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Supplementary data

Thermodynamic Properties (*S*(298), *Cp(T)*, Internal Rotations and Group Additivity Parameters in Vinyl and Phenyl Hydroperoxides

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SM 1: Total Energy and Internal Rotation Barriers about C—O Bond of Unsaturated Hydroperoxides

***trans* - $CH_3CH=CH—OOH$**			***cis* - $CH_3CH=CH—OOH$**		
Torsion Angle	Total energy[a]	Rotational barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]
0.0	-268.262306948	0.00	0.0	-268.257694902	2.65
15.0	-268.261819566	0.30	15.0	-268.257431774	2.82
30.0	-268.260166345	1.34	30.0	-268.256777160	3.23
45.0	-268.257915018	2.75	45.0	-268.256080902	3.66
60.0	-268.256037511	3.93	60.0	-268.256113836	3.64
75.0	-268.255396438	4.33	75.0	-268.256537585	3.38
90.0	-268.256442326	3.68	90.0	-268.257720267	2.64
105.0	-268.258586159	2.33	105.0	-268.259418555	1.57
120.0	-268.260477818	1.14	120.0	-268.260998677	0.58
135.0	-268.261466572	0.52	135.0	-268.261926886	0.00
150.0	-268.261422849	0.55	150.0	-268.261871280	0.03
165.0	-268.260713219	1.00	165.0	-268.261091754	0.52
180.0	-268.260224275	1.30	180.0	-268.260575194	0.84
195.0	-268.260696729	1.01	195.0	-268.261037536	0.55
210.0	-268.261557167	0.47	210.0	-268.261600642	0.20
225.0	-268.261730279	0.36	225.0	-268.261428905	0.31
240.0	-268.260865027	0.90	240.0	-268.260232849	1.06
255.0	-268.259186263	1.95	255.0	-268.258265992	2.29
270.0	-268.257298405	3.14	270.0	-268.256235287	3.57
285.0	-268.255926609	4.00	285.0	-268.256537745	3.38
300.0	-268.255857804	4.04	300.0	-268.256117615	3.64
315.0	-268.257311979	3.13	315.0	-268.256272230	3.54
330.0	-268.259555492	1.72	330.0	-268.256824936	3.20
345.0	-268.261475349	0.52	345.0	-268.257447004	2.81
360.0	-268.262307145	0.00	360.0	-268.257685515	2.66

[a]Electronic energies at 0 K. ZPVE and Thermal correction to 298 K are not included. Unit are in hartree. [b]Rotational barriers are calculated as the difference between the total energy of each conformer and that of the most stable conformer. Units in kcal/mole.

SM 1 (cont): Total Energy and Internal Rotation Barriers about C—O Bond of Unsaturated Hydroperoxides

$(CH_3)_2C=CH—OOH$				**$CH_3CH=C(CH_3)—OOH$**		
Torsion Angle	Relative Torsion Angle	Total energy[a]	Torsion Angle	Torsion Angle	Relative Torsion Angle	Total energy[a]
-133.92	0.0	-307.583985380	0.00	-55.63	-307.582469772	2.11
-118.92	15.0	-307.583493612	0.30	-40.63	-307.583143652	1.69
-103.92	30.0	-307.582261666	1.08	-25.63	-307.584427132	0.88
-88.924	45.0	-307.580809812	1.99	-10.63	-307.585410633	0.27
-73.924	60.0	-307.579527139	2.79	4.3711	-307.585453330	0.24
-58.924	75.0	-307.578507527	3.43	19.371	-307.584222720	1.01
-43.924	90.0	-307.577651210	3.97	34.371	-307.582171666	2.30
-28.924	105.0	-307.577165695	4.28	49.371	-307.580678094	3.24
-13.924	120.0	-307.577106785	4.31	64.371	-307.580352750	3.44
1.0763	135.0	-307.577032431	4.36	79.371	-307.580372256	3.43
16.076	150.0	-307.576968741	4.40	94.371	-307.580536718	3.33
31.076	165.0	-307.576978033	4.39	109.37	-307.580693945	3.23
46.076	180.0	-307.577307182	4.19	124.37	-307.580902927	3.09
61.076	195.0	-307.578023806	3.74	139.37	-307.580864738	3.12
76.076	210.0	-307.579692259	2.69	154.37	-307.580639407	3.26
91.076	225.0	-307.581017351	1.86	169.37	-307.580441060	3.39
106.08	240.0	-307.582464017	0.95	184.37	-307.580565388	3.31
121.08	255.0	-307.583621259	0.22	199.37	-307.581321238	2.83
136.08	270.0	-307.583974306	0.00	214.37	-307.582917793	1.83
151.08	285.0	-307.583333642	0.40	229.37	-307.584775124	0.67
166.08	300.0	-307.582115786	1.17	244.37	-307.585842298	0.00
181.08	315.0	-307.581541900	1.53	259.37	-307.585668844	0.10
181.08	330.0	-307.581531792	1.53	274.37	-307.584547499	0.81
196.08	345.0	-307.582287507	1.06	289.37	-307.583166432	1.68
211.08	360.0	-307.583479035	0.31	304.37	-307.582469829	2.11

