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Kinetic and modeling studies on ETBE pyrolysis behind reflected shock waves

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Abstract

The high temperature pyrolysis of ethyl *tert*-butyl ether (ETBE) was studied behind reflected shock waves coupled with the single-pulse method and UV (195 nm) absorption spectroscopy in the temperature range 1000–1500 K at total pressures ranging between 1.0 and 9.0 atm. The energies of ETBE and transition states for the reactions ETBE = *iso*-C₄H₈ + C₂H₅OH (1) and ETBE = C₂H₄ + *tert*-C₄H₉OH (2) were calculated at the MP4/cc-pVTZ//MP2/cc-pVTZ level of theory. A 170-reaction mechanism was constructed to explain the product distribution. From the UV absorption experiment, the rate coefficient $k_1 = 1.7 \times 10^{14} \text{exp}(-254.0 \text{ kJ mol}^{-1}/\text{RT}) \text{ s}^{-1}$ was found to reach its high-pressure limit.

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1. Introduction

Recently, biofuels have been expected to function as new energy resources. In particular, bioethanol prevails as a fuel in several countries. In the United States and Brazil, bioethanol itself is used as an automobile fuel. In Europe, on the other hand, ethyl *tert*-butyl ether (ETBE) synthesized from C_2H_5OH and *iso*- C_4H_8 is used. In Japan, a tentative sale of ETBE began in April 2007.

The gas-phase oxidation of pure ETBE has previously been investigated using a static reactor [1] and jet-stirred reactors [2,3]. Previous works concluded that the dominant initial thermal decomposition step of ETBE was the unimolecular elimination reaction, ETBE = *iso*-C₄H₈ + C₂H₅OH (1). In the present study, shock tube study of ETBE pyrolysis was performed at temperatures above 1000 K. A 170-reaction ETBE pyrolysis mechanism was constructed in order to explain the product distributions. The evidence for the new unimolecular elimination reaction

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 $ETBE = C_2H_4 + tert-C_4H_9OH$ (TBA) (2) was found by detecting TBA produced by the pyrolysis of ETBE. The pressure dependence of the rate coefficient for reaction (1) was examined by UV absorption experiments.

2. Experimental

All experiments were performed behind reflected shock waves. In the gas-analyzing experiments, the initial pressure (P_1) was fixed at 50 torr, while in the UV absorption experiments, it ranged between 100 and 300 torr. The Ar (Teisan Co. and Iwatani), specified to be 99.999% pure, was used without further purification. The ETBE (Sigma– Aldrich, Inc.), specified to be 99% pure, was frozen, degassed a number of times, and purified by trap-to-trap distillation before use.

Two shock tubes were used in this study. The first was a magic-hole-type with 4.1 cm i.d. [4]. The reacted gas mixtures were extracted into a pre-evacuated vessel (50 cm³) through the valve near the end plate and analyzed by three serially connected gas-chromatographs, each with a TCD. The gas-chromatographic analysis, which was similar to

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that in the study conducted by Hidaka et al. [5], was used to determine the concentrations of reactant and products. The amounts of reactant and products were determined within an uncertainty of 4%. The effective heating time t_e (reaction time), which was defined as the amount of time between the arrival point of the reflected shock front and the 80% point in the fall from the reflected shock front pressure as shown in Fig. 1, was determined using the method described previously [6,7]. The modeling methodology for this comparison is shown in detail in previous reports [8,9].

The second was a standard-type shock tube connected to a UV absorption system. This tube consisted of three sections [10]. The high-pressure section was made of a steel tube 1.5 m long and with an inner diameter of 10 cm. The low-pressure section was made of stainless steel and had a rectangular cross-section of 7.2 by 3.8 cm. For smooth flow of the driver gas from the round high-pressure section to the low-pressure section, we employed a conversion section of 30 cm in length. Observation windows were located 3.8 m downstream from the diaphragm positioned between the high-pressure section and the conversion section. The end plate for the reflected shock wave was located 1 cm from the observation windows. The total length of lowpressure section was 3.8 m. UV light obtained from a deuterium lamp passed through a path of 7.2 cm in length in the shock tube at the observation station and was dispersed into 195 nm by a monochromator (half-width = 1.6 nm). It was detected by a photo-multiplier (R208, Hamamatsu photonics). The UV absorption profile that we observed was analyzed using absorbance, $\log(I_f/I_t)$. The extinction coefficients at 195 nm were measured for several compounds expected to be the main products of UV absorption under our experimental conditions. We found that iso-



Fig. 1. A typical pressure profile with the definition of effective heating time.

