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Supplementary data

Thermochemical Properties, Rotation Barriers and Group Additivity for Unsaturated Oxygenated Hydrocarbons and Radicals Resulting from Reaction of Vinyl and Phenyl Radical Systems with O_2

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SM 1: Total Energies[a] at 298 K

Species	B3LYP/ 6-311G(d,p)	ZPVE[b]	Therm corr[c]	Species	B3LYP/ 6-311G(d,p)	ZPVE[b]	Therm corr[c]
OHCH=O	-189.748657227	21.25	23.82	$C_6H_5C(=CH_2)CH=O$	-422.785339355	89.29	95.25
$CH_2=CHCH_2CH_2CH_3$	-196.316268921	85.59	90.30	$C_6H_5OCH=O$	-384.677886963	85.89	91.34
$CH_2=C=CH_2$	-116.451873779	36.08	38.67	$C_6H_5C(=CH_2)CH_3$	-348.726989746	101.04	106.11
$CH_2=CHCH_2CH=O$	-231.105224609	55.76	60.003	$C_6H_5C(=CH_2)OH$	-384.691040039	86.40	91.78
$CH_2(OH)_2$	-190.890090942	35.98	38.93	$Y(C_6H_6)=O$	-307.313415527	64.543	68.81
$CH(OH)_2CH=O$	-304.219451904	41.29	45.36	$Y(C_5H_5)C(OH)=O$	-382.550201416	67.56	72.47
$CH_3OCH=O$	-228.997528076	38.19	41.35	$Y(C_5H_5O)CH=O$	-382.514404297	66.82	71.81
$CH_2=CHC(OH)=O$	-228.775207520	35.36	39.23	$Y(C_5H_5)OCH=O$	-382.515350342	66.75	71.57
$CH_2=CHCH(CHO)CH=O$	-344.426208496	61.43	66.84	$CH_3OCH=O$	-228.997528076	38.19	41.35
$CH_2=CHCH(CHO)C\equiv CH$	-307.240936279	61.51	66.94	$CH_2=CHCH=O$	-191.842590332	38.34	41.67
$CH_2=C=CH_2$	-116.451873779	36.08	38.67	$CH(OH)_2CH=O$	-304.219451904	41.29	45.36
$CH(OH)_2CH=O$	-304.219451904	41.29	45.36	$Y(C_5H_6O)$	-269.189971924	61.70	65.39
$CH_3C(OH)_2CH=O$	-343.497619629	58.20	63.23	$Y(C_5H_5\bullet)$ (cyclopentadienyl)	-193.354248047	48.74	52.32
$CH_2=CHCH(CHO)CH=CH_2$	-308.448669434	76.47	82.11	Furanj1	-229.265411377	35.63	38.56
$CH_2=CHC(OH)_2CH=CH_2$	-345.593536377	76.70	82.22	Furanj2	-229.265213013	35.85	38.76
$CH_2=C(OH)_2$	-228.979919434	38.32	41.70	$Y(C_6H_5\bullet)=O$	-306.721008301	57.22	61.12
$CH_2=CHCH(CH_3)CH=CH_2$	-234.393524170	88.38	93.61	$Y(C_5H_5)C(O\bullet)=O$	-381.910003662	58.51	63.45
$CH_2=C(CH=O)CH=CH_2$	-269.191528320	59.15	63.86	$C_6H_5C\bullet=O$	-344.811096191	61.03	65.59
$CH_2=C(CH=O)C\equiv CH$	-267.984375000	44.30	48.73	$Y(C5O)C\bullet=O$	-381.890716553	59.13	64.09
$CH_2=CHCH(OH)CH=CH_2$	-270.351135254	73.96	78.84	$Y(C5)OC\bullet=O$	-381.891601562	59.09	64.11
$CH_2=C(OH)CH=O$	-267.082916260	41.79	45.48	$CH_3OC\bullet=O$	-228.362701416	30.59	34.21
$CH_2=CHOCH=CH_2$	-231.083282471	55.60	59.87	$CH_2=C\bullet CH=O$	-191.182113647	29.25	32.83
$CH_2=CHCH=O$	-191.842590332	38.339	41.67	$CH_2=CHC\bullet=O$	-191.214782715	30.61	33.96
$C_6H_5C(OH)_2CH_3$	-461.114532471	103.64	110.03	$CH_2=CHC\bullet(CH=O)C\equiv CH$	-306.650756836	53.97	59.13
$C_6H_5C(CH_2)CH=CH_2$	-386.805786133	104.16	-110.28	$C\bullet(OH)_2CH=O$	-303.622192383	34.05	37.76
$C_6H_5C(CH_3)_2CH=O$	-463.235534668	121.15	128.37	$CH_2=CHC\bullet(CH=O)CH=O$	-343.830718994	54.31	59.33
$C_6H_5CH=O$	-345.439910889	68.71	73.25	$O\bullet CH=O$	-189.092697144	12.29	14.79
$CH_3C_6H_4CH=O$	-384.714080811	85.71	90.88	$CH_2=CHC(O\bullet)=O$	-228.238479614	29.47	32.81

[a]Total energy calculation are based on the geometries optimized at B3LYP/6-311G(d,p) level of theory (ZPVE's and thermal corrections to 298 K are included) in hartrees; 1 hartree = 627.51 kcal/mol. [b]ZVPE scaled by .97 in kcal mol^{-1}; [c]values in kcal mol^{-1}

SM 2: Geometry Parameters[a]

Structure		Bond length (angstrom)		Bond angle (degree)		Dihedral angle (degree)
$CH(OH)_2CH=O$						
C						
C	1	r21=1.531				
O	2	r32=1.202	1	a321=121.38		
O	1	r41=1.387	2	a412=111.22	3	d4123=4.9
O	1	r51=1.415	2	a512=103.55	3	d5123=-118.0
H	1	r61=1.099	2	a612=110.03	3	d6123=123.6
H	2	r72=1.105	1	a721=116.02	4	d7214=-177.4
H	4	r84=0.969	1	a841=106.87	2	d8412=-24.5
H	5	r95=0.963	1	a951=107.39	2	d9512=179.2
$CH_2=CHCH(CH=O)CH=O$						
C						
C	1	r21=1.534				
C	2	r32=1.498	1	a321=113.57		
C	3	r43=1.327	2	a432=123.84	1	d4321=118.07
C	2	r52=1.534	1	a521=107.90	3	d5213=-126.8
O	5	r65=1.199	2	a652=124.36	1	d6521=122.89
H	1	r71=1.112	2	a712=114.52	3	d7123=-176.3
H	2	r82=1.101	1	a821=104.95	7	d8217=-54.66
H	3	r93=1.084	2	a932=115.82	1	d9321=-61.92
H	4	r104=1.083	3	a1043=121.39	2	d10432=179.9
H	4	r114=1.086	3	a1143=121.94	2	d11432=0.004
H	5	r125=1.112	2	a1252=114.52	1	d12521=-56.8
O	1	r131=1.199	2	a1312=124.36	3	d13123=3.935
$CH_3C(OH)_2CH=O$						
C						
C	1	r21=1.524				
C	2	r32=1.539	1	a321=112.32		
O	3	r43=1.202	2	a432=121.61	1	d4321=-125.63
O	2	r52=1.393	1	a521=108.77	3	d5213=-121.9
O	2	r62=1.424	1	a621=111.43	3	d6213=113.6
H	1	r71=1.091	2	a712=110.61	3	d7123=-60.2
H	1	r81=1.093	2	a812=108.91	3	d8123=-179.5
H	1	r91=1.091	2	a912=110.78	3	d9123=61.7
H	3	r103=1 .10	2	a1032=115.96	1	d10321=56.3
H	5	r115=0.96	2	a1152=106.79	1	d11521=145.
H	6	r126=0.96	2	a1262=106.83	1	d12621=69.9
$CH_2=CHCH(CH=O)CH=CH_2$						
C						
C	1	r21=1.329				
C	2	r32=1.512	1	a321=124.53		
C	3	r43=1.512	2	a432=111.68	1	d4321=-127.2
C	4	r54=1.329	3	a543=124.52	2	d5432=127.2
C	3	r63=1.533	2	a632=108.96	1	d6321=112.2
O	6	r76=1.201	3	a763=124.16	2	d7632=-118.8
H	1	r81=1.085	2	a812=121.73	3	d8123=0.6
H	1	r91=1.083	2	a912=121.37	3	d9123=-179.7
H	2	r102=1.088	3	a1023=115.94	4	d10234=53.1
H	3	r113=1.092	2	a1132=110.28	1	d11321=-4.2
H	4	r124=1.088	3	a1243=115.95	2	d12432=-53.1
H	5	r135=1.083	4	a1354=121.38	3	d13543=179.7
H	5	r145=1.085	4	a1454=121.73	3	d14543=-0.6
H	6	r156=1.113	3	a1563=114.65	2	d15632=61.1
$CH_2=CHCH_2CH=O$						
C						
C	1	r21=1.328				
C	2	r32=1.505	1	a321=124.58		
C	3	r43=1.519	2	a432=112.30	1	d4321=-118.3
O	4	r54=1.202	3	a543=124.39	2	d5432=132.3
H	1	r61=1.085	2	a612=121.69	3	d6123=-0.6
H	1	r71=1.083	2	a712=121.44	3	d7123=179.8
H	2	r82=1.088	3	a823=116.17	4	d8234=61.07
H	3	r93=1.100	2	a932=109.36	1	d9321=123.8
H	3	r103=1.091	2	a1032=112.12	1	d10321=3.9
H	4	r114=1.113	3	a1143=114.78	2	d11432=-47.9

[a]Distances in angstroms and angles in degrees. Geometry parameters optimized at the B3LYP/6- 311G(d,p) level of theory.

SM 2: Geometry Parameters[a]

Structure		Bond length (angstrom)		Bond angle (degree)		Dihedral angle (degree)
$CH_2=CHC(OH)_2CH=CH_2$						
C						
C	1	r21=1.328				
C	2	r32=1.514	1	a321=125.17		
C	3	r43=1.514	2	a432=110.61	1	d4321=114.2
C	4	r54=1.328	3	a543=125.17	2	d5432=114.1
O	3	r63=1.418	2	a632=107.96	1	d6321=-6.07
O	3	r73=1.418	2	a732=109.89	1	d7321=-126.
H	1	r81=1.082	2	a812=121.05	3	d8123=-0.78
H	1	r91=1.084	2	a912=121.12	3	d9123=179.1
H	2	r102=1.085	3	a1023=113.39	4	d10234=-66.1
H	4	r114=1.085	3	a1143=113.40	2	d11432=-66.1
H	5	r125=1.084	4	a1254=121.12	3	d12543=179.1
H	5	r135=1.082	4	a1354=121.06	3	d13543=-0.76
H	6	r146=0.964	3	a1463=106.51	2	d14632=176.0
H	7	r157=0.964	3	a1573=106.50	2	d15732=55.2
$CH_2=C(OH)_2$						
C						
C	1	r21=1.327				
O	2	r32=1.367	1	a321=122.83		
O	2	r42=1.367	1	a421=122.83	3	d4213=180.
H	1	r51=1.079	2	a512=119.94	3	d5123=-7.4
H	1	r61=1.079	2	a612=119.94	3	d6123=172.5
H	3	r73=0.965	2	a732=108.19	1	d7321=136.6
H	4	r84=0.965	2	a842=108.19	1	d8421=136.6
$CH_2=CHCH(CH_3)CH=CH_2$						
C						
C	1	r21=1.329				
C	2	r32=1.511	1	a321=125.29		
C	3	r43=1.511	2	a432=110.44	1	d4321=-119.71
C	4	r54=1.329	3	a543=125.29	2	d5432=119.702
H	1	r61=1.084	2	a612=121.66	3	d6123=-179.4
H	1	r71=1.085	2	a712=121.60	3	d7123=0.6
H	2	r82=1.089	3	a823=115.46	4	d8234=60.7
H	3	r93=1.095	2	a932=108.35	1	d9321=-1.1
H	4	r104=1.089	3	a1043=115.46	2	d10432=-60.7
H	5	r115=1.084	4	a1154=121.66	3	d11543=179.5
H	5	r125=1.085	4	a1254=121.60	3	d12543=-0.6
C	3	r133=1.544	2	a1332=110.50	1	d13321=117.7
H	13	r1413=1.09	3	a14133=110.89	2	d141332=61.2
H	13	r1513=1.09	3	a15133=110.66	2	d151332=-58.4
H	13	r1613=1.09	3	a16133=110.66	2	d161332=-179.0´
$CH_2=C(CH=O)CH=CH_2$						
C						
C	1	r21=1.336				
C	2	r32=1.467	1	a321=127.73		
C	3	r43=1.343	2	a432=121.71	1	d4321=176.3
C	3	r53=1.499	2	a532=120.67	1	d5321=-4.09
O	5	r65=1.208	3	a653=124.13	2	d6532=177.8
H	1	r71=1.082	2	a712=123.50	3	d7123=-0.03
H	1	r81=1.083	2	a812=120.41	3	d8123=-179.8
H	2	r92=1.087	1	a921=117.94	7	d9217=179.55
H	4	r104=1.083	3	a1043=119.98	2	d10432=179.9
H	4	r114=1.084	3	a1143=121.73	2	d11432=-0.02
H	5	r125=1.106	3	a1253=115.94	2	d12532=-2.67
$CH_2=CHCH=O$						
C						
C	1	r21=1.333				
C	2	r32=1.475	1	a321=121.25		
O	3	r43=1.208	2	a432=124.31	1	d4321=-179.9
H	1	r51=1.086	2	a512=120.95	3	d5123=0.001
H	1	r61=1.083	2	a612=122.29	3	d6123=179.9
H	2	r72=1.085	1	a721=122.41	5	d7215=-179.9
H	3	r83=1.112	2	a832=114.49	1	d8321=-0.0

[a]Distances in angstroms and angles in degrees. Geometry parameters optimized at the B3LYP/6- 311G(d,p) level of theory.

SM 2(cont): Geometry Parameters[a]

Structure	Bond length (angstrom)		Bond angle (degree)		Dihedral angle (degree)
CH_2=C(CH=O)C≡CH					
C					
C	1	r21=1.326			
C	2	r32=1.513	1	a321=125.62	
C	3	r43=1.546	2	a432=111.88	1 d4321=-135.4
O	4	r54=1.198	3	a543=123.89	2 d5432=-18.08
H	1	r61=1.084	2	a612=121.99	3 d6123=0.5
H	1	r71=1.083	2	a712=120.70	3 d7123=-179.7
H	2	r82=1.084	3	a823=113.65	4 d8234=44.0624
H	3	r93=1.105	2	a932=107.84	1 d9321=112.126
H	4	r104=1.109	3	a1043=114.05	2 d10432=163.8
C	3	r113=1.459	2	a1132=115.69	1 d11321=-8.1
C	11	r1211=1.201	3	a12113=178.02	2 d121132=-132.8
H	12	r1312=1.062	11	a131211=179.60	3 d1312113=-174.0
CH_2=CHCH(OH)CH=CH_2					
C					
C	1	r21=1.345			
C	2	r32=1.467	1	a321=121.49	
C	3	r43=1.336	2	a432=127.09	1 d4321=179.9
C	2	r52=1.491	1	a521=115.58	3 d5213=179.9
O	5	r65=1.207	2	a652=126.54	1 d6521=179.9
H	1	r71=1.083	2	a712=121.95	3 d7123=-0.0
H	1	r81=1.084	2	a812=121.17	3 d8123=179.9
H	3	r93=1.087	2	a932=114.18	1 d9321=-0.0
H	4	r104=1.083	3	a1043=120.00	2 d10432=179.9
H	4	r114=1.080	3	a1143=121.98	2 d11432=0.0
H	5	r125=1.111	2	a1252=113.04	1 d12521=0.05
CH_2=CHOCH=CH_2					
C					
C	1	r21=1.327			
O	2	r32=1.367	1	a321=121.87	
C	3	r43=1.367	2	a432=118.44	1 d4321=179.9
C	4	r54=1.327	3	a543=121.87	2 d5432=180.
H	1	r61=1.082	2	a612=121.33	3 d6123=-0.0
H	1	r71=1.080	2	a712=119.77	3 d7123=179.9
H	2	r82=1.087	1	a821=122.99	6 d8216=-179.9
H	4	r94=1.087	5	a945=122.99	3 d9453=180.
H	5	r105=1.080	4	a1054=119.77	3 d10543=180.
H	5	r115=1.082	4	a1154=121.33	3 d11543=0.
CH_2=CHCH(CH=O)C≡CH					
C					
C	1	r21=1.326			
C	2	r32=1.513	1	a321=125.62	
C	3	r43=1.546	2	a432=111.88	1 d4321=-135.45
O	4	r54=1.198	3	a543=123.89	2 d5432=-18.08
H	1	r61=1.084	2	a612=121.99	3 d6123=0.49
H	1	r71=1.083	2	a712=120.70	3 d7123=-179.74
H	2	r82=1.084	3	a823=113.65	4 d8234=44.06
H	3	r93=1.105	2	a932=107.84	1 d9321=112.12
H	4	r104=1.109	3	a1043=114.05	2 d10432=163.80
C	3	r113=1.459	2	a1132=115.69	1 d11321=-8.10
C	11	r1211=1.201	3	a12113=178.02	2 d121132=-132.80
H	12	r1312=1.062	11	a131211=179.6	3 d1312113=-174.00

[a]Distances in angstroms and angles in degrees. Geometry parameters optimized at the B3LYP/6- 311G(d,p) level of theory.

SM 2 (cont): Geometry Parameters[a]

Structure	Bond length (angstrom)		Bond angle (degree)		Dihedral angle (degree)	
$C_6H_5C(OH)_2CH_3$						
C						
C	1	r21=1.393				
C	2	r32=1.393	1	a321=120.33		
C	3	r43=1.396	2	a432=120.28	1	d4321=0.1
C	4	r54=1.398	3	a543=119.15	2	d5432=0.02
C	5	r65=1.392	4	a654=120.48	3	d6543=-0.086
C	4	r74=1.527	3	a743=121.38	2	d7432=-178.4
C	7	r87=1.529	4	a874=112.11	3	d8743=97.6
O	7	r97=1.418	8	a978=110.94	4	d9784=119.4
O	7	r107=1.420	8	a1078=105.51	4	d10784=-121.4
H	1	r111=1.084	2	a1112=120.21	3	d11123=-179.9
H	2	r122=1.084	1	a1221=120.02	6	d12216=179.6
H	3	r133=1.081	2	a1332=120.52	1	d13321=179.3
H	5	r145=1.083	4	a1454=119.23	7	d14547=-2.1
H	6	r156=1.084	5	a1565=119.75	4	d15654=179.8
H	8	r168=1.090	7	a1687=110.73	4	d16874=58.8
H	8	r178=1.090	7	a1787=109.94	4	d17874=-61.7
H	8	r188=1.094	7	a1887=109.46	4	d18874=178.0
H	9	r199=0.963	7	a1997=106.78	8	d19978=54.520
H	10	r2010=0.965	7	a20107=106.87	8	d201078=178.2
$C_6H_5C(=CH_2)CH=CH_2$						
C						
C	1	r21=1.393				
C	2	r32=1.390	1	a321=120.26		
C	3	r43=1.402	2	a432=120.91	1	d4321=0.3
C	4	r54=1.402	3	a543=118.14	2	d5432=-0.9
C	5	r65=1.391	4	a654=120.94	3	d6543=1.05
C	4	r74=1.488	3	a743=121.43	2	d7432=178.9
C	7	r87=1.480	4	a874=116.96	3	d8743=144.3
C	8	r98=1.333	7	a987=125.31	4	d9874=139.9
C	7	r107=1.342	4	a1074=121.82	3	d10743=-35.1
H	1	r111=1.084	2	a1112=120.23	3	d11123=179.7
H	2	r122=1.084	1	a1221=120.04	6	d12216=-179.
H	3	r133=1.083	2	a1332=119.74	1	d13321=-178.
H	5	r145=1.084	4	a1454=119.33	3	d14543=179.8
H	6	r156=1.084	5	a1565=119.70	4	d15654=179.3
H	8	r168=1.088	7	a1687=115.74	4	d16874=-38.9
H	9	r179=1.084	8	a1798=121.27	7	d17987=178.2
H	9	r189=1.084	8	a1898=121.62	7	d18987=-2.4
H	10	r1910=1.083	7	a19107=121.13	4	d191074=176.0
H	10	r2010=1.083	7	a20107=121.65	4	d201074=-4.07
$C_6H_5C(CH_3)_2CH=O$						
C						
C	1	r21=1.393				
C	2	r32=1.390	1	a321120.14		
C	3	r43=1.403	2	a432121.19	1	d4321=0.01
C	4	r54=1.398	3	a543117.97	2	d5432=0.47
C	5	r65=1.394	4	a654120.93	3	d6543=-0.7
C	4	r74=1.537	3	a743118.94	2	d7432=-179.2
C	7	r87=1.542	4	a874113.00	3	d8743=-171.6
C	7	r97=1.538	8	a978109.93	4	d9784=124.42
C	7	r107=1.533	8	a1078=106.16	9	d10789=119.3
O	10	r1110=1.20	7	a11107=125.31	8	d111078=121.6
H	1	r121=1.084	2	a1212=120.32	3	d12123=179.9
H	2	r132=1.084	1	a1321=120.16	6	d13216=179.6
H	3	r143=1.084	2	a1432=119.21	1	d14321=179.8
H	5	r155=1.082	4	a1554=120.35	7	d15547=-0.7
H	6	r166=1.084	5	a1665=119.51	4	d16654=-179.6
H	8	r178=1.093	7	a1787=112.09	9	d17879=-178.1
H	8	r188=1.092	7	a1887=110.79	9	d18879=60.8
H	8	r198=1.092	7	a1987=109.92	9	d19879=-57.9
H	9	r209=1.092	7	a2097=110.06	8	d20978=-63.4
H	9	r219=1.090	7	a2197=111.53	8	d21978=176.2
H	9	r229=1.092	7	a2297=110.50	8	d22978=56.7
H	10	r2310=1.112	7	a23107=113.75	8	d231078=58.2

[a]Distances in angstroms and angles in degrees. Geometry paramet ers optimized at the B3LYP/6-311G(d,p) level of theory.

SM 2 (cont): Geometry Parameters[a]

Structure	Bond length (angstrom)		Bond angle (degree)		Dihedral angle (degree)	
$C_6H_5CH=O$						
C						
C	1	r21=1.393				
C	2	r32=1.391	1	a321=119.70		
C	3	r43=1.398	2	a432=120.18	1	d4321=-0.01
C	4	r54=1.400	3	a543=119.84	2	d5432=0.025
C	5	r65=1.388	4	a654=119.93	3	d6543=-0.01
C	4	r74=1.481	3	a743=119.83	2	d7432=-179.
O	7	r87=1.209	4	a874=124.88	3	d8743=179.9
H	1	r91=1.084	2	a912=119.80	3	d9123=-179.9
H	2	r102=1.083	1	a1021=120.10	6	d10216=179.9
H	3	r113=1.085	2	a1132=120.32	1	d11321=-179.9
H	5	r125=1.083	4	a1254=118.46	3	d12543=179.9
H	6	r136=1.084	5	a1365=120.08	4	d13654=179.9
H	7	r147=1.112	4	a1474=114.39	3	d14743=-0.08
$C_6H_5CH=CH_2$						
C						
C	1	r21=1.3917				
C	2	r32=1.3921	1	a321=120.03		
C	3	r43=1.4028	2	a432=121.26	1	d4321=-0.00
C	4	r54=1.4042	3	a543=117.92	2	d5432=0.01
C	5	r65=1.3884	4	a654=120.89	3	d6543=-0.01
C	4	r74=1.4712	3	a743=118.91	2	d7432=-179.9
H	1	r81=1.0849	2	a812=120.32	3	d8123=-179.9
H	2	r92=1.0847	1	a921=120.15	6	d9216=179.9
H	3	r103=1.085	2	a1032=119.67	1	d10321=179.9
H	5	r115=1.083	4	a1154=119.87	3	d11543=179.9
H	6	r126=1.084	5	a1265=119.65	4	d12654=-179.9
C	7	r137=1.335	4	a1374=127.64	3	d13743=179.9
H	13	r1413=1 .083	7	a14137=120.79	4	d141374=-179.9
H	13	r1513=1.084	7	a15137=122.81	4	d151374=-0.028
H	7	r167=1.087	4	a1674=114.41	3	d16743=-0.08
$C_6H_5OCH=O$						
C						
C	1	r21=1.394				
C	2	r32=1.392	1	a321=120.35		
C	3	r43=1.390	2	a432=119.18	1	d4321=0.3
C	4	r54=1.392	3	a543=121.18	2	d5432=0.42
C	5	r65=1.394	4	a654=119.09	3	d6543=-0.9
O	4	r74=1.393	3	a743=117.75	2	d7432=177.8
C	7	r87=1.365	4	a874=118.39	3	d8743=123.9
O	8	r98=1.189	7	a987=122.03	4	d9874=175.1
H	1	r101=1.083	2	a1012=120.09	3	d10123=179.9
H	2	r112=1.083	1	a1121=120.13	6	d11216=179.7
H	3	r123=1.083	2	a1232=121.66	1	d12321=-179.9
H	5	r135=1.083	4	a1354=120.07	3	d13543=177.5
H	6	r146=1.083	5	a1465=119.48	4	d14654=179.9
H	8	r158=1.103	7	a1587=112.53	4	d15874=-5.3
$CH_3C_6H_4CH=O$						
C						
C	1	r21=1.405				
C	2	r32=1.397	1	a321=118.43		
C	3	r43=1.391	2	a432=120.76	1	d4321=0.
C	4	r54=1.396	3	a543=120.39	2	d5432=0.
C	5	r65=1.401	4	a654=119.24	3	d6543=0.
C	5	r75=1.478	4	a754=120.14	3	d7543=180.
O	7	r87=1.209	5	a875=125.00	4	d8754=180.
C	2	r92=1.507	1	a921=120.35	6	d9216=180.
H	1	r101=1.085	2	a1012=119.29	9	d10129=0.
H	3	r113=1.084	2	a1132=119.45	9	d11329=0.
H	4	r124=1.085	3	a1243=120.06	2	d12432=180.
H	6	r136=1.083	5	a1365=118.46	4	d13654=180.
H	7	r147=1.112	5	a1475=114.33	4	d14754=0.
H	9	r159=1.094	2	a1592=111.02	1	d15921=59.5
H	9	r169=1.094	2	a1692=111.02	1	d16921=-59.5
H	9	r179=1.091	2	a1792=111.54	1	d17921=179.9

[a]Distances in angstroms and angles in degrees. Geometry paramet ers optimized at the B3LYP/6-311G(d,p) level of theory.

SM 2 (cont): Geometry Parameters[a]

Structure		Bond length (angstrom)		Bond angle (degree)		Dihedral angle (degree)
$C_6H_5C(=CH_2)CH=O$						
C						
C	1	r21=1.392				
C	2	r32=1.392	1	a321=120.21		
C	3	r43=1.402	2	a432=120.77	1	d4321=-0.3
C	4	r54=1.402	3	a543=118.37	2	d5432=0.7
C	5	r65=1.391	4	a654=120.82	3	d6543=-0.7
C	4	r74=1.482	3	a743=120.70	2	d7432=-179.1
H	1	r81=1.083	2	a812=120.17	3	d8123=-179.7
H	2	r92=1.084	1	a921=120.09	6	d9216=-179.7
H	3	r103=1.084	2	a1032=119.33	1	d10321=-178.5
H	5	r115=1.084	4	a1154=119.26	3	d11543=178.0
H	6	r126=1.084	5	a1265=119.72	4	d12654=179.8
C	7	r137=1.339	4	a1374=123.90	3	d13743=136.9
C	7	r147=1.501	4	a1474=118.15	3	d14743=-44.0
O	14	r1514=1.207	7	a15147=124.52	4	d151474=177.7
H	13	r1613=1.083	7	a16137=119.48	4	d161374=178.7
H	13	r1713=1.083	7	a17137=122.17	4	d171374=-2.0
H	14	r1814=1.109	7	a18147=114.85	4	d181474=-3.3
$C_6H_5C(=CH_2)OH$						
C						
C	1	r21=1.392				
C	2	r32=1.392	1	a321=120.19		
C	3	r43=1.403	2	a432=120.73	1	d4321=0.2
C	4	r54=1.402	3	a543=118.49	2	d5432=-0.6
C	5	r65=1.390	4	a654=120.66	3	d6543=0.7
C	4	r74=1.482	3	a743=120.23	2	d7432=179.8
C	7	r87=1.336	4	a874=124.75	3	d8743=-145.1
O	7	r97=1.376	4	a974=116.10	3	d9743=31.610
H	1	r101=1.084	2	a1012=120.22	3	d10123=179.8
H	2	r112=1.084	1	a1121=120.12	6	d11216=179.5
H	3	r123=1.084	2	a1232=119.65	1	d12321=178.0
H	5	r135=1.083	4	a1354=119.25	3	d13543=-177.8
H	6	r146=1.084	5	a1465=119.66	4	d14654=-179.7
H	8	r158=1.081	7	a1587=120.29	4	d15874=-179.1
H	8	r168=1.080	7	a1687=120.91	4	d16874=3.5
H	9	r179=0.963	7	a1797=108.64	4	d17974=25.9
$C_6H_5C(=CH_2)CH_3$						
C						
C	1	r21=1.390				
C	2	r32=1.393	1	a321=120.33		
C	3	r43=1.404	2	a432=121.51	1	d4321=-0.0
C	4	r54=1.406	3	a543=117.12	2	d5432=0.0
C	5	r65=1.387	4	a654=121.46	3	d6543=-0.0
C	4	r74=1.490	3	a743=120.73	2	d7432=-179.9
C	7	r87=1.339	4	a874=123.05	3	d8743=179.9
C	7	r97=1.512	4	a974=117.73	3	d9743=-0.03
H	1	r101=1.084	2	a1012=120.49	3	d10123=-179.9
H	2	r112=1.084	1	a1121=120.14	6	d11216=179.9
H	3	r123=1.082	2	a1232=118.52	1	d12321=-179.9
H	5	r135=1.082	4	a1354=119.99	3	d13543=179.9
H	6	r146=1.084	5	a1465=119.51	4	d14654=179.9
H	8	r158=1.083	7	a1587=120.73	9	d15879=-0.0
H	8	r168=1.082	7	a1687=123.22	9	d16879=179.9
H	9	r179=1.094	7	a1797=111.53	4	d17974=59.8
H	9	r189=1.094	7	a1897=111.53	4	d18974=-59.8
H	9	r199=1.090	7	a1997=110.53	4	d19974=-179.9

[a]Distances in angstroms and angles in degrees. Geometry paramet ers optimized at the B3LYP/6-311G(d,p) level of theory.

