Supporting Information of

"Discriminating Dissociative Photoionization and Thermal Decomposition Products of Ethylene Glycol by Synchrotron VUV Photoionization Mass Spectrometry and Theoretical Calculations"

Hong Wang,[1] Jiwen Guan,[1]* Jiao Gao,[2] Yanbo Li,[3] Jinyang Zhang,[4] Xiaobin Shan,[1] Zhandong Wang[1,4]*

[1]National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, P. R. China

[2]Dalian Institute of Chemical Physics, Dalian, 116023 P. R. China;

[3]State Key Laboratory of Fire Science, University of Science and Technology of China, Hefei, Anhui 230026, PR China
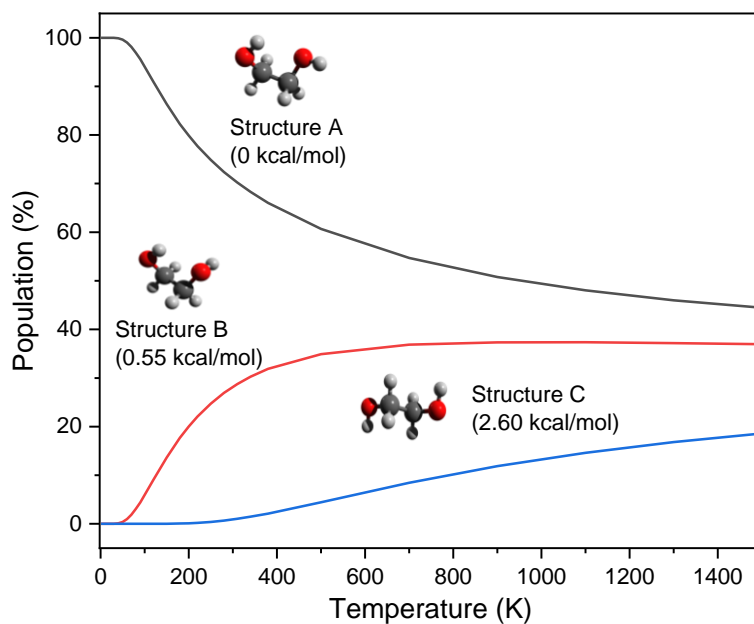
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Figure 1S. Boltzmann distribution of the three conformers (structure A, structure B and structure C) of ethylene glycol. The energies of the three structures are calculated at the G4 method. The energies are relative to the lowest energy (structure A).
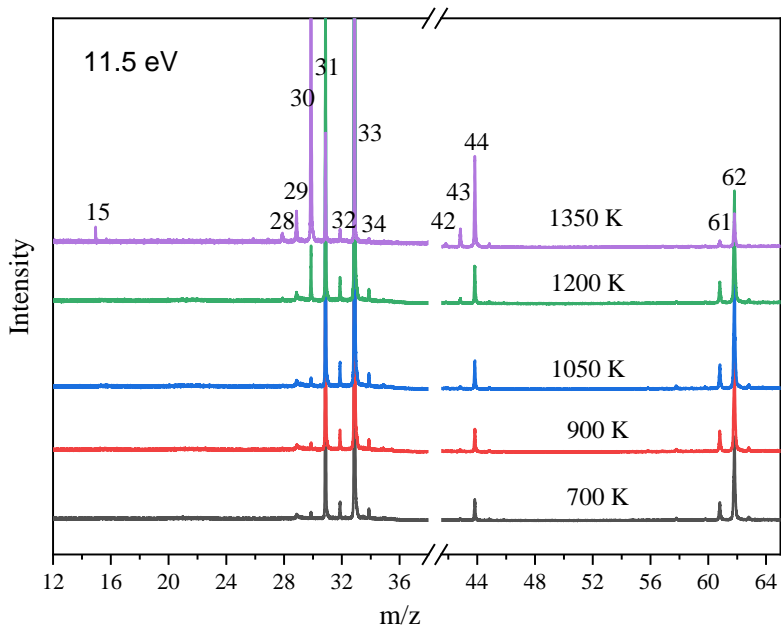

Figure 2S. The photoionization mass spectra of ethylene glycol at 11.5 eV as function of pyrolysis temperature.