C₄H₈ and ETBE only contributed to the UV absorption profile at 195 nm. The equations for the extinction coefficients of *iso*-C₄H₈ and ETBE were $\varepsilon_{UV}(iso$ -C₄H₈) = $3.44 \times 10^6 \text{ cm}^2 \text{ mol}^{-1}$ and $\varepsilon_{UV}(\text{ETBE}) = -2.83 \times 10^6 +$ $2770 \times T \text{ (K) cm}^2 \text{ mol}^{-1}$, respectively. The extinction coefficient of C₂H₄ was about 1/30 that of *iso*-C₄H₈ at 1300 K. The influence of C₂H₄ concentration on the UV absorption profile at 195 nm was negligible.

Thermochemical data for H₂O were adopted from the JANAF table [11]. The heat of formations of ETBE, TBA, C₂H₅ and OH were adopted from tables reported by Dunphy et al. [12], NIST [13], Brouard et al. [14] and Ruscic et al. [15], respectively. Thermochemical data for H, H₂, CH₃, CH₄, C₂H₄, CH₂O and CH₃CHO were adopted from NIST [13]. Thermochemical data for C₂H₅O, C₂H₅OH, C₂H₆O (acetone), iso-C₄H₈ and tert-C₄H₉ were adopted from Burcat [16]. Thermochemical data for r1ETBE(C₂H₅OC(CH₃)₂CH₂), r2ETBE(CH₂-CH₂OC(CH₃)₃), r3ETBE(CH₃CHOC(CH₃)₃), r4ETBE- $(C_2H_5OC(CH_3)_2)$, tert-C₄H₉O, rdMTBE $(CH_2OC(CH_3)_3)$, $r1TBA(HOC(CH_3)_2CH_2)$ and $r2TBA(HOC(CH_3)_2)$ were estimated using group values shown in [17] and group additivity method reported by Benson [17]; Cp values at 1500 K not found in [17] were assumed from those in similar species. Thermochemical data of ETBE and associated radicals are shown in Table 1. Shock temperature was calculated by the measured velocity, assuming no chemical reactions and full relaxation of the chemical species.

The computer calculations used in this study were essentially the same as those described by Hidaka et al. [18]. We used a computer routine consisting of the Gear-type integration of the set of differential equations describing the chemical kinetics under constant density conditions for the reflected shock waves. Reverse reactions were automatically included in the computer program through equilibrium constants computed from the thermochemical data.

Sensitive spectra (pS) were calculated in order to determine the importance of each reaction. The pS adopted was defined as pSij = log[(computed quantity)j'/(computedquantity)j]/log[(parameter)i'/(parameter)i], where the primesdenote the parameters*i*and computed quantities*j*for acomputer simulation in which the value of one parameter

Table	1	
Therm	ochemical	data

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	ΔH_{f298}° (kJ/mol)	S°_{298} (J/mol K)	300 K	C _p (J/mol K) 500 K	1000 K	1500 K
ETBE	-325.1	386.4	149.3	232.3	348.9	403.9
rlETBE	-144.9	406.5	147.0	227.6	335.1	378.6 ^a
r2ETBE	-149.3	399.3	147.1	225.5	336.0	384.4
r3ETBE	-155.6	401.0	141.8	219.8	330.7	382.9
r4ETBE	-123.0	351.1	120.0	185.6	293.0	357.9 ^a
tert-C ₄ H ₉ O	-86.9	309.2	106.6	160.9	240.3	273.6
rdMTBE	-116.0	393.9	134.7	198.3	287.0	324.4 ^a
tert-C ₄ H ₉	55.0	322.4	82.8	126.3	202.9	240.1

^a Assumed value.

has been changed from a reference value (unprimed quantity and parameter) [19]. The computed quantity and parameter were the concentration of reactant or products obtained by simulation and the rate coefficient, respectively.

