



Elucidating the flame chemistry of monoglyme via experimental and modeling approaches

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ABSTRACT

This study is concerning the flame chemistry of monoglyme ($\text{CH}_3\text{OCH}_2\text{CH}_2\text{OCH}_3$), an oxygenated compound recognized as a clean diesel additive and an ignition improver. Speciation diagnosis was performed for two low-pressure premixed flames fueled by monoglyme with different equivalence ratios ($\phi = 1.0$ and 1.5) using the technique of photoionization molecular-beam mass spectrometry (PI-MBMS). Dozens of flame intermediates including some reactive species were quantitatively probed from the monoglyme flames. A kinetic model was proposed for the first time for the combustion of this fuel and validated against the flame structure measurements. By combining experimental observations and modeling interpretations, it has been revealed that under flame conditions, the fuel consumption is dominated by hydrogen abstractions from the central ($-\text{CH}_2\text{CH}_2-$) moiety of monoglyme. Subsequent β -scissions of the resulting fuel radical lead to the formation of fuel-specific intermediates, methyl vinyl ether and methoxy acetaldehyde. The species pool detected in monoglyme flames differs much from that of dimethyl ether (DME, CH_3OCH_3) flames, though a monoglyme molecule is symmetrically composed of two DME fuel radicals. This could be attributed to the presence of the central carbon-to-carbon (C–C) bond in monoglyme. Further modeling analyses suggest that the C–C contents together with the stoichiometry of fuel mixtures can impact the concentrations of benzene precursors under premixed flame conditions.

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1. Introduction

The industrial utilization of oxygenated fuels has been proven as one pathway towards the goal of satisfying increasing energy demands while minimizing environmental impacts [1]. Glycol ethers were initially noted because they could improve ignition properties of diesel fuels in engines. A coal-derived syngas commercial product, CENTANERTM, exhibits a high cetane number, which is actually a 20/80 mixture of monoglyme ($\text{CH}_3\text{OCH}_2\text{CH}_2\text{OCH}_3$) and diglyme ($\text{CH}_3\text{OCH}_2\text{CH}_2\text{OCH}_2\text{CH}_2\text{OCH}_3$) [2]. Glycol ethers possessing suitable physical properties can be well blended into diesel fuels [3]. It has been proven by a series of engine studies [2–7] that glycol ethers as additives can inhibit particulate matter (PM) emissions from diesel engines under different operation conditions. Besides, Liotta and Montalvo [3] found that glycol ethers are more effective in reducing PM emissions than alcohols at the same fuel oxygen content in fuel mixtures. To account for such emission reduction effects, kinetic

understanding [8,9] for the combustion of glycol ethers is needed, which however has been barely investigated to the best of our knowledge. In the present work the combustion kinetics of the simplest glycol ether, monoglyme, whose molecular structure is shown in Fig. 1, is targeted. It is noted that a monoglyme molecule is symmetrically composed of two methoxymethyl (CH_3OCH_2-) moieties, the fuel radical of the widely-used and-investigated dimethyl ether (DME, CH_3OCH_3). Compared to DME, the central carbon-to-carbon (C–C) bond in monoglyme can be expected to result in a distinct intermediates pool in respects of types and concentrations.

In the present study, speciation measurements were performed for two premixed flames with different equivalence ratios using the technique of molecular-beam mass spectrometry (MBMS). A kinetic model was constructed as a first-of-its-kind effort to reproduce the experimental flame structures and to interpret the reactions responsible for the fuel consumption and intermediate formations. To explore the effects of the C–C structure in similar ether fuels (or fuel mixtures) on species concentrations, further modeling analyses were performed for different binary blended flames fueled by simple unbranched saturated ethers and ethane (C_2H_6).

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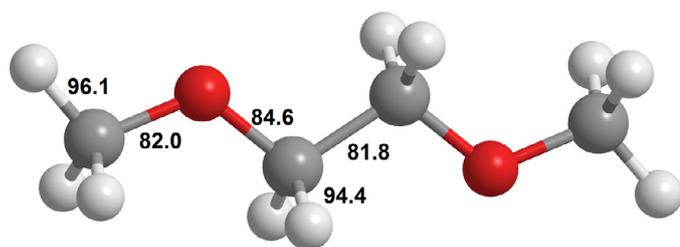


Fig. 1. Molecular structure of monoglyme and bond dissociation energies (BDEs) calculated in the current work. (Unit, kcal/mol).

2. Experimental method

The measurements for flame structures were conducted at the National Synchrotron Radiation Laboratory (NSRL), Hefei, China. The experimental setup and procedures have been well documented in [10,11]. Briefly, the apparatus includes a McKenna burner, a molecular beam sampling system and a time-of-flight mass spectrometer (TOFMS) with the synchrotron vacuum ultraviolet (VUV) light being the ionization source. Detailed conditions for the investigated flames are provided in Table 1. The premixed flames of monoglyme, with equivalence ratios of 1.0 and 1.5, were stabilized on a 6.0-cm-diameter stainless steel burner. The pressures in the flame chamber were respectively controlled at 20.0 and 30.0 Torr for the two flames, respectively, to maximize the flame thickness and the stand-off distance while maintaining flame stability. Gas flow rates were controlled separately by mass flow controllers, while the flow rate of liquid monoglyme into the vaporizer (kept at 373 K) was metered by a chromatography pump. During the experiments, the temperature of the burner cooling water was set at 303 K.