[a]Electronic energies at 0 K. ZPVE and Thermal correction to 298 K are not included. Unit are in hartree. [b]Rotational barriers are calculated as the difference between the total energy of each conformer and that of the most stable conformer. Units in kcal/mole.

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SM 2: Total Energy and Internal Rotation Barriers about O—O Bond of Unsaturated Hydroperoxides

trans - $CH_3CH=CHO—OH$			*cis* - $CH_3CH=CHO—OH$		
Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational Barrier[b]
0.0	-268.252958229	5.53	0.0	-268.253396912	5.40
15.0	-268.254081788	4.82	15.0	-268.254465429	4.73
30.0	-268.255965419	3.64	30.0	-268.256259157	3.60
45.0	-268.258073894	2.32	45.0	-268.258275181	2.34
60.0	-268.259876096	1.19	60.0	-268.260004486	1.25
75.0	-268.261049105	0.45	75.0	-268.261140967	0.54
90.0	-268.261537587	0.14	90.0	-268.261621537	0.24
105.0	-268.261468419	0.19	105.0	-268.261567410	0.27
120.0	-268.261105943	0.41	120.0	-268.261208323	0.50
135.0	-268.260680012	0.68	135.0	-268.260800556	0.75
150.0	-268.260412584	0.85	150.0	-268.260554752	0.91
165.0	-268.260419710	0.84	165.0	-268.260583283	0.89
180.0	-268.260690906	0.67	180.0	-268.260874442	0.71
195.0	-268.261118014	0.41	195.0	-268.261320215	0.43
210.0	-268.261533243	0.15	210.0	-268.261753918	0.15
225.0	-268.261771100	0.00	225.0	-268.262006698	0.00
240.0	-268.261691965	0.05	240.0	-268.261940992	0.04
255.0	-268.261186524	0.36	255.0	-268.261459254	0.34
270.0	-268.260211149	0.97	270.0	-268.260507980	0.94
285.0	-268.258792543	1.8	285.0	-268.259118233	1.81
300.0	-268.257058954	2.95	300.0	-268.257424889	2.87
315.0	-268.255255909	4.08	315.0	-268.255666996	3.97
330.0	-268.253727830	5.04	330.0	-268.254174020	4.91
345.0	-268.252858760	5.59	345.0	-268.253319652	5.45
360.0	-268.252958302	5.53	360.0	-268.253396915	5.40

[a]Electronic energies at 0 K. ZPVE and Thermal correction to 298 K are not included. Unit are in hartree. [b]Rotational barriers are calculated as the difference between the total energy of each conformer and that of the most stable conformer. Units in kcal/mole.

SM 2 (cont): Total Energy and Internal Rotation Barriers about O—O Bond of Unsaturated Hydroperoxides