3. Theoretical calculations

All quantum chemical calculations were performed using the GAUSSIAN 03 program package [20]. The geometries of the reactant, products, and transition states were optimized at the MP2/cc-pVTZ level of approximation. Vibrational frequencies were calculated using the analytical second derivatives at the same level of the geometry optimization in order to confirm the stationary structures and correct for the zero-point vibrational energy. Single point energy calculations were performed at the MP4/ccpVTZ//MP2/cc-pVTZ level in order to estimate the energy of the compounds.

4. Results

4.1. Theoretical calculations

The transition states of reactions (1) and (2), TS1 and 2, which form a four-centered structure, were found by quantum chemical calculations. The relative energies of TS1 and 2 calculated from the reactant are shown in Fig. 2 along with a concise optimized structural diagram. The relative energies calculated were over 70 kJ mol⁻¹ lower than the ΔH_0° of reactions (3)–(6), estimated from heats of formation as described in Table 2. This suggests that the dominant initial decomposition steps of ETBE were unimolecular elimination reactions.

4.2. Product distribution

The reactant and product distributions obtained by the pyrolysis of 3% ETBE diluted in Ar are shown in Fig. 3a. In this Letter, the distributions of ETBE, *iso*-C₄H₈, C₂H₆O(acetone), C₂H₅OH, TBA, H₂, CH₄ and CH₃CHO are shown to estimate rate coefficients relating to ETBE pyrolysis. The distributions of C₂H₂, C₂H₄, C₂H₆, a-C₃H₄-(allene), p-C₃H₄(propyne), C₃H₆ and C₃H₈, on the other hand, depend mainly on the subsequent reactions, so they are not shown in this Letter.

4.3. UV absorption at 195 nm

The typical time-dependent absorbance at 195 nm, $log(I_f/I_t)$, is shown in Fig. 4a. Under the conditions of our UV absorption experiments, the main absorbers were *iso*-C₄H₈ and ETBE, as shown in Fig. 4a.

5. Discussion

5.1. Construction of an ETBE pyrolysis mechanism

An ETBE pyrolysis mechanism, which included 170reactions, was constructed in order to reproduce the reactant and product distributions obtained by the single pulse method. The mechanism constructed is shown in Table 2. The distributions of C₂H₅OH and TBA are sensitive to reactions (1) and (2), as seen in Fig. 3b. C₂H₅OH and TBA are produced only via unimolecular elimination reactions (1) and (2), respectively. The activation energies of the rate coefficients for reactions (1) and (2) were adopted from the E_0 obtained from quantum chemical calculations. Those pre-exponential factors were estimated to reproduce the distributions of C₂H₅OH and TBA. The distribution of



Fig. 2. Potential energy diagrams of ETBE unimolecular elimination reactions with geometries of TS1 and 2.

