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Thermal Dissociation of Ethylene Glycol Vinyl Ether

Authors: Xueliang Yang, John H. Kiefer and Robert S. Tranter

Supplementary information Table S1

Summary of the shock conditions of EGVE decomposition with second order rate constants of reactions R_1 and R_2 of Table 1.

P_1/Torr	T_2/°C	P_2/Torr	T_2/K	k_{R1}(cm^3/mol/s)	k_{R2}(cm^3/mol/s)
		1% EGVE in Kr at 120 Torr			
8.93	24.80	122.00	1203.00	8.28E+09	9.77E+09
8.56	24.80	124.00	1251.00	1.41E+10	1.99E+10
8.17	24.80	122.00	1287.00	2.17E+10	3.33E+10
7.86	24.80	123.00	1331.00	3.45E+10	5.57E+10
7.46	24.80	120.00	1361.00	4.56E+10	7.64E+10
7.20	24.80	122.00	1413.00	7.00E+10	1.24E+11
6.88	24.80	122.00	1465.00	1.00E+11	1.88E+11
6.68	24.80	123.00	1513.00	1.33E+11	2.61E+11
6.46	24.80	122.00	1540.00	1.52E+11	3.07E+11
6.24	24.80	122.00	1580.00	1.82E+11	3.82E+11
6.02	24.80	122.00	1631.00	2.20E+11	4.84E+11
6.06	24.80	126.00	1650.00	2.33E+11	5.23E+11
5.84	24.80	121.00	1663.00	2.43E+11	5.50E+11
5.64	24.80	120.00	1695.00	2.64E+11	5.89E+11
5.64	24.80	122.00	1714.00	2.76E+11	6.55E+11
5.64	24.80	122.00	1716.00	2.77E+11	6.59E+11
5.65	24.80	122.00	1717.00	2.78E+11	6.61E+11
5.64	24.80	122.00	1718.00	2.78E+11	6.63E+11

5.61	26.20	122.00	1733.00	4.05E+11	6.62E+11
		1% EGVE in Kr at 60 Torr			
3.98	26.20	57.00	1248.00	1.35E+10	2.54E+10
3.80	26.20	56.00	1283.00	1.97E+10	3.83E+10
3.63	26.20	56.00	1330.00	3.51E+10	7.07E+10
3.50	26.20	57.00	1370.00	4.44E+10	9.65E+10
3.51	26.20	59.00	1411.00	6.14E+10	1.47E+11
3.30	26.20	58.00	1464.00	8.88E+10	2.21E+11
3.11	26.20	57.00	1513.00	1.34E+11	2.93E+11
3.05	26.20	58.00	1557.00	1.70E+11	3.82E+11
2.89	26.20	57.00	1606.00	2.09E+11	5.20E+11
3.06	25.50	61.00	1607.00	1.92E+11	5.23E+11
2.79	26.20	56.00	1616.00	1.99E+11	5.47E+11
2.75	26.20	56.00	1639.00	2.40E+11	6.10E+11
2.70	25.50	56.00	1661.00	2.39E+11	6.73E+11
2.64	26.20	55.00	1677.00	2.53E+11	6.42E+11
2.72	26.20	57.00	1679.00	2.55E+11	7.27E+11
2.58	26.20	55.00	1712.00	2.85E+11	8.29E+11
2.57	26.20	55.00	1715.00	2.88E+11	8.38E+11
2.60	25.50	57.00	1729.00	3.01E+11	8.83E+11
		0.5% EGVE in Kr at 120 Torr			
8.87	25.90	123.00	1259.00	1.56E+10	2.21E+10
8.40	25.90	119.00	1285.00	1.68E+10	2.58E+10
8.10	25.90	120.00	1328.00	2.66E+10	4.28E+10
7.85	25.90	122.00	1380.00	4.27E+10	7.30E+10
7.62	25.90	121.00	1406.00	5.78E+10	1.02E+11