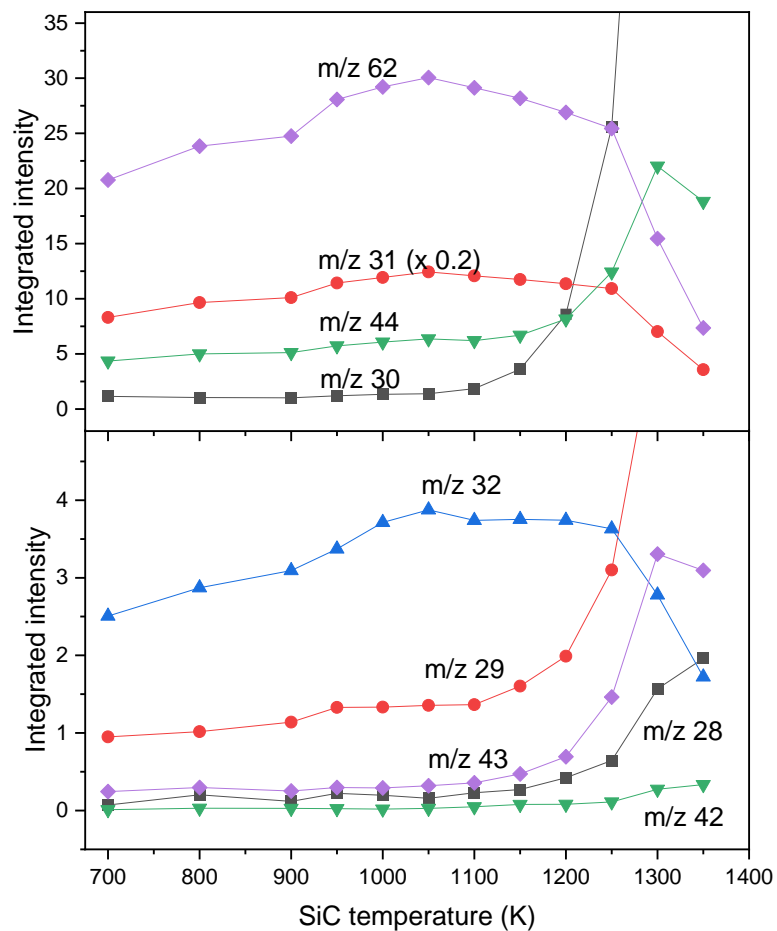Figure 3S. Integrated ion signal intensities of pyrolysis products of ethylene glycol as function of pyrolysis temperature. The mass spectra are taken at 11.5 eV.
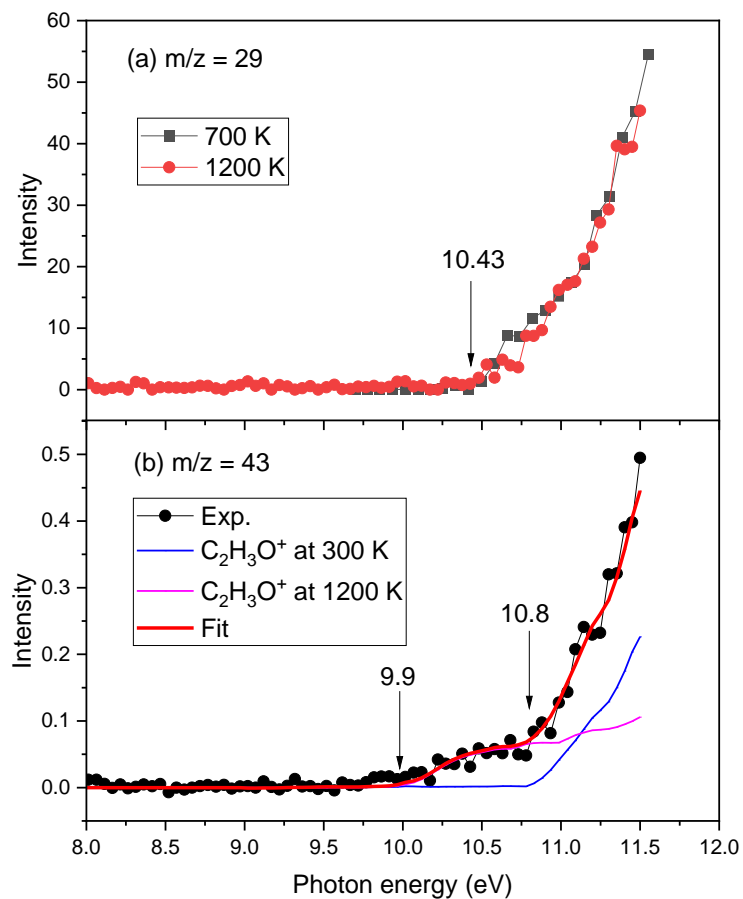
Figure 4S. Photoionization spectra of ethylene glycol at the channel of (a) m/z = 29 with the temperature of the SiC reactor at 700 K and 1200 K, (b) m/z = 43. The dot line is experimental PIE curves, the solid lines are reference PIE curves, the red line is overall fit.