Table 2 Elementary reactions and rate coefficient expressions

No.	Reaction	A	n	E_{a}	ΔH_0	Reference
(1)	$ETBE = iso-C_4H_8 + C_2H_5OH$	$1.70 imes 10^{14}$	0.00	254,000	55,200	This work
(2)	$ETBE = C_2H_4 + TBA$	5.00×10^{13}	0.00	265,000	56,900	This work
(3)	$ETBE = r4ETBE + CH_3$	2.50×10^{16}	0.00	337,000	337,000	This work
(4)	$ETBE = tert - C_4 H_9 O + C_2 H_5$	$8.00 imes 10^{15}$	0.00	334,000	334,000	This work
(5)	$ETBE = rdMTBE + CH_3$	$8.00 imes 10^{15}$	0.00	344,000	344,000	See text
(6)	$ETBE = tert - C_4H_9 + C_2H_5O$	$8.00 imes 10^{15}$	0.00	348,000	348,000	See text
(7)	$ETBE + H = r1ETBE + H_2$	$3.00 imes 10^{14}$	0.00	49,000	-64,100	See text
(8)	$ETBE + H = r2ETBE + H_2$	$1.00 imes 10^{14}$	0.00	49,800	-50,600	See text
(9)	$ETBE + H = r3ETBE + H_2$	7.00×10^{13}	0.00	22,600	-54,800	See text
(10)	$ETBE + CH_3 = r1ETBE + CH_4$	3.00×10^{12}	0.00	65,700	-58,200	See text
(11)	$ETBE + CH_3 = r2ETBE + CH_4$	1.00×10^{12}	0.00	66,500	-43,900	See text
(12)	$ETBE + CH_3 = r3ETBE + CH_4$	$7.00 imes 10^{11}$	0.00	39,300	-48,100	See text
(13)	$r1ETBE = iso-C_4H_8 + C_2H_5O$	5.00×10^{14}	0.00	116,000	116,000	Assume
(14)	$r2ETBE = tert-C_4H_9O + C_2H_4$	5.00×10^{14}	0.00	98,300	98,300	Assume
(15)	$r3ETBE = tert-C_4H_9 + CH_3CHO$	1.00×10^{12}	0.00	26,400	26,400	Assume
(16)	$r4ETBE = C_2H_6O + C_2H_5$	1.00×10^{12}	0.00	12,600	12,600	Assume
(17)	$rdMTBE = tert-C_4H_9 + CH_2O$	2.50×10^{14}	0.00	82,800	45,600	[20]
(18)	$TBA = iso-C_4H_8 + H_2O$	8.00×10^{13}	0.00	266,000	42,700	See text
(19)	$TBA = r2TBA + CH_3$	2.50×10^{16}	0.00	337,000	342,000	See text
(20)	$TBA + H = r1TBA + H_2$	$3.00 imes 10^{14}$	0.00	49,000	-42,300	See text
(21)	$TBA + CH_3 = r1TBA + CH_4$	3.00×10^{12}	0.00	65,700	-35,600	See text
(22)	$r2TBA = H + C_2H_6O$	1.00×10^{12}	0.00	104,000	104,000	Assume
(23)	$r1TBA = OH + iso-C_4H_8$	5.00×10^{14}	0.00	140,000	140,000	Assume
(24)	$C_2H_5O = CH_3 + CH_2O$	1.32×10^{20}	-2.02	86,800	40,200	[21]
(25)	$C_2H_5O = CH_3CHO + H$	5.43×10^{15}	-0.69	93,000	60,700	[21]
(26)	tert-C ₄ H ₉ = iso -C ₄ H ₈ + H	5.66×10^{11}	0.70	141,000	140,000	[21]
(27)	$tert-C_4H_9O = C_2H_6O + CH_3$	1.59×10^{22}	-2.55	70,500	16,300	[21]

Rate coefficients in the form, $AT^{n}\exp(-E_{a}/RT)$, in cm, mol, J and K units. Heat of reactions, ΔH_{0}° , in J/mol unit.