7.36	25.90	123.00	1458.00	8.35E+10	1.55E+11
7.15	25.90	123.00	1494.00	1.19E+11	2.20E+11
6.92	25.90	121.00	1520.00	1.38E+11	2.60E+11
6.70	25.90	122.00	1566.00	1.71E+11	3.39E+11
6.42	25.60	123.00	1630.00	2.19E+11	4.60E+11
6.50	25.90	124.00	1631.00	2.20E+11	4.62E+11
6.30	25.90	123.00	1662.00	2.42E+11	5.23E+11
6.22	25.60	123.00	1669.00	2.47E+11	5.37E+11
6.11	25.90	122.00	1692.00	2.62E+11	5.83E+11
6.11	25.90	123.00	1704.00	2.70E+11	6.06E+11
6.07	25.60	123.00	1713.00	2.75E+11	6.24E+11

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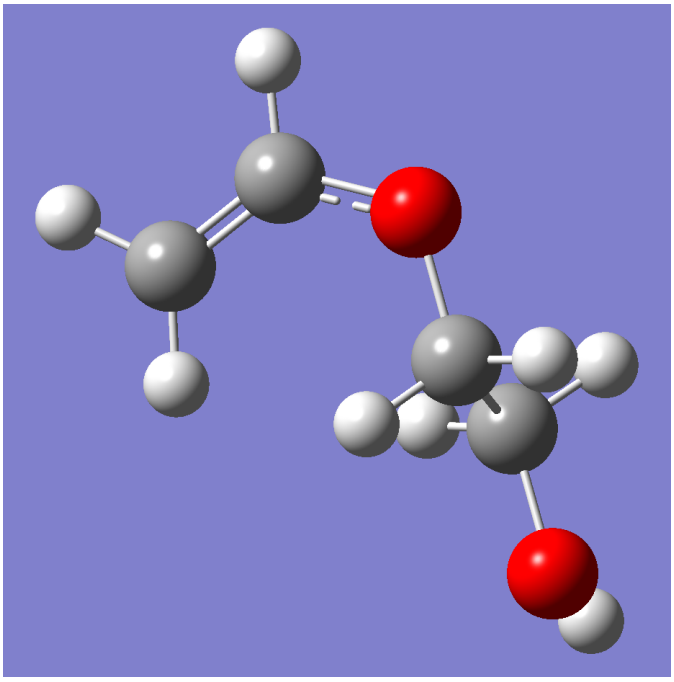
Supplementary information Table S2

Structures, vibrational frequencies, zero-point energy levels and moments of inertia for three conformers of EGVE and a PES for EGVE +H at the G3B3 level.

Note: All vibrational frequencies and energies presented below are unscaled. A scaling factor of 0.964 is normal for G3B3 calculations and should be applied when using the values presented below.

EGVE-1



Cartesian Coordinates

C	0.58842	1.915071	0.34994
C	-0.30858	1.538326	-0.56636
O	-0.49131	0.322069	-1.14876
C	0.378672	-0.74783	-0.78334
C	-0.09194	-1.44537	0.490597
O	0.825949	-2.50678	0.724871
H	0.592431	2.947124	0.680985
H	1.324836	1.251476	0.788421
H	-1.03482	2.237754	-0.97256
H	1.41014	-0.39457	-0.66964
H	0.348946	-1.45476	-1.61661

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H	-1.11751	-1.81375	0.335662
H	-0.11387	-0.73133	1.326319
H	0.541635	-2.97843	1.521479

Moments of inertia in GHz

7.7809206 1.9410732 1.6989921

Vibrational frequencies in cm^{-1}

77.9321	128.3027	171.7679
246.2065	315.2688	327.5577
451.6850	613.3909	712.9449
823.8962	831.9774	919.6494
1000.1641	1015.0202	1051.4432
1088.0275	1184.1419	1241.8194
1256.0017	1272.3012	1326.8932
1374.2854	1393.6871	1460.9152
1484.3120	1542.9917	1563.0676
1713.1070	3010.7364	3046.8970
3068.5592	3132.1348	3191.6904
3205.4808	3274.2001	3763.4922

