by SEO (Barcelona, Spain), with a minimum purity of 99.998%, was used to achieve the pressure required to maintain the reacting mixture in the liquid phase at every temperature.

The commercial acidic resin used was K-2631 produced by Bayer. The resin had an exchange capacity, determined by titration against standard base, of 4.6–4.8 meq of H^+ per g of dry resin. Before use, the cation exchanger was washed with water to remove impurities and then dried at 110°C for 12 h. The residual water content in the resin, measured by Karl-Fischer titration, was less than 2.9 wt%.

2.2 Apparatus

Experiments were carried out in a stainless steel autoclave of $3 \times 10^{-4}\,\mathrm{m}^3$ capacity (Autoclave Engineers, USA) operating in batch mode. The reaction medium was agitated at 500 rpm by a magnetic-drive turbine. The temperature inside the autoclave could be controlled to within ±0.2 K of the set point by thermostatic water that flowed through the jacket. Further information on the apparatus is described elsewhere [2].

2.3. Analysis

The analysis of the reaction mixture consisting of TAME, methanol, 2M2B, 2M1B, TAA and traces of dimers of isoamylenes was done on a gas chromatograph (HP5880) with a flame ionization detector. Samples was taken out of the reactor by a liquid sampling valve (Valco 4-CL4WE), which injected 0.2 µl of pressurized liquid into the chromatograph. A 50 m × 0.2 mm × 0.5 µm (length × id × film thickness) of methyl silicone capillary column (PONA-HP 19091S-001) was used for analysis. The injector and detector were kept at 355 and 523 K, respectively. The oven temperature was programmed with a 7-min initial hold at 313 K, followed by a $10\,\mathrm{K} \times \mathrm{min}^{-1}$ ramp up to 463 K, and held for 10 min. Helium, pure 99.999% (SEO, Barcelona, Spain), was used as the carrier gas with a flow rate of $30\,\mathrm{ml\,min}^{-1}$.

2.4. Procedure

A calculated amount of TAME and about 10 g of dried resin was charged into the open reactor. After the reactor was checked for leaks, the agitation was switched on and the reacting mixture reached the desired temperature; the pressure was set at 700 kPa. Then, the reaction was allowed to achieve equilibrium, which was checked by taking out several samples at successive intervals until a constant composition was obtained. To be sure that true equilibrium was reached, different initial compositions were used in some experiments either by using an initial amount of methanol or by changing the temperature of a reacting mixture that was already supposed to be at equilibrium.

3. Results and discussion

A set of 15 experiments was carried out in the temperature range 313.2–353.2 K at 700 kPa. Table 1 shows the experimental temperature and results. The second and third experiments at 333.2 K were performed using an excess of methanol, 10% and 20% molar. Calculations were done only for reactions (1) and (2) because the third (isomerization) is a linear combination of the first two reactions. However, as the equilibrium constants for a reaction and its reverse are reciprocals of each other, the equilibrium constants for the TAME synthesis (forward reactions) were obtained by raising the respective equilibrium constants for the TAME cracking (reverse reaction) to the -1 power. The activity coefficients of the compounds, γ, were estimated by the UNIFAC prediction method [3–6], whose validity for reacting system of lighter tertiary ethers, such as methyl *tert*-butyl ether and ethyl *tert*-butyl ether has already been checked [7–9]. All the species present were considered in the UNIFAC predictions. However, TAA and dimers of isoamylenes were not considered because they were detected in very small amounts and did not alter the UNIFAC predictions. The values of

Table 1
Equilibrium constants for TAME syntheses from 2M1B and 2M2B determined using TAME decomposition equilibrium data

Temperature/K	K_x^1	K_x^2	K_y^1	K_y^2	K^1	K^2	Average K^1	Average K^2
	408.5	39.9	0.26	0.25	104	10.1		
313.2	366.4	35.4	0.26	0.26	94.2	9.1	98	9.4
	365.1	35.3	0.26	0.26	94.0	9.0		
	245.7	24.5	0.27	0.27	66.5	6.6		
323.2	248.2	24.5	0.27	0.27	66.6	6.6	65	6.4
	226.7	22.3	0.27	0.27	60.9	6.0		
	158.1	16.2	0.28	0.28	44.7	4.6		
333.2	127.8	13.2	0.30	0.30	38.2	3.9	39	4.0
	110.2	11.6	0.32	0.31	35.0	3.6		
	103.0	11.0	0.29	0.29	30.2	3.21		
343.2	98.8	10.4	0.29	0.29	28.8	3.0	29.4	3.1
	101.0	10.6	0.29	0.29	29.2	3.0		
	64.9	7.2	0.30	0.30	19.5	2.2		
353.2	68.6	7.6	0.30	0.30	20.6	2.3	19.6	2.2
	62.3	7.0	0.30	0.30	18.8	2.1		