SM 2 (cont): Geometry Parameters[a]

Structure		Bond length (Angstrom)		Bond angle (degree)		Dihedral angle (degree)
$CH_3OCH=O$						
C						
O	1	r21=1.435				
C	2	r32=1.348	1	a321=116.52		
O	3	r43=1.192	2	a432=122.80	1	d4321=-179.9
H	1	r51=1.087	2	a512=105.90	3	d5123=-179.9
H	1	r61=1.093	2	a612=111.23	3	d6123=61.5
H	1	r71=1.093	2	a712=111.23	3	d7123=-61.3
H	3	r83=1.107	2	a832=113.10	1	d8321=0.00
$Y(C_6H_6)=O$						
C						
C	1	r21=1.469				
C	2	r32=1.349	1	a321=121.38		
C	3	r43=1.456	2	a432=122.61	1	d4321=-0.007
C	4	r54=1.340	3	a543=120.73	2	d5432=-0.002
C	5	r65=1.497	4	a654=121.66	3	d6543=0.005
O	1	r71=1.217	6	a716=120.68	5	d7165=179.9
H	2	r82=1.083	1	a821=116.40	6	d8216=-179.9
H	3	r93=1.085	2	a932=119.54	1	d9321=179.9
H	4	r104=1.083	3	a1043=118.47	2	d10432=-179.9
H	5	r115=1.085	6	a1156=117.69	1	d11561=179.9
H	6	r126=1.097	5	a1265=110.24	4	d12654=122.69
H	6	r136=1.097	5	a1365=110.23	4	d13654=-122.6
$Y(C_5H_5)C(OH)=O$						
C						
C	1	r21=1.343				
C	2	r32=1.470	1	a321=109.52		
C	3	r43=1.343	2	a432=109.57	1	d4321=0.2
C	4	r54=1.515	3	a543=108.60	2	d5432=1.2
C	5	r65=1.520	4	a654=114.65	3	d6543=-128.2
O	6	r76=1.201	5	a765=126.35	4	d7654=126.8
O	6	r86=1.356	5	a865=110.89	4	d8654=-54.5
H	1	r91=1.079	5	a915=123.41	4	d9154=-177.5
H	2	r102=1.082	1	a1021=126.04	5	d10215=178.9
H	3	r113=1.082	2	a1132=124.51	1	d11321=-179.8
H	4	r124=1.079	5	a1245=123.28	1	d12451=178.9
H	5	r135=1.102	4	a1354=108.22	3	d13543=114.1
H	8	r148=0.968	6	a1486=106.42	5	d14865=-179.4
$Y(C_5H_5O)CH=O$						
C						
O	1	r21=1.442				
C	2	r32=1.360	1	a321=115.94		
C	3	r43=1.341	2	a432=123.09	1	d4321=-23.5
C	4	r54=1.457	3	a543=118.18	2	d5432=-4.7
C	1	r61=1.507	2	a612=112.50	3	d6123=40.1
C	1	r71=1.523	6	a716=113.03	5	d7165=-151.1
O	7	r87=1.201	1	a871=123.06	6	d8716=-46.9
H	1	r91=1.106	7	a917=106.76	8	d9178=74.64
H	3	r103=1.082	4	a1034=124.95	5	d10345=170.57
H	4	r114=1.080	3	a1143=119.92	2	d11432=-178.4
H	5	r125=1.084	4	a1254=119.31	3	d12543=-162.4
H	6	r136=1.082	1	a1361=117.60	7	d13617=30.052
H	7	r147=1.109	1	a1471=114.02	6	d14716=1 33.52
$Y(C_5H_5)OCH=O$						
O						
C	1	r21=1.441				
C	2	r32=1.513	1	a321=116.66		
C	3	r43=1.342	2	a432=108.54	1	d4321=-135.5
C	4	r54=1.476	3	a543=109.56	2	d5432=3.9
C	2	r62=1.513	3	a623=103.38	4	d6234=-6.0
C	1	r71=1.354	2	a712=116.08	3	d7123=61.4
O	7	r87=1.192	1	a871=122.08	2	d8712=179.9
H	2	r92=1.097	3	a923=108.25	4	d9234=108.6
H	3	r103=1.080	2	a1032=123.27	6	d10326=178.2
H	4	r114=1.082	3	a1143=126.23	2	d11432=-175.8
H	5	r125=1.082	4	a1254=124.20	3	d12543=-179.8
H	6	r136=1.080	2	a1362=123.27	3	d13623=-178.2
H	7	r147=1.103	1	a1471=113.20	2	d14712=0.1

[a]Distances in angstroms and angles in degrees. Geometry paramet ers optimized at the B3LYP/6-311G(d,p) level of theory.

SM 2 (cont): Geometry Parameters[a]

Structure		Bond length (angstrom)		Bond angle (degree)		Dihedral angle (degree)
$CH_3OC\bullet=O$						
C						
O	1	r21=1.445				
C	2	r32=1.334	1	a321=116.00		
O	3	r43=1.181	2	a432=126.92	1	d4321=-179.9
H	1	r51=1.087	2	a512=105.36	3	d5123=179.9
H	1	r61=1.090	2	a612=110.44	3	d6123=61.08
H	1	r71=1.090	2	a712=110.44	3	d7123=-61.1
$CH_2=C\bullet CH=O$						
C						
C	1	r21=1.314				
C	2	r32=1.462	1	a321=132.53		
O	3	r43=1.204	2	a432=126.97	1	d4321=179.9
H	1	r51=1.093	2	a512=121.39	3	d5123=-0.03
H	1	r61=1.086	2	a612=122.47	3	d6123=-179.9
H	3	r73=1.118	2	a732=111.92	1	d7321=0.0
$CH_2=CHC\bullet=O$						
C	1	r21=1.333				
C	2	r32=1.476	1	a321=120.40		
O	3	r43=1.185	2	a432=128.33	1	d4321=180.
H	1	r51=1.084	2	a512=120.57	3	d5123=0.
H	1	r61=1.083	2	a612=121.77	3	d6123=180.
H	2	r72=1.089	1	a721=122.38	5	d7215=180.
$CH_2=CHC\bullet(CH=O)C\equiv CH$						
C						
C	1	r21=1.355				
C	2	r32=1.426	1	a321=125.53		
C	3	r43=1.474	2	a432=118.77	1	d4321=179.99
O	4	r54=1.215	3	a543=123.66	2	d5432=0.0330
H	1	r61=1.084	2	a612=121.65	3	d6123=0.0293
H	1	r71=1.082	2	a712=120.87	3	d7123=-179.9
H	2	r82=1.085	3	a823=114.33	4	d8234=0.0217
H	4	r94=1.106	3	a943=114.95	2	d9432=-179.9
C	3	r103=1.401	2	a1032=123.31	1	d10321=-0.01
C	10	r1110=1.211 3		a11103=178.24	2	d111032=175.5
H	11	r1211=1.062 10		a121110=179.87	3	d1211103=172.7
$C\bullet(OH)_2CH=O$						
C						
C	1	r21=1.409				
O	2	r32=1.255	1	a321=117.84		
O	1	r41=1.330	2	a412=118.71	3	d4123=-0.01
O	1	r51=1.331	2	a512=124.44	3	d5123=-179.9
H	2	r62=1.096	1	a621=118.49	4	d6214=-179.9
H	4	r74=0.982	1	a741=103.24	2	d7412=0.02
H	5	r85=0.966	1	a851=108.88	2	d8512=179.9
$CH_2=CHC\bullet(CH=O)CH=O$						
C						
C	1	r21=1.470				
C	2	r32=1.413	1	a321=118.23		
C	3	r43=1.365	2	a432=126.37	1	d4321=-179.9
C	2	r52=1.466	1	a521=116.30	3	d5213=-179.9
O	5	r65=1.216	2	a652=126.17	1	d6521=179.96
H	1	r71=1.108	2	a712=115.16	3	d7123=179.99
H	3	r83=1.086	2	a832=114.39	1	d8321=-0.009
H	4	r94=1.083	3	a943=120.00	2	d9432=179.97
H	4	r104=1.080	3	a1043=121.38	2	d10432=-0.005
H	5	r115=1.109	2	a1152=113.94	1	d11521=0.029
O	1	r121=1.216	2	a1212=124.44	3	d12123=-0.006

[a]Distances in angstroms and angles in degrees. Geometry paramet ers optimized at the B3LYP/6-311G(d,p) level of theory.

SM 2 (cont): Geometry Parameters[a]

Structure	Bond length (angstrom)		Bond angle (degree)		Dihedral angle (degree)	
Furanj1						
C						
C	1	r21=1.356				
C	2	r32=1.445	1	a321=107.19		
C	3	r43=1.354	2	a432=103.40	1	d4321=-0.03
O	4	r54=1.328	3	a543=114.12	2	d5432=0.01
H	1	r61=1.075	2	a612=134.65	3	d6123=-179.9
H	2	r72=1.079	1	a721=126.33	5	d7215=-179.9
H	3	r83=1.076	2	a832=128.45	1	d8321=179.9
Furanj2						
C						
C	1	r21=1.362				
C	2	r32=1.421	1	a321=103.75		
C	3	r43=1.348	2	a432=109.81	1	d4321=-0.01
O	4	r54=1.375	3	a543=107.86	2	d5432=-0.007
H	1	r61=1.077	2	a612=132.98	3	d6123=-179.9
H	2	r72=1.077	1	a721=127.27	5	d7215=-179.9
H	4	r84=1.074	3	a843=135.61	2	d8432=-179.9
Y(C_6H_5•)=O						
C						
C	1	r21=1.452				
C	2	r32=1.374	1	a321=120.94		
C	3	r43=1.407	2	a432=120.25	1	d4321=0.02
C	4	r54=1.407	3	a543=120.68	2	d5432=-0.03
C	5	r65=1.374	4	a654=120.25	3	d6543=0.02
O	1	r71=1.251	6	a716=121.53	5	d7165=179.9
H	2	r82=1.083	1	a821=116.86	6	d8216=179.9
H	3	r93=1.084	2	a932=120.30	1	d9321=-179.9
H	4	r104=1.083	3	a1043=119.65	2	d10432=179.9
H	5	r115=1.084	6	a1156=120.30	1	d11561=-179.9
H	6	r126=1.083	5	a1265=122.17	4	d12654=179.9
C_6H_5C•=O						
C						
C	1	r21=1.399				
C	2	r32=1.391	1	a321=119.80		
C	3	r43=1.397	2	a432=119.87	1	d4321=0.003
C	4	r54=1.403	3	a543=120.22	2	d5432=-0.02
C	5	r65=1.388	4	a654=119.68	3	d6543=0.029
C	4	r74=1.481	3	a743=119.31	2	d7432=179.9
O	7	r87=1.186	4	a874=128.52	3	d8743=179.8
H	1	r91=1.084	2	a912=119.78	3	d9123=179.9
H	2	r102=1.083	1	a1021=120.09	6	d10216=-179.9
H	3	r113=1.083	2	a1132=121.13	1	d11321=179.9
H	5	r125=1.083	4	a1254=119.03	3	d12543=-179.9
H	6	r136=1.084	5	a1365=120.05	4	d13654=179.9

[a]Distances in angstroms and angles in degrees. Geometry paramet ers optimized at the B3LYP/6-311G(d,p) level of theory.

SM 2 (cont): Geometry Parameters[a]

Structure	Bond length (angstrom)		Bond angle (degree)		Dihedral angle (degree)	
Y(C_5H_5)C(O•)=O						
C						
C	1	r21=1.372				
C	2	r32=1.433	1	a321=109.46		
C	3	r43=1.371	2	a432=109.05	1	d4321=0.7
C	4	r54=1.505	3	a543=108.53	2	d5432=-2.7
C	5	r65=1.601	4	a654=104.32	3	d6543=-109.3
O	6	r76=1.205	5	a765=122.80	4	d7654=-176.1
O	6	r86=1.281	5	a865=106.24	4	d8654=3.7
H	1	r91=1.080	5	a915=123.68	4	d9154=-178.7
H	2	r102=1.08	1	a1021=125.59	5	d10215=-177.4
H	3	r113=1.08	2	a1132=125.08	1	d11321=-178.3
H	4	r124=1.07	5	a1245=124.40	1	d12451=-175.1
H	5	r135=1.09	4	a135=117.53	3	d13543=133.02
Y(C_5H_5O)C•=O						
C						
O	1	r21=1.425				
C	2	r32=1.356	1	a321=116.38		
C	3	r43=1.343	2	a432=123.17	1	d4321=21.68
C	4	r54=1.452	3	a543=118.18	2	d5432=4.559
C	1	r61=1.492	2	a612=113.41	3	d6123=-38.2
C	1	r71=1.595	6	a716=109.38	5	d7165=-91.4
O	7	r87=1.176	1	a871=123.74	6	d8716=-66.7
H	1	r91=1.091	6	a916=113.42	5	d9165=151.9
H	3	r103=1.082	4	a1034=124.95	5	d10345=-171.0
H	4	r114=1.080	3	a1143=119.94	2	d11432=178.69
H	5	r125=1.083	4	a1254=119.49	3	d12543=164.28
H	6	r136=1.082	1	a1361=118.28	2	d13612=-153.1
Y(C_5H_5)OC•=O						
C						
C	1	r21=1.510				
C	2	r32=1.340	1	a321=108.49		
C	3	r43=1.480	2	a432=109.49	1	d4321=3.5
C	1	r51=1.509	2	a512=103.70	3	d5123=-5.3
O	1	r61=1.452	2	a612=112.79	3	d6123=-127.7
C	6	r76=1.334	1	a761=116.68	2	d7612=-121.4
O	7	r87=1.181	6	a876=127.24	1	d8761=-179.9
H	1	r91=1.098	2	a912=109.82	3	d9123=111.9
H	2	r102=1.080	1	a1021=123.27	5	d10215=177.4
H	3	r113=1.081	2	a1132=126.27	1	d11321=-176.5
H	4	r124=1.081	3	a1243=124.24	2	d12432=179.9
H	5	r135=1.080	1	a1351=123.27	2	d13512=-177.4

[a]Distances in angstroms and angles in degrees. Geometry paramet ers optimized at the B3LYP/6-311G(d,p) level of theory.

SM 3: Vibrational Frequencies[a] (cm^{-1})

Molecules	Frequencies ν[a]
$CH(OH)_2CH=O$	133.1, 250.7, 291.6, 361.2, 436.2, 551.8, 733.3, 839.1, 978.6, 1070.0, 1134.0, 1219.7, 1310.6, 1376.3, 1402.2, 1478.2, 1822.8, 2953.7, 2996.7, 3723.2, 3823.8
$CH_2=CHCH(CH=O)CH=O$	63.9, 64.9, 145.8, 213.8, 232.8, 294.6, 412.9, 557.3, 665.0, 765.1, 777.2, 881.2, 929.7, 961.0, 982.7, 1020.3, 1097.2, 1187.8, 1210.5, 1288.2, 1328.8, 1402.1, 1426.8, 1464.5, 1714.8, 1800.8, 1838.5, 2861.3, 2881.7, 2982.6, 3128.3, 3174.3, 3216.0
$CH_3C(OH)_2CH=O$	115.3, 168.2, 226.7, 277.4, 317.5, 374.2, 396.0, 475.2, 526.5, 645.0, 829.4, 895.4, 950.1, 993.2, 1084.7, 1148.1, 1200.0, 1326.6, 1371.2, 1408.3, 1437.3, 1485.7, 1496.9, 1821.6, 2948.6, 3037.4, 3106.3, 3121.9, 3718.6, 3809.2
$CH_2=CHCH(CH=O)CH=CH_2$	59.1, 59.2, 113.7, 209.3, 270.5, 286.8, 434.3, 469.3, 507.5, 628.3, 685.2, 911.1, 930.1, 954.8, 956.3, 1016.0, 1026.0, 1028.3, 1031.5, 1117.1, 1182.7, 1250.1, 1286.5, 1323.6, 1332.2, 1416.6, 1450.0, 1456.5, 1694.2, 1704.2, 1816.9, 2859.3, 3074.6, 3120.6, 3125.2, 3134.2, 3135.5, 3216.2726, 3216.6
$CH_2=CHC(OH)_2CH=CH_2$	89.4, 104.1, 288.6, 288.8, 309.9, 346.3, 390.2, 422.7, 437.6, 541.8, 627.5, 669.9, 708.3, 778.1, 972.1, 973.6, 979.1, 993.7, 1007.1, 1032.4, 1037.9, 1166.8, 1172.9, 1313.4, 1317.6, 1317.7, 1366.5, 1441.2, 1452.2, 1702.3, 1703.4, 3140.7, 3141.1, 3161.7, 3162.1, 3233.7, 3233.8, 3812.6, 3814.0
$CH_2=CHCH=O$	171.9, 319.0, 572.3, 612.2, 919.4, 996.5, 1028.3, 1040.3, 1166.0, 1294.9, 1389.4, 1453.3, 1679.7, 1785.6, 2866.2, 3130.8, 3170.2, 3222.3
$CH_2=C(OH)_2$	276.3, 453.9, 486.9, 539.0, 599.2, 731.2, 817.4, 925.5, 971.6, 1234.7, 1238.9, 1318.6, 1420.9, 1769.9, 3183.0, 3281.6, 3776.6, 3782.1
$CH_2=CHCH(CH_3)CH=CH_2$	78.9, 105.8, 229.7, 256.2, 295.1, 308.5, 434.3, 501.6, 647.1, 720.6, 830.8, 915.8, 942.2, 944.6, 977.1, 1017.2, 1031.8, 1035.2, 1059.8, 1169.7, 1204.5, 1296.7, 1320.0, 1322.9, 1329.7, 1402.8, 1452.7, 1455.7, 1497.8, 1498.4, 1699.2, 1709.2, 3022.8, 3028.6, 3087.6, 3100.2, 3107.8, 3113.7, 3126.5, 3127.3, 3207.6, 3208.1
$CH_2=C(CHO)CH=CH_2$	131.0, 162.5, 253.1, 367.9, 393.3, 443.8, 657.1, 668.9, 781.2, 800.9, 964.1, 964.8, 985.9, 1022.4, 1037.9, 1078.2, 1336.5, 1355.9, 1396.7, 1428.2, 1472.5, 1641.0, 1692.3, 1786.9, 2874.6, 3126.8, 3139.1, 3154.1, 3223.9, 3256.5
$CH_2=CHOCH=CH_2$	84.0, 109.5, 230.0, 488.9, 520.7, 687.6, 715.3, 857.2, 861.4, 861.8, 963.7, 976.8, 1032.5, 1205.3, 1212.6, 1330.9, 1353.7, 1420.9, 1433.0, 1685.6, 1736.7, 3135.5, 3143.3, 3165.6, 3166.3, 3257.7, 3257.8
$CH_2=CHCH(OH)CH=CH_2$	98.5, 145.4, 243.8, 318.7, 360.8, 368.8, 543.5, 585.9, 612.9, 714.5, 888.3, 956.3, 960.1, 986.2, 999.0, 1029.4, 1038.8, 1052.9, 1158.0, 1271.2, 1281.6, 1311.4, 1338.4, 1414.4, 1437.8, 1438.0, 1697.0, 1709.7, 2990.6, 3127.1, 3133.3, 3143.0, 3145.5, 3223.5, 3224.0, 3788.8
$CH_3OCH=O$	-63.2, 179.5, 344.5, 634.4, 1031.0, 1041.4, 1123.2, 1169.5, 1240.1, 1421.3, 1482.5, 1496.7, 1497.7, 1855.8, 2930.6, 3026.0, 3092.5, 3152.3
$CH_2CHCH(CH=O)C\equiv CH$	60.5, 94.9, 150.3, 204.4, 247.9, 378.1, 492.2, 525.6, 599.2, 670.4, 698.5, 711.2, 751.8, 961.5, 966.4, 999.9, 1026.4, 1051.6, 1126.0, 1231.1, 1286.6, 1333.8, 1406.4, 1443.9, 1709.6, 1821.7, 2222.9, 2907.4, 2938.8, 3138.7, 3172.8, 3224.6, 3475.3
$CH_2=C(CH=O)C\equiv CH$	146.7, 158.5, 254.9, 310.3, 468.0, 561.8, 678.4, 690.3, 693.9, 739.0, 774.5, 958.8, 970.3, 1026.5, 1294.8, 1391.3, 1448.4, 1656.4, 1801.2, 2217.6, 2884.0, 3144.2, 3241.1, 3477.0
$CH_2=CHCH_2CH=O$	63.26, 110.97, 276.62, 416.64, 510.02, 626.42, 770.06, 937.87, 955.57, 993.12, 1030.50, 1049.99, 1155.52, 1223.62, 1282.72, 1330.01, 1422.24, 1445.60, 1462.47, 1707.48, 1820.37, 2857.05, 2986.05, 3096.00, 3125.13, 3133.72, 3215.74,
$Y(C_5H_5)C(OH)=O$	32.55, 133.55, 193.49, 411.65, 433.47, 527.89, 585.07, 643.24, 705.08, 714.75, 725.12, 820.50, 846.04, 900.75, 957.88, 960.57, 976.15, 1018.15, 1036.36, 1107.02, 1128.42, 1142.63, 1208.27, 1256.74, 1308.95, 1356.72, 1395.03, 1562.04, 1645.25, 1829.40, 2987.20, 3195.19, 3206.72, 3235.58, 3239.80, 3758.43
$Y(C_5H_5O)CH=O$	75.57, 84.82, 209.13, 329.29, 384.20, 448.77, 562.39, 611.11, 633.65, 732.15, 784.41, 824.23, 906.57, 933.23, 977.44, 990.51, 998.87, 1060.90, 1095.05, 1101.06, 1179.67, 1243.94, 1299.85, 1331.48, 1372.13, 1393.68, 1437.00, 1621.75, 1694.43, 1826.21, 2897.23, 2911.30, 3173.19, 3195.70, 3203.47, 3218.84,
$Y(C_5H_5)OCH=O$	100.18, 120.62, 127.28, 306.75, 350.49, 474.75, 552.82, 681.37, 731.14, 753.03, 801.84, 859.34, 894.75, 964.83, 969.22, 987.29, 1030.34, 1051.71, 1056.53, 1106.31, 1107.59, 1155.72, 1234.79, 1310.81, 1349.23, 1388.67, 1419.61, 1565.53, 1646.59, 1851.42, 2983.02, 3034.45, 3196.54, 3206.56, 3226.69, 3231.37

[a]Frequencies are calculated at B3LYP/6-311 level of theory.

SM3 (cont): Vibrational Frequencies[a] (cm^{-1})

Molecules	Frequencies ν[a]
$C_6H_5OCH=O$	152.9, 302.1, 398.5, 424.1, 449.1, 541.3, 630.2, 673.6, 708.7, 774.7, 843.5, 882.2, 921.5, 978.3, 1000.8, 1017.0, 1037.2, 1044.6, 1095.5, 1112.0, 1181.4, 1187.7, 1232.3, 1326.3, 1347.6, 1407.9, 1487.1, 1521.5, 1633.9, 1639.3, 1857.1, 2981.6, 3170.9, 3179.4, 3187.8, 3195.4, 59.7, 127.0, 3201.3
$C_6H_5C(CH=O)=CH_2$	59.2, 116.4, 122.4, 213.6, 290.7, 358.4, 392.1, 415.4, 502.8, 551.7, 634.6, 659.0, 707.8, 719.6, 790.4, 811.5, 856.0, 925.3, 945.2, 981.5, 989.7, 1005.3,1016.3, 1039.3, 1049.3, 1102.2, 1121.8, 1183.9, 1206.2, 1285.5, 1324.8, 1355.1, 1416.1, 1432.3, 1476.8, 1527.0, 1615.6, 1643.4, 1659.3, 1789.3, 2906.6, 3145.1, 3161.6, 3166.7, 3176.0, 3183.1, 3192.3, 3238.3
$C_6H_5C(OH)_2CH_3$	48.6, 129.5, 211.5, 254.7, 297.4, 327.6, 339.1, 365.7, 413.0, 422.5, 494.2, 515.4, 582.5, 610.5, 635.0, 718.1, 736.5, 779.8, 865.4, 910.9, 941.3, 946.8, 991.2, 1006.3, 1018.0, 1042.0, 1053.3, 1092.3, 1115.4, 1167.4, 1181.9, 1188.3, 1203.7, 1327.0, 1339.4, 1349.3, 1401.4, 1416.3, 1479.7, 1481.9, 1496.6, 1526.6, 1626.4, 1647.1, 3035.8, 3108.3, 3132.1, 3160.3, 3170.0, 3182.1, 3190.2, 3208.5, 3796.5, 3815.1
$C_6H_5C(=CH_2)CH=CH_2$	60.4, 104.1, 130.3, 227.3, 290.5, 347.7, 379.6, 417.8, 471.5, 527.5, 629.8, 640.2, 694.0, 715.8, 758.1, 773.6, 796.5, 859.6, 905.6, 929.5, 939.5, 952.6, 984.3, 1003.5, 1016.5, 1032.2, 1049.4, 1090.7, 1102.4, 1121.5, 1182.4, 1205.4, 1285.4, 1318.9, 1332.3, 1355.5, 1434.1, 1453.5, 1477.7, 1526.2, 1615.3, 1643.7, 1658.3, 1687.4, 3126.8, 3136.8, 3145.0, 3159.7, 3167.1, 3177.0, 3183.2, 3190.4, 3219.2, 3230.0
$C_6H_5C(CH_3)_2CH=O$	45.1712, 67.4533, 123.3751, 201.1980, 232.3457, 264.5411, 294.6710, 307.9790, 325.4132, 362.9875, 385.3833, 416.2486, 498.1502, 545.3619, 634.7822, 648.1830, 718.5845, 740.6084, 777.1340, 835.0899, 860.4637, 913.3619, 934.7146, 956.1532, 986.7171, 1006.6052, 1015.8882, 1018.2715, 1042.5856, 1052.2429, 1104.1722, 1125.0801, 1182.0116, 1184.8551, 1214.1755, 1229.9720, 1256.8653, 1324.9159, 1361.5549, 1399.4556, 1403.1972, 1426.1813, 1476.1035, 1487.1526, 1488.5668, 1508.0678, 1511.9388, 1528.8173, 1622.5095, 1643.7437, 1805.1173, 2866.8254, 3029.4879, 3040.4446, 3096.3728, 3099.2736, 3106.4514, 3120.6596, 3161.3615, 3168.0606, 3177.7726, 3188.4460, 3198.4488
$C_6H_5CH=O$	122.3, 220.5, 241.6, 419.4, 442.5, 469.5, 631.2, 663.2, 707.6, 764.9, 838.0, 866.0, 943.1, 996.2, 1015.8, 1016.9, 1039.4, 1043.5, 1100.8, 1183.5, 1187.6, 1223.7, 1334.6, 1351.5, 1420.5, 1486.2, 1521.1, 1624.4, 1641.6, 1783.6, 2873.5, 3158.0, 3168.4, 3179.4, 3189.6, 3196.5
$C_6H_5C(=CH_2)OH$	77.8164, 145.2172, 216.4201, 358.3417, 386.6724, 387.5545, 421.8260, 515.8712, 571.6101, 627.6971, 639.2967, 714.7375, 729.6232, 760.9114, 788.8409, 851.4888, 862.4696, 938.2986, 971.3077, 986.4726,1005.8988, 1015.1444, 1047.9546, 1103.6944, 1122.0632, 1183.4003, 1203.6383, 1262.5972, 1312.7481, 1343.1420, 1353.8735, 1427.7336, 1476.7821, 1525.1802, 1616.1146, 1644.3383, 1708.6430, 3162.3495, 3166.9977, 3169.3403, 3178.3189, 3186.8308, 3193.5391, 3260.6021, 3815.0561,
$C_6H_5C(=CH_2)CH_3$	-55.4, 153.1, 241.7, 246.9, 383.1, 406.3, 418.6, 456.4, 541.7, 551.2, 635.8, 679.3, 717.8, 747.0, 797.7, 846.4, 914.0, 927.5, 935.9, 975.2, 999.3, 1015.3,1025.0,1053.4, 1069.6,1115.3,1136.4, 1184.7,1217.1,1302.9, 1328.8,1362.2,1414.7,1445.1, 1478.1, 1486.9, 1503.9, 1532.4, 1616.9, 1644.6, 1687.1, 3020.9, 3067.5, 3111.5, 3150.0, 3160.8, 3169.3, 3184.1, 3193.9, 3200.6, 3228.6
$CH_3C_6H_4CH=O$	-2.14, 96.85, 187.30, 197.37, 314.22, 350.01, 409.78, 423.65, 498.53, 613.88, 653.57, 727.24, 769.78, 824.53, 856.95, 860.25, 967.60, 998.43, 1009.15, 1034.71, 1038.57, 1061.60, 1134.56, 1189.73, 1227.03, 1234.58, 1331.10, 1339.15, 1415.81, 1418.59, 1446.92, 1487.22, 1497.22, 1539.34, 1611.41, 1650.46, 1779.70, 2869.90, 3027.18, 3076.54, 3109.01, 3154.22, 3159.39, 3172.11, 3191.31,
$C_6H_5CH=CH_2$	36.2, 205.3, 235.5, 411.9, 446.5448.6, 561.5, 635.0, 655.4, 710.5, 787.4, 798.7, 849.8, 927.6, 930.1, 976.2, 998.8, 1014.9, 1029.9, 1040.2, 1056.2, 1111.9, 1182.7, 1205.3, 1226.6, 1318.1, 1345.4, 1362.5, 1451.8, 1483.2, 1528.6, 1618.1, 1644.4, 1690.5, 3128.9, 3143.1, 3157.1, 3163.6, 3173.5, 3182.3, 3190.6, 3222.4
$Y(C_6H_6)=O$	57.2, 270.8, 444.8, 455.8, 494.2, 541.2, 578.8, 724.4, 743.4, 814.6, 944.6, 945.9, 953.8, 998.0, 998.4, 1026.7, 1159.6, 1192.1, 1193.1, 1242.9, 1333.9, 1398.9, 1408.2, 1443.9, 1608.9, 1693.5, 1746.0, 3014.8, 3033.7, 3153.3, 3158.4, 3183.3, 3190.8

[a]Frequencies are calculated at the B3LYP/6-311g(d,p) level of theory.

SM3 (cont): Vibrational Frequencies[a] (cm^{-1})

Molecules	Frequencies ν[a]
$CH_3OC\bullet=O$	65.8, 220.3, 318.7, 617.7, 990.3, 1115.2, 1170.6, 1217.1, 1475.9, 1491.8, 1498.1, 1878.7, 3050.3, 3127.8, 3161.7
$CH_2=C\bullet CH=O$	73.8, 242.3, 437.8, 561.5, 860.8, 947.0, 988.6, 1089.2,1370.8, 1418.9, 1691.2, 1773.6, 2796.8, 3045.4, 3164.3
$CH_2=CHC\bullet=O$	147.27, 311.41, 543.88, 640.64, 881.83, 1004.19, 1017.28, 1102.23, 1288.25, 1423.03, 1669.89, 1898.41, 3109.48, 3144.15, 3233.71
$CH_2CHC\bullet(CH=O)C\equiv CH$	144.1, 145.5, 178.5, 216.0, 285.1, 392.7, 491.0, 546.0, 604.1, 634.9, 663.2, 681.4, 791.7, 924.4, 997.3, 1025.8, 1034.6, 1193.9, 1284.5, 1321.2, 1424.4, 1436.1, 1561.6, 1699.8, 2115.7, 2937.0, 3143.7, 3173.0, 3237.2, 3467.3
$C\bullet(OH)_2CH=O$	268.2, 276.3, 346.5, 463.2, 524.2, 664.7, 711.5, 869.9, 932.3, 1180.0, 1255.3, 1318.3, 1480.5, 1524.0, 1640.9, 3042.9, 3524.6, 3797.4
$CH_2=CHC\bullet(CH=O)CH=O$	116.7, 172.6, 235.2, 246.0, 259.0, 367.5, 419.8, 487.9, 603.2, 750.2, 830.6, 932.1, 969.8, 1027.8, 1034.4, 1037.6, 1182.9, 1289.8, 1365.1, 1434.5, 1436.4, 1469.4, 1541.8, 1669.2, 1738.4, 2890.2, 2914.9, 3150.2, 3156.6, 3261.6
Furanj1	481.1, 606.4, 708.3, 780.8, 863.4, 865.2, 873.4, 1013.1, 1043.4,1106.3, 1180.6, 1246.5, 1376.6, 1472.0, 1591.8, 3259.2, 3296.2, 3304.6
Furanj2	546.3, 616.6, 700.1, 759.7, 842.3, 864.6, 872.1, 1027.2, 1060.6,1155.6, 1188.9, 1250.2, 1391.8, 1507.0, 1564.0, 3273.5, 3293.5, 3315.2
$Y(C_6H_5\bullet)=O$	190.4, 379.4, 445.6, 483.9, 531.3, 597.5, 656.1, 802.2, 804.0, 804.9, 928.0, 984.0, 987.6, 999.7, 1008.9, 1088.6, 1163.4, 1164.7, 1271.7, 1336.8, 1419.2, 1442.9, 1481.1, 1546.3, 1587.4, 3165.9, 3171.8, 3187.6, 3195.2, 3198.5
$Y(C_5H_5)C(O\bullet)=O$	89.3, 117.1, 171.2, 329.8, 396.7, 443.1, 545.8, 665.4, 699.9, 770.6, 818.5, 822.7, 844.3, 930.9, 957.4, 966.4, 1014.1, 1032.0, 1060.5, 1107.2, 1130.8, 1216.9, 1271.3, 1333.5, 1425.3, 1448.2, 1541.6, 1762.4, 3098.2, 3207.6, 3221.0, 3236.5, 3252.7
$Y(C_5H_5O)C\bullet=O$	84.9, 116.9, 220.8, 339.6, 373.0, 454.5, 525.1, 582.3, 638.9, 698.7, 741.6, 795.6, 878.9, 935.6, 970.8, 979.6, 993.4, 1039.8,1108.8, 1171.3, 1193.8, 1254.5, 1342.4, 1388.4, 1444.3, 1602.5, 1680.3, 1917.2, 3082.4, 3176.7, 3201.6, 3203.8, 3222.7
$Y(C_5H_5)OC\bullet=O$	28.5, 122.4, 198.1, 303.9, 343.9, 432.2, 550.2, 645.1, 723.4, 752.0, 802.3, 847.9, 919.8, 965.8, 967.1, 980.6, 1041.0, 1051.7, 1110.1, 1125.9, 1151.3, 1252.3, 1312.8, 1322.7, 1388.8, 1581.8, 1656.0, 1388.8, 1581.8, 1656.0, 3209.4, 3231.3, 3235.8
$C_6H_5C\bullet=O$	112.7, 206.6, 242.1, 416.7, 441.0, 469.0, 624.0, 635.9, 704.7, 767.8, 805.4, 865.8, 954.3, 996.3, 1017.5, 1018.1, 1044.4, 1099.0, 1160.9, 1184.9, 1199.5, 1331.4, 1348.1, 1478.5, 1511.4, 1618.1, 1634.2, 1890.2, 3166.4, 3176.3, 3183.4, 3191.9, 3195.6716

[a]Frequencies are calculated at the B3LYP/6-311g(d,p) level of theory.