Zero Point Energy: 0.119107 Hartree un-scaled

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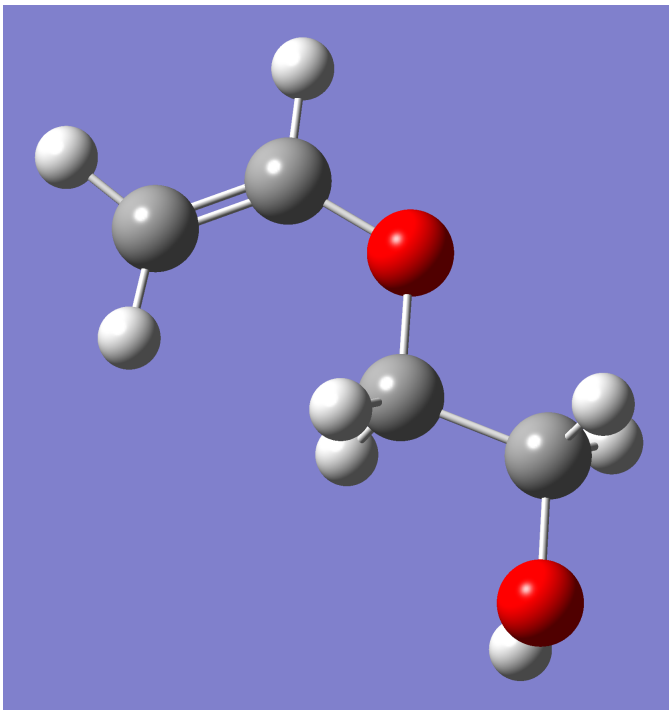
EGVE-2

EGVE-1 from reference conformer III at G3B3 level



Cartesian Coordinates

C	1.672446	1.355843	-1.1124
C	0.542746	0.857045	-1.6227
O	-0.45118	0.189836	-0.97928
C	-0.29766	-0.02016	0.419405
C	-1.52567	-0.78395	0.908209
O	-1.44517	-1.04807	2.301555
H	2.365563	1.865708	-1.77142
H	1.945455	1.278851	-0.06641
H	0.296349	0.946773	-2.67732
H	0.613993	-0.59623	0.626685
H	-0.21191	0.948242	0.937393
H	-1.57415	-1.75717	0.411661
H	-2.43719	-0.22884	0.641535
H	-1.56964	-0.20888	2.771088

Moments of inertia in GHz

12.0535953 1.5662532 1.4163407

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Vibrational frequencies in cm^{-1}

94.8385	118.5188	155.0531
249.0471	322.2895	342.6224
437.5251	604.9096	714.0366
824.2549	836.2363	960.6008
998.1953	1038.0131	1070.8231
1094.6210	1119.2965	1224.5585
1251.5011	1319.1924	1359.4735
1376.2077	1412.0804	1448.8649
1471.2455	1537.1232	1551.7207
1714.8957	3004.7588	3025.4923
3065.4394	3122.6032	3193.7064
3208.8408	3276.8906	3742.5793

Zero Point Energy: 0.119121 Hartree un-scaled

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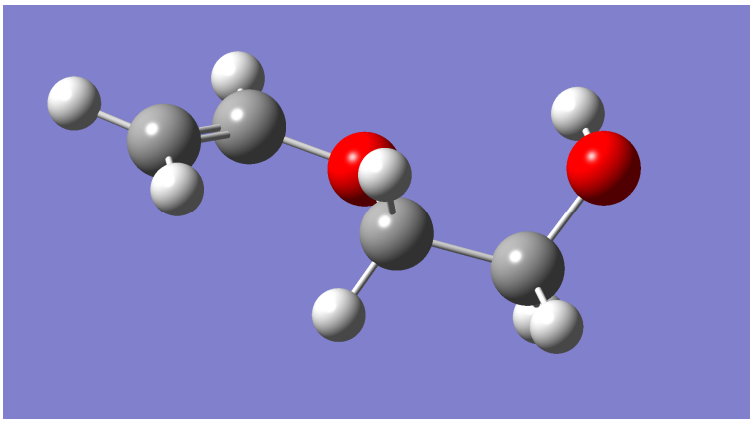
EGVE-3