$(CH_3)_2C=CHO—OH$				$CH_3CH=C(CH_3)O—OH$			
Torsion angle	Relative Torsion angle	Total energy[a]	Rotational barrier[b]	Torsion angle	Relative Torsion angle	Total energy[a]	Rotational barrier[b]
-132.41	0.0	-307.583978803	0.00	126.80	0.0	-307.585910337	0.00
-117.41	15.0	-307.583864469	0.071	141.80	15.0	-307.585682980	0.14
-102.41	30.0	-307.583353472	0.39	156.80	30.0	-307.585254177	0.41
-87.41	45.0	-307.582425010	0.97	171.80	45.0	-307.584817442	0.68
-72.41	60.0	-307.581117828	1.79	186.80	60.0	-307.584522806	0.87
-57.41	75.0	-307.579553814	2.77	201.80	75.0	-307.584457096	0.91
-42.41	90.0	-307.577953302	3.78	216.80	90.0	-307.584634387	0.80
-27.41	105.0	-307.576642218	4.60	231.80	105.0	-307.584991530	0.57
-12.41	120.0	-307.575989646	5.01	246.80	120.0	-307.585379919	0.33
2.59	135.0	-307.576240006	4.85	261.80	135.0	-307.585580400	0.20
17.59	150.0	-307.577386593	4.13	276.80	150.0	-307.585363069	0.34
32.59	165.0	-307.579113162	3.05	291.80	165.0	-307.584549648	0.85
47.59	180.0	-307.580926193	1.91	306.80	180.0	-307.583066905	1.78
62.59	195.0	-307.582380338	1.00	321.80	195.0	-307.581027768	3.06
77.59	210.0	-307.583239807	0.46	336.80	210.0	-307.578803580	4.46
92.59	225.0	-307.583487164	0.30	351.80	225.0	-307.576935987	5.63
107.59	240.0	-307.583279355	0.43	366.80	240.0	-307.575959133	6.24
122.59	255.0	-307.582869953	0.69	381.80	255.0	-307.576159808	6.11
137.59	270.0	-307.582495523	0.93	396.80	270.0	-307.577543760	5.25
152.59	285.0	-307.582338562	1.03	411.80	285.0	-307.579638178	3.93
167.59	300.0	-307.582474046	0.94	426.80	300.0	-307.581892982	2.52
182.59	315.0	-307.582851373	0.70	441.80	315.0	-307.583801053	1.32
197.59	330.0	-307.583338755	0.40	456.80	330.0	-307.585094607	0.51
212.59	345.0	-307.583766418	0.13	471.80	345.0	-307.585764308	0.09
227.59	360.0	-307.583978809	0.00	486.80	360.0	-307.585910341	0.00

[a]Electronic energies at 0 K. ZPVE and Thermal correction to 298 K are not included. Unit are in hartree. [b]Rotational barriers are calculated as the difference between the total energy of each conformer and that of the most stable conformer. Units in kcal/mole.

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SM 3: Total Energy and Internal Rotation Barriers about C—C Bond.

trans - CH_3—CH=CHOOH			*cis* - CH_3—CH=CHOOH		
Torsion Angle	Total energy[a]	Rotational barrier[b]	Torsion angle	Total energy[a]	Rotational barrier[b]
0.0	-268.261740667	0.00	0.0	-268.259500864	1.31
15.0	-268.261064645	0.431	15.0	-268.260133871	0.91
30.0	-268.259862381	1.18	30.0	-268.261000558	0.37
45.0	-268.258750742	1.88	45.0	-268.261589159	0.00
60.0	-268.258503487	2.03	60.0	-268.261542707	0.03
75.0	-268.259352690	1.50	75.0	-268.260882311	0.44
90.0	-268.260635316	0.70	90.0	-268.260013734	0.98
105.0	-268.261571014	0.11	105.0	-268.259464027	1.33
120.0	-268.261751612	0.00	120.0	-268.259497489	1.31
135.0	-268.261116104	0.39	135.0	-268.260092158	0.94
150.0	-268.259921525	1.14	150.0	-268.260940221	0.40
165.0	-268.258769125	1.87	165.0	-268.261563186	0.01
180.0	-268.258506501	2.03	180.0	-268.261568090	0.01
195.0	-268.259395176	1.48	195.0	-268.260925719	0.41
210.0	-268.260701076	0.66	210.0	-268.260034731	0.97
225.0	-268.261610990	0.08	225.0	-268.259462878	1.33
240.0	-268.261729976	0.01	240.0	-268.259510106	1.30
255.0	-268.261033498	0.45	255.0	-268.260131200	0.91
270.0	-268.259823750	1.21	270.0	-268.260969522	0.38
285.0	-268.258722742	1.90	285.0	-268.261565585	0.01
300.0	-268.258516461	2.03	300.0	-268.261578241	0.00
315.0	-268.259384736	1.48	315.0	-268.260973806	0.38
330.0	-268.260661138	0.68	330.0	-268.260084556	0.94
345.0	-268.261588341	0.10	345.0	-268.259475560	1.32
360.0	-268.261740281	0.00	360.0	-268.259500993	1.31

[a]Electronic energies at 0 K. ZPVE and Thermal correction to 298 K are not included. Unit are in hartree. [b]Rotational barriers are calculated as the difference between the total energy of each conformer and that of the most stable conformer. Units in kcal/mole.