SM4: Moment of Inertia[a]

	I_a [b]	I_b	I_c
$C(OH)_2CH=O$	11.22	4.35	3.13
$CH_2=CHCH(CH=O)CH=O$	2.92	2.46	1.52
$CH_3C(OH)_2CH=O$	5.06	2.91	2.88
$CH_2=CHCH(CHO)CH=CH_2$	2.63	2.34	1.40
$CH_2=CHC(OH)_2CH=CH_2$	4.24	1.96	1.84
$CH_2=CHCH=O$	48.20	4.65	4.24
$CH_2=C(OH)_2$	10.75	10.09	5.29
$CH_2=CHCH(CH_3)CH=CH_2$	4.81	2.51	1.86
$CH_2=C(CHO)CH=CH_2$	4.28	4.07	2.08
$CH_2=CHOCH=CH_2$	35.13	2.50	2.33
$CH_2=CHCH(OH)CH=CH_2$	7.31	2.35	1.97
$CH_3OCH=O$	47.52	4.69	4.38
$CH_2CHCH(CH=O)C\equiv CH$	3.33	2.35	1.46
$CH_2=C(CH=O)C\equiv CH$	4.97	3.48	2.05
$CH_2=CHCH_2CH=O$	16.70	2.51	2.44
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$C_6H_5OCH=O$	4.99	0.97	0.83
$C_6H_5C(CH=O)=CH_2$	3.34	0.81	0.69
$C_6H_5C(OH)_2CH_3$	2.71	0.95	0.82
$C_6H_5C(=CH_2)CH=CH_2$	3.13	0.86	0.70
$C_6H_5C(CH_3)_2CH=O$	2.05	0.79	0.66
$C_6H_5CH=O$	5.25	1.56	1.20
$C_6H_5C(=CH_2)OH$	3.72	0.94	1.19
$C_6H_5C(=CH_2)CH_3$	3.61	1.21	0.91
$C_6H_5CH=CH_2$	5.20	1.53	1.18
$CH_3C_6H_4CH=O$	5.01	0.98	0.82
$Y(C_6H_6)=O$	5.19	2.68	1.79
$Y(C_5H_5)C(OH)=O$	4.49	1.64	1.30
$Y(C_5H_5)OCH=O$	4.92	1.36	1.29
$Y(C_5H_5O)CH=O$	4.95	1.59	1.23

[a]Optimized at the B3LYP/6 -311g(d,p) level of theory. [b]Units in GHz

SM4: Moment of Inertia[a]

	I_a [b]	I_b	I_c
$CH_3OC\bullet=O$	59.03	4.69	4.46
$CH_2=C\bullet CH=O$	70.32	4.46	4.19
$CH_2=CHC\bullet=O$	61.32	4.65	4.33
$CH_2CHC\bullet(CH=O)C\equiv CH$	3.44	2.36	1.39
$C\bullet(OH)_2CH=O$	11.21	4.35	3.13
$CH_2=CHC\bullet(CH=O)CH=O$	4.21	2.10	1.40
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Furanj1	10.52	9.18	4.90
Furanj2	10.60	9.18	4.92
$Y(C_6H_5\bullet)=O$	5.52	2.78	1.85
$Y(C_5H_5)C(O\bullet)=O$	4.38	1.54	1.88
$Y(C_5H_5O)C\bullet=O$	3.95	1.79	1.49
$Y(C_5H_5)OC\bullet=O$	7.24	1.17	1.04
$C_6H_5C\bullet=O$	5.42	1.22	1.57

[a]Optimized at the B3LYP/6 -311g(d,p) level of theory. [b]Units in GHz

SM5: Total Energy and Internal Rotation Barriers about C—C bonds in $C_6H_5C(OH)_2$ —CH_3, $C_6H_5C(—CH_3)_2CH=O$, $CH_2=CHCH(—CH_3)CH=CH_2$ and $CH_3—C(OH)_2CH=O$

$C_6H_5C(OH)_2—CH_3$			$C_6H_5C(—CH_3)_2CH=O$			$CH_2=CHCH(—CH_3)CH=CH_2$			$CH_3—C(OH)_2CH=O$		
Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion angle	Total energy[a]	Rotational barrier[b]	Torsion angle	Total energy[a]	Rotational barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]
0.0	-461.331104003	3.71	0.0	-463.517917143	2.64	0.0	-234.621137251	3.27	0.0	-343.588739609	2.86
15.0	-461.332276048	2.98	15.0	-463.517880420	2.66	15.0	-234.621860833	2.82	15.0	-343.589264236	2.54
30.0	-461.334450280	1.61	30.0	-463.519238390	1.81	30.0	-234.623715482	1.65	30.0	-343.590887860	1.52
45.0	-461.336348008	0.42	45.0	-463.520991169	0.71	45.0	-234.625536482	0.51	45.0	-343.592533007	0.48
60.0	-461.337024930	0.00	60.0	-463.522102528	0.01	60.0	-234.626351541	0.00	60.0	-343.593301348	0.00
75.0	-461.336159792	0.54	75.0	-463.522115908	0.00	75.0	-234.625771438	0.36	75.0	-343.592840279	0.29
90.0	-461.334090676	1.84	90.0	-463.521068453	0.66	90.0	-234.624080217	1.42	90.0	-343.591382334	1.21
105.0	-461.331923568	3.20	105.0	-463.519299366	1.77	105.0	-234.622148514	2.63	105.0	-343.589670637	2.28
120.0	-461.331095749	3.72	120.0	-463.517913395	2.64	120.0	-234.621144595	3.26	120.0	-343.588738420	2.87
135.0	-461.332242896	3.00	135.0	-463.517889547	2.66	135.0	-234.621805172	2.85	135.0	-343.589309185	2.51
150.0	-461.334471772	1.60	150.0	-463.519254401	1.80	150.0	-234.623675217	1.68	150.0	-343.590989350	1.45
165.0	-461.336393949	0.39	165.0	-463.520993335	0.71	165.0	-234.625541530	0.51	165.0	-343.592603711	0.44
180.0	-461.337018129	0.00	180.0	-463.522096235	0.02	180.0	-234.626353762	0.00	180.0	-343.593307064	0.00
195.0	-461.336080906	0.59	195.0	-463.522129087	0.00	195.0	-234.625730659	0.39	195.0	-343.592811007	0.31
210.0	-461.334005209	1.89	210.0	-463.521109512	0.64	210.0	-234.623999572	1.47	210.0	-343.591348894	1.23
225.0	-461.331895012	3.22	225.0	-463.519348715	1.74	225.0	-234.622090393	2.67	225.0	-343.589646220	2.30
240.0	-461.331095498	3.72	240.0	-463.517962655	2.61	240.0	-234.621138500	3.27	240.0	-343.588735376	2.87
255.0	-461.332228068	3.01	255.0	-463.517828617	2.69	255.0	-234.621810049	2.85	255.0	-343.589331560	2.49
270.0	-461.334451400	1.61	270.0	-463.519083899	1.91	270.0	-234.623631931	1.70	270.0	-343.591034798	1.42
285.0	-461.336375057	0.40	285.0	-463.520863728	0.79	285.0	-234.625485670	0.54	285.0	-343.592652926	0.41
300.0	-461.337021123	0.00	300.0	-463.522069940	0.03	300.0	-234.626348271	0.00	300.0	-343.593311559	0.00
315.0	-461.336099012	0.58	315.0	-463.522125257	0.00	315.0	-234.625777967	0.36	315.0	-343.592745967	0.35
330.0	-461.333995530	1.90	330.0	-463.521065030	0.66	330.0	-234.624043933	1.45	330.0	-343.591268979	1.28
345.0	-461.331852289	3.24	345.0	-463.519287672	1.78	345.0	-234.622092826	2.67	345.0	-343.589622848	2.31
360.0	-461.331103911	3.71	360.0	-463.517917143	2.64	360.0	-234.621136767	3.27	360.0	-343.588739402	2.86

[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/mol.

SM6: Total Energy and Internal Rotation Barriers about C—C_b and C—C_d bonds in CH_3—C_6H_4CH=O and C_6H_5C(—CH_3)=CH_2

CH_3—C_6H_4CH=O			C_6H_5C(—CH_3)=CH_2		
Torsion Angle	Total Energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]
0.0	-384.904091718	0.0574	0.0	-348.976363007	1.97
15.0	-384.904110781	0.0455	15.0	-348.977151086	1.48
30.0	-384.904153680	0.01859	30.0	-348.978513041	0.62
45.0	-384.904177626	0.003563	45.0	-348.979509744	0.00
60.0	-384.904183305	0.0000	60.0	-348.979485064	0.01
75.0	-384.904176982	0.00396	75.0	-348.978646985	0.54
90.0	-384.904151209	0.02014	90.0	-348.977504303	1.26
105.0	-384.904109961	0.04602	105.0	-348.976556150	1.85
120.0	-384.904091750	0.05745	120.0	-348.976374492	1.97
135.0	-384.904107500	0.04756	135.0	-348.977141151	1.48
150.0	-384.904150988	0.02028	150.0	-348.978448147	0.66
165.0	-384.904176900	0.00402	165.0	-348.979471197	0.02
180.0	-384.904183251	0.000	180.0	-348.979513066	0.00
195.0	-384.904176921	0.00400	195.0	-348.978661709	0.53
210.0	-384.904151055	0.02023	210.0	-348.977477636	1.27
225.0	-384.904108478	0.04695	225.0	-348.976527162	1.87
240.0	-384.904091753	0.05745	240.0	-348.976395145	1.95
255.0	-384.904110297	0.04581	255.0	-348.977207590	1.44
270.0	-384.904152347	0.01942	270.0	-348.978509075	0.63
285.0	-384.904176309	0.004390	285.0	-348.979490193	0.01
300.0	-384.904182682	0.000391	300.0	-348.979508937	0.00
315.0	-384.904177580	0.003592	315.0	-348.978722854	0.49
330.0	-384.904153657	0.018604	330.0	-348.977600992	1.19
345.0	-384.904110801	0.045497	345.0	-348.976605408	1.82
360.0	-384.904091721	0.057470	360.0	-348.976363104	1.97

[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 mol^{-1}.

SM7: Total Energy and Internal Rotation Barriers about C—OH bonds in CH_2=CHC(—OH)CH=CH_2 and $C_6H_5CH_2$—OH and C—O bonds in CH_3—OCH=O

CH_2=CHCH(—OH)CH=CH_2			$C_6H_5CH_2$—OH				CH_3—OCH=O		
Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]
0.000	-270.516533078	3.44	-172.0	0.0	-346.783866152	1.80	0.0	-229.060379902	0.00
15.00	-270.518213126	2.39	-157.0	15.0	-346.783745073	1.88	15.0	-229.060336112	0.0274
30.00	-270.520008722	1.26	-142.0	30.0	-346.783372070	2.11	30.0	-229.060216572	0.1025
45.00	-270.521385995	0.39	-127.0	45.0	-346.783132539	2.26	45.0	-229.060065822	0.1971
60.00	-270.522022205	0.00	-112.0	60.0	-346.783476844	2.05	60.0	-229.059991111	0.2439
75.00	-270.521765924	0.16	-97.0	75.0	-346.784484901	1.41	75.0	-229.060047174	0.2088
90.00	-270.520682553	0.84	-82.0	90.0	-346.785724165	0.64	90.0	-229.060198021	0.1141
105.0	-270.519004240	1.89	-67.0	105.0	-346.786597833	0.09	105.0	-229.060329020	0.03193
120.0	-270.517148708	3.05	-52.0	120.0	-346.786729429	0.00	120.0	-229.060379922	0.00
135.0	-270.517184875	3.03	-37.0	135.0	-346.786049418	0.43	135.0	-229.060335380	0.02793
150.0	-270.518606570	2.14	-22.0	150.0	-346.784848802	1.19	150.0	-229.060209711	0.1068
165.0	-270.519665083	1.48	-7.0	165.0	-346.783715630	1.90	165.0	-229.060056869	0.2027
180.0	-270.520071838	1.22	7.9	180.0	-346.783766053	1.87	180.0	-229.059990702	0.2442
195.0	-270.519853970	1.36	22.9	195.0	-346.784923152	1.14	195.0	-229.060056927	0.2026
210.0	-270.519245848	1.74	37.9	210.0	-346.786107078	0.40	210.0	-229.060209854	0.1067
225.0	-270.518588342	2.15	52.9	225.0	-346.786744855	0.00	225.0	-229.060335303	0.02798
240.0	-270.518275870	2.35	67.9	240.0	-346.786565171	0.11	240.0	-229.060379928	0.00
255.0	-270.518481649	2.22	82.9	255.0	-346.785657530	0.68	255.0	-229.060329111	0.03187
270.0	-270.519090462	1.84	97.9	270.0	-346.784414791	1.46	270.0	-229.060198026	0.1141
285.0	-270.519740892	1.43	112.9	285.0	-346.783436211	2.07	285.0	-229.060047192	0.2087
300.0	-270.520071761	1.22	127.9	300.0	-346.783136159	2.26	300.0	-229.059991402	0.2438
315.0	-270.519811610	1.38	142.9	315.0	-346.783394029	2.10	315.0	-229.060065832	0.1970
330.0	-270.518885457	1.96	157.9	330.0	-346.783761769	1.87	330.0	-229.060216608	0.1024
345.0	-270.517531959	2.81	172.9	345.0	-346.783861470	1.81	345.0	-229.060336155	0.02745
360.0	-270.516538004	3.44	187.9	360.0	-346.783866433	1.80	360.0	-229.060379981	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 mol^{-1}.

SM8: Total Energy and Internal Rotation Barriers about C—OH bonds in $CH(—OH)_2CH=O$, $CH_3C(—OH)_2CH=O$, $CH_2=CHC(—OH)_2CH=CH_2$ and $C_6H_5C(—OH)_2CH_3$

$CH(—OH)_2CH=O$			$CH_3C(—OH)_2CH=O$				$CH_2=CHC(—OH)_2CH=CH_2$			$C_6H_5C(—OH)_2CH_3$		
Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]
0.0	-304.258853358	5.07	69.942	0.0	-343.591931656	0.84663	0.0	-345.741487046	5.1708	0.0	-461.332543387	2.7863
15.0	-304.260423780	4.09	84.942	15.0	-343.591958804	0.82959	15.0	-	-	15.0	-461.334158801	1.7726
30.0	-304.262626146	2.71	99.942	30.0	-343.592016916	0.79312	30.0	-345.741618490	5.0884	30.0	-461.335755739	0.77050
45.0	-304.264785173	1.35	114.94	45.0	-343.592277647	0.62951	45.0	-345.742555383	4.5005	45.0	-461.336807162	0.11072
60.0	-304.266300394	0.40	129.94	60.0	-343.592752887	0.33130	60.0	-345.743001919	4.2202	60.0	-461.336983612	0.0000
75.0	-304.266944832	0.00	144.94	75.0	-343.593192342	0.055533	75.0	-345.743045198	4.1931	75.0	-461.336294820	0.43222
90.0	-304.266837833	0.06	159.94	90.0	-343.593280840	0.0000	90.0	-345.743067983	4.1788	90.0	-461.335053097	1.2114
105.0	-304.266340936	0.37	174.94	105.0	-343.592680258	0.37687	105.0	-345.743533979	3.8864	105.0	-461.333789766	2.0042
120.0	-304.265941825	0.63	189.94	120.0	-343.591232186	1.2856	120.0	-345.744749869	3.1234	120.0	-461.333005570	2.4963
135.0	-304.265922694	0.64	204.94	135.0	-343.589076042	2.6386	135.0	-345.746532137	2.0050	135.0	-461.332855609	2.5904
150.0	-304.266241748	0.44	219.94	150.0	-343.586716487	4.1192	150.0	-345.748312223	0.88798	150.0	-461.333193233	2.3785
165.0	-304.266623318	0.20	234.94	165.0	-343.584909858	5.2529	165.0	-345.749476655	0.15729	165.0	-461.333667743	2.0807
180.0	-304.266724675	0.13	249.94	180.0	-343.584214690	5.6891	180.0	-345.749727308	0.0000	180.0	-461.334024076	1.8571
195.0	-304.266308392	0.39	264.94	195.0	-343.584579133	5.4604	195.0	-345.749140985	0.36792	195.0	-461.334055154	1.8376
210.0	-304.265355181	0.99	279.94	210.0	-343.585506864	4.8782	210.0	-345.747909941	1.1404	210.0	-461.333654292	2.0892
225.0	-304.264115508	1.77	294.94	225.0	-343.586452396	4.2849	225.0	-345.746405371	2.0845	225.0	-461.332886558	2.5709
240.0	-304.262932205	2.51	309.94	240.0	-343.587111129	3.8716	240.0	-345.745143879	2.8761	240.0	-461.331992966	3.1317
255.0	-304.262047650	3.07	324.94	255.0	-343.587434155	3.6689	255.0	-345.744493432	3.2843	255.0	-461.331223046	3.6148
270.0	-304.261432897	3.45	339.94	270.0	-343.587645871	3.5360	270.0	-345.744470135	3.2989	270.0	-461.330590666	4.0116
285.0	-304.260854906	3.82	354.94	285.0	-343.588078852	3.2643	285.0	-345.744712715	3.1467	285.0	-461.330023598	4.3675
300.0	-304.260132054	4.27	369.94	300.0	-343.588902835	2.7472	300.0	-345.744858074	3.0555	300.0	-461.330493125	4.0728
315.0	-304.259277560	4.81	384.94	315.0	-343.589980447	2.0710	315.0	-345.744605350	3.2141	315.0	-461.330696319	3.9453
330.0	-304.258530354	5.28	399.94	330.0	-343.590995958	1.4338	330.0	-345.743846750	3.6901	330.0	-461.330854028	3.8464
345.0	-304.258265832	5.44	414.94	345.0	-343.591672979	1.0089	345.0	-345.742729290	4.3913	345.0	-461.331396684	3.5059
360.0	-304.258853407	5.07	429.94	360.0	-343.591931739	0.84657	360.0	-345.741490311	5.1688	360.0	-461.332543395	2.7863

[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 mol^{-1}.

SM9: Total Energy and Internal Rotation Barriers about C_d—OH bonds in CH_2=C(—OH)CH=CH_2, CH_2=C(—OH)$_2$, C_6H_5C(—OH)=CH_2 and CH_2=C(—OH)CH=O

CH_2=C(—OH)CH=CH_2				CH_2=C(—OH)$_2$			C_6H_5C(—OH)=CH_2			CH_2=C(—OH)CH=O		
Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]
156.9	0.0	-231.221029639	1.56	0.0	-229.040942771	1.16745	0.0	-384.879753497	1.73	0.0	-267.136275080	6.47
171.9	15.0	-231.220595661	1.83	15.0	-229.040648745	1.35196	15.0	-384.880745018	1.11	15.0	-267.135728455	6.82
186.9	30.0	-231.220551142	1.86	30.0	-229.039714971	1.93791	30.0	-384.880958496	0.98	30.0	-267.134249100	7.74
201.9	45.0	-231.221017975	1.57	45.0	-229.038211483	2.88137	45.0	-384.880253372	1.42	45.0	-267.132263090	8.99
216.9	60.0	-231.220755229	1.73	60.0	-229.036593732	3.89652	60.0	-384.878780517	2.35	60.0	-267.130425642	10.14
231.9	75.0	-231.219668879	2.41	75.0	-229.035526857	4.56599	75.0	-384.877005061	3.46	75.0	-267.129453371	10.75
246.9	90.0	-231.218196815	3.34	90.0	-229.035549624	4.55171	90.0	-384.875626483	4.32	90.0	-267.129883052	10.48
261.9	105.0	-231.216991508	4.09	105.0	-229.036736477	3.80695	105.0	-384.875368832	4.49	105.0	-267.131883049	9.23
276.9	120.0	-231.216632104	4.32	120.0	-229.038657044	2.60177	120.0	-384.876869091	3.54	120.0	-267.135228188	7.13
291.9	135.0	-231.217356838	3.86	135.0	-229.040611673	1.37522	135.0	-384.879037222	2.18	135.0	-267.139306583	4.57
306.9	150.0	-231.218944189	2.87	150.0	-229.042009351	0.498165	150.0	-384.881078906	0.90	150.0	-267.143095206	2.19
321.9	165.0	-231.220870190	1.66	165.0	-229.042667164	0.0853809	165.0	-384.882364098	0.10	165.0	-267.145687142	0.57
336.9	180.0	-231.222530330	0.62	180.0	-229.042803227	0.00000	180.0	-384.882523859	0.00	180.0	-267.146596891	0.00
351.9	195.0	-231.223483827	0.02	195.0	-229.042667080	0.0854336	195.0	-384.882364080	0.10	195.0	-267.145687467	0.57
366.9	210.0	-231.223520999	0.00	210.0	-229.042009266	0.498218	210.0	-384.881078949	0.90	210.0	-267.143095236	2.19
381.9	225.0	-231.222634679	0.55	225.0	-229.040611620	1.37526	225.0	-384.879037435	2.18	225.0	-267.139306639	4.57
396.9	240.0	-231.221016863	1.57	240.0	-229.038657081	2.60175	240.0	-384.876868669	3.54	240.0	-267.135228215	7.13
411.9	255.0	-231.219090666	2.78	255.0	-229.036736404	3.80699	255.0	-384.875368092	4.49	255.0	-267.131883029	9.23
426.9	270.0	-231.217455198	3.80	270.0	-229.035549596	4.55173	270.0	-384.875626652	4.32	270.0	-267.129883026	10.48
441.9	285.0	-231.216650333	4.31	285.0	-229.035526429	4.56626	285.0	-384.877004950	3.46	285.0	-267.129453256	10.75
456.9	300.0	-231.216926869	4.13	300.0	-229.036594446	3.89607	300.0	-384.878780645	2.34	300.0	-267.130425612	10.14
471.9	315.0	-231.218084426	3.41	315.0	-229.038211734	2.88121	315.0	-384.880253277	1.42	315.0	-267.132263119	8.99
486.9	330.0	-231.219559756	2.48	330.0	-229.039714467	1.93823	330.0	-384.880958503	0.98	330.0	-267.134249088	7.74
501.9	345.0	-231.220696775	1.77	345.0	-229.040648753	1.35195	345.0	-384.880744913	1.11	345.0	-267.135728603	6.82
516.9	360.0	-231.221029638	1.56	360.0	-229.040942803	1.16743	360.0	-384.879753485	1.73	360.0	-267.136275123	6.47

[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 mol^{-1}.

SM10: Total Energy and Internal Rotation Barriers about C_d—O bonds in CH_2=CH—OCH=CH_2 and C—O bonds in Y(C_5H_5)— OCH=O and C_b—O bonds in C_6H_5—OCH=O

CH_2=CH—OCH=CH_2			Y(C_5H_5)—OCH=O				C_6H_5—OCH=O		
Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]
0.0	-231.204941630	0.75	61.4	0.0	-382.649627033	0.00	0.0	-420.802148061	2.72
15.0	-231.205907294	0.15	76.4	15.0	-382.649172610	0.28	15.0	-420.803390399	1.94
30.0	-231.205515985	0.39	91.4	30.0	-382.648009847	1.01	30.0	-420.805165449	0.82
45.0	-231.203958832	1.37	106.4	45.0	-382.646693917	1.84	45.0	-420.806278186	0.13
60.0	-231.201939714	2.64	121.4	60.0	-382.645461330	2.61	60.0	-420.806486240	0.00
75.0	-231.200405637	3.60	136.4	75.0	-382.644610241	3.14	75.0	-420.806171971	0.19
90.0	-231.199950716	3.89	151.4	90.0	-382.644502526	3.21	90.0	-420.805930573	0.34
105.0	-231.200554491	3.51	166.4	105.0	-382.645301495	2.71	105.0	-420.806117501	0.23
120.0	-231.201851374	2.69	181.4	120.0	-382.646444890	1.99	120.0	-420.806456529	0.01
135.0	-231.203473941	1.67	196.4	135.0	-382.647351271	1.42	135.0	-420.806374796	0.07
150.0	-231.204905890	0.78	211.4	150.0	-382.647985474	1.03	150.0	-420.805417665	0.67
165.0	-231.205830338	0.20	226.4	165.0	-382.648382810	0.78	165.0	-420.803628721	1.79
180.0	-231.206149238	0.00	241.4	180.0	-382.648490504	0.71	180.0	-420.802147691	2.72
195.0	-231.205830386	0.20	256.4	195.0	-382.648273980	0.85	195.0	-420.803628712	1.79
210.0	-231.204905636	0.78	271.4	210.0	-382.647787118	1.15	210.0	-420.805417611	0.67
225.0	-231.203473972	1.67	286.4	225.0	-382.647054142	1.61	225.0	-420.806374859	0.07
240.0	-231.201851311	2.69	301.4	240.0	-382.646033916	2.25	240.0	-420.806456703	0.01
255.0	-231.200554618	3.51	316.4	255.0	-382.644925064	2.95	255.0	-420.806117427	0.23
270.0	-231.199950569	3.89	331.4	270.0	-382.644434803	3.25	270.0	-420.805929800	0.35
285.0	-231.200405205	3.60	346.4	285.0	-382.644742661	3.06	285.0	-420.806171994	0.19
300.0	-231.201939808	2.64	361.4	300.0	-382.645598903	2.52	300.0	-420.806486421	0.00
315.0	-231.203958969	1.37	376.4	315.0	-382.646762620	1.79	315.0	-420.806278203	0.13
330.0	-231.205516004	0.39	391.4	330.0	-382.648026914	1.00	330.0	-420.805165460	0.82
345.0	-231.205907319	0.15	406.4	345.0	-382.649178384	0.28	345.0	-420.803390502	1.94
360.0	-231.204941648	0.75	421.4	360.0	-382.649627072	0.00	360.0	-420.802148144	2.72

[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 mol^{-1}.

SM11: Total Energy and Internal Rotation Barriers about C—CH=O bonds in CH_2=$CHCH_2$—CH=O, CH_2=CHCH(CH=CH_2)—CH=O and CH_2=CHCH(CH=O)—CH=O

CH_2=$CHCH_2$—CH=O			CH_2=CHCH(CH=CH_2)—CH=O				CH_2=CHCH(CH=O)—CH=O			
Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational barrier[b]
0.0	-231.227304155	1.16	61.1	0.0	-308.621125217	0.68	122.8	0.0	-344.537658296	1.47
15.0	-231.227548342	1.00	76.1	15.0	-308.620789065	0.89	137.8	15.0	-344.537376586	1.65
30.0	-231.228095729	0.66	91.1	30.0	-308.619962137	1.41	152.8	30.0	-344.536460883	2.22
45.0	-231.228581744	0.36	106.1	45.0	-308.619108063	1.95	167.8	45.0	-344.535780778	2.65
60.0	-231.228749032	0.25	121.1	60.0	-308.618661720	2.23	182.8	60.0	-344.535363564	2.91
75.0	-231.228510074	0.40	136.1	75.0	-308.618938639	2.05	197.8	75.0	-344.535649301	2.73
90.0	-231.227976607	0.73	151.1	90.0	-308.620015024	1.38	212.8	90.0	-344.538766537	0.78
105.0	-231.227421530	1.08	166.1	105.0	-308.621289080	0.58	227.8	105.0	-344.539281020	0.45
120.0	-231.227206753	1.22	181.1	120.0	-308.622086245	0.08	242.8	120.0	-344.539475004	0.33
135.0	-231.227513122	1.03	196.1	135.0	-308.622218132	0.00	257.8	135.0	-344.539550378	0.28
150.0	-231.228243963	0.57	211.1	150.0	-308.621782388	0.27	272.8	150.0	-344.539705889	0.19
165.0	-231.228964506	0.11	226.1	165.0	-308.621219602	0.62	287.8	165.0	-344.539913107	0.06
180.0	-231.229154035	0.00	241.1	180.0	-308.620973286	0.78	302.8	180.0	-344.540010910	0.00
195.0	-231.228463472	0.43	256.1	195.0	-308.621233959	0.61	317.8	195.0	-344.539854531	0.09
210.0	-231.227083738	1.29	271.1	210.0	-308.621785770	0.27	332.8	210.0	-344.539507843	0.31
225.0	-231.225718445	2.15	286.1	225.0	-308.622208428	0.00	347.8	225.0	-344.539444347	0.35
240.0	-231.225125751	2.52	301.1	240.0	-308.622138401	0.05	362.8	240.0	-344.539608414	0.25
255.0	-231.225431327	2.33	316.1	255.0	-308.621496432	0.45	377.8	255.0	-344.539370405	0.40
270.0	-231.226297334	1.79	331.1	270.0	-308.620333144	1.18	392.8	270.0	-344.538450855	0.97
285.0	-231.227279159	1.17	346.1	285.0	-308.619120564	1.94	407.8	285.0	-344.537136124	1.80
300.0	-231.227953617	0.75	361.1	300.0	-308.618648828	2.24	422.8	300.0	-344.536180777	2.40
315.0	-231.228129653	0.64	376.1	315.0	-308.619045566	1.99	437.8	315.0	-344.536092266	2.46
330.0	-231.227884912	0.79	391.1	330.0	-308.619933303	1.43	452.8	330.0	-344.536652537	2.10
345.0	-231.227493388	1.04	406.1	345.0	-308.620793244	0.89	467.8	345.0	-344.537312997	1.69
360.0	-231.227304178	1.16	421.1	360.0	-308.621125139	0.68	482.8	360.0	-344.537658668	1.47

[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 mol^{-1}.