The flame gases were sampled along the axis of the flame by a quartz nozzle (with a 40° included angle and a 200 μm orifice at the tip) and then entered the ionization region of the mass spectrometer. The formed molecular beam was crossed by the dispersed VUV light from the synchrotron, and photo-ions were collected and mass-analyzed by the TOFMS with a mass resolution ($m/\Delta m$) up to 3500, which enables separations of species pairs with the same mass number but different molecular weights. To exclude interferences from the fuel photo-fragmentations in the identification and quantification for flame intermediates, the absolute photoionization cross sections (PICSSs) of monoglyme were derived by making relative measurements with respect to propene (C_3H_6) [12]. The measured results for the parent fuel ion and major fragmentations are provided in Fig. S1 in the Supplemental Material, according to which the ionization energy (IE) of monoglyme is about 9.3 eV, in line with the value from the NIST database [13]. The appearance energies (AEs) for major fragmentations were also obtained.

For the species identification, the photon energy was scanned with the sampling position fixed at a specific position to obtain the photoionization efficiency (PIE) spectra. Examples in Fig. 2 show the presence of two intermediates specific to the consumption of monoglyme, as will be discussed below. After the

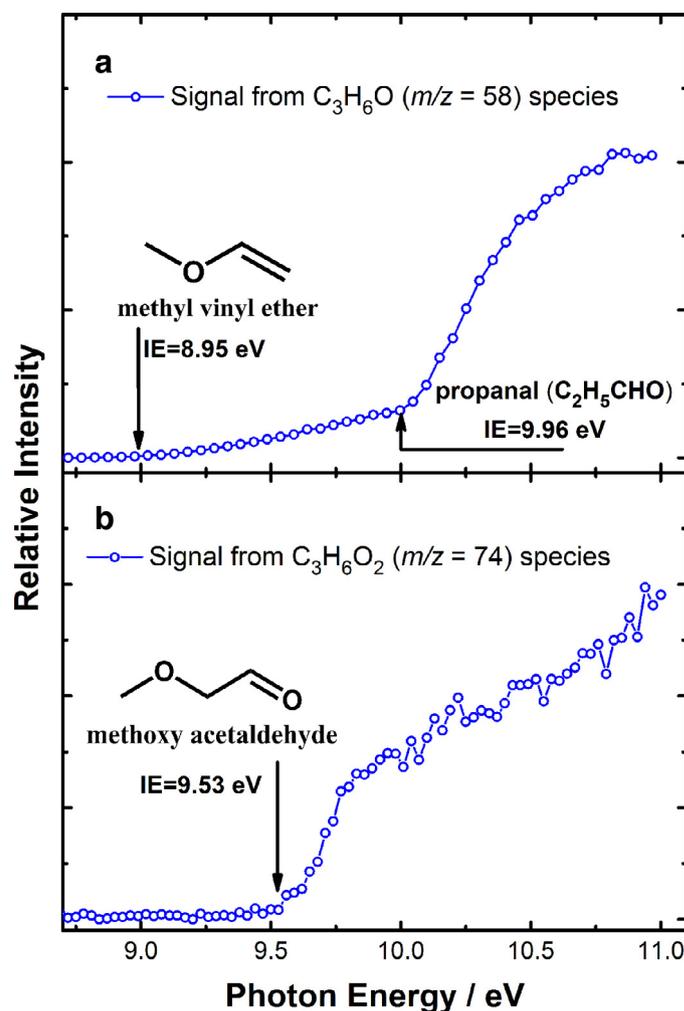


Fig. 2. The PIE curves for (a) C_3H_6O species with $m/z=58$ and (b) $C_3H_6O_2$ species with $m/z=74$ in the stoichiometric monoglyme flame at 2.0 mm away from the burner, with the photon energy ranging from 8.7 to 11.0 eV.

deduction of the signal of the fuel fragmentation, the presence of methyl vinyl ether ($CH_3OCH=CH_2$) can be suggested by the onset around 8.95 eV in the PIE curve for the C_3H_6O ($m/z=58$) species, consistent with the ionization energy (IE) value provided in the NIST database [13]. Another threshold at about 10.0 eV corresponds to the IE of propanal (C_2H_5CHO), a common intermediate in flames fueled by oxygenates. While for the $C_3H_6O_2$ ($m/z=74$) species the threshold of 9.53 eV matches the IE for methoxy acetaldehyde (CH_3OCH_2CHO), which was theoretically calculated using the same method adopted by Moshhammer et al. [14] with an uncertainty of 0.2 eV. For the quantification, by fixing the photon energy while gradually changing the sampling position, the integrated ion intensities for a specific mass were recorded as a function of the distance from the burner surface, which were subsequently converted to species mole fraction profiles by following the

Table 1
Detailed flame conditions in the present study.

Flame	Equivalence ratio	Pressure (Torr)	D_M^a (g/s/cm ²)	Gaseous flow rate (slm ^b)		
				Monoglyme	O ₂	Ar
1	1.0	20.0	0.00214	0.231	1.269	0.500
2	1.5	30.0	0.00228	0.321	1.179	0.500

^a Total mass flux.

^b Standard liter per minute.

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