K_y^i calculated by the relations

$$K_y^1 = \frac{\gamma_{\mathrm{TAME}}}{\gamma_{\mathrm{M}}\gamma_{\mathrm{2M1B}}} \tag{4}$$

$$K_y^2 = \frac{\gamma_{\mathrm{TAME}}}{\gamma_{\mathrm{M}}\gamma_{\mathrm{2M2B}}} \tag{5}$$

showed the strong non-ideal behaviour of the system, methanol being the most non-ideal compound.

The thermodynamic equilibrium constant for a liquid-phase reaction of a non-ideal system, considering pure liquid at its equilibrium vapour pressure as the standard state, is given by

$$K = \prod_{j=1}^{s} (a'_j)_e^{\nu_j} = \prod_{j=1}^{s} (\gamma_j)_e^{\nu_j}(x_j)_e^{\nu_j} = \prod_{j=1}^{s} (\gamma_j)_e^{\nu_j} \prod_{j=1}^{s} (x_j)_e^{\nu_j} = K_y K_x \tag{6}$$

The effect of the pressure on the equilibrium constant was neglected because the Poynting corrector factor was estimated to be less than 0.5%, which is far less than the experimental uncertainty in K. As a result, K was assumed to be only a function of temperature. It is worth noting that the K^1 and K^2 values of Table 1 follow the general trend of lowering when temperature is increased, as expected for exothermic reactions. Tables 2 and 3 show a comparison of the equilibrium constants obtained with those found in the literature. The K values of the present work are given with the confidence

Table 2
Comparison of equilibrium constants of TAME synthesis from 2M1B with literature data

Temperature/K	Present work	Bravo et al. [10]	Rikho and Krause [11]	Lovisi and Piccoli [12]
313.2	98 ± 25	129	–	–
323.2	65 ± 14	85	–	119
333.2	39 ± 20	56	–	82
343.2	29 ± 3	39	–	55
353.2	20 ± 4	27	22	43

Table 3
Comparison of equilibrium constants of TAME synthesis from 2M2B with literature data

Temperature/K	Present work	Bravo et al. [10]	Rikho and Krause [11]	Lovisi and Piccoli [12]
313.2	9.4 ± 2.6	11.1	–	–
323.2	6.4 ± 1.7	7.8	–	10
333.2	4.0 ± 2.2	5.6	–	7.5
343.2	3.1 ± 0.4	4.4	–	5.6
353.2	2.2 ± 0.4	3.3	2.5	4.6

interval for a 95% probability level. As can been seen, the values obtained are slightly lower than those of Bravo et al. [10] and Rikho and Krause [11]. Experimental error could explain this discrepancy. The values, however, are much lower than that of Lovisi and Piccoli [12]. In this case, experimental error does not explain the differences and systematic errors are likely. We will return to this point after calculating the standard enthalpy changes of reactions.

The dependence of K on temperature can be deduced by intergration of the van't Hoff equation. As a starting point, by considering previous results for MTBE and ETBE [2, 9], we will accept the fact that standard reaction enthaply changes of the two reactions are functions of temperature (Kirchoff equation). Assuming that the constant-pressure heat capacities are given by the third degree polynomials shown in Table 4, integration of the Kirchoff equation yields the well-known expression

$$\ln K - \frac{a}{R}\ln T - \frac{b}{2R}T - \frac{c}{6R}T^2 - \frac{d}{12R}T^3 = \ln K + f(T) = I_{\mathrm{H}} - \frac{I_{\mathrm{K}}}{RT} \tag{7}$$

where

$$a = \sum v_j a_j;\ b = \sum v_j b_j;\ c = \sum v_j c_j;\ d = \sum v_j d_j; \tag{8}$$