SM12: Total Energy and Internal Rotation Barriers about C—CH=O bonds in $CH(OH)_2$—CH=O and $CH_3C(OH)_2$—CH=O

$CH(OH)_2$—CH=O				$CH_3C(OH)_2$—CH=O			
Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational barrier[b]	Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational barrier[b]
-177.4	0.0	-304.266741290	0.00	56.364	0.0	-343.593297151	0.00
-162.4	15.0	-304.266172291	0.35	71.365	15.0	-343.592548166	0.47
-147.4	30.0	-304.264712263	1.27	86.365	30.0	-343.590920416	1.49
-132.4	45.0	-304.262920774	2.39	101.36	45.0	-343.588916011	2.75
-117.4	60.0	-304.261372301	3.37	116.36	60.0	-343.587204903	3.82
-102.4	75.0	-304.260473493	3.93	131.36	75.0	-343.586287857	4.39
-87.43	90.0	-304.260294397	4.04	146.36	90.0	-343.586117042	4.50
-72.43	105.0	-304.260511309	3.91	161.36	105.0	-343.586186515	4.46
-57.43	120.0	-304.260694080	3.79	176.36	120.0	-343.585977187	4.59
-42.43	135.0	-304.260664981	3.81	191.36	135.0	-343.585245785	5.05
-27.43	150.0	-304.260403605	3.97	206.36	150.0	-343.588567511	2.96
-12.43	165.0	-304.260079425	4.18	221.36	165.0	-343.587749884	3.48
2.57	180.0	-304.260033024	4.21	236.36	180.0	-343.587116777	3.87
17.57	195.0	-304.260489812	3.92	251.36	195.0	-343.587177440	3.84
32.57	210.0	-304.261362667	3.37	266.36	210.0	-343.588611777	2.94
47.57	225.0	-304.262282264	2.79	281.36	225.0	-343.590555822	1.72
62.57	240.0	-304.262835108	2.45	296.36	240.0	-343.593078442	0.13
77.57	255.0	-304.262776413	2.48	311.36	255.0	-343.593224603	0.04
92.57	270.0	-304.262189520	2.85	326.36	270.0	-343.592090537	0.75
107.57	285.0	-304.261519551	3.27	341.36	285.0	-343.590135086	1.98
122.57	300.0	-304.261296722	3.41	356.36	300.0	-343.588698630	2.88
137.57	315.0	-304.261902051	3.03	371.36	315.0	-343.589253123	2.53
152.57	330.0	-304.264245772	1.56	386.36	330.0	-343.591191859	1.32
167.57	345.0	-304.266064757	0.42	401.36	345.0	-343.592810152	0.30
182.57	360.0	-304.266741292	0.00	416.36	360.0	-343.593297064	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 mol^{-1}.

SM13: Total Energy and Internal Rotation Barriers about C—CH=O bonds in $Y(C_5H_5O)$—CH=O and $C_6H_5C(CH_3)_2$—CH=O and about C—C(OH)O bonds in $Y(C_5H_5)$—C(OH)=O

$Y(C_5H_5O)$—CH=O				$C_6H_5C(CH_3)_2$—CH=O			$Y(C_5H_5)$—C(OH)=O			
Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]	Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational barrier[b]
-46.897	0.0	-382.636991717	0.00	0.0	-463.520028274	2.32	-54.5	0.0	-382.677113003	0.00
-31.897	15.0	-382.636687050	0.19	15.0	-463.521339892	1.50	-39.5	15.0	-382.677008477	0.06
-16.897	30.0	-382.635770045	0.76	30.0	-463.522695604	0.65	-24.5	30.0	-382.676819250	0.18
-1.8970	45.0	-382.634198883	1.75	45.0	-463.523579197	0.09	-9.5	45.0	-382.676674434	0.27
13.103	60.0	-382.632195324	3.01	60.0	-463.523738538	0.00	5.4	60.0	-382.676621326	0.30
28.103	75.0	-382.630172083	4.28	75.0	-463.523232439	0.31	20.4	75.0	-382.676587873	0.33
43.103	90.0	-382.628685418	5.21	90.0	-463.522392689	0.84	35.4	90.0	-382.676524184	0.37
58.103	105.0	-382.628286238	5.46	105.0	-463.521577559	1.35	50.4	105.0	-382.676434946	0.42
73.103	120.0	-382.629135766	4.93	120.0	-463.521015901	1.70	65.4	120.0	-382.676430457	0.42
88.103	135.0	-382.630709361	3.94	135.0	-463.520835098	1.82	80.4	135.0	-382.676514783	0.37
103.10	150.0	-382.632162459	3.03	150.0	-463.521144431	1.62	95.4	150.0	-382.676583747	0.33
118.10	165.0	-382.632913003	2.56	165.0	-463.521775750	1.23	110.4	165.0	-382.676614773	0.31
133.10	180.0	-382.632775824	2.64	180.0	-463.522229655	0.94	125.4	180.0	-382.676653306	0.28
148.10	195.0	-382.631822308	3.24	195.0	-463.521923810	1.13	140.4	195.0	-382.676758082	0.22
163.10	210.0	-382.630478295	4.08	210.0	-463.520787623	1.85	155.4	210.0	-382.676943649	0.10
178.10	225.0	-382.629616763	4.62	225.0	-463.519448340	2.69	170.4	225.0	-382.677100808	0.007
193.10	240.0	-382.629782565	4.52	240.0	-463.518474569	3.30	185.4	240.0	-382.677011358	0.06
208.10	255.0	-382.630722754	3.93	255.0	-463.518422594	3.33	200.4	255.0	-382.676494945	0.38
223.10	270.0	-382.631996665	3.13	270.0	-463.519092672	2.91	215.4	270.0	-382.675780749	0.83
238.10	285.0	-382.633327728	2.29	285.0	-463.519874187	2.42	230.4	285.0	-382.675317167	1.12
253.10	300.0	-382.634575201	1.51	300.0	-463.520267326	2.17	245.4	300.0	-382.675322819	1.12
268.10	315.0	-382.635639443	0.84	315.0	-463.520114546	2.27	260.4	315.0	-382.675779549	0.83
283.10	330.0	-382.636420273	0.35	330.0	-463.519660728	2.55	275.4	330.0	-382.676458241	0.41
298.10	345.0	-382.636871147	0.07	345.0	-463.519431225	2.70	290.4	345.0	-382.676963534	0.09
313.10	360.0	-382.636991707	0.00	360.0	-463.520028218	2.32	305.4	360.0	-382.677113057	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 mol^{-1}.

SM14: Total Energy and Internal Rotation Barriers about C_d—C bonds in CH_2=CH—CH_2CH=O and CH_2=CH—CH(CH=O)CH=O

CH_2=CH—CH_2CH=O				CH_2=CH—CH(CH=O)CH=O		
Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]
-118.3	0.0	-231.228129907	0.00	0.0	-344.536314317	0.83
-103.3	15.0	-231.227845812	0.17	15.0	-344.536243382	0.88
-88.3	30.0	-231.227181834	0.59	30.0	-344.535963893	1.05
-73.3	45.0	-231.226523133	1.00	45.0	-344.535520240	1.33
-58.3	60.0	-231.226309165	1.14	60.0	-344.534945690	1.69
-43.3	75.0	-231.226601372	0.96	75.0	-344.534318611	2.08
-28.3	90.0	-231.226915442	0.76	90.0	-344.533818115	2.40
-13.3	105.0	-231.226720674	0.88	105.0	-344.533585281	2.54
1.6	120.0	-231.225987530	1.34	120.0	-344.533553533	2.56
16.6	135.0	-231.225057309	1.92	135.0	-344.533657214	2.50
31.6	150.0	-231.224641644	2.18	150.0	-344.534093065	2.23
46.6	165.0	-231.226514705	1.01	165.0	-344.534722552	1.83
61.6	180.0	-231.226303575	1.14	180.0	-344.535356248	1.43
76.6	195.0	-231.226639349	0.93	195.0	-344.535837510	1.13
91.6	210.0	-231.227344457	0.49	210.0	-344.536174107	0.92
106.6	225.0	-231.227952901	0.11	225.0	-344.536307547	0.84
121.6	240.0	-231.228121123	0.00	240.0	-344.536296083	0.84
136.6	255.0	-231.227702136	0.26	255.0	-344.536378322	0.79
151.6	270.0	-231.226759953	0.86	270.0	-344.536861668	0.49
166.6	285.0	-231.225650058	1.55	285.0	-344.537447016	0.12
181.6	300.0	-231.225049721	1.93	300.0	-344.537646679	0.00
196.6	315.0	-231.225465100	1.67	315.0	-344.537315249	0.20
211.6	330.0	-231.226600811	0.96	330.0	-344.536667853	0.61
226.6	345.0	-231.227818912	0.19	345.0	-344.536303061	0.84
241.6	360.0	-231.228129907	0.00	360.0	-344.536314339	0.83

[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 mol^{-1}.

SM15: Total Energy and Internal Rotation Barriers about C_d—C bonds in CH_2=CH—$C(CH_3)$CH=CH_2 and CH_2=CH—C(CH=O)CH=CH_2

CH_2=CH—$C(CH_3)$CH=CH_2				CH_2=CH—C(CH=O)CH=CH_2			
Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational barrier[b]	Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational barrier[b]
119.70	0.0	-234.626356412	0.0000	112.2	0.0	-308.621122913	0.07
134.70	15.0	-234.625973966	0.24	127.2	15.0	-308.620766862	0.30
149.70	30.0	-234.624866320	0.93	142.2	30.0	-308.619904879	0.84
164.70	45.0	-234.623508322	1.78	157.2	45.0	-308.618801669	1.53
179.70	60.0	-234.622697229	2.29	172.2	60.0	-308.618117207	1.96
194.70	75.0	-234.623057866	2.07	187.2	75.0	-308.618455056	1.75
209.70	90.0	-234.624339709	1.26	202.2	90.0	-308.619552703	1.06
224.70	105.0	-234.625597967	0.47	217.2	105.0	-308.620673696	0.36
239.70	120.0	-234.626105783	0.15	232.2	120.0	-308.621247929	0.00
254.70	135.0	-234.625641345	0.44	247.2	135.0	-308.621084353	0.10
269.70	150.0	-234.624428742	1.21	262.2	150.0	-308.620414394	0.52
284.70	165.0	-234.623128940	2.02	277.2	165.0	-308.619746988	0.94
299.70	180.0	-234.622373902	2.49	292.2	180.0	-308.619261168	1.24
314.70	195.0	-234.622496190	2.42	307.2	195.0	-308.618688517	1.60
329.70	210.0	-234.623506380	1.78	322.2	210.0	-308.618346149	1.82
344.70	225.0	-234.624818380	0.96	337.2	225.0	-308.618700425	1.59
359.70	240.0	-234.625783022	0.36	352.2	240.0	-308.619395376	1.16
374.70	255.0	-234.626001050	0.22	367.2	255.0	-308.619974642	0.79
389.70	270.0	-234.625439878	0.57	382.2	270.0	-308.620235296	0.63
404.70	285.0	-234.624433607	1.20	397.2	285.0	-308.620139758	0.69
419.70	300.0	-234.623723024	1.65	412.2	300.0	-308.619907615	0.84
434.70	315.0	-234.623962918	1.50	427.2	315.0	-308.619909895	0.84
449.70	330.0	-234.624930517	0.89	442.2	330.0	-308.620356694	0.56
464.70	345.0	-234.625934886	0.26	457.2	345.0	-308.620910743	0.21
479.70	360.0	-234.626356351	0.00	472.2	360.0	-308.621122990	0.07

[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 mol^{-1}.

SM16: Total Energy and Internal Rotation Barriers about C_d—C bonds in CH_2=CH—CH(OH)CH=CH_2 and CH_2=CH—$C(OH)_2$CH=CH_2

CH_2=CH—CH(OH)CH=CH_2			CH_2=CH—$C(OH)_2$CH=CH_2		
Torsion Angle	Total energy[a]	Rotational barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]
0.0	-270.521850565	0.02	0.0	-345.749681007	0.00
15.0	-270.521882502	0.00	15.0	-345.748880572	0.50
30.0	-270.520655229	0.77	30.0	-345.747267459	1.51
45.0	-270.518949271	1.84	45.0	-345.744979362	2.95
60.0	-270.517943134	2.47	60.0	-345.742744003	4.35
75.0	-270.518265844	2.27	75.0	-345.741969706	4.84
90.0	-270.519302093	1.62	90.0	-345.743989359	3.57
105.0	-270.520207837	1.05	105.0	-345.746417839	2.04
120.0	-270.520491756	0.87	120.0	-345.748204577	0.92
135.0	-270.520019591	1.17	135.0	-345.748979755	0.44
150.0	-270.518953636	1.83	150.0	-345.748654937	0.64
165.0	-270.517939564	2.47	165.0	-345.747590482	1.31
180.0	-270.517734537	2.60	180.0	-345.746738106	1.84
195.0	-270.518291003	2.25	195.0	-345.746693824	1.87
210.0	-270.519315405	1.61	210.0	-345.746889995	1.75
225.0	-270.520375005	0.94	225.0	-345.746622608	1.92
240.0	-270.521010717	0.54	240.0	-345.745663462	2.52
255.0	-270.520906665	0.61	255.0	-345.744236161	3.41
270.0	-270.519894822	1.24	270.0	-345.743012272	4.18
285.0	-270.518132387	2.35	285.0	-345.742926911	4.23
300.0	-270.516359535	3.46	300.0	-345.744318331	3.36
315.0	-270.516357381	3.46	315.0	-345.746496514	1.99
330.0	-270.518323431	2.23	330.0	-345.748471034	0.76
345.0	-270.520503407	0.86	345.0	-345.749593373	0.05
360.0	-270.521850616	0.02	360.0	-345.749681307	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 mol^{-1}.

SM17: Total Energy and Internal Rotation Barriers about C_d—C_d bonds in $C_6H_5CH(=CH_2)$—CH=CH_2, CH_2=C—(CH=O)CH=CH_2 and CH_2=C(OH)—CH=CH_2

$C_6H_5CH(=CH_2)$—CH=CH_2				CH_2=C—(CH=O)CH=CH_2			CH_2=C(OH)—CH=CH_2			
Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational barrier[b]
139.9	0.0	-387.059871064	1.20	0.0	-269.318038851	0.00	169.5	0.0	-231.221034334	0.00
154.9	15.0	-387.059445833	1.47	15.0	-269.318002690	0.02	184.5	15.0	-231.220258946	0.48
169.9	30.0	-387.058289279	2.19	30.0	-269.317400547	0.40	199.5	30.0	-231.220814348	0.13
184.9	45.0	-387.057423626	2.74	45.0	-269.315845001	1.37	214.5	45.0	-231.219166396	1.17
199.9	60.0	-387.057373305	2.77	60.0	-269.313641447	2.76	229.5	60.0	-231.216168701	3.05
214.9	75.0	-387.057390132	2.76	75.0	-269.311890262	3.85	244.5	75.0	-231.212806108	5.16
229.9	90.0	-387.056680753	3.20	90.0	-269.311616180	4.03	259.5	90.0	-231.211307102	6.10
244.9	105.0	-387.057957602	2.40	105.0	-269.312797815	3.28	274.5	105.0	-231.212296033	5.48
259.9	120.0	-387.055725961	3.80	120.0	-269.314558749	2.18	289.5	120.0	-231.214104820	4.34
274.9	135.0	-387.053602664	5.13	135.0	-269.316019545	1.26	304.5	135.0	-231.215677634	3.36
289.9	150.0	-387.054008474	4.88	150.0	-269.316708767	0.83	319.5	150.0	-231.216406404	2.90
304.9	165.0	-387.056276234	3.46	165.0	-269.316698764	0.84	334.5	165.0	-231.216087816	3.10
319.9	180.0	-387.058973204	1.76	180.0	-269.316558162	0.93	349.5	180.0	-231.215148389	3.69
334.9	195.0	-387.061004437	0.49	195.0	-269.316698722	0.84	364.5	195.0	-231.214840326	3.88
349.9	210.0	-387.061789082	0.00	210.0	-269.316708671	0.83	379.5	210.0	-231.215742886	3.32
364.9	225.0	-387.061149877	0.40	225.0	-269.316019389	1.26	394.5	225.0	-231.216392100	2.91
379.9	240.0	-387.059106044	1.68	240.0	-269.314559758	2.18	409.5	240.0	-231.216096091	3.09
394.9	255.0	-387.055965556	3.65	255.0	-269.312798022	3.28	424.5	255.0	-231.214802454	3.91
409.9	270.0	-387.052270669	5.97	270.0	-269.311616192	4.03	439.5	270.0	-231.212989171	5.04
424.9	285.0	-387.054650695	4.48	285.0	-269.311891367	3.85	454.5	285.0	-231.211503632	5.98
439.9	300.0	-387.053317205	5.31	300.0	-269.313641364	2.76	469.5	300.0	-231.211838150	5.77
454.9	315.0	-387.054947140	4.29	315.0	-269.315844655	1.37	484.5	315.0	-231.214769116	3.93
469.9	330.0	-387.057243312	2.85	330.0	-269.317400230	0.40	499.5	330.0	-231.218097455	1.84
484.9	345.0	-387.059081162	1.69	345.0	-269.318003050	0.02	514.5	345.0	-231.220346528	0.43
499.9	360.0	-387.059871247	1.20	360.0	-269.318038803	0.00	529.5	360.0	-231.221034186	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 mol^{-1}.

SM18: Total Energy and Internal Rotation Barriers about C_d—CH=O bonds in CH_2=CH—CH=O, CH_2=CHC(=CH_2)—CH=O, C_6H_5C(=CH_2)—CH=O and CH_2=C(OH)—CH=O

CH_2=CH—CH=O			CH_2=CHC(=CH_2)—CH=O			C_6H_5C(=CH_2)—CH=O			CH_2=C(OH)—CH=O		
Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]
0.0	-191.819126941	6.44	0.0	-269.318038842	2.54	0.0	-422.978719035	1.53	0.0	-267.146597050	0.00
15.0	-191.820842025	5.36	15.0	-269.317907630	2.62	15.0	-422.977921871	2.03	15.0	-267.145539573	0.66
30.0	-191.824188953	3.26	30.0	-269.316981574	3.20	30.0	-422.976161285	3.14	30.0	-267.142400241	2.63
45.0	-191.826244018	1.97	45.0	-269.315141837	4.36	45.0	-422.973598912	4.75	45.0	-267.137312314	5.82
60.0	-191.825633037	2.35	60.0	-269.312662275	5.91	60.0	-422.970610381	6.62	60.0	-267.130726981	9.95
75.0	-191.823138181	3.92	75.0	-269.310335953	7.37	75.0	-422.967950562	8.29	75.0	-267.123959450	14.20
90.0	-191.820604227	5.51	90.0	-269.309347096	7.99	90.0	-422.969110655	7.56	90.0	-267.120289009	16.50
105.0	-191.819626575	6.12	105.0	-269.310340557	7.37	105.0	-422.970332107	6.80	105.0	-267.122220344	15.29
120.0	-191.821681078	4.83	120.0	-269.312912850	5.76	120.0	-422.973006892	5.12	120.0	-267.125925562	12.97
135.0	-191.824965034	2.77	135.0	-269.316229738	3.67	135.0	-422.976190036	3.12	135.0	-267.129317000	10.84
150.0	-191.827481776	1.19	150.0	-269.319287393	1.76	150.0	-422.978978485	1.37	150.0	-267.131879850	9.23
165.0	-191.828925686	0.29	165.0	-269.321360521	0.45	165.0	-422.980754601	0.26	165.0	-267.133442463	8.25
180.0	-191.829388622	0.00	180.0	-269.322090622	0.00	180.0	-422.981170084	0.00	180.0	-267.133964952	7.92
195.0	-191.828925679	0.29	195.0	-269.321360448	0.45	195.0	-422.980060539	0.69	195.0	-267.133442116	8.25
210.0	-191.827481766	1.19	210.0	-269.319287218	1.76	210.0	-422.977535281	2.28	210.0	-267.131879646	9.23
225.0	-191.824965036	2.77	225.0	-269.316229743	3.67	225.0	-422.974047880	4.47	225.0	-267.129316992	10.84
240.0	-191.821681226	4.83	240.0	-269.312911393	5.76	240.0	-422.973006858	5.12	240.0	-267.125925581	12.97
255.0	-191.819626670	6.12	255.0	-269.310340765	7.37	255.0	-422.970332543	6.80	255.0	-267.122220558	15.29
270.0	-191.820604285	5.51	270.0	-269.309347417	7.99	270.0	-422.969110381	7.56	270.0	-267.120289029	16.50
285.0	-191.823138279	3.92	285.0	-269.310336044	7.37	285.0	-422.969910213	7.06	285.0	-267.123959534	14.20
300.0	-191.825633336	2.35	300.0	-269.312662416	5.91	300.0	-422.972281314	5.57	300.0	-267.130727104	9.95
315.0	-191.826244001	1.97	315.0	-269.315141827	4.36	315.0	-422.975023643	3.85	315.0	-267.137312596	5.82
330.0	-191.824189021	3.26	330.0	-269.316981566	3.20	330.0	-422.977225732	2.47	330.0	-267.142400043	2.63
345.0	-191.820842027	5.36	345.0	-269.317907634	2.62	345.0	-422.978493214	1.68	345.0	-267.145539563	0.66
360.0	-191.819126546	6.44	360.0	-269.318038849	2.54	360.0	-422.978718570	1.53	360.0	-267.146597055	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 mol^{-1}.

SM19: Total Energy and Internal Rotation Barriers about C_b—C bonds in C_6H_5—CH_2OH, C_6H_5—$C(OH)_2CH_3$ and C_6H_5—$C(CH_3)_2CH$=O

C_6H_5—CH_2OH			C_6H_5—$C(OH)_2CH_3$				C_6H_5—$C(CH_3)_2CH$=O		
Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]
0.0	-346.785541686	0.77	97.60	0.0	-461.337010193	0.007	0.0	-463.523613010	0.04
15.0	-346.784510424	1.42	112.60	15.0	-461.336442509	0.36	15.0	-463.523680678	0.00
30.0	-346.783531956	2.03	127.60	30.0	-461.335336755	1.05	30.0	-463.522969121	0.44
45.0	-346.782876093	2.44	142.60	45.0	-461.334130301	1.81	45.0	-463.521975312	1.07
60.0	-346.783169822	2.26	157.60	60.0	-461.333248105	2.36	60.0	-463.520898151	1.74
75.0	-346.784099665	1.68	172.60	75.0	-461.332277049	2.97	75.0	-463.519412339	2.67
90.0	-346.784890852	1.18	187.60	90.0	-461.330645319	4.00	90.0	-463.518979404	2.95
105.0	-346.785546664	0.77	202.60	105.0	-461.329501106	4.72	105.0	-463.520299137	2.12
120.0	-346.786088676	0.43	217.60	120.0	-461.330825377	3.89	120.0	-463.521771346	1.19
135.0	-346.786564557	0.13	232.60	135.0	-461.333209976	2.39	135.0	-463.522236686	0.90
150.0	-346.786778271	0.00	247.60	150.0	-461.335368779	1.03	150.0	-463.522175681	0.94
165.0	-346.786442487	0.21	262.60	165.0	-461.336669901	0.22	165.0	-463.522610271	0.67
180.0	-346.785555094	0.76	277.60	180.0	-461.337022940	0.00	180.0	-463.523562986	0.07
195.0	-346.784433276	1.47	292.60	195.0	-461.336438891	0.36	195.0	-463.523650235	0.02
210.0	-346.783425762	2.10	307.60	210.0	-461.335101755	1.20	210.0	-463.522791575	0.55
225.0	-346.782848611	2.46	322.60	225.0	-461.333847893	1.99	225.0	-463.521789303	1.18
240.0	-346.783185146	2.25	337.60	240.0	-461.333062696	2.48	240.0	-463.520780264	1.82
255.0	-346.784001670	1.74	352.60	255.0	-461.332113764	3.08	255.0	-463.519503555	2.62
270.0	-346.784755379	1.27	367.60	270.0	-461.330702235	3.96	270.0	-463.518915587	2.99
285.0	-346.785430277	0.84	382.60	285.0	-461.329504310	4.71	285.0	-463.520068743	2.26
300.0	-346.786034650	0.46	397.60	300.0	-461.330523901	4.07	300.0	-463.521781962	1.19
315.0	-346.786570737	0.13	412.60	315.0	-461.333065545	2.48	315.0	-463.522241831	0.90
330.0	-346.786773002	0.00	427.60	330.0	-461.335485308	0.96	330.0	-463.522200397	0.92
345.0	-346.786394782	0.24	442.60	345.0	-461.336768684	0.16	345.0	-463.522800936	0.55
360.0	-346.785542023	0.77	457.60	360.0	-461.337010167	0.008	360.0	-463.523612127	0.04

[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 mol^{-1}.

SM 20: Total Energy and Internal Rotation Barriers about C_b—CH=O bonds in C_6H_5—CH=O, and $CH_3C_6H_4$—CH=O

C_6H_5—CH=O				$CH_3C_6H_4$—CH=O		
Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational Barrier[b]
90.00	0.0	-345.582684964	4.52	0.0	-384.904183312	0.00
105.0	15.0	-345.581909499	3.75	15.0	-384.903389682	0.49
120.0	30.0	-345.579668676	1.97	30.0	-384.901098383	1.93
135.0	45.0	-345.576233139	0.51	45.0	-384.897566222	4.15
150.0	60.0	-345.572159044	0.00	60.0	-384.893344456	6.80
165.0	75.0	-345.568477554	0.39	75.0	-384.889477385	9.22
180.0	90.0	-345.566877615	0.84	90.0	-384.887755806	10.30
195.0	105.0	-345.568506513	0.39	105.0	-384.889461806	9.23
210.0	120.0	-345.572153728	0.00	120.0	-384.893270573	6.84
225.0	135.0	-345.576196833	0.51	135.0	-384.897464150	4.21
240.0	150.0	-345.579632817	1.97	150.0	-384.901038789	1.97
255.0	165.0	-345.581896870	3.75	165.0	-384.903367240	0.51
270.0	180.0	-345.582684977	4.52	180.0	-384.904183265	0.00
285.0	195.0	-345.581897386	3.57	195.0	-384.903367213	0.51
300.0	210.0	-345.579632895	1.77	210.0	-384.901038773	1.97
315.0	225.0	-345.576196835	0.36	225.0	-384.897502942	4.19
330.0	240.0	-345.572159044	0.01	240.0	-384.893322995	6.81
345.0	255.0	-345.568477554	0.47	255.0	-384.889511852	9.20
360.0	270.0	-345.566877615	0.84	270.0	-384.887764410	10.30
375.0	285.0	-345.568506513	0.47	285.0	-384.889429746	9.25
390.0	300.0	-345.572153728	0.01	300.0	-384.893344492	6.80
405.0	315.0	-345.576196833	0.36	315.0	-384.897566222	4.15
420.0	330.0	-345.579632817	1.77	330.0	-384.901098269	1.93
435.0	345.0	-345.581896870	3.57	345.0	-384.903389663	0.49
450.0	360.0	-345.582684977	4.52	360.0	-384.904183308	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 mol^{-1}.

SM 21: Total Energy and Internal Rotation Barriers about C_b—C_d bonds in C_6H_5—CH=CH_2, C_6H_5—C(=CH_2)OH, C_6H_5—C(=CH_2)CH=CH_2 and C_6H_5—C(=CH_2)CH=O

C_6H_5—CH=CH_2				C_6H_5—C(=CH_2)OH			C_6H_5—C(=CH_2)CH=CH_2			C_6H_5—C(CH_3)=CH_2				C_6H_5—C(=CH_2)CH=O		
Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]	Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational barrier[b]	Torsion Angle	Total energy[a]	Rotational barrier[b]
179.9	0.0	-309.660909299	0.00	0.0	-384.877998688	1.87	0.0	-387.057309392	1.59	180	0.000	-348.979059187	0.36	0.0	-422.978719035	1.53
194.9	15.0	-309.660797789	0.07	15.0	-384.880130130	0.53	15.0	-387.056353563	2.19	195	15.00	-348.979381629	0.15	15.0	-422.977921871	2.03
209.9	30.0	-309.660212522	0.43	30.0	-384.880987711	0.00	30.0	-387.056889415	1.86	210	30.00	-348.979629571	0.00	30.0	-422.976161285	3.14
224.9	45.0	-309.658816617	1.31	45.0	-384.880221984	0.48	45.0	-387.057435843	1.51	225	45.00	-348.979146070	0.30	45.0	-422.973598912	4.75
239.9	60.0	-309.656719830	2.62	60.0	-384.878336378	1.66	60.0	-387.056791330	1.92	240	60.00	-348.978015329	1.01	60.0	-422.970610381	6.62
254.9	75.0	-309.654693265	3.90	75.0	-384.876418952	2.86	75.0	-387.055609135	2.66	255	75.00	-348.976670710	1.85	75.0	-422.967950562	8.29
269.9	90.0	-309.653866582	4.42	90.0	-384.875724854	3.30	90.0	-387.055028421	3.02	270	90.00	-348.976108031	2.21	90.0	-422.969110655	7.56
284.9	105.0	-309.654733324	3.87	105.0	-384.876638402	2.73	105.0	-387.055892007	2.48	285	105.0	-348.976721844	1.82	105.0	-422.970332107	6.80
299.9	120.0	-309.656706781	2.63	120.0	-384.878538181	1.53	120.0	-387.057745673	1.32	300	120.0	-348.978023747	1.01	120.0	-422.973006892	5.12
314.9	135.0	-309.658801508	1.32	135.0	-384.880308740	0.42	135.0	-387.059392862	0.28	315	135.0	-348.979152908	0.30	135.0	-422.976190036	3.12
329.9	150.0	-309.660214173	0.43	150.0	-384.880985843	0.00	150.0	-387.059852297	0.00	330	150.0	-348.979632619	0.00	150.0	-422.978978485	1.37
344.9	165.0	-309.660797980	0.07	165.0	-384.880093635	0.56	165.0	-387.058895378	0.60	345	165.0	-348.979365870	0.16	165.0	-422.980754601	0.26
359.9	180.0	-309.660909269	0.00	180.0	-384.877960546	1.89	180.0	-387.057245995	1.63	360	180.0	-348.979058965	0.36	180.0	-422.981170084	0.00
374.9	195.0	-309.660801403	0.06	195.0	-384.880093426	0.56	195.0	-387.056346860	2.19	375	195.0	-348.979365887	0.16	195.0	-422.980060539	0.69
389.9	210.0	-309.660226385	0.42	210.0	-384.880985746	0.00	210.0	-387.056876762	1.86	390	210.0	-348.979632744	0.00	210.0	-422.977535281	2.28
404.9	225.0	-309.658824406	1.30	225.0	-384.880308424	0.42	225.0	-387.057436795	1.51	405	225.0	-348.979153001	0.30	225.0	-422.974047880	4.47
419.9	240.0	-309.656734562	2.62	240.0	-384.878538006	1.53	240.0	-387.056811023	1.90	420	240.0	-348.978023496	1.01	240.0	-422.973006858	5.12
434.9	255.0	-309.654752336	3.86	255.0	-384.876639106	2.73	255.0	-387.055574500	2.68	435	255.0	-348.976721706	1.82	255.0	-422.970332543	6.80
449.9	270.0	-309.653867470	4.41	270.0	-384.875721748	3.30	270.0	-387.055046254	3.01	450	270.0	-348.976107182	2.21	270.0	-422.969110381	7.56
464.9	285.0	-309.654673177	3.91	285.0	-384.876418912	2.86	285.0	-387.055973351	2.43	465	285.0	-348.976671005	1.85	285.0	-422.969910213	7.06
479.9	300.0	-309.656691984	2.64	300.0	-384.878336788	1.66	300.0	-387.057776538	1.30	480	300.0	-348.978015406	1.01	300.0	-422.972281314	5.57
494.9	315.0	-309.658793948	1.32	315.0	-384.880222280	0.48	315.0	-387.059396597	0.28	495	315.0	-348.979146156	0.30	315.0	-422.975023643	3.85
509.9	330.0	-309.660200169	0.44	330.0	-384.880988002	0.00	330.0	-387.059852229	0.00	510	330.0	-348.979629467	0.00	330.0	-422.977225732	2.47
524.9	345.0	-309.660794270	0.07	345.0	-384.880130119	0.53	345.0	-387.058917847	0.58	535	345.0	-348.979381529	0.15	345.0	-422.978493214	1.68
539.9	360.0	-309.660909064	0.00	360.0	-384.877998642	1.87	360.0	-387.057309157	1.59	540	360.0	-348.979059123	0.36	360.0	-422.978718570	1.53

[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 mol^{-1}.