SM 3 (cont): Total Energy and Internal Rotation Barriers about C—C Bond

$(CH_3)CH_3$—C=CHOOH			CH_3—CH=C(CH_3)OOH				CH_3CH=C(—CH_3)OOH			
Torsion angle	Total energy[a]	Rot. barrier[b]	Torsion angle	Relative Torsion angle	Total energy[a]	Rot. barrier[b]	Torsion angle	Relative Torsion angle	Total energy[a]	Rot. barrier[b]
0.0	-307.583985298	0.00	110.91	0.0	-307.585916345	0.00	0.54630	0.0000	-307.585916230	0.00
15.0	-307.583556131	0.27	125.91	15.0	-307.585617002	0.18	15.546	15.000	-307.585576769	0.21
30.0	-307.582560857	0.89	140.91	30.0	-307.584814330	0.69	30.546	30.000	-307.584562319	0.85
45.0	-307.581548206	1.53	155.91	45.0	-307.583901580	1.26	45.546	45.000	-307.583286368	1.65
60.0	-307.581073176	1.82	170.91	60.0	-307.583528637	1.49	60.546	60.000	-307.582694654	2.02
75.0	-307.581454349	1.58	185.91	75.0	-307.584002903	1.20	75.546	75.000	-307.583353433	1.60
90.0	-307.582482456	0.94	200.91	90.0	-307.584906451	0.63	90.546	90.000	-307.584553234	0.85
105.0	-307.583520923	0.29	215.91	105.0	-307.585672071	0.15	105.55	105.00	-307.585525030	0.24
120.0	-307.583983300	0.00	230.91	120.0	-307.585911862	0.00	120.55	120.00	-307.585915324	0.00
135.0	-307.583625657	0.22	245.91	135.0	-307.585543267	0.23	135.55	135.00	-307.585590531	0.20
150.0	-307.582650879	0.83	260.91	150.0	-307.584709635	0.75	150.55	150.00	-307.584576546	0.84
165.0	-307.581583507	1.50	275.91	165.0	-307.583847964	1.29	165.55	165.00	-307.583296562	1.64
180.0	-307.581072058	1.82	290.91	180.0	-307.583529880	1.49	180.55	180.00	-307.582693818	2.02
195.0	-307.581525138	1.54	305.91	195.0	-307.583973724	1.22	195.55	195.00	-307.583354628	1.60
210.0	-307.582634161	0.84	320.91	210.0	-307.584839451	0.67	210.55	210.00	-307.584591150	0.83
225.0	-307.583634916	0.22	335.91	225.0	-307.585624886	0.18	225.55	225.00	-307.585563464	0.22
240.0	-307.583983867	0.00	350.91	240.0	-307.585915577	0.00	240.55	240.00	-307.585915989	0.00
255.0	-307.583559375	0.26	365.91	255.0	-307.585566206	0.22	255.55	255.00	-307.585560244	0.22
270.0	-307.582604818	0.86	380.91	270.0	-307.584713154	0.75	270.55	270.00	-307.584544723	0.86
285.0	-307.581591008	1.50	395.91	285.0	-307.583836235	1.30	285.55	285.00	-307.583273705	1.65
300.0	-307.581076268	1.82	410.91	300.0	-307.583532796	1.49	300.55	300.00	-307.582696047	2.02
315.0	-307.581443494	1.59	425.91	315.0	-307.584006573	1.19	315.55	315.00	-307.583384034	1.59
330.0	-307.582500378	0.93	440.91	330.0	-307.584872164	0.65	330.55	330.00	-307.584595350	0.82
345.0	-307.583564150	0.26	455.91	345.0	-307.585629033	0.18	345.55	345.00	-307.585551826	0.22
360.0	-307.583985288	0.00	470.91	360.0	-307.585916349	0.00	360.55	360.00	-307.585916188	0.00

[a]Electronic energies at 0 K. ZPVE and Thermal correction to 298 K are not included. Unit are in hartree. [b]Rotational barriers are calculated as the difference between the total energy of each conformer and that of the most stable conformer. Units in kcal/mole.