Table 4
Constants for the equaton $c_p/\mathrm{J\,mol^{-1}\,K^{-1}} = a + b(T/\mathrm{K}) + c(T/\mathrm{K})^2 + d(T/\mathrm{K})^3$

Compound	a_i	b_i	$c_i \times 10^2$	$d_i \times 10^5$
Methanol[a]	1391.6	−12.364	3.781	−3.719
2M1B[b]	−107.501	2.141774	−0.634436	0.7287577384
2M2B[b]	−73.8206	1.79621	−0.531408	0.6216732173
TAME[c]	46258.36	−443.401	1.420576	−15.137236

[a] Calculated from Gallant [13] by fitting of a third-order equation.
[b] Estimated by the Rowlinson–Bondi method [14].
[c] Obtained in a calorimetric reactor [15].

with the a_j, b_j, c_j and d_j values of Table 4. The constants I_K and I_H of each reaction can be calculated from the temperature dependence relationship for the corresponding experimental equilibrium constants. By fitting Eq. (7) to the data of Table 1, we obtain I_K from the slope and I_H from the intercept, with regression coefficients of 0.999999 for both reactions. Thus, the expressions derived from Eq. (7) for the temperature dependence are

$$\ln K^1 = -265554.756 + 424875.69\,T^{-1} + 5409.46 \ln T - 26.0512\,T + 0.0278467\,T^2 - 1.48721 \times 10^{-5}\,T^3 \quad (9)$$

$$\ln K^2 = -26536.79 + 424297.56\,T^{-1} + 5405.41 \ln T - 26.0304\,T + 0.027826\,T^2 - 1.4862 \times 10^{-5}\,T^3 \quad (10)$$

The K values are also well correlated (regression coefficients of 0.996 and 0.994) by the following relations, deduced by assuming that the standard enthalpy changes of both reactions are independent of temperature

$$K^1 = 7.16 \times 10^{-5}\,\mathrm{e}^{4420.75/T} \quad (11)$$

$$K^2 = 2.48 \times 10^{-5}\,\mathrm{e}^{4017.076/T} \quad (12)$$

The better correlation obtained by Eqs. (9) and (10) confirms the fact that standard enthalpy changes of reactions depend on temperature. Taking into consideration the well-known thermodynamic relations

$$\Delta H^\ominus = I_K + aT + \frac{b}{2}T^2 + \frac{c}{3}T^3 + \frac{d}{4}T^4 \quad (13)$$

$$\Delta S^\ominus = R \ln K + \frac{\Delta H^\ominus}{T} \quad (14)$$

and

$$\Delta G^\ominus = -RT \ln K = \Delta H^\ominus - T\Delta S^\ominus \quad (15)$$

we can obtain the standard molar changes of the reaction $\Delta_r H^\ominus$, $\Delta_r S^\ominus$ and $\Delta_r G^\ominus$ as functions of temperature for both reactions. For reaction 1, we obtain

$$\Delta_r H^\ominus = -3532416.4 + 44974.26T - 216.5896T^2 + 0.4630349T^3 - 3.709399 \times 10^{-4}T^4 \quad (16)$$

$$\Delta_r G^\ominus = -3532416.4 + 220776.24T - 44974.25T\ln T + 216.58967T^2 - 0.2315174T^3 + 1.2364663 \times 10^{-4}T^4 \quad (17)$$

$$\Delta_r S^\ominus = -175801.98 + 44974.25\ln T - 433.17934T + 0.6945523T^2 - 4.9458653 \times 10^{-4}T^3 \quad (18)$$

At 298.2 K we have, giving the errors as the standard deviation, the following values

$$\Delta_r H^\ominus(1) = -(35.8 \pm 1.3)\,\mathrm{kJ\,mol^{-1}}$$

$$\Delta_r G^\ominus(1) = -(13.1 \pm 1.4)\,\mathrm{kJ\,mol^{-1}}$$

$$\Delta_r S^\ominus(1) = -(76.4 \pm 0.4)\,\mathrm{J\,mol^{-1}\,K^{-1}}$$

Table 5 shows a comparison of the standard molar enthalpy change of the TAME synthesis from 2M1B with those theoretical (from $\Delta_f H^\ominus$ values in Table 6) and experimental values found in the literature. As can be seen, the value of this work is in good agreement with those calculated from the enthalpy of formation of the components, which accounts for the validity of the methodology used. However, by reaction calorimetry at 343 K [15] a range of values from −37 to −39 kJ mol^{-1} was obtained in experiments for the forward and reverse reaction, which supports the previous conclusion. From Eq. (16), it can be deduced that the existing effect of temperature on the standard enthalpy is small, about 0.3 kJ mol^{-1} per 10 K. At this point, it is interesting to reconsider the equilibrium constant of Lovisi and Piccoli [12], because the standard enthalpy change they deduced seems rather low.