SM22: Total Energy and Internal Rotation Barriers about O—CH=O bonds in CH_3O—CH=O, C_6H_5O—CH=O, $Y(C_5H_5)O$—CH=O and $Y(C_5H_5)C(OH)=O$

CH_3O—CH=O			C_6H_5O—CH=O			$Y(C_5H_5)O$—CH=O				$Y(C_5H_5)C(OH)=O$			
Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational barrier[b]	Torsion Angle	Relative Torsion Angle	Total energy[a]	Rotational barrier[b]
0.0	-229.060379969	4.99	0.0	-420.806423626	1.63	179.8	0.0	-382.649627014	1.59	-179.4	0.0	-382.677113356	0.00
15.0	-229.059848555	5.32	15.0	-420.805294433	2.33	194.8	15.0	-382.648886842	2.05	-164.4	15.0	-382.675981465	0.71
30.0	-229.058014359	6.47	30.0	-420.804704691	2.70	209.8	30.0	-382.646614691	3.48	-149.4	30.0	-382.672548400	2.86
45.0	-229.054936615	8.40	45.0	-420.802036093	4.38	224.8	45.0	-382.643091619	5.69	-134.4	45.0	-382.667435753	6.07
60.0	-229.051130093	10.79	60.0	-420.798675034	6.49	239.8	60.0	-382.639200572	8.13	-119.4	60.0	-382.661884285	9.55
75.0	-229.047651299	12.97	75.0	-420.795500635	8.48	254.8	75.0	-382.636216783	10.00	-104.4	75.0	-382.657469785	12.32
90.0	-229.046022818	14.00	90.0	-420.793731430	9.59	269.8	90.0	-382.635303958	10.57	-89.4	90.0	-382.655543043	13.53
105.0	-229.047454079	13.10	105.0	-420.794484677	9.12	284.8	105.0	-382.636794036	9.64	-74.4	105.0	-382.656330222	13.04
120.0	-229.051705360	10.43	120.0	-420.797765720	7.06	299.8	120.0	-382.640067836	7.58	-59.4	120.0	-382.658896838	11.43
135.0	-229.057322532	6.91	135.0	-420.801952556	4.43	314.8	135.0	-382.644112864	5.05	-44.4	135.0	-382.662027980	9.46
150.0	-229.062940409	3.38	150.0	-420.805710826	2.07	329.8	150.0	-382.648027778	2.59	-29.4	150.0	-382.664797892	7.72
165.0	-229.066923150	0.88	165.0	-420.808205961	0.51	344.8	165.0	-382.651030460	0.70	-14.4	165.0	-382.666646386	6.56
180.0	-229.068333024	0.00	180.0	-420.809020427	0.00	359.8	180.0	-382.652160121	0.00	0.58	180.0	-382.667349966	6.12
195.0	-229.066923166	0.88	195.0	-420.808205966	0.51	374.8	195.0	-382.651061491	0.69	15.5	195.0	-382.672071385	3.16
210.0	-229.062940407	3.38	210.0	-420.805710936	2.07	389.8	210.0	-382.648079548	2.56	30.5	210.0	-382.669654139	4.68
225.0	-229.057322767	6.91	225.0	-420.801952539	4.43	404.8	225.0	-382.644171541	5.01	45.5	225.0	-382.665741778	7.13
240.0	-229.051705355	10.43	240.0	-420.797765745	7.06	419.8	240.0	-382.640123037	7.55	60.5	240.0	-382.661307483	9.91
255.0	-229.047454078	13.10	255.0	-420.794484653	9.12	434.8	255.0	-382.636830633	9.62	75.5	255.0	-382.657676456	12.19
270.0	-229.046022795	14.00	270.0	-420.793731453	9.59	449.8	270.0	-382.635308319	10.57	90.5	270.0	-382.656243941	13.09
285.0	-229.047651262	12.97	285.0	-420.795500690	8.48	464.8	285.0	-382.636187307	10.02	105.6	285.0	-382.657924907	12.04
300.0	-229.051130139	10.79	300.0	-420.798674652	6.49	479.8	300.0	-382.639147962	8.16	120.6	300.0	-382.662236028	9.33
315.0	-229.054936519	8.40	315.0	-420.802036105	4.38	494.8	315.0	-382.643035641	5.72	135.6	315.0	-382.667664464	5.93
330.0	-229.058014346	6.47	330.0	-420.804704857	2.70	509.8	330.0	-382.646571010	3.50	150.6	330.0	-382.672602775	2.83
345.0	-229.059848579	5.32	345.0	-420.806224021	1.75	524.8	345.0	-382.648864999	2.06	165.6	345.0	-382.675796324	0.82
360.0	-229.060379990	4.99	360.0	-420.806423610	1.63	539.8	360.0	-382.649627069	1.59	180.6	360.0	-382.677113508	0.0000

[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 mol^{-1}.

SM23: Total Energy and Internal Rotation Barriers about C—O and O—C·=O bonds in CH_3—OC·=O

CH_3—OC·=O			CH_3O—C·=O		
Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational Barrier[b]
0.0	-228.400571536	0.021243	0.0	-228.401149684	5.0201e-06
15.0	-228.400571515	0.021256	15.0	-228.400165616	0.61752
30.0	-228.400571180	0.021466	30.0	-228.397499387	2.2906
45.0	-228.400588298	0.010725	45.0	-228.393853817	4.5782
60.0	-228.400605252	8.5969e-05	60.0	-228.390114628	6.9246
75.0	-228.400591720	0.0085774	75.0	-228.387345591	8.6622
90.0	-228.400572160	0.020852	90.0	-228.386408325	9.2504
105.0	-228.400571138	0.021493	105.0	-228.387557599	8.5292
120.0	-228.400571611	0.021196	120.0	-228.390381488	6.7572
135.0	-228.400571664	0.021163	135.0	-228.394021284	4.4731
150.0	-228.400571257	0.021418	150.0	-228.397479200	2.3033
165.0	-228.400589407	0.010029	165.0	-228.399855428	0.81216
180.0	-228.400605389	0.0000	180.0	-228.400605397	0.34155
195.0	-228.400589412	0.010026	195.0	-228.399855426	0.81216
210.0	-228.400571257	0.021418	210.0	-228.397479142	2.3033
225.0	-228.400571670	0.021159	225.0	-228.394021241	4.4732
240.0	-228.400571614	0.021194	240.0	-228.390381395	6.7572
255.0	-228.400571144	0.021489	255.0	-228.387557687	8.5291
270.0	-228.400572157	0.020853	270.0	-228.386408346	9.2503
285.0	-228.400591725	0.0085743	285.0	-228.387345704	8.6621
300.0	-228.400605256	8.3459e-05	300.0	-228.390114590	6.9246
315.0	-228.400588308	0.010718	315.0	-228.393853816	4.5782
330.0	-228.400571185	0.021463	330.0	-228.397499257	2.2907
345.0	-228.400571556	0.021231	345.0	-228.400165436	0.61763
360.0	-228.400571612	0.021195	360.0	-228.401149692	0.0000

[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 mol^{-1}.

SM 24: Total Energy and Internal Rotation Barriers about C_d—C· bonds in CH_2=CHC·(CH=O)CH=O, C·—OH bond in C·$(OH)_2$CH=O and C·—CH=O bond in C·$(OH)_2$CH=O

CH_2=CH—C·(CH=O)CH=O			C·(—OH)$_2$CH=O			C·$(OH)_2$—CH=O		
Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational Barrier[b]
0.0	-343.921375160	0.0000	0.0	-303.644634797	1.8746	0.0	-303.647622324	0.0000
15.0	-343.920087441	0.80806	15.0	-303.644183146	2.1580	15.0	-303.645552110	1.2991
30.0	-343.916464825	3.0813	30.0	-303.642927877	2.9457	30.0	-303.639652101	5.0014
45.0	-343.911219932	6.3725	45.0	-303.641139387	4.0680	45.0	-303.631042720	10.404
60.0	-343.905267854	10.107	60.0	-303.639269198	5.2415	60.0	-303.621347494	16.488
75.0	-343.899632031	13.644	75.0	-303.637941473	6.0747	75.0	-303.611925433	22.400
90.0	-343.897119426	15.221	90.0	-303.637825937	6.1472	90.0	-303.604170664	27.266
105.0	-343.900076395	13.365	105.0	-303.639175796	5.3001	105.0	-303.599849069	29.978
120.0	-343.905789720	9.7800	120.0	-303.641466075	3.8630	120.0	-303.598786832	30.645
135.0	-343.911838832	5.9841	135.0	-303.643916252	2.3254	135.0	-303.621679762	16.279
150.0	-343.916895794	2.8108	150.0	-303.645922555	1.0665	150.0	-303.627787153	12.447
165.0	-343.920220951	0.72428	165.0	-303.647193163	0.26915	165.0	-303.631606402	10.050
180.0	-343.921375120	2.5100e-05	180.0	-303.647622081	0.0000	180.0	-303.632902377	9.2369
195.0	-343.920220939	0.72429	195.0	-303.647192889	0.26932	195.0	-303.631606437	10.050
210.0	-343.916896015	2.8107	210.0	-303.645922534	1.0665	210.0	-303.627786983	12.447
225.0	-343.911838933	5.9841	225.0	-303.643916269	2.3254	225.0	-303.621679926	16.279
240.0	-343.905789529	9.7801	240.0	-303.641465903	3.8631	240.0	-303.613821947	21.210
255.0	-343.900076247	13.365	255.0	-303.639175817	5.3001	255.0	-303.605342965	26.531
270.0	-343.897118293	15.221	270.0	-303.637825928	6.1472	270.0	-303.598206531	31.009
285.0	-343.899632359	13.644	285.0	-303.637941496	6.0747	285.0	-303.594368017	33.418
300.0	-343.905267950	10.107	300.0	-303.639269567	5.2413	300.0	-303.621347336	16.488
315.0	-343.911220034	6.3724	315.0	-303.641139381	4.0680	315.0	-303.631042741	10.404
330.0	-343.916465027	3.0812	330.0	-303.642927873	2.9457	330.0	-303.639652290	5.0013
345.0	-343.920087593	0.80796	345.0	-303.644183172	2.1579	345.0	-303.645552087	1.2991
360.0	-343.921375202	-2.6355e-05	360.0	-303.644634802	1.8745	360.0	-303.647622297	1.6943e-05

[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 mol^{-1}.

SM25: Total Energy and Internal Rotation Barriers about C—C(O·)=O in (YC_5H_5)—C(O·)=O, C—O and O—C·=O bonds in (YC_5H_5)O—C·=O

(YC_5H_5)—C(O·)=O			(YC_5H_5)—OC·=O			(YC_5H_5)O—C·=O		
Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational Barrier[b]
0.0	-382.006546590	0.068372	0.0	-381.987477195	1.3238	0.0	-381.989907576	0.0000
15.0	-382.005998362	0.41239	15.0	-381.988143611	0.90562	15.0	-381.988899159	0.63279
30.0	-382.002935708	2.3342	30.0	-381.988819289	0.48163	30.0	-381.986159346	2.3521
45.0	-382.001214457	3.4143	45.0	-381.989363816	0.13993	45.0	-381.982368429	4.7309
60.0	-382.000881543	3.6232	60.0	-381.989586810	0.0000	60.0	-381.978521459	7.1449
75.0	-382.001501637	3.2341	75.0	-381.989398893	0.11792	75.0	-381.975671074	8.9335
90.0	-382.005441962	0.76154	90.0	-381.988851726	0.46127	90.0	-381.974647028	9.5761
105.0	-382.006655548	0.0000	105.0	-381.988146091	0.90407	105.0	-381.975731361	8.8957
120.0	-382.005712886	0.59153	120.0	-381.987449545	1.3412	120.0	-381.978537288	7.1350
135.0	-382.003645112	1.8891	135.0	-381.987064572	1.5827	135.0	-381.982204255	4.8339
150.0	-382.003890125	1.7353	150.0	-381.987163692	1.5205	150.0	-381.985697109	2.6421
165.0	-382.005070601	0.99457	165.0	-381.987608791	1.2412	165.0	-381.988128089	1.1166
180.0	-382.006566375	0.055957	180.0	-381.988107140	0.92851	180.0	-381.988987983	0.57705
195.0	-382.006120064	0.33602	195.0	-381.988477294	0.69623	195.0	-381.988128152	1.1166
210.0	-382.003620033	1.9048	210.0	-381.988738641	0.53223	210.0	-381.985696980	2.6422
225.0	-381.999377910	4.5668	225.0	-381.988924089	0.41586	225.0	-381.982204559	4.8337
240.0	-382.000879693	3.6244	240.0	-381.988987142	0.37630	240.0	-381.978538161	7.1344
255.0	-382.001441297	3.2720	255.0	-381.988895279	0.43394	255.0	-381.975731667	8.8955
270.0	-382.005683101	0.61022	270.0	-381.988692289	0.56132	270.0	-381.974646962	9.5762
285.0	-382.006655425	7.7184e-05	285.0	-381.988414497	0.73564	285.0	-381.975671088	8.9335
300.0	-382.005768593	0.55657	300.0	-381.988020310	0.98299	300.0	-381.978522481	7.1443
315.0	-382.003970857	1.6847	315.0	-381.987522425	1.2954	315.0	-381.982368659	4.7307
330.0	-382.003893697	1.7331	330.0	-381.987124542	1.5451	330.0	-381.986159401	2.3520
345.0	-382.004956508	1.0662	345.0	-381.987079815	1.5732	345.0	-381.988899153	0.63280
360.0	-382.006546913	0.068170	360.0	-381.987477211	1.3238	360.0	-381.989907548	1.7570e-05

[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 mol^{-1}.

SM26: Total Energy and Internal Rotation Barriers about C—C·=O in $(YC_5H_5O)C\cdot=O$, and C_b—C·=O bonds in $C_6H_5C\cdot=O$

(YC_5H_5O)—C·=O			C_6H_5—C·=O		
Torsion Angle	Total energy[a]	Rotational Barrier[b]	Torsion Angle	Total energy[a]	Rotational Barrier[b]
0.0	-381.983687900	2.7668	0.0	-344.928479782	0.0000
15.0	-381.982852435	3.2911	15.0	-344.928104899	0.23524
30.0	-381.982454488	3.5408	30.0	-344.927014333	0.91958
45.0	-381.982320327	3.6250	45.0	-344.925366668	1.9535
60.0	-381.982682637	3.3976	60.0	-344.923542345	3.0983
75.0	-381.983928350	2.6159	75.0	-344.922083964	4.0134
90.0	-381.985708977	1.4986	90.0	-344.921412758	4.4346
105.0	-381.986780459	0.82619	105.0	-344.921703042	4.2525
120.0	-381.986742066	0.85029	120.0	-344.922998286	3.4397
135.0	-381.985944290	1.3509	135.0	-344.924924511	2.2310
150.0	-381.984682840	2.1425	150.0	-344.926774336	1.0702
165.0	-381.983190650	3.0788	165.0	-344.928038228	0.27708
180.0	-381.981964375	3.8483	180.0	-344.928479766	1.0040e-05
195.0	-381.981641177	4.0511	195.0	-344.928038214	0.27709
210.0	-381.982210342	3.6940	210.0	-344.926774316	1.0702
225.0	-381.983267933	3.0303	225.0	-344.924924511	2.2310
240.0	-381.984582961	2.2051	240.0	-344.922998514	3.4396
255.0	-381.986013354	1.3076	255.0	-344.921702938	4.2525
270.0	-381.987242099	0.53651	270.0	-344.921412488	4.4348
285.0	-381.987991597	0.066192	285.0	-344.922083922	4.0135
300.0	-381.988097081	0.0000	300.0	-344.923542455	3.0982
315.0	-381.987520219	0.36199	315.0	-344.925366763	1.9535
330.0	-381.986384750	1.0745	330.0	-344.927014371	0.91956
345.0	-381.984975050	1.9591	345.0	-344.928104935	0.23522
360.0	-381.983688113	2.7667	360.0	-344.928479778	2.5100e-06

[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 mol^{-1}.

SM27: Coefficient of Truncated Fourier Series. Representation Expansions for Internal Rotation Potentials[a]

species	$C(OH)_2CH=O$		$CH_2=CHCH(CH=O)CH=O$		$CH_3C(OH)_2CH=O$			$CH_2=C(CHO)CH=CH_2$	
	C—CH=O	C—OH	C_d—C	C—CH=O	C—C	C—OH	C—CH=O	C_d—C_d	C_d—CH=O
a_0	2,8700	2,1664	1,2598	1,1935	1,3962	2,4614	2,5161	1,7777	4,3158
a_1	-1,2944	1,8966	-0,4603	1,1951	0,0162	-1,9576	-1,0347	-0,1854	0,8649
a_2	-0,6827	0,4144	-0,1267	-0,2054	0,0175	0,7489	-0,4268	-1,8092	-3,3623
a_3	-0,8049	0,5678	0,1921	-0,5642	1,4320	-0,4616	-0,8933	-0,3489	0,3621
a_4	-0,1074	0,0197	0,0362	-0,2876	-0,0176	0,0564	-0,2887	0,4621	0,3060
a_5	-0,0250	4,1875e-3	-0,0270	0,1450	-0,0140	-2,4648e-3	0,0833	0,0775	0,0313
a_6	0,0131	7,3078e-3	-0,0284	0,0647	0,0408	1,0010e-3	0,1146	0,0246	-6,7784e-4
a_7	0,0214	1,0865e-3	-3,4918e-3	-0,0584	-2,5805e-3	-4,5372e-4	-0,1113	-9,2794e-3	4,3630e-3
b_1	0,3990	-1,6570	0,9579	0,1119	2,9203e-3	-1,4275	1,4643	7,6416e-5	-3,7211e-5
b_2	-0,3482	-0,5771	-0,1278	0,1069	3,0156e-3	0,0425	-0,5653	-3,3700e-5	8,8274e-5
b_3	-0,1625	0,0441	-0,0247	-0,0390	0,1176	0,3563	-0,5010	-7,4341e-5	-3,9137e-5
b_4	0,0676	-4,3944e-3	-0,1234	-0,0768	3,5959e-4	-7,7114e-3	0,4465	1,4872e-5	-6,9277e-5
b_5	0,0564	7,7655e-3	-0,0394	-0,0522	1,9850e-3	0,0186	-0,1458	4,6012e-6	7,8551e-5
b_6	0,0470	3,1725e-3	7,0775e-3	0,0510	0,0223	-7,7797e-3	0,1368	7,8838e-5	3,3382e-6
b_7	0,0195	2,3011e-3	-0,0104	0,0673	2,5231e-4	2,6087e-3	-8,5459e-3	9,8437e-5	-7,6353e-5

species	$CH_2=CHC(OH)_2CH=CH_2$		$CH_2=CHCH=O$	$CH_2=C(OH)_2$	$CH_2=CHCH(CH_3)CH=CH_2$		$CH_2=C(OH)CH=CH_2$		$CH_2=CHOCH=CH_2$
	C_d—C	C—OH	C_d—CH=O	C_d—OH	C_d—C	C—OH	C_d—C_d	C_d—OH	C_d—O
a_0	2,1266	3,0591	3,4026	2,3448	1,1359	1,6008	3,2938	2,3588	1,6292
a_1	0,0344	1,9389	1,2544	0,8273	-0,3011	-6,5961e-3	-1,0846	0,3671	-0,0252
a_2	-1,5422	-0,5936	-1,2449	-2,0008	0,1402	-4,4539e-4	-1,8769	-1,2043	-1,8969
a_3	-1,0300	0,6504	1,9013	-0,2360	-0,9892	1,6326	-0,8224	0,1678	0,1027
a_4	0,2936	0,1039	1,0005	0,2196	-0,0457	-2,2471e-5	0,4465	-0,0113	0,2929
a_5	0,1146	-1,8531e-3	-0,0104	-3,1587e-3	0,0308	9,2433e-3	0,1268	-0,0339	0,1738
a_6	0,0491	0,0136	0,0728	0,0158	0,0245	0,0354	0,0427	-0,0361	0,1195
a_7	-0,0485	-3,9124e-3	0,0723	-1,8773e-3	6,9051e-3	-2,1042e-4	-0,0309	-0,0271	0,0761
b_1	-0,2050	0,4452	2,9705e-5	-2,0871e-6	0,1341	-0,0132	-0,1974	0,1571	-1,6657e-5
b_2	0,6476	0,3708	3,0551e-6	2,1464e-5	0,2135	5,2421e-4	-0,7113	-1,2530	7,1158e-6
b_3	0,0291	0,0464	-5,8876e-6	-6,5899e-6	-0,2066	0,1157	-0,4883	0,4473	1,7041e-5
b_4	-0,1212	0,1128	4,9177e-9	-2,9173e-5	-0,0336	-3,8235e-4	0,4262	0,2378	2,6396e-5
b_5	-0,0168	0,0522	-1,9489e-5	-6,8317e-5	7,0194e-3	-0,0126	0,1994	0,0678	-1,7209e-5
b_6	0,0457	0,0294	-8,3284e-6	-3,0603e-5	0,0151	7,2883e-3	0,1380	0,0304	-2,6188e-5
b_7	0,0272	0,0139	2,3812e-5	3,3938e-5	5,0954e-4	-7,0002e-4	-0,0116	8,2268e-3	-3,3096e-6

species	$CH_2=CHCH_2CH=O$		$CH_3OCH=O$		$CH_2=CHCH(OH)CH=CH_2$		$CH_2=CHCH(CH=O)CH=CH_2$	
	C_d—C	C—CH=O	C—O	O—CH=O	C_d—C	C—OH	C_d—C	C—CH=O
a_0	0.9230	0.9823	0,1154	7,9329	1,6083	1,7468	0,8949	1,0022
a_1	-0.1636	-0.0949	-1,3086e-3	1,7791	-0,1183	-0,0932	-0,1936	0,6792
a_2	-0.1436	-0.3469	-3,0910e-3	-5,7320	-0,1082	0,3624	-0,0803	-0,2863
a_3	-0.4492	0.6509	-0,1224	0,7182	-1,1821	1,0303	-0,4702	-0,7439
a_4	-0.2730	-0.0612	3,3286e-3	0,2979	-0,2418	0,0389	-0,1316	0,0102
a_5	0.0966	0.0248	1,5593e-3	-3,9727e-3	-0,0283	0,1141	0,0588	0,0252
a_6	-0.0229	4.7740e-3	7,0865e-3	-0,0213	0,0549	0,1330	-0,0131	9,4480e-3
a_7	0.0208	-4.8926e-4	-4,1335e-4	5,8692e-3	0,0381	0,0170	0,0185	-0,0119
b_1	0.1577	-0.5072	2,2449e-5	1,2006e-5	-0,1368	-0,2749	-0,0191	0,0350
b_2	-0.5636	0.2029	1,0005e-5	-1,7078e-5	-0,4383	-0,4369	0,5555	-8,0987e-3
b_3	0.1895	0.0316	6,9324e-6	1,2379e-5	-0,2756	0,1276	-0,2377	-0,0343
b_4	0.0856	-0.0294	-1,5312e-5	-7,1677e-7	-0,0674	0,0882	-0,1044	2,1822e-3
b_5	-0.0548	0.0180	4,0348e-7	-1,0975e-5	0,0661	-0,1117	0,0106	0,0231
b_6	0.0977	-7.1842e-3	-9,8284e-6	1,5838e-5	0,0201	0,0317	4,9142e-3	8,9172e-4
b_7	-0.0704	4.7914e-3	1,7761e-5	-1,0975e-5	0,0108	5,5957e-3	0,0181	-5,3262e-3

[a]Units in kcal/mol. Values of rotation barriers calculated at B3LYP/6-31G(d,p) level are used to calculate the coefficients

SM 28: Coefficient of Truncated Fourier Series. Representation Expansions for Internal Rotation Potentials[a]

species	$C_6H_5OCH=O$		$C_6H_5C(CH=O)=CH_2$		$C_6H_5C(OH)_2CH_3$			$C_6H_5C(=CH_2)CH=CH_2$	
	C_b—O	O—CH=O	C_b—C_d	C_d—CH=O	C_b—C	C—OH	C—C	C_b—C_d	C_d—C_d
a_0	0,7492	4,8079	1,0348	4,0938	2,0977	2,3954	1,8016	1,6205	2,8623
a_1	0,0568	0,3872	0,0327	0,6726	-0,0257	0,0505	1,7847e-3	-8,7685e-3	0,1280
a_2	1,0021	-4,3716	0,0103	-3,4336	-2,0589	-0,1618	7,9840e-3	-0,6874	-1,1108
a_3	0,0234	0,4874	1,4034e-3	-0,0346	1,0795e-3	0,4010	1,8552	-8,6019e-4	-0,4632
a_4	0,7048	0,4114	1,1231	0,1202	-0,0799	0,0890	-7,3530e-3	0,7070	-0,1597
a_5	-0,0249	-0,0388	0,0245	0,2109	0,0139	0,0308	-5,1685e-3	-0,0106	0,0436
a_6	0,1545	-7,3250e-3	0,2101	-0,0339	0,0485	3,4155e-3	0,0580	-8,4669e-3	-0,2095
a_7	-0,0125	0,0216	-5,0616e-3	-0,0720	0,0233	-0,0263	1,3082e-3	1,6779e-3	0,0633
b_1	-2,4060e-5	0,0126	2,5821e-5	0,1366	-0,0448	-1,3926	-0,0112	5,6173e-3	-0,0776
b_2	6,5950e-6	0,0243	4,5600e-5	0,4601	-0,4211	-0,9913	3,1900e-4	0,7122	-1,4133
b_3	4,9534e-5	0,0344	-3,2604e-5	-0,1233	-0,0155	0,0153	-0,1356	-2,5735e-3	1,1066
b_4	4,7984e-6	0,0421	1,0586e-5	6,4685e-3	0,5126	0,0303	-2,7865e-4	0,3827	-0,2597
b_5	-5,3974e-5	0,0470	3,2619e-5	-0,0387	0,0404	-0,0244	-0,0131	-4,3019e-4	-0,0550
b_6	1,5838e-5	0,0486	9,2323e-6	-0,0179	-0,1634	-0,0372	-0,0156	0,0982	0,2188
b_7	6,2464e-5	0,0469	-6,5475e-5	0,1324	-3,5109e-3	-5,0878e-3	-3,0714e-3	2,9489e-3	-7,2090e-3

species	$C_6H_5C(CH_3)_2CH=O$			$C_6H_5CH=CH_2$	$C_6H_5C(=CH_2)OH$		$C_6H_5C(=CH_2)CH_3$		$C_6H_5CH=O$
	C_b—C	C—C	C—CH=O	C_b—C_d	C_b—C_d	C_d—OH	C_b—C_d	C_d—C	C_b—CH=O
a_o	1,2460	1,2932	1,7424	1,7594	1,3435	2,1517	0,7689	0,9655	1,5186
a_1	-0,0276	8,3718e-3	-0,0424	4,9628e-3	0,0378	0,0941	2,9473e-3	-0,0136	2,1042e-3
a_2	-1,2216	-0,0174	-0,1229	-2,2044	-1,1308	-1,8740	-0,9603	3,7986e-4	1,8596
a_3	-7,4660e-3	1,3061	0,7005	-5,8546e-3	-0,0276	0,6844	-4,3574e-3	0,9824	2,0521e-3
a_4	0,2547	0,0180	0,0176	0,4457	1,0260	0,3883	0,4948	8,3320e-4	1,1177
a_5	0,0249	1,0656e-3	0,0251	5,4393e-3	0,0444	0,0114	6,2888e-3	0,0175	2,1027e-3
a_6	-0,2274	0,0394	9,9240e-4	-4,0349e-3	0,3181	0,1005	0,0304	0,0215	-7,5399e-3
a_7	-0,0157	-3,6742e-3	7,4082e-3	-5,6533e-3	0,0147	0,0745	-2,1357e-3	3,3063e-3	2,0788e-3
b_1	-0,0237	-0,0140	-1,0657	-7,2333e-6	-1,1634e-4	-4,1989e-5	-3,4878e-5	0,0107	0,0260
b_2	0,0473	-9,1893e-3	-0,3311	-7,2172e-3	6,1567e-5	2,7846e-5	5,5983e-6	5,6687e-3	-8,8443e-6
b_3	-2,8210e-4	0,5869	-8,4512e-3	-8,8309e-6	1,3681e-4	2,2212e-5	4,0409e-5	-0,3082	0,0820
b_4	-0,3003	4,8129e-3	-0,1631	2,8596e-3	3,6098e-5	-5,8452e-5	-4,4288e-5	5,7770e-3	9,0991e-6
b_5	0,0104	-0,0126	0,0133	2,1343e-5	-1,6082e-4	-1,9257e-6	-4,2247e-5	4,8804e-3	0,0273
b_6	-0,0618	0,0426	-9,5173e-3	-2,1328e-5	-5,2241e-5	2,5838e-5	2,0005e-5	0,0329	-4,9951e-6
b_7	0,0154	3,9770e-3	-8,7340e-3	-8,4758e-5	1,6014e-4	-4,9127e-5	2,5558e-5	2,2807e-3	-9,4860e-3

species	$Y(C_5H_5)C(OH)=O$		$Y(C_5H_5)OCH=O$		$Y(C_5H_5O)CH=O$	$C_6H_5CH_2OH$	
	O=C—OH	C—C=O	C—O	O—CH=O	C—CH=O	C_b—C	C—OH
a_o	7.5258	0.3714	1.7310	5.5255	2.7680	1.1305	1.3170
a_1	-2.0441	0.0531	-0.0726	0.6287	-1.7163	-4.1359e-3	0.6854
a_2	-5.3951	-0.2270	-1.3946	-4.8712	-1.4289	-0.2509	0.3569
a_3	-0.4635	-0.2052	-0.2633	0.0719	0.3818	-3.0591e-3	-0.7082
a_4	0.4545	3.3452e-4	0.0625	0.1567	-0.0222	-0.1470	0.1225
a_5	-0.1013	4.6399e-3	-0.0239	0.0892	0.0123	9.2577e-3	-2.2315e-3
a_6	0.1389	-2.0842e-3	-0.0472	-0.0218	3.0583e-3	0.0307	0.0363
a_7	-0.1497	3.2364e-3	3.8748e-3	7.8961e-3	1.2999e-3	5.6978e-3	-4.4971e-3
b_1	0.5979	-0.1426	-0.0428	1.1145e-3	0.5663	-0.0250	-0.0954
b_2	-0.6629	-0.2349	0.0700	-0.0183	0.3688	1.1243	-0.1014
b_3	0.4930	0.0758	-9.1690e-3	4.0388e-4	-0.4547	3.7786e-3	0.3125
b_4	-0.3379	0.1042	-0.0329	1.1280e-3	0.0524	0.0835	-0.0759
b_5	0.1833	-6.4030e-3	4.0279e-3	7.4304e-4	0.0261	-0.0167	2.0615e-3
b_6	-0.1577	-1.9865e-3	0.0135	-1.8916e-4	-0.0282	-0.0335	-0.0400
b_7	0.1033	6.4116e-3	-4.1594e-3	2.0121e-4	7.9730e-3	-1.7721e-4	7.0777e-3

[a]Units in kcal/mol. Values of rotation barriers calculated at B3LYP/6-31G(d,p) level