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SM 4: Coefficient of Truncated Fourier Series. Representation Expansions for Internal Rotation Potentials[a] (O—O bond)

Species	a_0	a_1	a_2	a_3	a_4	a_5	a_6	a_7
tr-CH_3CH=CHOOH	1,8035	2,2251	1,2699	0,1962	0,0304	5,1478e-3	2,3703e-4	2,9853e-4
cis-CH_3CH=CHOOH	1,7967	2,1568	1,2316	0,1838	0,0273	5,8548e-3	1,0835e-3	-3,2548e-4
$(CH_3)_2C$=CHOOH	1,6845	-0,6992	-1,0948	0,1327	-0,0275	3,9528e-3	7,9453e-5	1,5288e-4
CH_3CH=$C(CH_3)$OOH	1,9614	-1,1234	-1,0657	0,2342	-1,1273e-3	-4,0065e-3	-2,0422e-3	1,0305e-3
	b_1	b_2	b_3	b_4	b_5	b_6	b_7	
tr-CH_3CH=CHOOH	-0,3988	-0,6125	0,0216	4,4268e-3	5,4217e-3	6,2500e-4	4,4489e-4	
cis-CH_3CH=CHOOH	-0,3300	-0,5974	0,0238	2,7980e-3	4,5803e-3	8,0000e-4	1,8159e-5	
$(CH_3)_2C$=CHOOH	1,5636	-1,0691	0,1355	6,5021e-3	-3,0603e-3	6,6050e-4	-3,3129e-4	
CH_3CH=$C(CH_3)$OOH	-2,1855	1,1954	0,0397	-0,0363	-2,0529e-3	-6,1808e-4	-5,8256e-4	

[a] Units in kcal/mole. Values of rotation barriers calculated at B3LYP/6-31G(d,p) level for CH_2=CH—OOH and $CH_3C{\equiv}C$—OOH and B3LYP/3-2G for Phenyl-OOH are used to calculate the coefficients.

SM 5: Coefficient of Truncated Fourier Series. Representation Expansions for Internal Rotation Potentials[a] (C—O bond)

Species	a_0	a_1	a_2	a_3	a_4	a_5	a_6	a_7
tr-CH_3CH=CHOOH	1,8549	0,5729	-1,4136	-1,2055	0,1689	-3,4367e-3	0,0356	-0,0147
cis-CH_3CH=CHOOH	2,0929	1,6704	-0,6010	-0,6272	0,2566	-0,1349	-0,0350	0,0167
$(CH_3)_2C$=CHOOH	2,2854	-1,4359	0,1291	-0,4331	-0,1689	-0,1122	-0,0140	-0,0320
CH_3CH=$C(CH_3)$OOH	2,0564	-1,4197	0,2864	0,9244	0,2719	-0,0373	-0,0171	0,0391
	b_1	b_2	b_3	b_4	b_5	b_6	b_7	
tr-CH_3CH=CHOOH	0,0813	-0,1152	-0,1375	-0,0197	0,0325	0,0246	-0,0133	
cis-CH_3CH=CHOOH	-0,1880	0,1173	0,0959	-0,0695	-0,0552	0,0279	0,0428	
$(CH_3)_2C$=CHOOH	1,4847	-0,5534	-0,4751	-0,0592	-6,8831e-3	-0,0329	-0,0527	
CH_3CH=$C(CH_3)$OOH	0,1472	0,0125	-0,0523	-9,7709e-3	0,0315	-0,0224	-3,7448e-3	

[a]Units in kcal/mole. Values of rotation barriers calculated at B3LYP/6-31G(d,p) level for CH_2=CH—OOH and $CH_3C{\equiv}C$—OOH and B3LYP/3-2G for Phenyl-OOH are used to calculate the coefficients.