 C_2H_6O was sensitive to reactions (1), (3), (4), (8) and (9). The radicals r4ETBE and tert-C₄H₉O produced by reactions (3) and (4) unimolecularly decomposed to produce C₂H₆O via reactions (16) and (27). The radical r2ETBE produced by reactions (8) and (11) also produced C_2H_6O via reactions (14) and (27). The rate coefficients for reactions (3) and (4) were determined by fixing those for reactions (1) and (2) to the value estimated above. The activation energies were adopted from the heat of reactions at 0 K. The pre-exponential factors were estimated in order to reproduce C_2H_6O distribution, and the difference between their pre-exponential factors was determined based on the number of CH₃ groups contributing to reactions (3) and (4). The uncertainties of the rate coefficients for reactions (3) and (4) were within 5% in the case of reaction (8) with uncertainty of 50%. The rate coefficients for reactions (5) and (6) were adopted by assuming values similar to those of reactions (3) and (4), because none of the experimental data had any sensitivity to them. The product distributions of H₂, CH₄ and CH₃CHO were sensitive to the secondary reactions of ETBE, as seen in Fig. 3b. The rate coefficients for reactions (7)-(12) were estimated to reproduce the product distributions of H₂, CH₄ and CH₃CHO. They seemed to be much more sensitive to experimental results in the oxidation system. We will determine the rate coefficients of the secondary reaction of ETBE accurately in the near future in our work that includes the oxidation mechanism. The rate coefficient for reaction (18) was estimated by a shock tube study coupled with UV absorption spectroscopy conducted at 195 nm using 0.01-0.08% TBA in Ar and ab initio calculation, and the details of this experiment will be published in the near future. The same rate coefficient values as in reactions (3), (7) and (10) were adopted for reactions (19), (20) and (21), respectively. No experimental data was sensitive to the rate coefficients for reactions (13)–(16), (22) and (23), so we assumed those rate coefficients. We adopted the published values of Curran [21] as the rate coefficients for reactions (24)–(27).

From the ETBE pyrolysis mechanism that we constructed, we saw that 50% of the ETBE was consumed by 70 µs at 1300 K under the gas-chromatographic experimental condition. About 85% of the ETBE decomposed unimolecularly, while about 15% of the ETBE reacted with H and CH₃. C₂H₅OH and TBA were each only produced directly via reaction (1) or (2). About 82% of the iso- C_4H_8 was produced via reaction (1), and about 17% was produced via reactions (6), (7), (9), (10) and (12). About 82% of the C_2H_6O was produced via reactions (3) and (4), and about 15% was produced via reactions (8) and (11). About 15% of the CH₄ was produced via reactions (10)-(12), while about 85% was produced by subsequent reactions. About 63% of the CH₃CHO was produced via reactions (6), (7), (9), (10) and (12), and about 37% was produced via the secondary reactions of C₂H₅OH. About 55% of the H₂ was produced via reactions (7)-(9), while about 45% was produced by subsequent reactions.



Fig. 3. (a) Product distribution measured with 3% ETBE diluted in Ar at $P_1 = 50$ torr. Solid lines are the simulated results using ETBE pyrolysis mechanism constructed in the present study. The effective heating times are 1410 µs (900 K), 1360 µs (1000 K), 1310 µs (1100 K), 1270 µs (1200 K), 1230 µs (1300 K), 1180 µs (1400 K) and 1130 µs (1500 K), respectively. (b) Sensitive spectra (pS) [19] for ETBE, *iso*-C₄H₈, C₂H₅OH, TBA, H₂, C₂H₆O, CH₄ and CH₃CHO concentration at 1200 K and 1270 µs for 3% ETBE diluted in Ar.

5.2. Pressure dependence of the rate coefficient for reaction (1)

The pressure dependence of the rate coefficient for reaction (1) was examined by monitoring the ETBE pyrolysis at 195 nm under the condition ranging from 0.0167% to 0.05% ETBE in Ar. As seen in Fig. 4a, absorption was measured from the initial part of the ETBE pyrolysis. From the ETBE pyrolysis mechanism that we constructed, 93% of the ETBE was consumed by reactions (1)–(6), and the remaining 7% of the ETBE was consumed by reactions (7)–(12) at 200 μ s under the conditions shown in Fig. 4a. The influence of secondary reactions was so small under the conditions of UV absorption experiments that we analyzed the pyrolysis of ETBE using simple first order equations, as shown below, coupled with the Lambert–Beer equation,

$$\begin{split} [\text{ETBE}] &= [\text{ETBE}]_0 \exp\{-(k(iso\text{-}C_4\text{H}_8) + k(\text{others})t) \\ [iso\text{-}C_4\text{H}_8] &= -k(iso\text{-}C_4\text{H}_8) / (k(iso\text{-}C_4\text{H}_8) \\ &+ k(\text{others}))[\text{ETBE}]_0 \\ [1 - \exp\{-(k(iso\text{-}C_4\text{H}_8) + k(\text{others}))t\}], \end{split}$$

where $k(iso-C_4H_8)$ and k(others) signify the rate coefficients producing $iso-C_4H_8$ and other products, respectively. The estimated rate coefficients are shown in Fig. 5, with the