SM 29: Coefficient of Truncated Fourier Series. Representation Expansions for Internal Rotation Potentials[a]

species	$CH_3OC\cdot=O$		$C_6H_5C\cdot=O$	$CH_2=CHC\cdot(CH=O)CH=O$	$C\cdot(OH)_2)CH=O$	
	C—O	O—C·=O	C_b—C·=O	C_d—C·	C·—OH	C·—CH=O
a_0	0.0158	4.6142	2.1603	6.8264	3.3664	15.6589
a_1	1.0725e-4	-0.0294	-0.1002	0.1407	1.0853	-4.7318
a_2	3.4014e-4	-4.5455	-2.2375	-7.3772	-2.5840	-12.6201
a_3	9.4341e-3	-0.1072	0.1126	-0.1201	-0.1475	0.5206
a_4	-2.3218e-4	0.0905	0.0624	0.7108	0.1724	1.8315
a_5	-2.8944e-4	-0.0119	-0.0145	-5.8855e-3	7.6524e-4	-0.2071
a_6	-5.2344e-3	1.4795e-3	0.0187	-0.2012	-0.0195	0.0900
a_7	4.4067e-4	-0.0132	6.6503e-4	-0.0114	-8.4719e-4	-0.7256
b_1	2.1957e-6	1.2005e-5	-9.2284e-6	8.9551e-6	5.7120e-6	-0.2404
b_2	1.3874e-6	-3.4620e-6	-1.4684e-6	2.0138e-5	3.2906e-5	-1.2836
b_3	2.2180e-6	-4.0821e-5	2.4820e-5	2.7867e-5	-4.1199e-6	0.7580
b_4	1.8373e-6	-1.5151e-5	1.0830e-5	7.2661e-7	-2.1601e-6	1.7248
b_5	1.4799e-6	5.5235e-6	-3.1614e-5	1.6907e-5	-1.2847e-5	-1.1561
b_6	1.5133e-6	-1.7495e-5	-5.8284e-6	8.3825e-7	2.2505e-5	-1.2054
b_7	2.0475e-6	-2.8099e-6	2.8920e-5	-1.4193e-5	1.5872e-6	0.8295

species	$Y(C_5H_5)C(O\cdot)=O$	$Y(C_5H_5O)C\cdot=O$	$Y(C_5H_5)OC\cdot=O$	
	C—C=O	C—C·=O	C—O	O—C·=O
a_o	1.6039	2.1299	0.8374	4,8567
a_1	-0.0365	-0.3268	5.1398e-4	-0.1776
a_2	-0.3975	1.0941	0.3206	-4.6427
a_3	0.0969	-0.2385	0.1879	-0.0992
a_4	-1.1191	0.0356	-0.0203	0.0753
a_5	0.0508	0.0390	0.0102	-8.1107e-3
a_6	-0.0446	0.0484	-0.0123	-5.1179e-4
a_7	-0.1094	-0.0146	-1.5446e-3	-2.8516e-3
b_1	-0.0258	0.5333	-0.0266	1.1772e-4
b_2	1.0795	1.2671	-0.5780	5.6838e-6
b_3	-0.0300	-0.0113	4.2128e-3	1.9529e-5
b_4	-0.9488	-0.1055	-0.0165	2.8146e-5
b_5	0.0836	-0.0489	-0.0239	-1.1500e-4
b_6	0.0655	0.0328	1.8258e-3	-1.7500e-5
b_7	0.0273	9.3829e-3	-3.5573e-3	7.4874e-5

[a]Units in kcal/mol. Values of rotation barriers calculated at B3LYP/6-31G(d,p) level

SM30: Thermochemical Properties of species

1. $C(OH)_2CH=O$ (ideal Gas)

T (K)	Cp (cal/mol/K)					S (cal/mol/K)	[H(T) - H(0 K)] (kcal/mol)
	IR C(OH)2—CH=O	IR C(—OH)2CH=O	IR total	TVR	IR + TVR		
0.1	0.000	0.000	0.00	7.95	7.95	0.63	0.00
10	0.000	0.274	0.27	7.95	8.22	37.30	0.08
50	1.427	0.608	2.03	7.96	9.99	51.65	0.44
100	2.099	0.934	3.03	8.49	11.52	59.14	0.98
150	1.897	1.199	3.10	9.83	12.92	64.03	1.59
200	2.103	1.342	3.45	11.50	14.94	67.98	2.28
298.15	3.018	1.526	4.54	15.24	19.78	74.75	3.98
300	3.034	1.529	4.56	15.31	19.87	74.87	4.02
400	3.593	1.675	5.27	19.16	24.43	81.16	6.24
500	3.561	1.773	5.33	22.52	27.86	86.93	8.86
600	3.240	1.818	5.06	25.30	30.36	92.19	11.78
700	2.863	1.820	4.68	27.59	32.27	96.97	14.92
800	2.524	1.794	4.32	29.49	33.81	101.35	18.22
900	2.246	1.752	4.00	31.09	35.09	105.37	21.67
1000	2.025	1.701	3.73	32.47	36.19	109.10	25.24
1100	1.851	1.649	3.50	33.65	37.15	112.57	28.90
1200	1.714	1.598	3.31	34.68	37.99	115.82	32.66
1300	1.606	1.549	3.15	35.57	38.73	118.87	36.50
1400	1.518	1.504	3.02	36.35	39.38	121.75	40.40
1500	1.447	1.463	2.91	37.04	39.95	124.47	44.37
1600	1.389	1.425	2.81	37.64	40.46	127.05	48.39
1700	1.342	1.391	2.73	38.17	40.91	129.51	52.46
1800	1.302	1.361	2.66	38.64	41.31	131.85	56.57
1900	1.268	1.333	2.60	39.06	41.66	134.08	60.72
2000	1.239	1.308	2.55	39.43	41.98	136.22	64.90
2500	1.146	1.215	2.36	40.78	43.14	145.70	86.21
3000	1.097	1.156	2.25	41.59	43.85	153.61	107.97
3500	1.068	1.118	2.19	42.12	44.30	160.40	130.01
4000	1.049	1.091	2.14	42.47	44.61	166.33	152.25
4500	1.037	1.072	2.11	42.72	44.83	171.59	174.61
5000	1.028	1.058	2.09	42.91	44.99	176.32	197.07

2. $CH_2=CHCH(CH=O)CH=O$ (ideal Gas)

T (K)	Cp (cal/mol/K)						S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C_d—C	IR C—CH=O	IR C—CH=O	IR Total	TVR	IR + TVR		
0.1	0.00	0.00	0.00	0	7.95	7.95	3.83	0.00
10	0.03	0.61	0.61	1.27	7.94	9.22	40.44	0.09
50	1.89	2.44	2.44	6.78	8.28	15.06	53.29	0.57
100	3.35	1.86	1.86	7.07	10.62	17.70	59.64	1.38
150	3.46	1.70	1.70	6.87	13.18	20.06	64.38	2.33
200	3.05	1.76	1.76	6.59	15.90	22.50	68.49	3.39
298.15	2.40	1.90	1.90	6.20	21.99	28.21	75.83	5.87
300	2.39	1.90	1.90	6.20	22.12	28.32	75.96	5.92
400	1.99	1.88	1.88	5.76	28.38	34.15	83.07	9.05
500	1.74	1.78	1.78	5.31	33.87	39.18	89.90	12.72
600	1.56	1.67	1.67	4.90	38.46	43.37	96.40	16.86
700	1.44	1.56	1.56	4.57	42.28	46.86	102.55	21.38
800	1.35	1.47	1.47	4.31	45.48	49.80	108.35	26.21
900	1.29	1.40	1.40	4.09	48.19	52.29	113.81	31.32
1000	1.24	1.34	1.34	3.93	50.49	54.42	118.96	36.66
1100	1.20	1.29	1.29	3.79	52.45	56.25	123.83	42.20
1200	1.17	1.25	1.25	3.68	54.13	57.82	128.43	47.90
1300	1.15	1.22	1.22	3.59	55.57	59.17	132.79	53.75
1400	1.13	1.19	1.19	3.52	56.81	60.34	136.94	59.73
1500	1.11	1.17	1.17	3.46	57.89	61.35	140.87	65.82
1600	1.10	1.15	1.15	3.41	58.82	62.23	144.62	72.00
1700	1.09	1.13	1.13	3.36	59.63	63.00	148.19	78.26
1800	1.08	1.12	1.12	3.32	60.34	63.67	151.61	84.59
1900	1.07	1.11	1.11	3.29	60.97	64.27	154.87	90.99
2000	1.06	1.10	1.10	3.26	61.52	64.79	158.00	97.44
2500	1.04	1.06	1.06	3.17	63.49	66.66	171.92	130.35
3000	1.02	1.04	1.04	3.11	64.64	67.76	183.59	163.98
3500	1.01	1.03	1.03	3.08	65.38	68.46	193.60	198.05
4000	1.012	1.02	1.02	3.05	65.87	68.93	202.35	232.40
4500	1.00	1.01	1.01	3.04	66.21	69.26	210.12	266.96
5000	1.00	1.01	1.01	3.02	66.46	69.49	217.11	301.65

3. $CH_3C(OH)_2CH=O$ (ideal Gas)

T (K)	Cp (cal/mol/K)						S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C—C	IR C—OH	IR C—CH=O	IR Total	TVR	IR + TVR		
0.1	0.000	0.000	0.01	0.01	7.95	7.96	1.43	0.00
10	0.022	0.000	0.01	0.03	7.95	7.98	41.59	0.08
50	0.046	0.227	0.38	0.65	7.98	8.63	54.54	0.41
100	0.630	1.281	1.31	3.22	9.13	12.35	61.55	0.93
150	1.227	1.790	1.76	4.78	11.54	16.32	67.27	1.64
200	1.618	1.923	2.03	5.57	14.21	19.78	72.40	2.54
298.15	1.966	1.979	2.39	6.34	19.65	25.99	81.36	4.79
300	1.968	1.980	2.40	6.35	19.76	26.11	81.52	4.84
400	1.989	2.039	2.61	6.64	25.10	31.73	89.72	7.74
500	1.886	2.073	2.65	6.61	29.72	36.32	97.22	11.15
600	1.757	2.063	2.56	6.38	33.55	39.93	104.10	14.97
700	1.637	2.017	2.42	6.07	36.72	42.79	110.41	19.11
800	1.535	1.950	2.26	5.74	39.38	45.12	116.23	23.51
900	1.452	1.874	2.10	5.43	41.65	47.08	121.61	28.13
1000	1.385	1.798	1.96	5.15	43.60	48.75	126.62	32.92
1100	1.330	1.725	1.84	4.90	45.29	50.19	131.30	37.87
1200	1.285	1.657	1.74	4.68	46.76	51.44	135.69	42.95
1300	1.248	1.596	1.65	4.50	48.04	52.54	139.83	48.15
1400	1.218	1.541	1.58	4.34	49.16	53.49	143.74	53.45
1500	1.192	1.492	1.51	4.20	50.14	54.34	147.43	58.85
1600	1.171	1.448	1.46	4.08	51.00	55.08	150.95	64.32
1700	1.152	1.410	1.41	3.97	51.76	55.73	154.29	69.86
1800	1.137	1.375	1.37	3.88	52.43	56.31	157.48	75.46
1900	1.123	1.344	1.33	3.80	53.03	56.83	160.53	81.12
2000	1.111	1.317	1.30	3.73	53.56	57.29	163.44	86.83
2500	1.071	1.217	1.20	3.49	55.47	58.96	176.38	115.93
3000	1.048	1.156	1.14	3.34	56.63	59.97	187.21	145.68
3500	1.034	1.116	1.10	3.25	57.37	60.62	196.49	175.83
4000	1.025	1.089	1.07	3.19	57.87	61.06	204.60	206.26
4500	1.019	1.071	1.06	3.15	58.22	61.37	211.80	236.87
5000	1.014	1.057	1.05	3.12	58.48	61.59	218.28	267.61

4. $CH_2=CHCH(CH=O)CH=CH_2$ (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=C	IR C—C=O	IR Total	TVR	IR + TVR		
0.1	0.00	0.00	0.00	0.00	7.95	7.95	4.01	0.00
10	0.49	0.49	0.06	1.05	7.95	9.00	42.26	0.08
50	2.13	2.13	1.68	5.93	8.24	14.17	60.74	0.54
100	2.77	2.77	2.35	7.89	10.61	18.50	71.89	1.36
150	2.73	2.73	2.43	7.89	13.64	21.53	79.94	2.35
200	2.48	2.48	2.35	7.30	16.89	24.20	86.44	3.50
298.15	2.01	2.01	2.10	6.11	24.09	30.20	97.03	6.16
300	2.00	2.00	2.09	6.09	24.23	30.32	97.22	6.21
400	1.68	1.68	1.84	5.21	31.68	36.89	106.70	9.58
500	1.49	1.49	1.65	4.62	38.22	42.84	115.45	13.57
600	1.36	1.36	1.50	4.23	43.66	47.89	123.61	18.12
700	1.28	1.28	1.40	3.95	48.20	52.15	131.23	23.13
800	1.22	1.22	1.32	3.75	52.01	55.76	138.36	28.53
900	1.17	1.17	1.26	3.61	55.25	58.86	145.05	34.26
1000	1.14	1.14	1.22	3.50	58.03	61.53	151.33	40.28
1100	1.12	1.12	1.19	3.42	60.41	63.83	157.26	46.55
1200	1.10	1.10	1.16	3.36	62.47	65.83	162.86	53.04
1300	1.08	1.08	1.14	3.30	64.25	67.55	168.16	59.71
1400	1.07	1.07	1.12	3.26	65.79	69.05	173.20	66.54
1500	1.06	1.06	1.10	3.23	67.13	70.36	177.98	73.51
1600	1.05	1.05	1.09	3.20	68.30	71.50	182.53	80.61
1700	1.05	1.05	1.08	3.18	69.32	72.50	186.88	87.81
1800	1.04	1.04	1.07	3.16	70.22	73.38	191.03	95.11
1900	1.04	1.04	1.06	3.14	71.01	74.15	195.00	102.48
2000	1.03	1.03	1.06	3.12	71.71	74.84	198.81	109.93
2500	1.02	1.02	1.04	3.07	74.22	77.29	215.74	148.02
3000	1.01	1.01	1.02	3.05	75.71	78.76	229.95	187.06
3500	1.01	1.01	1.02	3.03	76.66	79.68	242.14	226.69
4000	1.00	1.00	1.01	3.02	77.29	80.31	252.81	266.70
4500	1.00	1.00	1.01	3.01	77.74	80.75	262.29	306.97
5000	1.00	1.00	1.00	3.00	78.06	81.06	270.81	347.43

5. CH_2=CHC(OH)$_2$CH=CH_2 (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=C	IR C—OH	IR C—OH	IR Total	TVR	IR + TVR		
0.1	0.000	0.00	0.00	0.00	0.00	7.95	7.95	3.57	0.00
10	0.00	0.00	0.00	0.00	0.01	7.95	7.96	40.17	0.08
50	1.65	1.65	0.02	0.02	3.35	7.99	11.34	54.63	0.47
100	2.75	2.75	0.45	0.45	6.42	9.50	15.92	63.86	1.14
150	2.92	2.92	1.03	1.03	7.92	12.71	20.63	71.14	2.05
200	2.95	2.95	1.52	1.52	8.95	16.47	25.42	77.65	3.20
298.15	2.82	2.82	2.39	2.39	10.43	24.38	34.81	89.40	6.15
300	2.82	2.82	2.40	2.40	10.46	24.53	34.99	89.62	6.22
400	2.60	2.60	3.01	3.01	11.23	32.11	43.34	100.72	10.15
500	2.38	2.38	3.21	3.21	11.18	38.43	49.61	110.98	14.81
600	2.18	2.18	3.12	3.12	10.60	43.52	54.12	120.34	20.01
700	2.01	2.01	2.90	2.90	9.83	47.65	57.48	128.86	25.59
800	1.86	1.86	2.66	2.66	9.04	51.09	60.13	136.65	31.48
900	1.74	1.74	2.42	2.42	8.33	54.01	62.34	143.80	37.61
1000	1.64	1.64	2.22	2.22	7.72	56.52	64.24	150.42	43.94
1100	1.56	1.56	2.04	2.04	7.21	58.70	65.91	156.58	50.45
1200	1.49	1.49	1.90	1.90	6.78	60.60	67.38	162.34	57.11
1300	1.43	1.43	1.78	1.78	6.42	62.26	68.68	167.75	63.92
1400	1.38	1.38	1.68	1.68	6.12	63.72	69.84	172.85	70.85
1500	1.34	1.34	1.60	1.60	5.87	65.00	70.87	177.68	77.88
1600	1.30	1.30	1.53	1.53	5.66	66.12	71.79	182.26	85.02
1700	1.27	1.27	1.47	1.47	5.48	67.12	72.60	186.62	92.24
1800	1.25	1.25	1.42	1.42	5.33	68.00	73.33	190.77	99.53
1900	1.22	1.22	1.37	1.37	5.20	68.78	73.98	194.74	106.90
2000	1.20	1.20	1.34	1.34	5.08	69.47	74.56	198.53	114.33
2500	1.13	1.13	1.21	1.21	4.70	72.00	76.70	215.37	152.19
3000	1.09	1.09	1.14	1.14	4.48	73.53	78.01	229.44	190.89
3500	1.07	1.07	1.10	1.10	4.35	74.51	78.86	241.52	230.12
4000	1.05	1.05	1.08	1.08	4.26	75.17	79.43	252.07	269.70
4500	1.04	1.04	1.06	1.06	4.20	75.64	79.84	261.44	309.53
5000	1.03	1.03	1.05	1.05	4.15	75.98	80.14	269.87	349.53

6. CH_2=CHCH=O (ideal gas)

T (K)	Cp (cal/mol/K)				S (cal/mol/K)	[H(T) -H(0K)] (kcal/mol)
	IR C=C—C=O	IR Total	TVR	TVR + IR		
0.1	0.00	0.00	7.95	7.95	-3.63	0.00
10	0.00	0.00	7.95	7.95	32.96	0.08
50	1.09	1.09	7.96	9.05	46.32	0.42
100	1.57	1.57	8.47	10.04	52.89	0.89
150	1.87	1.87	9.48	11.35	57.18	1.43
200	2.23	2.23	10.81	13.04	60.64	2.04
298.15	2.82	2.82	14.07	16.89	66.49	3.50
300	2.83	2.83	14.14	16.97	66.60	3.53
400	3.07	3.07	17.69	20.76	71.94	5.42
500	3.08	3.08	20.88	23.96	76.87	7.66
600	2.97	2.97	23.59	26.56	81.42	10.19
700	2.80	2.80	25.86	28.66	85.63	12.96
800	2.62	2.62	27.79	30.41	89.54	15.91
900	2.44	2.44	29.44	31.88	93.17	19.03
1000	2.28	2.28	30.85	33.13	96.57	22.28
1100	2.13	2.13	32.06	34.19	99.765	25.65
1200	2.01	2.01	33.11	35.12	102.75	29.12
1300	1.89	1.89	34.01	35.9	105.58	32.67
1400	1.80	1.80	34.79	36.59	108.25	36.30
1500	1.72	1.72	35.48	37.2	110.79	39.99
1600	1.64	1.64	36.07	37.71	113.19	43.73
1700	1.58	1.58	36.59	38.17	115.47	47.53
1800	1.53	1.53	37.04	38.57	117.66	51.37
1900	1.48	1.48	37.44	38.92	119.74	55.24
2000	1.43	1.43	37.80	39.23	121.75	59.15
2500	1.29	1.29	39.07	40.36	130.61	79.08
3000	1.20	1.20	39.82	41.02	138.02	99.43
3500	1.15	1.15	40.30	41.45	144.36	120.06
4000	1.11	1.11	40.62	41.73	149.91	140.86
4500	1.09	1.09	40.84	41.93	154.84	161.78
5000	1.07	1.07	41.01	42.08	159.26	182.79

7. $CH_2=C(OH)_2$ (ideal Gas)

T (K)	Cp (cal/mol/K)					S (cal/mol/K)	[H(T) - H(0 K)] (kcal/mol)
	IR C_d(—OH)	IR C_d(—OH)	IR Total	TVR	TVR + IR		
0.1	0.000	0.000	0.00	7.95	7.95	0.00	0.00
10	0.000	0.000	0.00	7.95	7.95	35.05	0.08
50	0.094	0.094	0.19	7.95	8.14	47.87	0.40
100	0.910	0.910	1.82	8.15	9.97	53.99	0.85
150	1.710	1.710	3.42	9.14	12.56	58.49	1.41
200	2.194	2.194	4.39	10.78	15.17	62.44	2.10
298.15	2.540	2.540	5.08	14.55	19.63	69.28	3.82
300	2.542	2.542	5.08	14.62	19.71	69.40	3.85
400	2.562	2.562	5.12	18.19	23.31	75.51	6.01
500	2.465	2.465	4.93	21.11	26.04	80.96	8.48
600	2.323	2.323	4.65	23.43	28.07	85.85	11.19
700	2.171	2.171	4.34	25.30	29.64	90.26	14.08
800	2.026	2.026	4.05	26.86	30.91	94.27	17.11
900	1.896	1.896	3.79	28.19	31.99	97.95	20.26
1000	1.784	1.784	3.57	29.35	32.92	101.35	23.50
1100	1.687	1.687	3.37	30.37	33.74	104.51	26.84
1200	1.605	1.605	3.21	31.26	34.47	107.45	30.25
1300	1.535	1.535	3.07	32.06	35.13	110.22	33.73
1400	1.476	1.476	2.95	32.76	35.71	112.84	37.27
1500	1.425	1.425	2.85	33.38	36.23	115.30	40.87
1600	1.381	1.381	2.76	33.93	36.69	117.65	44.52
1700	1.343	1.343	2.69	34.42	37.11	119.87	48.21
1800	1.310	1.310	2.62	34.86	37.48	122.00	51.94
1900	1.282	1.282	2.56	35.25	37.81	124.02	55.70
2000	1.257	1.257	2.51	35.60	38.11	125.96	59.50
2500	1.169	1.169	2.34	36.88	39.22	134.57	78.85
3000	1.118	1.118	2.24	37.67	39.90	141.77	98.65
3500	1.087	1.087	2.17	38.17	40.35	147.95	118.72
4000	1.066	1.066	2.13	38.52	40.65	153.35	138.97
4500	1.051	1.051	2.10	38.77	40.87	158.14	159.35
5000	1.040	1.040	2.08	38.94	41.02	162.45	179.82

8. $CH_2=CHCH(CH_3)CH=CH_2$ (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=C	IR C—C	IR Total	TVR	IR + TVR		
0.1	0.00	0.00	0.00	0.00	7.95	7.95	1.79	0.00
10	0.05	0.05	0.02	0.12	7.95	8.07	40.58	0.08
50	2.63	2.63	0.14	5.40	8.09	13.48	58.05	0.51
100	2.35	2.35	0.93	5.63	10.02	15.65	67.88	1.23
150	2.32	2.32	1.47	6.12	12.77	18.88	74.78	2.09
200	2.31	2.31	1.78	6.41	15.83	22.24	80.61	3.12
298.15	2.15	2.15	2.09	6.39	23.10	29.49	90.67	5.64
300	2.15	2.15	2.09	6.39	23.25	29.64	90.85	5.70
400	1.91	1.91	2.14	5.97	31.14	37.11	100.26	9.04
500	1.71	1.71	2.05	5.48	38.21	43.68	109.12	13.09
600	1.56	1.56	1.92	5.04	44.17	49.21	117.47	17.74
700	1.44	1.44	1.79	4.68	49.18	53.86	125.31	22.90
800	1.36	1.36	1.67	4.39	53.45	57.84	132.68	28.49
900	1.29	1.29	1.57	4.16	57.11	61.27	139.62	34.45
1000	1.24	1.24	1.49	3.98	60.27	64.25	146.17	40.73
1100	1.21	1.21	1.42	3.84	63.01	66.85	152.37	47.29
1200	1.17	1.17	1.37	3.72	65.39	69.11	158.23	54.09
1300	1.15	1.15	1.32	3.62	67.46	71.08	163.80	61.10
1400	1.13	1.13	1.28	3.54	69.25	72.80	169.10	68.30
1500	1.11	1.11	1.25	3.48	70.82	74.30	174.14	75.66
1600	1.10	1.10	1.22	3.42	72.19	75.61	178.95	83.15
1700	1.09	1.09	1.20	3.38	73.39	76.77	183.55	90.77
1800	1.08	1.08	1.18	3.34	74.45	77.79	187.94	98.50
1900	1.07	1.07	1.16	3.30	75.38	78.69	192.15	106.33
2000	1.06	1.06	1.14	3.27	76.21	79.48	196.19	114.24
2500	1.04	1.04	1.09	3.17	79.18	82.35	214.20	154.76
3000	1.03	1.03	1.06	3.12	80.95	84.06	229.35	196.40
3500	1.02	1.02	1.04	3.08	82.07	85.15	242.37	238.72
4000	1.01	1.01	1.03	3.06	82.83	85.89	253.78	281.49
4500	1.01	1.01	1.02	3.04	83.36	86.40	263.91	324.57
5000	1.00	1.00	1.02	3.03	83.75	86.77	273.03	367.87

9. CH_2=C(CHO)CH=CH_2 (ideal Gas)

T (K)	Cp (cal/mol/K)					S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C_d—C_d	IR C_d—CH=O	IR Total	TVR	IR + TVR		
0.1	0.000	0.000	0.00	7.949	7.95	2.75	0.00
10	0.216	0.000	0.22	7.949	8.16	39.40	0.08
50	1.539	0.799	2.34	7.960	10.30	54.02	0.45
100	2.359	1.963	4.32	8.680	13.00	61.98	1.03
150	2.771	2.150	4.92	10.534	15.45	67.68	1.73
200	2.715	2.298	5.01	13.034	18.05	72.42	2.57
298.15	2.417	2.797	5.21	18.978	24.19	80.62	4.63
300	2.412	2.806	5.22	19.099	24.32	80.77	4.68
400	2.208	3.155	5.36	25.248	30.61	88.53	7.43
500	2.056	3.253	5.31	30.612	35.92	95.84	10.77
600	1.923	3.201	5.12	35.066	40.19	102.69	14.58
700	1.805	3.078	4.88	38.752	43.63	109.08	18.78
800	1.701	2.925	4.63	41.836	46.46	115.03	23.29
900	1.611	2.764	4.38	44.443	48.82	120.59	28.06
1000	1.534	2.607	4.14	46.663	50.80	125.80	33.04
1100	1.470	2.458	3.93	48.565	52.49	130.68	38.21
1200	1.414	2.322	3.74	50.199	53.94	135.28	43.53
1300	1.368	2.199	3.57	51.609	55.18	139.62	48.99
1400	1.328	2.088	3.42	52.828	56.24	143.72	54.56
1500	1.293	1.989	3.28	53.886	57.17	147.61	60.23
1600	1.264	1.901	3.16	54.808	57.97	151.31	65.99
1700	1.238	1.823	3.06	55.614	58.67	154.83	71.82
1800	1.216	1.753	2.97	56.321	59.29	158.19	77.72
1900	1.196	1.691	2.89	56.943	59.83	161.39	83.68
2000	1.179	1.635	2.81	57.493	60.31	164.46	89.69
2500	1.119	1.433	2.55	59.463	62.01	178.08	120.30
3000	1.084	1.310	2.39	60.631	63.02	189.46	151.58
3500	1.061	1.232	2.29	61.373	63.67	199.21	183.27
4000	1.046	1.179	2.22	61.870	64.09	207.73	215.21
4500	1.036	1.141	2.18	62.219	64.40	215.29	247.34
5000	1.028	1.114	2.14	62.472	64.61	222.09	279.59

10. CH_2=CHOCH=CH_2 (ideal Gas)

T (K)	Cp (cal/mol/K)					S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C_d—O	IR O—C_d	IR Total	TVR	IR + TVR		
0.1	0.00	0.00	0.00	7.95	7.95	0.00	.001
10	0.00	0.00	0.01	7.95	7.96	35.15	.08
50	2.76	2.76	5.53	8.08	13.61	51.03	.39
100	2.57	2.57	5.15	9.02	14.17	60.78	.82
150	2.18	2.18	4.36	10.52	14.88	66.59	1.31
200	2.03	2.03	4.06	12.66	16.72	71.06	1.88
298.15	2.00	2.00	4.01	17.96	21.97	78.57	3.38
300	2.00	2.00	4.01	18.07	22.08	78.70	3.41
400	2.03	2.03	4.06	23.50	27.56	85.71	5.50
500	2.00	2.00	4.00	28.15	32.15	92.28	8.09
600	1.92	1.92	3.85	31.97	35.82	98.40	11.10
700	1.83	1.83	3.67	35.12	38.79	104.09	14.46
800	1.73	1.73	3.48	37.77	41.25	109.38	18.11
900	1.65	1.65	3.30	40.04	43.34	114.32	22.00
1000	1.57	1.57	3.14	41.99	45.13	118.94	26.10
1100	1.50	1.50	3.01	43.67	46.68	123.28	30.39
1200	1.44	1.44	2.89	45.14	48.03	127.37	34.83
1300	1.39	1.39	2.79	46.41	49.20	131.24	39.41
1400	1.35	1.35	2.70	47.52	50.23	134.90	44.11
1500	1.31	1.31	2.63	48.49	51.12	138.38	48.91
1600	1.28	1.28	2.57	49.34	51.91	141.68	53.80
1700	1.25	1.25	2.51	50.09	52.60	144.84	58.77
1800	1.23	1.23	2.46	50.74	53.21	147.85	63.82
1900	1.21	1.21	2.42	51.32	53.74	150.73	68.92
2000	1.19	1.19	2.38	51.84	54.22	153.48	74.08
2500	1.12	1.12	2.25	53.69	55.94	165.75	100.50
3000	1.09	1.09	2.18	54.80	56.97	176.02	127.64
3500	1.06	1.06	2.13	55.50	57.63	184.84	155.23
4000	1.05	1.05	2.10	55.98	58.08	192.56	183.11
4500	1.03	1.03	2.08	56.31	58.39	199.41	211.19
5000	1.03	1.03	2.06	56.56	58.61	205.57	239.41

11. CH_2=C(OH)CH=O (ideal Gas)

T (K)	Cp (cal/mol/K)					S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C=C—OH	IR C=C—C=O	IR Total	TVR	IR + TVR		
0.1	0.000	0.000	0.00	7.95	7.95	0.34	0.00
10	0.000	0.000	0.00	7.95	7.95	36.95	0.08
50	0.001	0.801	0.80	7.95	8.75	50.00	0.41
100	0.112	1.586	1.70	8.28	9.97	56.46	0.88
150	0.472	1.683	2.16	9.52	11.68	60.77	1.42
200	0.853	1.726	2.58	11.45	14.03	64.41	2.06
298.15	1.366	1.820	3.19	15.87	19.05	70.86	3.68
300	1.373	1.821	3.19	15.95	19.15	70.98	3.72
400	1.700	1.906	3.61	20.21	23.81	77.05	5.87
500	1.997	2.003	4.00	23.79	27.79	82.73	8.46
600	2.311	2.134	4.45	26.73	31.17	88.05	11.41
700	2.623	2.301	4.92	29.13	34.05	93.03	14.67
800	2.895	2.485	5.38	31.13	36.51	97.70	18.21
900	3.100	2.668	5.77	32.83	38.59	102.09	21.96
1000	3.229	2.832	6.06	34.27	40.33	106.22	25.91
1100	3.286	2.968	6.25	35.52	41.77	110.11	30.02
1200	3.282	3.069	6.35	36.59	42.94	113.77	34.26
1300	3.233	3.136	6.37	37.52	43.89	117.23	38.60
1400	3.152	3.171	6.32	38.33	44.65	120.49	43.03
1500	3.051	3.177	6.23	39.04	45.26	123.58	47.53
1600	2.939	3.159	6.10	39.66	45.75	126.51	52.08
1700	2.823	3.122	5.94	40.20	46.14	129.28	56.67
1800	2.706	3.071	5.78	40.68	46.45	131.92	61.30
1900	2.594	3.009	5.60	41.10	46.70	134.43	65.96
2000	2.486	2.941	5.43	41.47	46.90	136.82	70.64
2500	2.045	2.564	4.61	42.82	47.43	147.33	94.25
3000	1.752	2.230	3.98	43.63	47.61	155.98	118.02
3500	1.558	1.969	3.53	44.15	47.67	163.31	141.85
4000	1.426	1.773	3.20	44.50	47.69	169.67	165.69
4500	1.334	1.627	2.96	44.74	47.70	175.29	189.54
5000	1.268	1.515	2.78	44.92	47.70	180.31	213.39