Cartesian Coordinates

C	-1.471330	1.455284	-1.210560
C	-1.123760	0.925575	-0.036610
O	-0.214640	-0.054370	0.205032
C	0.464580	-0.630940	-0.914970
C	1.367522	-1.721290	-0.371640
O	0.637550	-2.776310	0.237475
H	-2.218300	2.237075	-1.226080
H	-1.049000	1.148952	-2.157560
H	-1.565160	1.255566	0.897097
H	-0.269760	-1.050580	-1.611800
H	1.052904	0.138333	-1.430780
H	1.927674	-2.166920	-1.196750
H	2.087026	-1.282500	0.332183
H	0.100681	-2.390870	0.938957

Symbol	Bond		Angle		Dihedral
C					
C	1	1.33562			
O	2	1.36048	1	128.259	
C	3	1.42977	2	117.625	1 -1.306
C	4	1.51987	3	106.311	2 -177.250
O	5	1.41627	4	111.767	3 61.513
H	1	1.08381	2	118.911	3 -179.850
H	1	1.08362	2	123.747	3 0.143
H	2	1.08670	1	122.158	3 179.725
H	4	1.09812	3	109.556	2 -57.790

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H	4	1.09938	3	110.065	2	61.941
H	5	1.09493	4	109.431	3	179.710
H	5	1.10194	4	109.142	3	-62.397
H	6	0.97118	5	105.986	4	-53.882

Moments of inertia in GHz

10.5356404 1.7779567 1.6501429

Vibrational frequencies in cm^{-1}

74.7426	129.5734	220.2838
246.8433	323.4906	430.5304
511.8881	614.6171	716.1453
831.8184	845.8838	918.0464
996.0049	1006.1666	1043.6607
1103.0634	1143.0282	1233.4428
1256.6392	1277.8298	1369.6871
1403.6290	1416.1215	1454.4997
1467.5555	1528.3491	1532.1134
1716.6745	3006.0946	3026.6001
3076.3704	3107.4011	3194.8147
3209.6071	3278.5756	3731.5884

Zero Point Energy: 0.119475 Hartree un-scaled

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Comparison of the equilibrium energy of EGVE conformers.

	B3LYP/6-311++G(D,P)	Kcal/mol	G3B3(0K)	Kcal/mol
EGVE-1	-307.621507	3.640538	-307.414963	3.418416
EGVE-2	-307.623859	2.164746	-307.416908	2.198001
EGVE-3	-307.627309	0	-307.420411	0

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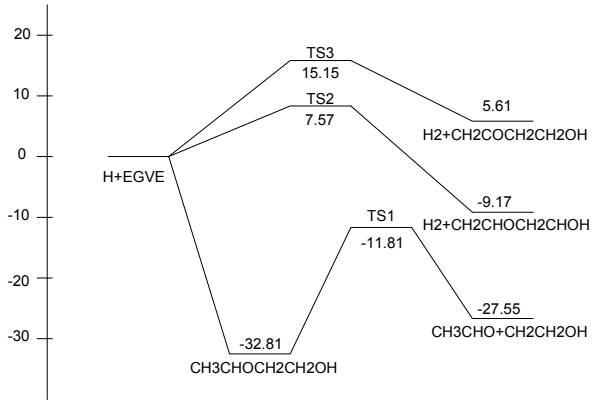
Potential Energy surface for H + EGVE at the G3B3 level.

Structures and pictures of the stationary points and transition states are given below.