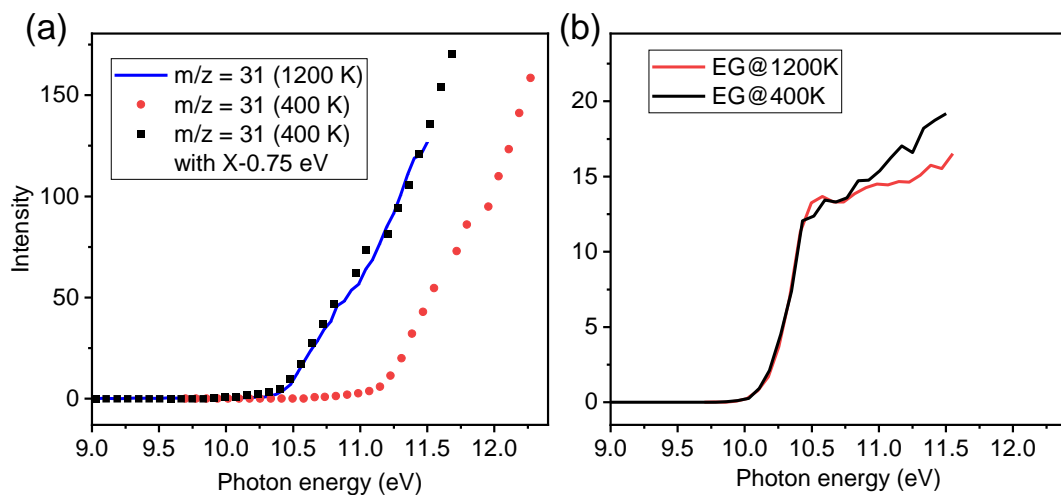Figure 5S. Photoionization spectra of products monitored at the channel (a) m/z = 31, (b) m/z = 62 for the pyrolysis of ethylene glycol at the temperature of 400 K and 1200 K.
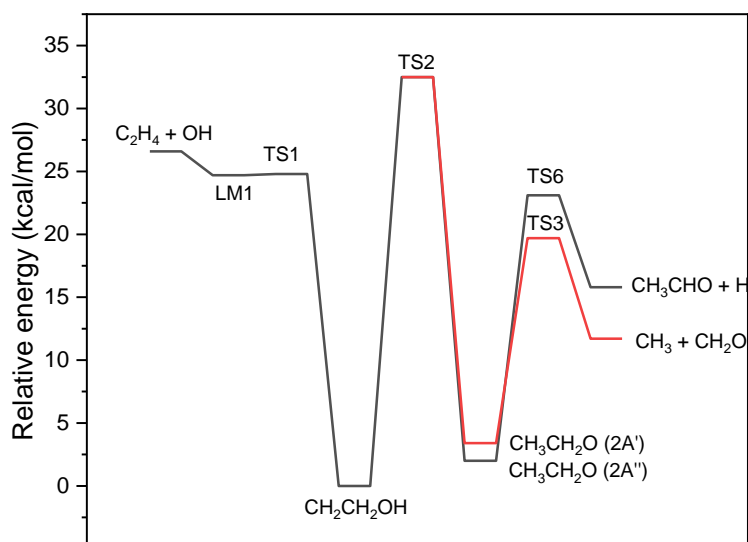

Figure 6S. Potential energy surface of the lowest energy reactions of C_2H_5O with the ZPE correction computed at the CCSD(T)/6-311+G(3df,2p)//B3LYP/6-311+G(3df,2p) level of theory. Taken from the Ref. 50 of the text.

Table 1S. Relative energies (eV) of the stable structures of the ethylene glycol cation calculated at the ωB97X-D/6-311++G(3df, 3pd) and G4 levels.

Structure number	Relative energy	
	ωB97X-D (ref. 19)	G4 (this work)
structure 1-1	9.46	9.79
structure 1-2	9.49	9.82
structure 1-3	9.49	9.82
structure 1-4	9.48	9.81
structure 1-5	9.46	9.79
structure 1-6	9.46	9.79
structure 2-1	10.17	10.28
structure 2-2	10.17	10.28
structure 2-3	10.21	10.32
structure 2-4	10.21	10.34
structure 2-5	10.18	-
structure 2-6	10.20	10.39
structure 2-7	10.15	-
structure 3-1	10.05	10.14
structure 3-2	10.04	10.12
structure 3-3	10.05	-
structure 4	10.15	10.38
structure 5	9.87	9.95
structure 6	9.69	9.74
structure 7-1	10.08	10.27
structure 7-2	10.41	10.57

Table 2S. Relative energies (eV) of the transition states (TSs) of ionized ethylene glycol calculated at the ωB97X-D/6-311++G(3df, 3pd) and G4 levels.

Structure number	Relative energy	
	ωB97X-D (ref. 19)	G4 (this work)
TS 1	9.57	9.90
TS 2	9.55	9.88
TS 3	9.57	9.90
TS 4	10.03	10.37
TS 5	9.54	9.87
TS 6	10.03	10.37
TS 7	9.96	10.28
TS 8	10.47	10.78
TS 9	9.95	-
TS 10	10.26	10.44
TS 11	10.07	10.15
TS 12	10.05	-
TS 13	10.06	-
TS 14	10.25	10.38
TS 15	10.24	10.36
TS 16	10.21	10.34
TS 17	10.21	-
TS 18	10.20	10.38
TS 19	10.18	10.31
TS 20	10.48	10.56
TS 21	10.25	-
TS 22	10.36	10.44
TS 23	10.37	-
TS 24	10.40	10.77
TS 25	9.98	9.98
TS 26	10.15	10.40
TS 27	10.41	10.58
TS 28	11.04	11.30
TS 29	11.45	11.66
TS 30	11.01	11.27
TS 31	11.08	11.26