12. CH_2=CHCH(OH)CH=CH_2 (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=C	IR C—OH	IR Total	TVR	IR + TVR		
0.1	0.00	0.00	0.00	0.00	7.95	7.95	2.26	0.00
10	0.00	0.00	0.00	0.00	7.95	7.95	38.86	0.08
50	1.44	1.44	0.03	2.92	7.98	10.90	52.31	0.46
100	3.20	3.20	0.94	7.34	9.16	16.50	59.90	1.13
150	3.66	3.66	2.35	9.67	11.58	21.25	66.08	2.07
200	3.51	3.51	3.10	10.12	14.58	24.69	71.59	3.22
298.15	2.95	2.95	3.09	8.98	21.46	30.44	81.10	5.92
300	2.94	2.94	3.08	8.96	21.60	30.55	81.27	5.97
400	2.46	2.46	2.57	7.49	28.67	36.15	89.91	9.32
500	2.11	2.11	2.15	6.36	34.77	41.13	97.90	13.19
600	1.85	1.85	1.86	5.57	39.78	45.35	105.32	17.52
700	1.67	1.67	1.66	5.01	43.91	48.92	112.23	22.24
800	1.54	1.54	1.52	4.61	47.38	51.98	118.68	27.29
900	1.44	1.44	1.42	4.31	50.33	54.64	124.73	32.62
1000	1.37	1.37	1.34	4.08	52.87	56.96	130.41	38.20
1100	1.31	1.31	1.29	3.91	55.08	58.98	135.76	44.00
1200	1.26	1.26	1.24	3.77	56.99	60.76	140.82	49.99
1300	1.23	1.23	1.21	3.66	58.66	62.32	145.61	56.15
1400	1.20	1.20	1.18	3.58	60.11	63.69	150.16	62.45
1500	1.17	1.17	1.16	3.50	61.39	64.89	154.49	68.88
1600	1.15	1.15	1.14	3.44	62.50	65.95	158.62	75.42
1700	1.14	1.14	1.12	3.39	63.49	66.88	162.55	82.06
1800	1.12	1.12	1.11	3.35	64.35	67.70	166.32	88.79
1900	1.11	1.11	1.10	3.31	65.12	68.43	169.92	95.60
2000	1.10	1.10	1.09	3.28	65.80	69.08	173.38	102.48
2500	1.06	1.06	1.05	3.18	68.26	71.43	188.78	137.66
3000	1.04	1.04	1.04	3.12	69.73	72.85	201.72	173.76
3500	1.03	1.03	1.02	3.08	70.68	73.76	212.84	210.43
4000	1.02	1.02	1.02	3.06	71.31	74.37	222.58	247.47
4500	1.01	1.01	1.01	3.04	71.76	74.80	231.24	284.77
5000	1.01	1.01	1.01	3.03	72.08	75.11	239.02	322.25

13. CH_2=C(OH)CH=CH_2 (ideal Gas)

T (K)	Cp (cal/mol/K)					S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C=C—OH	IR C—C=C	IR Total	TVR	IR + TVR		
0.1	0.000	0.000	0.00	7.95	7.95	0.43	0.00
10	0.000	0.029	0.03	7.95	7.98	37.04	0.08
50	0.011	1.556	1.57	7.96	9.53	51.02	0.40
100	0.475	1.598	2.07	8.64	10.71	57.88	0.93
150	1.473	1.671	3.14	10.49	13.63	62.69	1.54
200	2.372	1.830	4.20	12.98	17.19	67.05	2.30
298.15	3.112	2.350	5.46	18.60	24.06	75.10	4.33
300	3.116	2.361	5.48	18.71	24.18	75.25	4.37
400	3.041	2.860	5.90	24.14	30.04	82.93	7.10
500	2.752	3.091	5.84	28.70	34.54	90.05	10.33
600	2.455	3.082	5.54	32.40	37.93	96.59	13.97
700	2.201	2.938	5.14	35.43	40.57	102.58	17.90
800	1.997	2.741	4.74	37.98	42.72	108.09	22.06
900	1.834	2.536	4.37	40.15	44.52	113.18	26.43
1000	1.705	2.345	4.05	42.03	46.07	117.92	30.96
1100	1.601	2.176	3.78	43.66	47.43	122.34	35.64
1200	1.517	2.030	3.55	45.08	48.62	126.49	40.44
1300	1.449	1.905	3.35	46.32	49.67	130.40	45.36
1400	1.393	1.799	3.19	47.41	50.60	134.10	50.37
1500	1.346	1.708	3.05	48.36	51.42	137.60	55.47
1600	1.307	1.631	2.94	49.20	52.14	140.92	60.65
1700	1.274	1.565	2.84	49.95	52.78	144.09	65.90
1800	1.245	1.508	2.75	50.60	53.35	147.11	71.21
1900	1.221	1.458	2.68	51.18	53.86	149.99	76.57
2000	1.200	1.415	2.62	51.70	54.31	152.76	81.98
2500	1.128	1.268	2.40	53.57	55.97	165.03	109.59
3000	1.088	1.185	2.27	54.70	56.98	175.31	137.84
3500	1.064	1.134	2.20	55.43	57.63	184.13	166.50
4000	1.047	1.101	2.15	55.92	58.07	191.85	195.43
4500	1.036	1.079	2.11	56.26	58.38	198.70	224.55
5000	1.028	1.062	2.09	56.51	58.60	204.85	253.79

14. CH_3OCH=O (ideal Gas)

T (K)	Cp (cal/mol/K)					S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C—OC=O	IR COC—C=O	IR Total	TVR	IR + TVR		
0.1	0.000	0.000	0.00	7.95	7.95	-4.27	0.00
10	0.137	0.000	0.14	7.95	8.09	34.52	0.08
50	1.394	0.827	2.22	7.96	10.18	49.01	0.45
100	1.212	1.496	2.71	8.34	11.05	56.37	0.97
150	1.114	1.504	2.62	9.05	11.67	60.95	1.54
200	1.068	1.492	2.56	9.93	12.49	64.40	2.14
298.15	1.030	1.619	2.65	12.36	15.01	69.76	3.49
300	1.030	1.623	2.65	12.42	15.07	69.86	3.51
400	1.015	1.916	2.93	15.51	18.44	74.58	5.19
500	1.007	2.284	3.29	18.54	21.83	79.01	7.20
600	1.003	2.636	3.64	21.23	24.87	83.21	9.54
700	1.001	2.920	3.92	23.54	27.46	87.20	12.16
800	0.999	3.120	4.12	25.52	29.64	90.97	15.02
900	0.998	3.241	4.24	27.22	31.46	94.53	18.08
1000	0.997	3.296	4.29	28.68	32.97	97.90	21.30
1100	0.997	3.301	4.30	29.93	34.22	101.08	24.66
1200	0.996	3.268	4.26	31.00	35.27	104.08	28.14
1300	0.996	3.209	4.20	31.93	36.14	106.92	31.71
1400	0.996	3.131	4.13	32.73	36.86	109.61	35.36
1500	0.995	3.042	4.04	33.43	37.47	112.16	39.08
1600	0.995	2.947	3.94	34.03	37.98	114.58	42.85
1700	0.995	2.849	3.84	34.56	38.41	116.89	46.67
1800	0.995	2.752	3.75	35.03	38.77	119.08	50.53
1900	0.995	2.656	3.65	35.43	39.08	121.18	54.42
2000	0.995	2.564	3.56	35.79	39.35	123.18	58.34
2500	0.994	2.169	3.16	37.07	40.24	132.04	78.27
3000	0.994	1.885	2.88	37.83	40.71	139.41	98.51
3500	0.994	1.683	2.68	38.31	40.99	145.70	118.95
4000	0.994	1.539	2.53	38.64	41.17	151.18	139.49
4500	0.994	1.434	2.43	38.86	41.29	156.03	160.10
5000	0.994	1.356	2.35	39.02	41.37	160.38	180.77

15. $C_6H_5OCH{=}O$ (ideal Gas)

T (K)	Cp (cal/mol/K)					S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C_b—O	IR O—C=O	IR Total	TVR	IR + TVR		
0.1	0.14	0.00	0.14	7.95	8.09	8.17	0.00
10	0.26	0.02	0.28	7.95	8.23	46.16	0.08
50	1.92	1.70	3.62	8.49	12.11	62.30	0.48
100	1.63	1.81	3.44	10.50	13.94	71.15	1.13
150	1.50	2.17	3.67	13.55	17.22	77.32	1.90
200	1.47	2.45	3.92	17.35	21.27	82.74	2.86
298.15	1.49	2.47	3.96	26.00	29.96	92.66	5.38
300	1.49	2.47	3.95	26.17	30.13	92.85	5.43
400	1.47	2.27	3.74	34.80	38.54	102.52	8.87
500	1.42	2.13	3.55	42.08	45.63	111.76	13.09
600	1.37	2.06	3.43	47.94	51.37	120.49	17.96
700	1.32	2.03	3.35	52.65	56.00	128.67	23.33
800	1.28	2.02	3.30	56.49	59.78	136.33	29.13
900	1.24	2.01	3.25	59.66	62.91	143.49	35.27
1000	1.21	1.99	3.20	62.31	65.51	150.20	41.69
1100	1.18	1.97	3.15	64.55	67.70	156.51	48.36
1200	1.16	1.94	3.10	66.45	69.55	162.44	55.22
1300	1.14	1.90	3.05	68.08	71.12	168.04	62.26
1400	1.13	1.87	2.99	69.47	72.46	173.33	69.44
1500	1.11	1.82	2.94	70.68	73.61	178.35	76.74
1600	1.10	1.78	2.88	71.72	74.60	183.11	84.16
1700	1.09	1.74	2.83	72.63	75.46	187.64	91.66
1800	1.08	1.70	2.78	73.42	76.21	191.96	99.24
1900	1.07	1.66	2.74	74.12	76.86	196.08	106.90
2000	1.07	1.63	2.70	74.74	77.43	200.03	114.61
2500	1.04	1.47	2.52	76.93	79.45	217.50	153.88
3000	1.03	1.36	2.39	78.22	80.61	232.07	193.92
3500	1.02	1.28	2.30	79.04	81.34	244.54	234.42
4000	1.00	1.23	2.23	79.59	81.82	255.42	275.22
4500	0.99	1.18	2.17	79.97	82.14	265.07	316.21
5000	0.97	1.15	2.12	80.25	82.37	273.73	357.34

16. $C_6H_5C(CH{=}O){=}CH_2$ (ideal Gas)

T (K)	Cp (cal/mol/K)					S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C_b—C_d	IR C_d—CH=O	IR Total	TVR	IR + TVR		
0.1	0.00	0.00	0.00	7.95	7.95	9.22	0.00
10	0.02	0.00	0.02	7.95	7.97	47.20	0.08
50	1.43	1.05	2.48	8.98	11.46	61.62	0.46
100	1.96	1.76	3.72	12.03	15.75	70.84	1.14
150	2.20	2.22	4.42	16.03	20.45	78.01	2.04
200	2.34	2.63	4.97	20.73	25.70	84.51	3.19
298.15	2.31	3.02	5.33	31.20	36.52	96.57	6.24
300	2.30	3.02	5.32	31.41	36.73	96.80	6.31
400	2.07	3.05	5.12	41.74	46.86	108.59	10.50
500	1.84	2.98	4.82	50.48	55.30	119.81	15.62
600	1.66	2.88	4.54	57.54	62.08	130.37	21.51
700	1.52	2.77	4.30	63.26	67.56	140.25	28.00
800	1.42	2.66	4.08	67.95	72.04	149.47	34.98
900	1.34	2.54	3.89	71.86	75.75	158.10	42.38
1000	1.28	2.43	3.71	75.15	78.86	166.18	50.11
1100	1.24	2.31	3.55	77.93	81.48	173.77	58.13
1200	1.20	2.20	3.41	80.31	83.72	180.91	66.40
1300	1.17	2.10	3.28	82.35	85.62	187.64	74.87
1400	1.15	2.01	3.16	84.10	87.26	194.01	83.51
1500	1.13	1.92	3.06	85.62	88.68	200.05	92.31
1600	1.12	1.85	2.96	86.94	89.90	205.79	101.24
1700	1.10	1.78	2.88	88.09	90.97	211.25	110.29
1800	1.09	1.72	2.81	89.10	91.90	216.45	119.43
1900	1.08	1.66	2.74	89.98	92.72	221.43	128.67
2000	1.07	1.61	2.68	90.76	93.45	226.19	137.97
2500	1.04	1.42	2.46	93.55	96.01	247.28	185.40
3000	1.02	1.31	2.32	95.20	97.52	264.90	233.81
3500	0.99	1.23	2.22	96.24	98.47	279.99	282.82
4000	0.96	1.18	2.14	96.94	99.08	293.17	332.22
4500	0.93	1.14	2.07	97.43	99.50	304.85	381.87
5000	0.89	1.11	2.00	97.79	99.79	315.34	431.70

17. $C_6H_5C(OH)_2CH_3$ (ideal Gas)

T (K)	Cp (cal/mol/K)							S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C_b—C	IR C—OH	IR C—OH	IR C—C	IR Total	TVR	IR + TVR		
0.1	0.00	0.00	0.00	0.00	0.00	7.95	7.95	5.68	0.00
10	0.22	0.00	0.00	0.01	0.23	7.95	8.18	45.83	0.08
50	1.73	0.02	0.02	0.13	1.90	8.02	9.92	60.31	0.44
100	1.93	0.50	0.50	0.90	3.83	10.27	14.10	68.16	1.03
150	2.03	1.34	1.34	1.43	6.14	14.86	21.00	75.05	1.90
200	2.13	2.17	2.17	1.72	8.20	20.27	28.47	82.00	3.13
298.15	2.29	3.10	3.10	2.04	10.55	31.81	42.35	95.79	6.62
300	2.30	3.11	3.11	2.05	10.57	32.03	42.60	96.05	6.70
400	2.34	3.19	3.19	2.15	10.88	43.26	54.14	109.73	11.54
500	2.29	2.92	2.92	2.12	10.26	52.69	62.95	122.61	17.41
600	2.19	2.59	2.59	2.02	9.39	60.28	69.67	134.56	24.05
700	2.06	2.30	2.30	1.90	8.57	66.40	74.97	145.58	31.29
800	1.94	2.07	2.07	1.78	7.86	71.43	79.29	155.78	39.01
900	1.83	1.88	1.88	1.68	7.27	75.64	82.91	165.25	47.13
1000	1.73	1.74	1.74	1.59	6.79	79.22	86.01	174.08	55.58
1100	1.64	1.62	1.62	1.52	6.40	82.28	88.67	182.34	64.32
1200	1.57	1.53	1.53	1.45	6.07	84.92	90.99	190.11	73.30
1300	1.50	1.45	1.45	1.40	5.81	87.20	93.01	197.43	82.51
1400	1.45	1.39	1.39	1.35	5.59	89.19	94.78	204.34	91.90
1500	1.40	1.35	1.35	1.31	5.40	90.92	96.32	210.90	101.45
1600	1.36	1.30	1.30	1.28	5.25	92.43	97.68	217.13	111.15
1700	1.33	1.27	1.27	1.25	5.12	93.76	98.88	223.06	120.98
1800	1.29	1.24	1.24	1.23	5.00	94.94	99.94	228.72	130.93
1900	1.27	1.22	1.22	1.21	4.90	95.97	100.88	234.13	140.97
2000	1.24	1.19	1.19	1.19	4.82	96.89	101.71	239.31	151.10
2500	1.16	1.12	1.12	1.12	4.52	100.21	104.73	262.29	202.78
3000	1.09	1.08	1.08	1.08	4.34	102.20	106.54	281.51	255.63
3500	1.04	1.06	1.06	1.06	4.22	103.47	107.69	298.00	309.20
4000	0.98	1.04	1.04	1.05	4.12	104.32	108.44	312.42	363.25
4500	0.93	1.03	1.03	1.04	4.03	104.93	108.96	325.21	417.61
5000	0.87	1.03	1.03	1.03	3.95	105.36	109.32	336.70	472.18

18. $C_6H_5C(=CH_2)CH=CH_2$ (ideal Gas)

T (K)	Cp (cal/mol/K)					S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C_b—C_d	IR C_d—C_d	IR Total	TVR	IR + TVR		
0.1	0.00	0.00	0.00	7.95	7.95	6.42	0.00
10	0.06	0.00	0.06	7.95	8.01	44.39	0.08
50	1.59	1.22	2.81	8.85	11.66	59.19	0.47
100	2.03	2.02	4.05	12.01	16.06	68.53	1.15
150	2.48	2.60	5.07	16.32	21.39	75.93	2.09
200	2.91	3.03	5.95	21.49	27.44	82.80	3.30
298.15	3.12	3.44	6.56	33.24	39.80	95.83	6.60
300	3.12	3.44	6.56	33.47	40.03	96.08	6.68
400	2.77	3.38	6.16	45.13	51.29	108.95	11.26
500	2.37	3.12	5.50	54.95	60.45	121.22	16.86
600	2.05	2.83	4.88	62.88	67.76	132.75	23.28
700	1.81	2.55	4.36	69.30	73.67	143.52	30.37
800	1.64	2.31	3.95	74.60	78.55	153.58	37.98
900	1.52	2.11	3.63	79.03	82.66	162.98	46.05
1000	1.42	1.95	3.37	82.78	86.15	171.80	54.50
1100	1.35	1.82	3.17	85.98	89.15	180.09	63.26
1200	1.29	1.71	3.00	88.73	91.73	187.91	72.31
1300	1.25	1.62	2.87	91.10	93.97	195.29	81.60
1400	1.21	1.55	2.76	93.15	95.91	202.29	91.10
1500	1.19	1.48	2.67	94.93	97.59	208.93	100.77
1600	1.16	1.43	2.59	96.48	99.07	215.24	110.61
1700	1.14	1.38	2.53	97.83	100.36	221.26	120.58
1800	1.13	1.35	2.47	99.02	101.49	227.00	130.67
1900	1.11	1.31	2.42	100.07	102.49	232.50	140.87
2000	1.10	1.28	2.38	100.99	103.38	237.76	151.17
2500	1.06	1.18	2.24	104.31	106.55	261.13	203.72
3000	1.02	1.13	2.15	106.28	108.43	280.70	257.51
3500	0.99	1.09	2.08	107.53	109.61	297.48	312.04
4000	0.95	1.07	2.02	108.37	110.39	312.16	367.05
4500	0.90	1.05	1.96	108.96	110.92	325.18	422.39
5000	0.85	1.04	1.89	109.39	111.29	336.88	477.95

19. $C_6H_5C(CH_3)_2CH=O$ (ideal Gas)

T (K)	Cp (cal/mol/K)							S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C_b—C	IR C—C	IR C—C	IR C—CH=O	IR Total	TVR	IR + TVR		
0.1	0.00	0.00	0.00	0.00	0.00	7.95	7.95	4.38	0.00
10	0.52	0.11	0.11	0.01	0.75	7.95	8.70	46.43	0.08
50	1.91	0.24	0.24	1.51	3.90	8.23	12.13	62.30	0.50
100	2.64	1.10	1.10	2.35	7.19	11.98	19.17	72.63	1.26
150	2.86	1.60	1.60	3.03	9.09	17.40	26.49	81.72	2.40
200	2.73	1.87	1.87	3.36	9.84	23.15	32.99	90.12	3.89
298.15	2.34	2.10	2.10	3.24	9.78	35.54	45.31	105.35	7.73
300	2.33	2.10	2.10	3.23	9.76	35.78	45.55	105.63	7.82
400	2.03	2.06	2.06	2.77	8.93	48.35	57.29	120.12	12.97
500	1.81	1.93	1.93	2.35	8.03	59.29	67.32	133.80	19.22
600	1.65	1.79	1.79	2.04	7.26	68.34	75.59	146.64	26.38
700	1.53	1.66	1.66	1.81	6.65	75.79	82.44	158.68	34.29
800	1.43	1.55	1.55	1.64	6.17	82.00	88.17	169.94	42.83
900	1.36	1.46	1.46	1.52	5.80	87.23	93.03	180.51	51.89
1000	1.30	1.39	1.39	1.43	5.51	91.68	97.19	190.44	61.41
1100	1.26	1.34	1.34	1.35	5.29	95.47	100.76	199.80	71.31
1200	1.22	1.29	1.29	1.30	5.10	98.73	103.83	208.64	81.55
1300	1.19	1.25	1.25	1.26	4.95	101.53	106.49	217.00	92.06
1400	1.17	1.22	1.22	1.22	4.83	103.95	108.79	224.92	102.83
1500	1.15	1.19	1.19	1.19	4.73	106.05	110.78	232.46	113.81
1600	1.13	1.17	1.17	1.17	4.65	107.88	112.53	239.63	124.98
1700	1.12	1.15	1.15	1.15	4.57	109.48	114.05	246.46	136.31
1800	1.10	1.14	1.14	1.13	4.51	110.87	115.39	252.99	147.78
1900	1.09	1.12	1.12	1.12	4.46	112.11	116.56	259.24	159.38
2000	1.08	1.11	1.11	1.11	4.41	113.19	117.60	265.22	171.09
2500	1.03	1.07	1.07	1.07	4.24	117.08	121.31	291.82	230.91
3000	0.97	1.05	1.05	1.04	4.11	119.38	123.49	314.10	292.15
3500	0.91	1.03	1.03	1.03	4.01	120.84	124.85	333.22	354.26
4000	0.85	1.02	1.02	1.02	3.92	121.82	125.73	349.93	416.92
4500	0.78	1.02	1.02	1.02	3.83	122.50	126.34	364.76	479.95
5000	0.72	1.01	1.01	1.01	3.76	123.00	126.76	378.08	543.23

20. $C_6H_5CH=O$ (ideal Gas)

T (K)	Cp (cal/mol/K)				S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C_b—CH=O	IR Total	TVR	IR + TVR		
0.1	0.02	0.02	7.95	7.97	4.18	0.00
10	0.02	0.02	7.95	7.97	43.53	0.08
50	1.08	1.08	8.21	9.29	56.82	0.42
100	1.81	1.81	10.22	12.03	64.06	0.95
150	1.82	1.82	13.05	14.87	69.41	1.62
200	1.74	1.74	16.49	18.23	74.06	2.44
298.15	1.65	1.65	24.42	26.07	82.61	4.61
300	1.65	1.65	24.58	26.23	82.77	4.66
400	1.64	1.64	32.61	34.25	91.27	7.69
500	1.63	1.63	39.48	41.11	99.54	11.47
600	1.61	1.61	45.05	46.66	107.43	15.87
700	1.58	1.58	49.55	51.13	114.88	20.76
800	1.54	1.54	53.24	54.78	121.88	26.07
900	1.50	1.50	56.30	57.80	128.45	31.70
1000	1.46	1.46	58.87	60.33	134.62	37.61
1100	1.42	1.42	61.04	62.46	140.43	43.75
1200	1.38	1.38	62.89	64.27	145.91	50.09
1300	1.35	1.35	64.46	65.81	151.08	56.60
1400	1.32	1.32	65.82	67.14	155.98	63.25
1500	1.29	1.29	66.99	68.28	160.63	70.02
1600	1.27	1.27	68.01	69.27	165.05	76.90
1700	1.24	1.24	68.89	70.13	169.25	83.87
1800	1.22	1.22	69.66	70.89	173.27	90.92
1900	1.21	1.21	70.34	71.55	177.10	98.04
2000	1.19	1.19	70.94	72.13	180.78	105.23
2500	1.13	1.13	73.08	74.21	197.07	141.86
3000	1.10	1.10	74.33	75.43	210.70	179.30
3500	1.07	1.07	75.13	76.20	222.37	217.22
4000	1.06	1.06	75.66	76.72	232.57	255.46
4500	1.04	1.04	76.04	77.08	241.62	293.91
5000	1.03	1.03	76.31	77.34	249.75	332.52

21. $C_6H_5C(=CH_2)OH$ (ideal Gas)

T (K)	Cp (cal/mol/K)					S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C_b—C_d	IR C_d—OH	IR Total	TVR	IR + TVR		
0.1	0.02	0.00	0.02	7.95	7.97	6.76	0.00
10	0.44	0.00	0.44	7.95	8.39	44.50	0.08
50	1.20	0.03	1.23	8.13	9.36	58.13	0.43
100	1.87	0.93	2.80	10.12	12.93	65.52	0.98
150	2.13	2.14	4.27	13.84	18.11	71.65	1.75
200	2.23	2.67	4.90	18.54	23.44	77.49	2.79
298.15	2.24	2.68	4.92	28.89	33.81	88.59	5.59
300	2.24	2.68	4.92	29.09	34.01	88.80	5.66
400	2.12	2.46	4.58	39.04	43.62	99.73	9.55
500	1.96	2.26	4.22	47.28	51.50	110.18	14.32
600	1.82	2.09	3.90	53.85	57.76	120.01	19.80
700	1.69	1.94	3.63	59.12	62.75	129.20	25.83
800	1.58	1.81	3.39	63.43	66.82	137.76	32.32
900	1.49	1.71	3.20	67.02	70.22	145.76	39.17
1000	1.42	1.62	3.04	70.05	73.09	153.25	46.34
1100	1.36	1.54	2.90	72.64	75.54	160.28	53.78
1200	1.32	1.48	2.79	74.86	77.65	166.90	61.44
1300	1.28	1.42	2.70	76.78	79.48	173.15	69.30
1400	1.24	1.38	2.62	78.44	81.06	179.07	77.33
1500	1.22	1.34	2.55	79.88	82.44	184.68	85.50
1600	1.19	1.30	2.49	81.15	83.64	190.01	93.81
1700	1.17	1.27	2.45	82.25	84.70	195.09	102.23
1800	1.15	1.25	2.40	83.23	85.63	199.94	110.74
1900	1.14	1.23	2.37	84.08	86.45	204.58	119.35
2000	1.13	1.21	2.33	84.84	87.18	209.01	128.03
2500	1.08	1.14	2.22	87.58	89.80	228.72	172.34
3000	1.06	1.10	2.15	89.22	91.37	245.21	217.66
3500	1.04	1.07	2.11	90.26	92.36	259.35	263.61
4000	1.02	1.05	2.07	90.96	93.03	271.72	309.97
4500	1.00	1.04	2.04	91.45	93.50	282.69	356.61
5000	0.98	1.03	2.01	91.81	93.82	292.55	403.44

22. $C_6H_5C(=CH_2)CH_3$ (ideal Gas)

T (K)	Cp (cal/mol/K)					S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C_b—C_d	IR C_d—C	IR Total	TVR	IR + TVR		
0.1	0.15	0.00	0.15	7.95	8.10	6.75	0.00
10	0.12	0.05	0.17	7.95	8.12	46.94	0.08
50	1.80	0.34	2.14	8.15	10.29	61.54	0.45
100	1.67	1.30	2.97	10.52	13.49	69.51	1.03
150	1.62	1.83	3.45	14.52	17.97	75.71	1.81
200	1.64	2.07	3.71	19.39	23.10	81.48	2.84
298.15	1.64	2.08	3.72	30.27	33.98	92.49	5.63
300	1.64	2.08	3.71	30.48	34.20	92.70	5.70
400	1.56	1.88	3.44	41.33	44.77	103.80	9.66
500	1.48	1.69	3.16	50.58	53.74	114.60	14.60
600	1.39	1.53	2.93	58.14	61.07	124.92	20.35
700	1.33	1.42	2.75	64.31	67.06	134.67	26.77
800	1.27	1.34	2.61	69.44	72.04	143.86	33.73
900	1.23	1.28	2.50	73.74	76.25	152.51	41.15
1000	1.19	1.23	2.42	77.41	79.83	160.66	48.96
1100	1.17	1.19	2.36	80.54	82.89	168.35	57.10
1200	1.14	1.16	2.31	83.23	85.53	175.62	65.52
1300	1.13	1.14	2.26	85.55	87.81	182.51	74.19
1400	1.11	1.12	2.23	87.55	89.78	189.05	83.07
1500	1.10	1.10	2.20	89.30	91.50	195.27	92.14
1600	1.09	1.09	2.18	90.81	92.99	201.20	101.37
1700	1.08	1.08	2.16	92.14	94.30	206.85	110.73
1800	1.07	1.07	2.14	93.31	95.45	212.24	120.22
1900	1.06	1.06	2.13	94.34	96.46	217.41	129.82
2000	1.06	1.06	2.11	95.24	97.36	222.36	139.51
2500	1.03	1.04	2.07	98.49	100.56	244.40	189.06
3000	1.02	1.02	2.04	100.43	102.47	262.88	239.86
3500	1.01	1.02	2.02	101.65	103.68	278.75	291.41
4000	1.00	1.01	2.01	102.47	104.48	292.63	343.47
4500	0.98	1.01	1.99	103.05	105.04	304.96	395.86
5000	0.96	1.00	1.96	103.47	105.43	316.04	448.48

23. $C_6H_5CH=CH_2$ (ideal Gas)

T (K)	Cp (cal/mol/K)				S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C_b—C_d	IR Total	TVR	IR + TVR		
0.1	0.24	0.24	7.95	8.19	4.21	0.00
10	0.15	0.15	7.95	8.10	42.17	0.08
50	1.56	1.56	8.27	9.83	56.55	0.43
100	1.68	1.68	10.43	12.11	63.96	0.98
150	1.71	1.71	13.54	15.25	69.37	1.66
200	1.74	1.74	17.49	19.23	74.21	2.52
298.15	1.81	1.81	26.72	28.53	83.40	4.85
300	1.81	1.81	26.90	28.71	83.57	4.91
400	1.87	1.87	36.21	38.09	92.96	8.25
500	1.89	1.89	44.11	46.00	102.18	12.47
600	1.87	1.87	50.50	52.37	111.02	17.40
700	1.82	1.82	55.68	57.49	119.38	22.90
800	1.75	1.75	59.94	61.69	127.26	28.87
900	1.68	1.68	63.51	65.20	134.66	35.22
1000	1.62	1.62	66.54	68.15	141.62	41.89
1100	1.56	1.56	69.11	70.67	148.19	48.83
1200	1.50	1.50	71.32	72.82	154.39	56.01
1300	1.45	1.45	73.23	74.68	160.25	63.39
1400	1.41	1.41	74.88	76.28	165.81	70.94
1500	1.37	1.37	76.30	77.67	171.10	78.64
1600	1.34	1.34	77.55	78.88	176.12	86.47
1700	1.31	1.31	78.64	79.94	180.92	94.41
1800	1.28	1.28	79.59	80.87	185.49	102.45
1900	1.26	1.26	80.43	81.69	189.87	110.58
2000	1.24	1.24	81.17	82.41	194.06	118.79
2500	1.16	1.16	83.84	85.00	212.70	160.70
3000	1.11	1.11	85.42	86.53	228.31	203.61
3500	1.08	1.08	86.42	87.50	241.71	247.14
4000	1.06	1.06	87.09	88.16	253.43	291.06
4500	1.05	1.05	87.57	88.62	263.83	335.26
5000	1.04	1.04	87.91	88.95	273.18	379.65

24. $CH_2=CHCH_2CH=O$ (ideal Gas)

T (K)	Cp (cal/mol/K)					S (cal/mol/K)	[H(T) - H(0K)] (kcal/mol)
	IR C_d—C	IR C—CH=O	IR Total	TVR	IR + TVR		
0.1	0.00	0.00	0.00	7.95	7.95	0.62	0.00
10	0.44	0.00	0.45	7.95	8.40	38.34	0.08
50	0.90	2.07	2.97	8.00	10.98	52.74	0.47
100	2.23	3.05	5.28	8.89	14.16	61.42	1.09
150	2.67	2.82	5.48	10.49	15.97	67.50	1.84
200	2.58	2.43	5.01	12.49	17.50	72.26	2.68
298.15	2.13	1.92	4.04	17.30	21.34	79.82	4.58
300	2.12	1.91	4.03	17.40	21.43	79.95	4.62
400	1.77	1.63	3.40	22.60	26.00	86.64	6.99
500	1.55	1.46	3.01	27.26	30.27	92.82	9.81
600	1.40	1.35	2.76	31.21	33.96	98.59	13.03
700	1.31	1.28	2.58	34.52	37.11	104.00	16.59
800	1.24	1.22	2.46	37.33	39.80	109.08	20.43
900	1.19	1.18	2.38	39.73	42.11	113.86	24.53
1000	1.16	1.15	2.31	41.79	44.10	118.36	28.84
1100	1.13	1.13	2.26	43.56	45.82	122.61	33.34
1200	1.11	1.11	2.22	45.08	47.30	126.63	38.00
1300	1.09	1.09	2.19	46.40	48.59	130.44	42.79
1400	1.08	1.08	2.16	47.54	49.70	134.06	47.71
1500	1.07	1.07	2.14	48.53	50.67	137.50	52.73
1600	1.06	1.06	2.12	49.40	51.52	140.78	57.84
1700	1.05	1.06	2.11	50.15	52.26	143.91	63.03
1800	1.05	1.05	2.10	50.82	52.91	146.90	68.29
1900	1.04	1.04	2.09	51.40	53.49	149.77	73.61
2000	1.04	1.04	2.08	51.92	53.99	152.51	78.99
2500	1.02	1.02	2.05	53.76	55.81	164.74	106.48
3000	1.01	1.02	2.03	54.86	56.89	174.99	134.68
3500	1.01	1.01	2.02	55.55	57.57	183.80	163.30
4000	1.00	1.01	2.01	56.02	58.03	191.51	192.21
4500	1.00	1.00	2.01	56.35	58.35	198.36	221.31
5000	1.00	1.00	2.00	56.58	58.58	204.52	250.55