Total energies (hartree), and relative energies ΔE (kcal/mol) for reactants, transition states and products at G3B3 level

	G3B3(0K)	ΔE(Kcal/mol)
EGVE-3	-307.420411	
H	-0.501087	
H+EGVE-3	-307.921498	0
CH3CHOCH2CH2OH	-307.973793	-32.813157
TS1	-307.940315	-11.806964
CH2CHOCH2CHOH	-306.768635	
H2	-1.167475	
H2+CH2CHOCH2CHOH	-307.93611	-9.1684835
CH3CHO	-153.718196	
CH2CH2OH	-154.247211	
CH2CH2OH+CH3CHO	-307.965407	-27.551255
TS2	-307.909426	7.5747285



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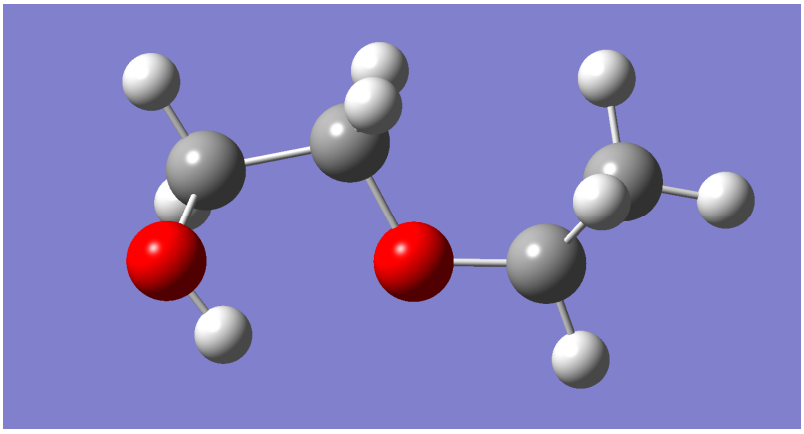
CH3CHOCH2CH2OH



C	-1.24737	1.624731	-1.16582
C	-0.5977	1.378295	0.157088
O	-0.51023	0.117732	0.694185
C	-0.29064	-0.98239	-0.19211
C	-0.21238	-2.22118	0.686192
O	-1.41472	-2.42186	1.408164
H	-1.21787	2.697168	-1.38374
H	-2.30756	1.31313	-1.18885
H	-0.74483	1.107689	-1.9936
H	-0.69546	2.112096	0.952265
H	-1.12515	-1.07731	-0.89864
H	0.64126	-0.83581	-0.75726
H	-0.06399	-3.10739	0.060299
H	0.654164	-2.13136	1.36079
H	-1.58652	-1.58454	1.870028

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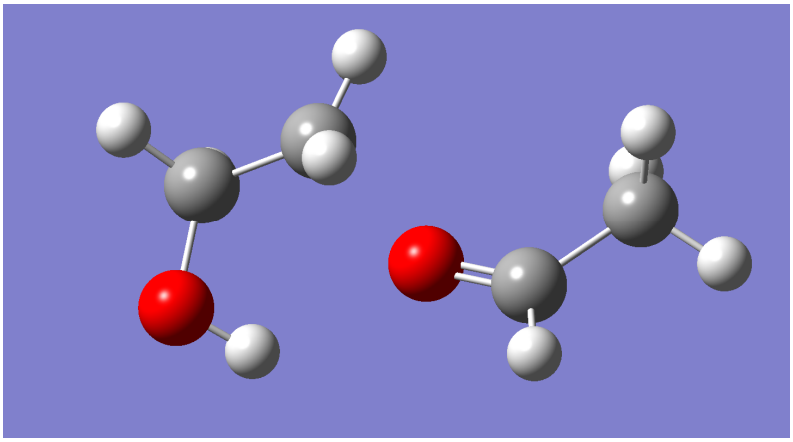
TS1



C	0	-0.42406	0.354595	0.107672
C	0	0.12578	-0.37227	1.297469
O	0	1.119474	0.065257	1.959285
C	0	2.916172	-0.29116	1.357113
C	0	3.614421	-0.06566	2.658908
O	0	3.11726	-0.925	3.66921
H	0	-1.4984	0.169495	-0.00684
H	0	0.060471	0.013707	-0.82305
H	0	-0.2467	1.430913	0.200828
H	0	-0.26328	-1.37915	1.514504
H	0	2.824937	-1.32322	1.025639
H	0	3.036753	0.448642	0.569926
H	0	4.689773	-0.27939	2.565555
H	0	3.519488	0.995975	2.942339
H	0	2.151421	-0.81332	3.620878