SM 6: Coefficient of Truncated Fourier Series. Representation Expansions for Internal Rotation Potentials[a] (C—C bond)

Species	a_0	a_1	a_2	a_3	a_4	a_5	a_6	a_7
tr-CH_3CH=CHOOH	0,9758	8,5308e-3	-0,0121	-1,0104	0,0120	-6,6120e-3	-3,0978e-3	0,0446
cis-CH_3CH=CHOOH	-5,9385e-4	-8,9110e-3	-5,3227e-3	4,6256e-3	0,0115	0,6704	0,6464	-8,0363e-3
$(CH_3)_2C$=CHOOH	0,9003	0,0197	-9,1270e-3	-0,9120	8,4476e-3	-0,0187	0,0136	-2,0436e-3
CH_3—CH=$C(CH_3)$OOH	0,7211	-0,0129	3,7430e-4	-0,7469	-5,7656e-5	0,0108	1,1800e-3	-9,8473e-3
CH_3CH=C(—CH_3)OOH	0,9258	-9,7228e-5	-6,7996e-3	-1,0019	7,1089e-3	-2,1819e-3	0,0828	2,2678e-4
	b_1	b_2	b_3	b_4	b_5	b_6	b_7	
tr-CH_3CH=CHOOH	-3,3004e-3	4,6459e-3	0,2525	-1,0378e-3	-2,6876e-4	-0,0175	1,3008e-3	
cis-CH_3CH=CHOOH	9,2626e-3	1,1352e-3	-0,2891	-3,1328e-3	-9,6256e-4	-9,6583e-4	-1,3059e-3	
$(CH_3)_2C$=CHOOH	9,1876e-3	-3,5135e-3	-0,0223	-3,5387e-3	7,5624e-3	0,0146	-8,5920e-4	
CH3—CH=$C(CH_3)$OOH	0,0271	-6,5803e-3	0,0420	-5,6745e-3	-9,1884e-3	-0,0104	1,9266e-3	
CH_3CH=C(—CH_3)OO H	1,7110e-3	2,2146e-3	8,4200e-3	2,2385e-3	-8,2969e-4	-0,0169	-2,2404e-3	

[a]Units in kcal/mole. Values of rotation barriers calculated at B3LYP/6-31G(d,p) level for CH_2=CH—OOH and $CH_3C{\equiv}C$—OOH and B3LYP/3-2G for Phenyl-OOH are used to calculate the coefficients.

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SM 7: Thermochemical Properties of *cis*–$CH_3CH=CHOOH$, *trans*–$CH_3CH=CHOOH$, $(CH_3)_2C=CHOOH$ and $CH_3CH=C(CH_3)OOH$

1. *cis*–$CH_3CH=CHOOH$ (ideal Gas)

T (K)	Cp (cal/mol/K)						S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C—C=COOH	IR CC=C—OOH	IR CC=CO—OH	IR Total	TVR	IR+TVR		
0.1	0,00	0,00	0,00	0,00	7,95	7,95	0.00	0.00
10	0,04	0,00	0,00	0,04	7,95	7,99	36.60	0.08
50	0,55	2,39	1,15	4,09	8,07	12,16	49.41	0.39
100	1,59	2,58	1,69	5,86	9,27	15,13	55.30	0.82
200	2,02	2,10	1,65	5,77	12,89	18,66	62.70	1.92
300	1,77	2,22	1,57	5,56	17,60	23,16	68.70	3.44
400	1,54	2,39	1,55	5,48	22,52	28,00	74.35	5.45
500	1,38	2,38	1,56	5,32	26,88	32,2	79.77	7.93
600	1,28	2,24	1,56	5,08	30,51	35,59	84.93	10.80
700	1,21	2,03	1,55	4,79	33,55	38,34	89.80	14.01
800	1,17	1,82	1,53	4,52	36,11	40,63	94.40	17.50
900	1,13	1,61	1,51	4,25	38,31	42,56	98.74	21.22
1000	1,11	1,43	1,48	4,02	40,20	44,22	102.84	25.15
1100	1,09	1,27	1,45	3,81	41,84	45,65	106.72	29.25
1200	1,07	1,13	1,41	3,61	43,27	46,88	110.39	33.51
1300	1,06	1,01	1,39	3,46	44,51	47,97	113.88	37.90
1400	1,05	0,90	1,36	3,31	45,60	48,91	117.20	42.41
1500	1,04	0,81	1,33	3,18	46,55	49,73	120.36	47.02
2000	1,02	0,51	1,23	2,76	49,85	52,61	134.19	71.21
2500	1,00	0,34	1,16	2,5	51,69	54,19	145.49	96.64
3000	0,98	0,25	1,12	2,35	52,80	55,15	155.00	122.78
3500	0,96	0,18	1,09	2,23	53,50	55,73	163.18	149.37
4000	0,92	0,14	1,07	2,13	53,98	56,11	170.35	176.25
4500	0,88	0,11	1,06	2,05	54,31	56,36	176.72	203.33
5000	0,83	0,09	1,04	1,96	54,56	56,52	182.45	230.55