Table 5
Standard molar enthalpy change of TAME synthesis from 2M1B in the liquid phase at 298.2 K

Reference	$\Delta_r H^\ominus$/kJ mol^{-1}
This study	−35.8
Theoretical [16]	−34.8
Theoretical [17]	−41.7
Lovisi and Piccoli [12]	−32.6

Table 6
Standard enthalpies of formation at 298.2 K in liquid state

Compound	$\Delta_f H^\ominus$/kJ mol^{-1}
TAME [16]	−334.9
TAME [17]	−341.8
Methanol [18]	−239.1
2M1B [18]	−61.0
2M2B [18]	−68.6

Table 7
Standard molar enthalpy change of TAME synthesis from 2M2B in the liquid phase at 298.2 K

Reference	$\Delta_r H^{\ominus}$/kJ mol^{-1}
This study	−32.8
Theoretical [16]	−27.2
Theoretical [17]	−34.1
Lovisi and Piccoli [12]	−24.5
Brockwell et al. [19]	−39.3 (independent of T)
Randriamahefa et al. [20]	−41.2 (independent of T)

For reaction (2), we obtain the expressions

$$\Delta_r H^{\ominus} = -3527609.9 + 44940.578T - 216.4167T^2 + 0.462691T^3 - 3.70688 \times 10^{-4}T^4 \qquad (19)$$

$$\Delta_r G^{\ominus} = -3527609.9 + 220626.87T - 44940.578T\ln T + 216.41674T^2 - 0.2313453T^3 + 1.2356266 \times 10^{-4}T^4 \qquad (20)$$

$$\Delta_r S^{\ominus} = -175686.3 + 44940.578\ln T - 432.83348T + 0.694036T^2 - 425066 \times 10^{-4}T^3 \qquad (21)$$

The values at 298.2 are

$$\Delta_r H^{\ominus} = -(32.8 \pm 1.4)\ \mathrm{kJ\,mol^{-1}}$$

$$\Delta_r G^{\ominus} = -(7.1 \pm 1.5)\ \mathrm{kJ\,mol^{-1}}$$

$$\Delta_r S^{\ominus} = -(86.5 \pm 0.4)\ \mathrm{J\,mol^{-1}\,K^{-1}}$$

A comparison of the standard molar enthaply change of the TAME synthesis from 2M2B with those theoretical and experimental values found in the literature is shown in Table 7. It can be seen that the value obtained in this work falls in the range of values predicted from the enthalpies of formation. Moreover, if the isomerization enthalpy is calculated from the formation enthaplies of the two amylenes, we obtain a value of 7.6 kJ mol^{-1}. However, the value that is obtained by combining the standard enthaply changes of TAME synthesis from the two amylenes is only 3 kJ mol^{-1}. The discrepancy can be explained by considering the experimental error for standard enthalpies which is obtained by subtraction of these two values. The other two enthalpies found in the literature show considerable divergence. The value quoted by Brockwell seems too high and that determined by Lovisi and Piccoli too low.

4. Conclusions

Conversions and, therefore, concentration at equilibrium for TAME synthesis from reactive amylenes and decomposition can be predicted from the respective equilibrium constant. As the reacting system behaves non-ideally, must be applied carry out the calculations.

The agreement between the standard enthaplies obtained in this work with those determined theoretically proves that the methodology used is correct. From the dispersion of the values (theoretical and experimental), however, more experimental work is needed to ascertain more reliable data.

From the temperature dependence relationship for the equilibrium constants, equations for the temperature dependence of standard enthalpies, entropies, and free energies of the TAME synthesis from reactive amylenes have been determined. These equations show that the variation of reaction standard enthalpies with temperature are significant although its effect is not very pronounced.

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