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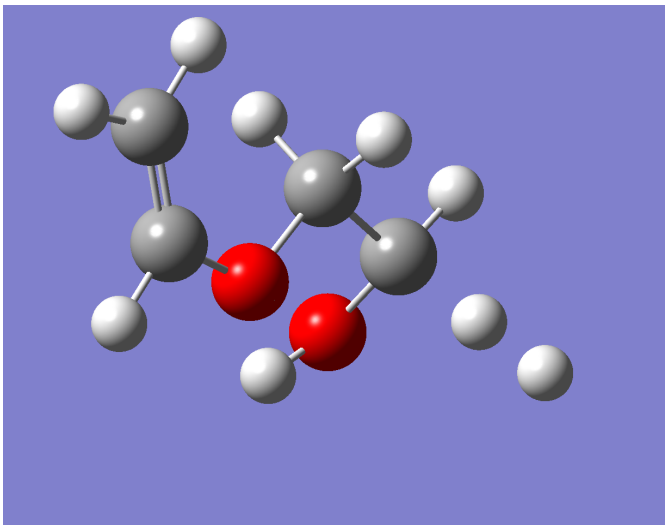
TS2



C	-2.5836	0.343681	-0.2964
C	-1.74377	-0.55961	0.214273
O	-0.39155	-0.46656	0.352373
C	0.242963	0.720376	-0.12432
C	1.72741	0.523568	0.098212
O	2.223001	-0.65856	-0.4293
H	-3.64202	0.113453	-0.3316
H	-2.2714	1.307841	-0.68012
H	-2.08273	-1.5177	0.597907
H	0.017573	0.849028	-1.19396
H	-0.12317	1.599934	0.422058
H	2.325974	1.362673	-0.26574
H	1.90012	0.55778	1.367293
H	1.573206	-1.3496	-0.21095
H	2.033333	0.608135	2.392817

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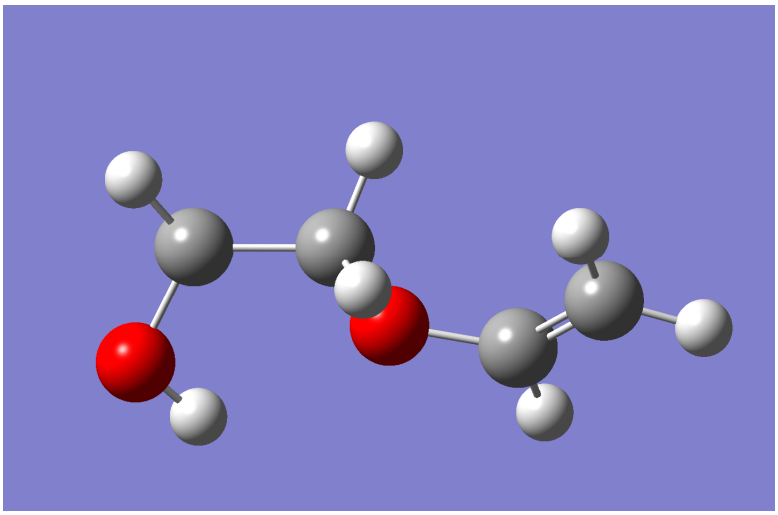
CH2CHOCH2CHOH



C	1.867689	0.497978	-0.21194
C	1.019273	-0.46826	-0.57299
O	-0.3369	-0.48633	-0.46014
C	-0.96495	0.634252	0.185451
C	-2.41818	0.318101	0.266826
O	-2.76944	-0.91946	0.726799
H	2.928717	0.351535	-0.37799
H	1.559593	1.434293	0.238029
H	1.358152	-1.39386	-1.03055
H	-0.49247	0.757333	1.178768
H	-0.79398	1.557372	-0.38455
H	-3.13386	1.090408	0.527118
H	-2.05265	-1.52537	0.466168