Fig. 4. (a) A typical absorbance profile in ETBE pyrolysis at 195 nm; shock conditions, 0.0167% ETBE diluted in Ar, $T_5 = 1231$ K, $P_5 = 8.1$ atm, $P_5 = 8.1 \times 10^{-5}$ mol cm⁻³. Sensitive spectra (pS) [19] for *iso*-C₄H₈ concentration in 200 µs and 800 µs at 1231 K for 0.0167% ETBE diluted in Ar.



Fig. 5. Arrhenius plots for $k(iso-C_4H_8)$ (\bigcirc ; $P_1 = 100$ torr, $P_5 = 2.5-3.0$ atm, 0.05% ETBE diluted in Ar, \Box ; $P_1 = 200$ torr, $P_5 = 5.0-6.1$ atm, 0.025% ETBE diluted in Ar, Δ ; $P_1 = 300$ torr, $P_5 = 8.1-8.9$ atm, 0.0167% ETBE diluted in Ar) and k (others) (\odot ; $P_1 = 100$ torr, $P_5 = 2.5-3.0$ atm, 0.05% ETBE diluted in Ar, \blacksquare ; $P_1 = 200$ torr, $P_5 = 5.0-6.1$ atm, 0.025% ETBE diluted in Ar, \blacksquare ; $P_1 = 200$ torr, $P_5 = 5.0-6.1$ atm, 0.025% ETBE diluted in Ar, \blacksquare ; $P_1 = 300$ torr, $P_5 = 8.1-8.9$ atm, 0.0167% ETBE diluted in Ar, \blacktriangle ; $P_1 = 300$ torr, $P_5 = 8.1-8.9$ atm, 0.0167% ETBE diluted in Ar, \blacktriangle ; $P_1 = 300$ torr, $P_5 = 8.1-8.9$ atm, 0.0167% ETBE diluted in Ar), -, $k_1 = 1.7 \times 10^{14} exp(-254.0 \text{ kJ mol}^{-1}/\text{RT}) s^{-1}$, estimated by gas chromatographic result, -----, $k_1 = 1.6 \times 10^{14} exp(-251.0 \text{ kJ mol}^{-1}/\text{RT})$, proposed by Glaude et al. [1], -----, the sum of k_2-k_5 estimated by gas chromatographic result.

Arrhenius expression of reaction (1) estimated by gas chromatographic results. At 200 μ s under the conditions shown in Fig. 4a, 90% of the *iso*-C₄H₈ was produced via reaction (1). The *k*(*iso*-C₄H₈) obtained was approximately *k*₁, and good agreement between UV absorption experiments at 2.5–8.9 atm and gas-chromatographic results was confirmed. The experimental results did not show pressuredependence, so we concluded that the rate coefficient for reaction (1) reached its high-pressure limit at 1 atm. We compared our k_1 value with that of Glaude et al. at 750–1150 K and 10 atm [2] and confirmed good agreement, as shown in Fig. 5. In UV absorption experiments, k(others) was also estimated simultaneously with k(iso-C₄H₈), but none of the reactions not producing *iso*-C₄H₈, namely reactions (2)–(5), were sensitive enough to the production of *iso*-C₄H₈ to be estimated accurately, as shown in Fig. 4b.

6. Conclusion

We constructed a 170-reaction mechanism including the new reaction (2). From the UV absorption experiments, we found that the rate coefficient for reaction (1) reached its high-pressure limit at 1 atm. The rate coefficient for reaction (1) estimated in the present study showed good agreement with the findings of Glaude et al. [2]. Detailed modeling for ETBE oxidation will be performed in the near future.

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