2. *trans*–$CH_3CH=CHOOH$ (ideal Gas)

T (K)	Cp (cal/mol/K)						S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C—C=COOH	IR CC=C—OOH	IR CC=CO—OH	IR Total	TVR	IR+TVR		
0.1	0,02	0,00	0,00	0,02	7,95	7,97	-.147	.001
10	0,00	0,00	0,02	0,02	7,95	7,97	36.46	.08
50	0,27	1,54	1,08	2,89	8,16	11,05	49.28	.39
100	1,19	2,55	1,44	5,18	9,67	14,85	55.33	.84
200	1,94	2,26	1,55	5,75	13,38	19,13	63.08	1.99
300	1,97	2,06	1,52	5,55	17,90	23,45	69.24	3.55
400	1,81	1,98	1,52	5,31	22,68	27,99	74.95	5.58
500	1,64	1,90	1,53	5,07	26,97	32,04	80.40	8.07
600	1,50	1,82	1,54	4,86	30,58	35,44	85.58	10.95
700	1,40	1,73	1,54	4,67	33,60	38,27	90.47	14.16
800	1,32	1,65	1,53	4,5	36,16	40,66	95.07	17.65
900	1,26	1,58	1,51	4,35	38,35	42,7	99.42	21.38
1000	1,22	1,51	1,48	4,21	40,24	44,45	103.52	25.32
1100	1,18	1,45	1,45	4,08	41,88	45,96	107.40	29.42
1200	1,15	1,40	1,42	3,97	43,31	47,28	111.08	33.69
1300	1,13	1,36	1,40	3,89	44,55	48,44	114.57	38.08
1400	1,11	1,32	1,37	3,8	45,64	49,44	117.89	42.59
1500	1,10	1,29	1,34	3,73	46,59	50,32	121.05	47.20
2000	1,05	1,16	1,24	3,45	49,88	53,33	134.89	71.41
2500	1,03	1,08	1,17	3,28	51,71	54,99	146.20	96.85
3000	1,01	0,99	1,13	3,13	52,81	55,94	155.71	123.00
3500	1,00	0,91	1,10	3,01	53,51	56,52	163.89	149.59
4000	0,97	0,83	1,08	2,88	53,99	56,87	171.06	176.48
4500	0,95	0,75	1,06	2,76	54,32	57,08	177.43	203.56
5000	0,92	0,68	1,05	2,65	54,56	57,21	183.17	230.78

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3. $(CH_3)_2C=CHOOH$ (ideal Gas)

T (K)	Cp (cal/mol/K)							S (cal/mol/K)	[H(T) -H(0K)] (kcal/mol)
	IR C—(C)C=C	IR C(—C)C=C	IR C=C—OOH	IR C=CO—OH	IR Total	TVR	TVR+IR		
0.1	0,00	0,00	0,00	0,00	0	7,95	7,95	-.25	0.00
10	0,11	0,11	0,03	0,00	0,25	7,95	8,20	36.35	0.08
50	0,37	0,37	0,92	1,80	3,46	8,16	11,62	49.18	0.39
100	1,35	1,35	1,34	2,54	6,58	10,17	16,75	55.32	0.85
200	2,03	2,03	2,03	2,06	8,15	15,60	23,75	63.92	2.13
300	1,95	1,95	2,19	1,78	7,87	21,63	29,50	71.24	3.99
400	1,74	1,74	2,24	1,68	7,4	27,86	35,26	78.20	6.47
500	1,56	1,56	2,23	1,63	6,98	33,47	40,45	84.92	9.54
600	1,43	1,43	2,16	1,60	6,62	38,23	44,85	91.36	13.13
700	1,33	1,33	2,06	1,57	6,29	42,25	48,54	97.49	17.16
800	1,26	1,267	1,96	1,53	6,01	45,67	51,68	103.29	21.56
900	1,21	1,21	1,86	1,49	5,77	48,60	54,37	108.78	26.28
1000	1,17	1,17	1,76	1,45	5,55	51,14	56,69	113.99	31.27
1100	1,15	1,15	1,67	1,42	5,39	53,33	58,72	118.92	36.50
1200	1,12	1,12	1,60	1,38	5,22	55,24	60,46	123.61	41.93
1300	1,10	1,10	1,53	1,35	5,08	56,90	61,98	128.06	47.54
1400	1,09	1,09	1,48	1,32	4,98	58,35	63,33	132.30	53.30
1500	1,08	1,08	1,43	1,29	4,88	59,61	64,49	136.35	59.20
2000	1,04	1,04	1,26	1,19	4,53	63,97	68,50	154.07	90.21
2500	1,02	1,02	1,17	1,12	4,33	66,39	70,72	168.58	122.86
3000	1,00	1,0	1,11	1,05	4,16	67,83	71,99	180.79	156.45
3500	0,98	0,98	1,07	0,98	4,01	68,76	72,77	191.31	190.61
4000	0,94	0,94	1,03	0,92	3,83	69,38	73,21	200.52	225.16
4500	0,91	0,91	0,98	0,85	3,65	69,81	73,46	208.71	259.96
5000	0,87	0,87	0,94	0,78	3,46	70,13	73,59	216.07	294.95

4. $CH_3CH=C(CH_3)OOH$ (ideal Gas)

T (K)	Cp (cal/mol/K)							S (cal/mol/K)	[H(T) -H(0K)] (kcal/mol)
	IR C—C=C	IR C(C)—OOH	IR C(C)O—O H	IR C(—C)OOH	IR Total	TVR	TVR+IR		
0.1	0,00	0,00	0,00	0,00	0	7,95	7,95	-0.34	0.00
10	0,03	0,00	0,00	0,01	0,04	7,95	7,99	36.26	0.08
50	1,06	1,00	1,14	0,23	3,43	8,14	11,57	49.08	0.40
100	1,85	1,40	1,56	1,11	5,92	10,25	16,17	55.25	0.85
200	2,09	2,04	1,59	1,84	7,56	15,57	23,13	63.86	2.14
300	1,83	2,43	1,52	1,87	7,65	21,65	29,3	71.18	3.99
400	1,58	2,56	1,49	1,72	7,35	27,93	35,28	78.15	6.47
500	1,42	2,47	1,50	1,57	6,96	33,55	40,51	84.89	9.56
600	1,31	2,30	1,51	1,45	6,57	38,31	44,88	91.34	13.16
700	1,24	2,11	1,51	1,36	6,22	42,31	48,53	97.47	17.19
800	1,18	1,94	1,51	1,29	5,92	45,71	51,63	103.28	21.60
900	1,15	1,79	1,50	1,24	5,68	48,63	54,31	108.78	26.32
1000	1,12	1,67	1,48	1,19	5,46	51,15	56,61	113.99	31.31
1100	1,09	1,58	1,46	1,16	5,29	53,34	58,63	118.93	36.54
1200	1,07	1,49	1,44	1,14	5,14	55,24	60,38	123.61	41.97
1300	1,06	1,43	1,41	1,12	5,02	56,90	61,92	128.07	47.58
1400	1,04	1,37	1,39	1,10	4,9	58,34	63,24	132.31	53.34
1500	1,02	1,33	1,37	1,09	4,81	59,60	64,41	136.35	59.24
2000	0,93	1,19	1,27	1,05	4,44	63,96	68,4	154.07	90.25
2500	0,82	1,11	1,20	1,03	4,16	66,38	70,54	168.58	122.89
3000	0,71	1,07	1,15	1,02	3,95	67,83	71,78	180.79	156.47
3500	0,62	1,03	1,11	1,01	3,77	68,75	72,52	191.30	190.63
4000	0,53	0,99	1,09	1,00	3,61	69,37	72,98	200.51	225.17
4500	0,46	0,95	1,07	0,99	3,47	69,81	73,28	208.70	259.97
5000	0,40	0,91	1,06	0,97	3,34	70,13	73,47	216.07	294.96