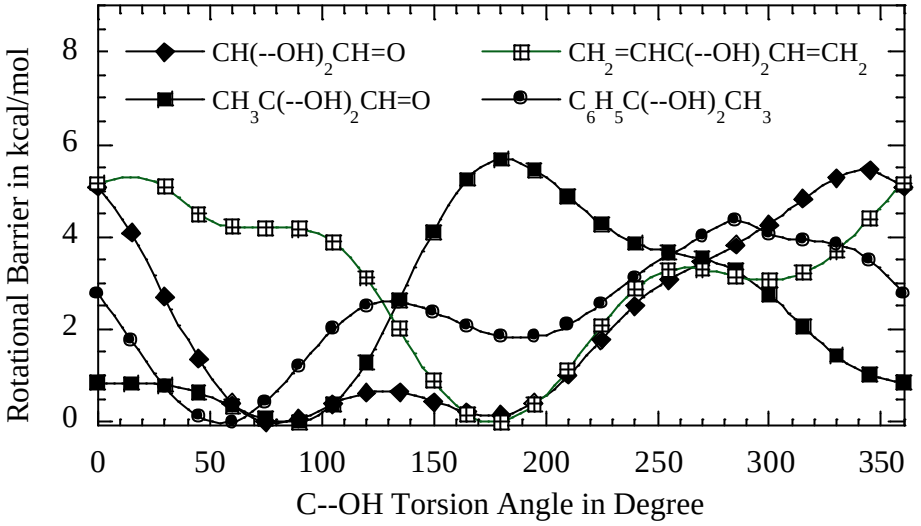

Fig. SM1: Potential barriers for internal rotations about C—OH bonds in $CH(—OH)_2CH=O$, $CH_3C(—OH)_2CH=O$, $CH_2=CHC(—OH)_2CH=CH_2$ and $C_6H_5C(—OH)_2CH_3$

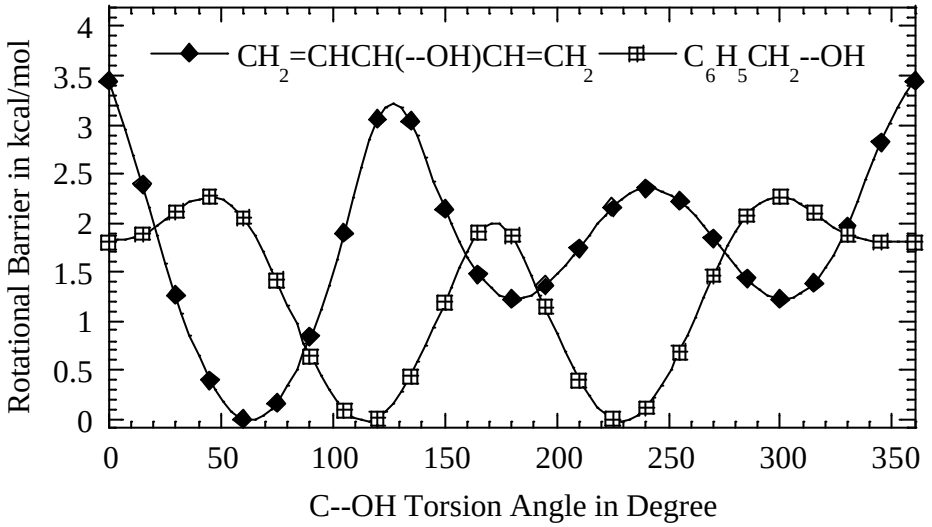

Fig. SM2: Potential barriers for internal rotations about C—OH bonds in $CH_2=CHC(—OH)CH=CH_2$ and $C_6H_5CH_2—OH$

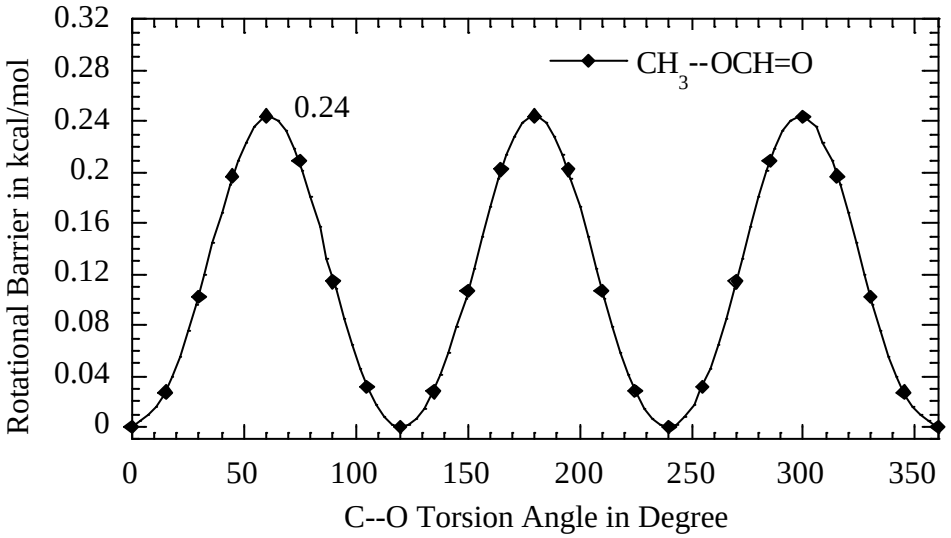

Fig. SM3: Potential barriers for internal rotations about C—O bonds in $CH_3—OCH=O$

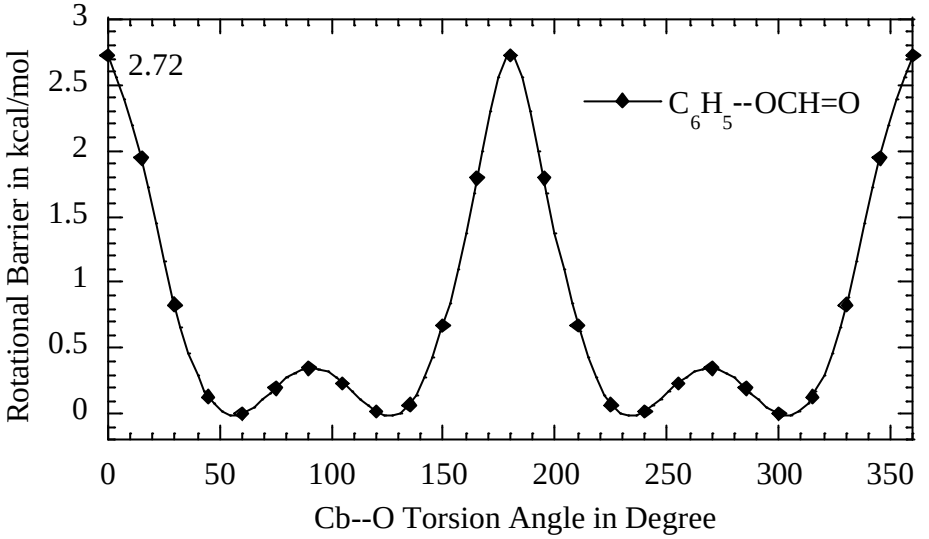

Fig. SM4: Potential barriers for internal rotations about C_b—O bonds in C_6H_5—OCH=O

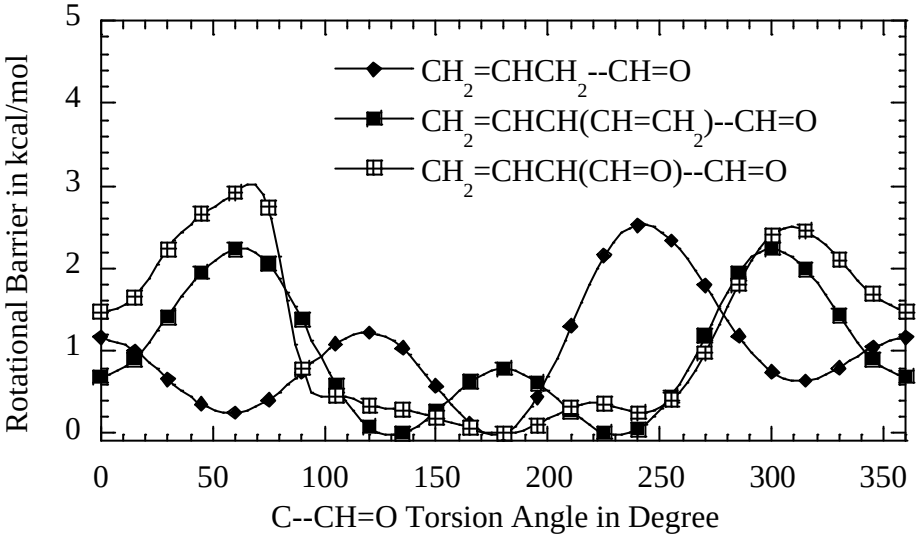

Fig. SM5: Potential barriers for internal rotations about C—CH=O bonds in CH_2=$CHCH_2$—CH=O, CH_2=CHCH(CH=CH_2)—CH=O and CH_2=CHCH(CH=O)—CH=O

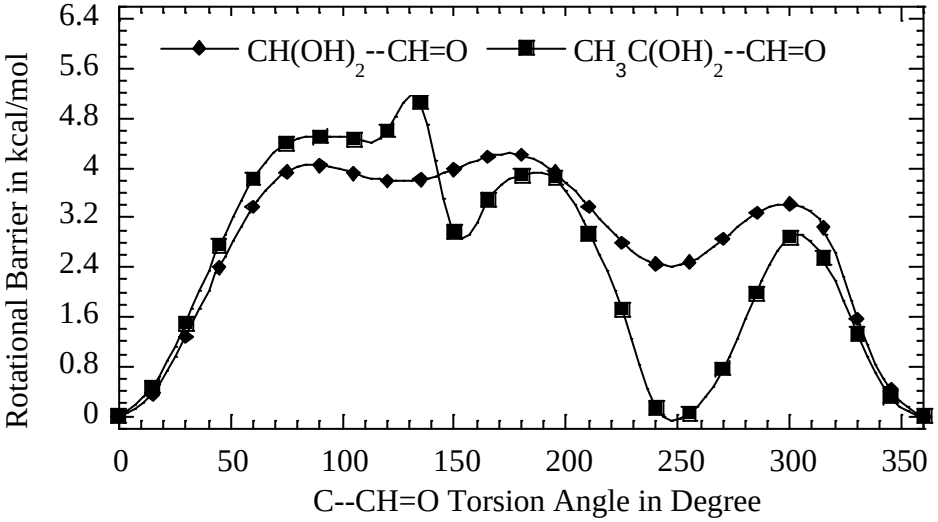

Fig. SM6: Potential barriers for internal rotations about C—CH=O bonds in $CH(OH)_2$—CH=O and $CH_3C(OH)_2$—CH=O

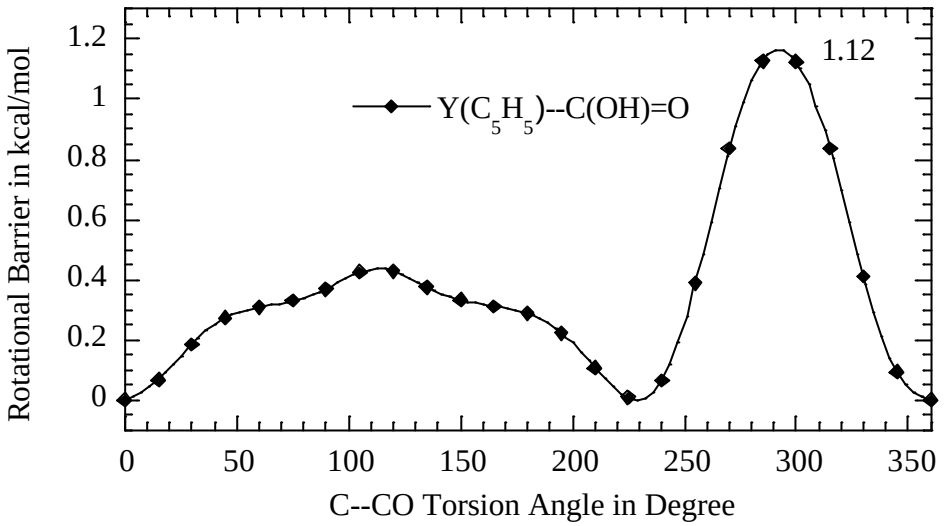

Fig. SM7: Potential barriers for internal rotations about C—C(OH)O bonds in $Y(C_5H_5)$—C(OH)=O

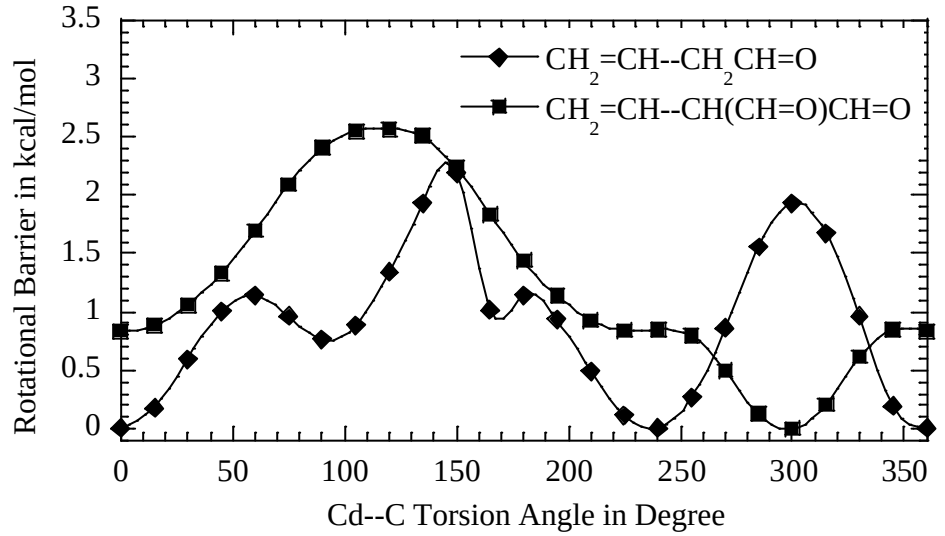

Fig. SM8: Potential barriers for internal rotations about C_d—C bonds in CH_2=CH—CH_2CH=O and CH_2=CH—CH(CH=O)CH=O

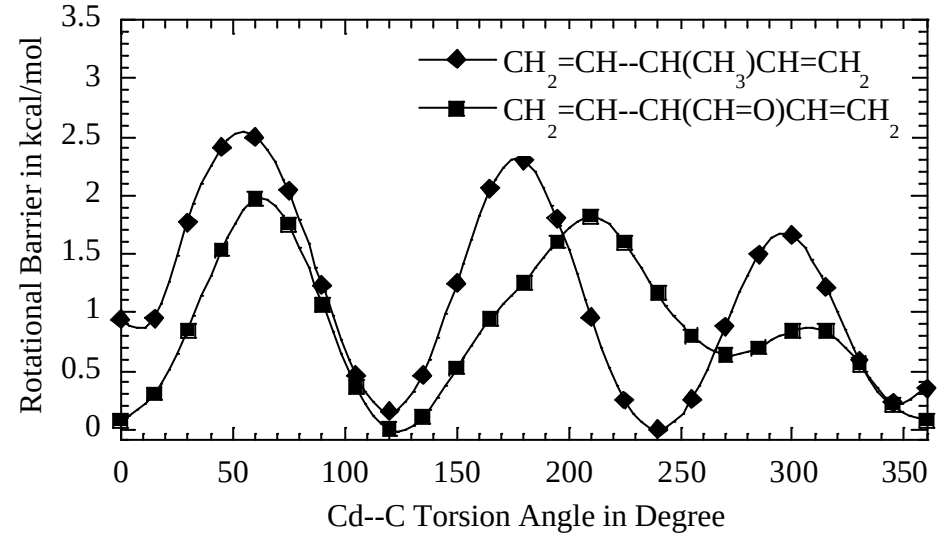

Fig. SM9: Potential barriers for internal rotations about C_d—C bonds in CH_2=CH—$C(CH_3)$CH=CH_2 and CH_2=CH—C(CH=O)CH=CH_2

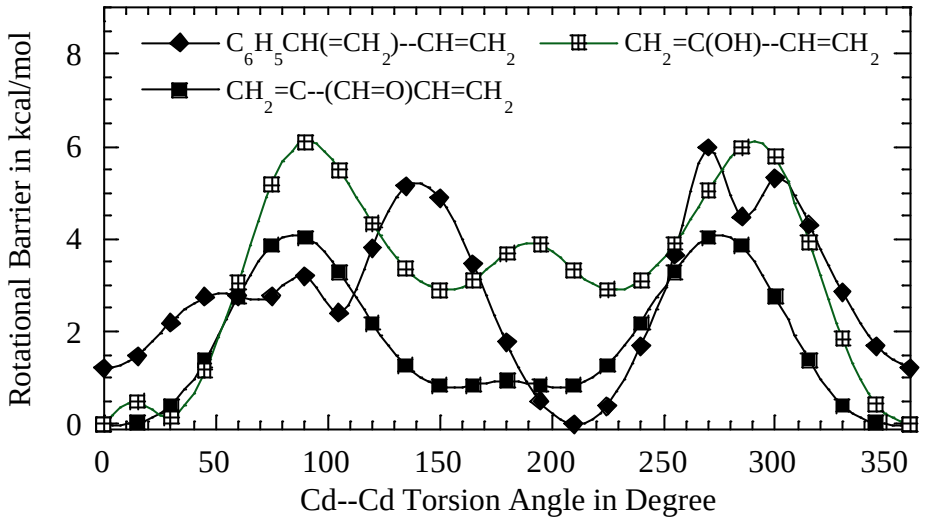

Fig. SM10: Potential barriers for internal rotations about C_d—C_d bonds in $C_6H_5CH(=CH_2)$—$CH=CH_2$, $CH_2=C$—$(CH=O)CH=CH_2$ and $CH_2=C(OH)$—$CH=CH_2$

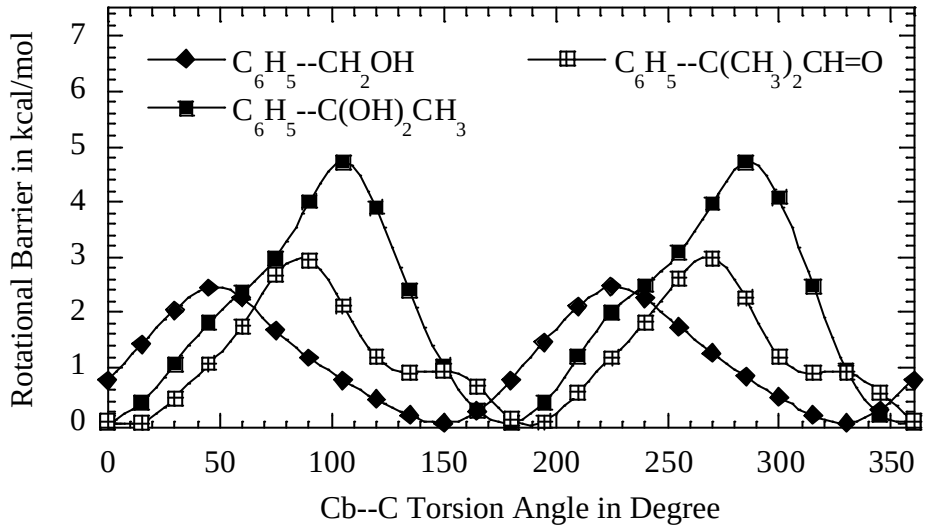

Fig. SM11: Potential barriers for internal rotations about C_b—C bonds in C_6H_5—CH_2OH, C_6H_5—$C(OH)_2CH_3$ and C_6H_5—$C(CH_3)_2CH=O$

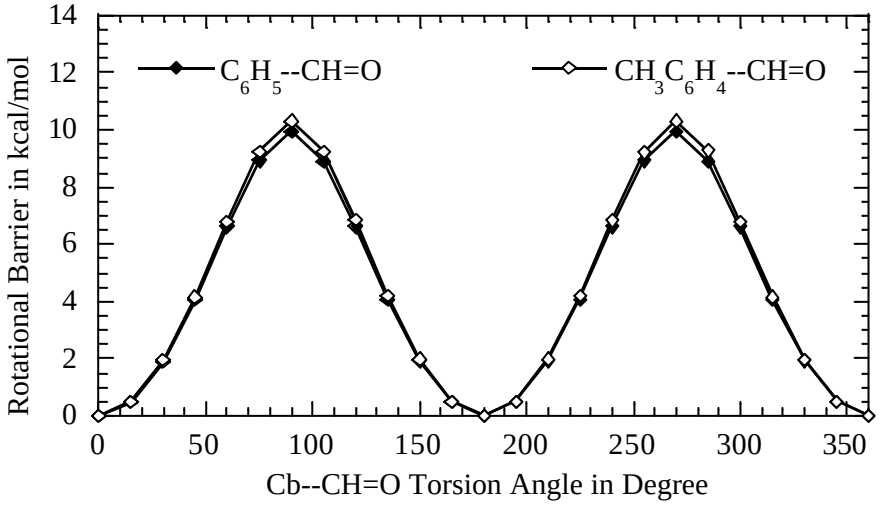

Fig. SM12: Potential barriers for internal rotations about C_b—CH=O bonds in C_6H_5—CH=O, and $CH_3C_6H_4$—CH=O

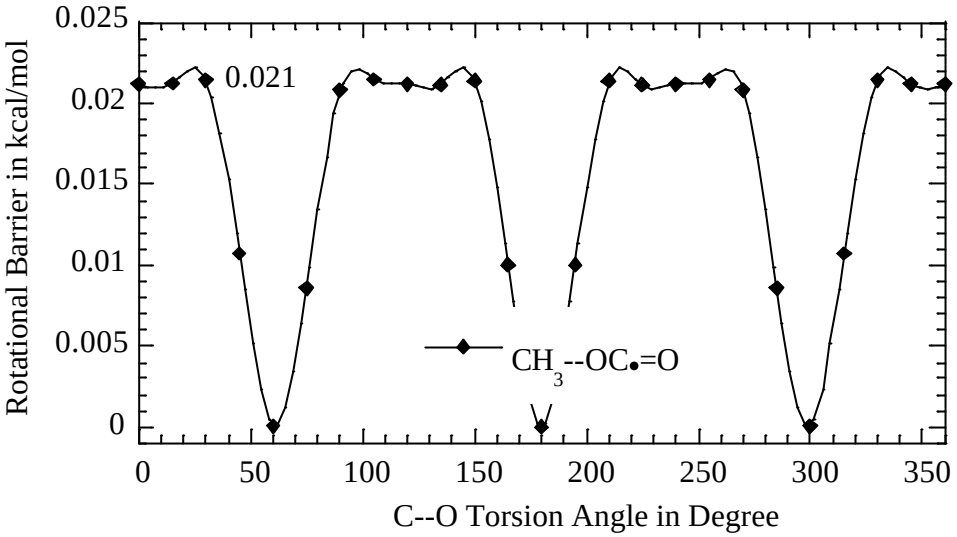

Fig. SM13: Potential barriers for internal rotations about C—O bonds in CH_3—OC•=O

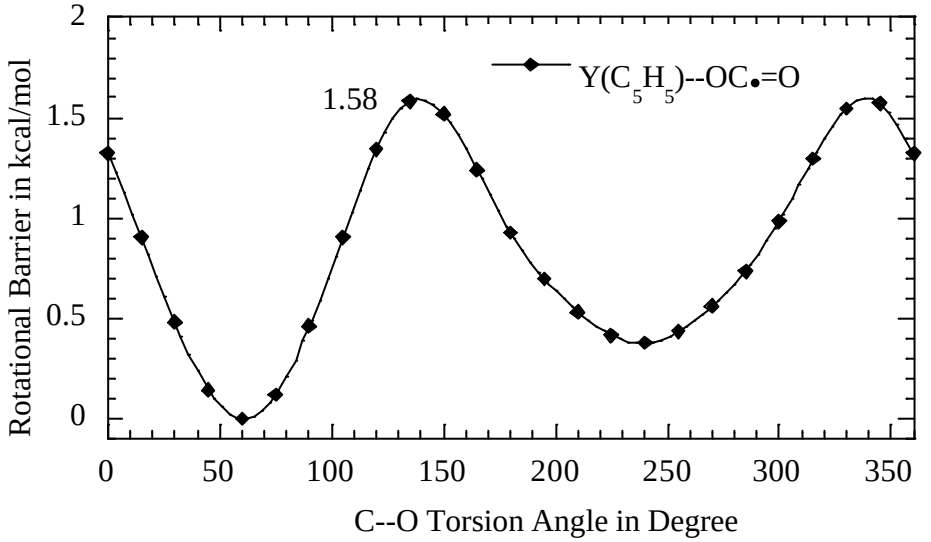

Fig. SM14: Potential barriers for internal rotations about C—O bonds in $Y(C_5H_5)$—OC•=O

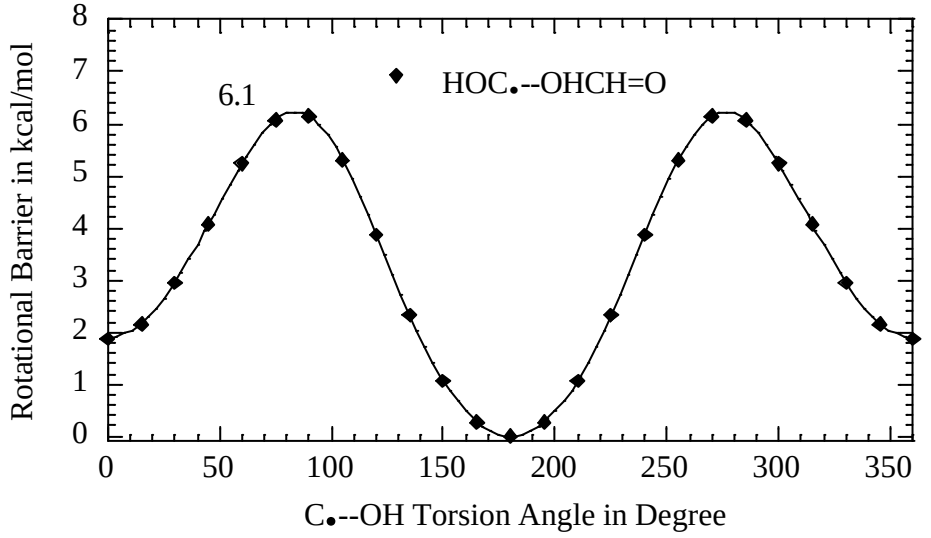

Fig. SM15: Potential barriers for internal rotations about C•—OH bonds in C•$(OH)_2$CH=O

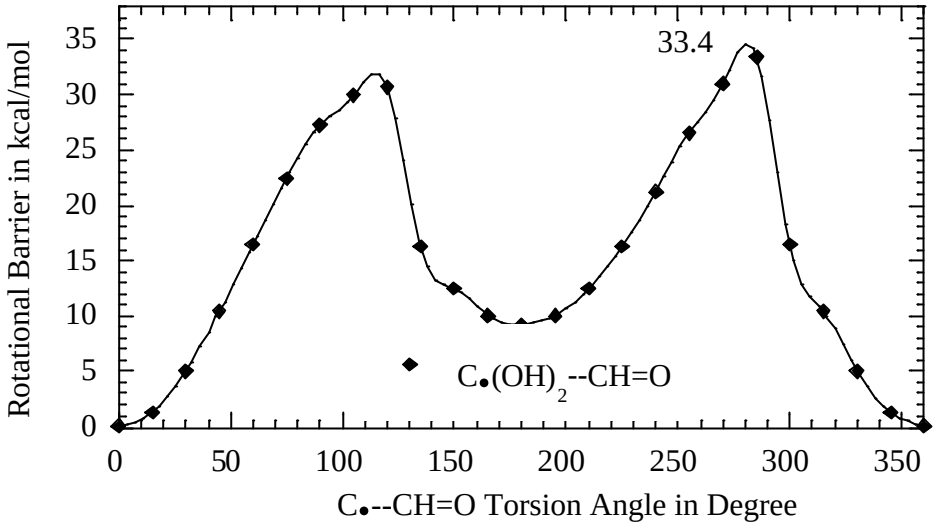

Fig. SM16: Potential barriers for internal rotations about C•—CH=O bonds in C•$(OH)_2$CH=O

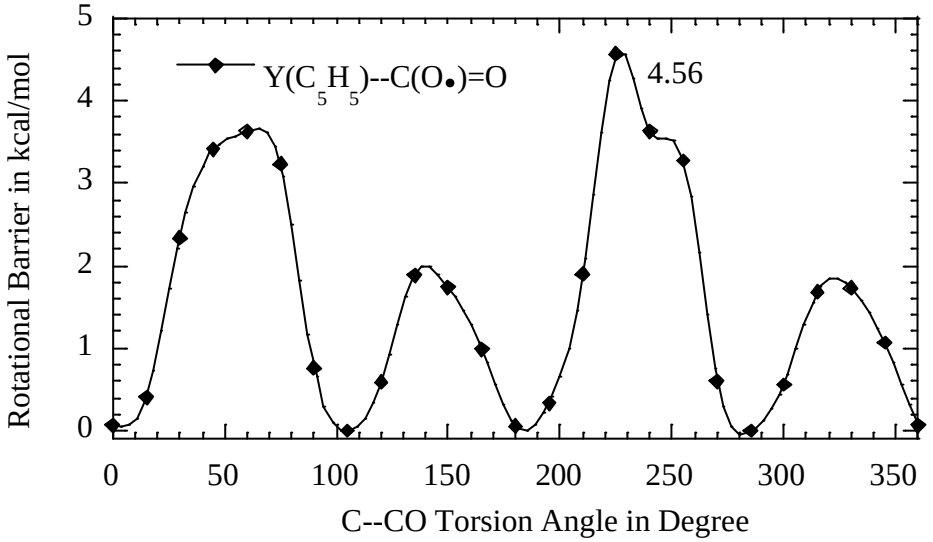

Fig. SM17: Potential barriers for internal rotations about C—CO bond in Y(C_5H_5)—C(O•)=O

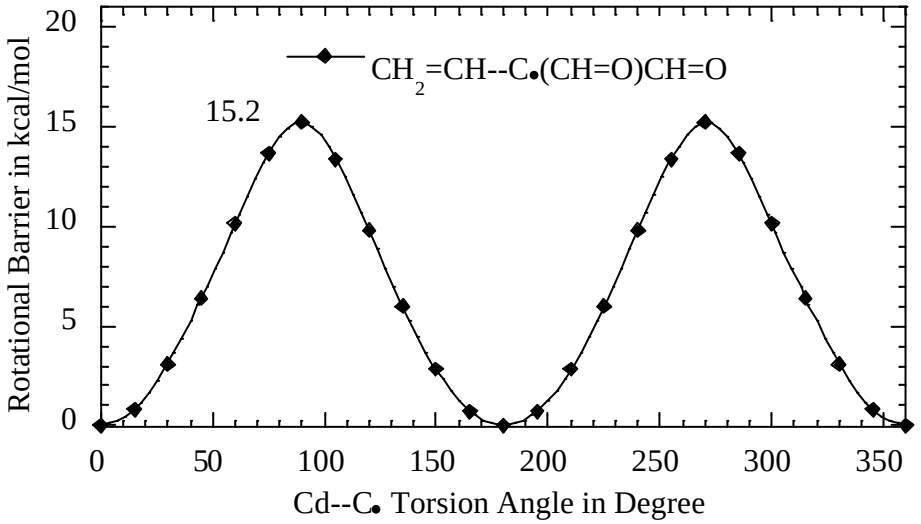

Fig. SM18: Potential barriers for internal rotations about C_d—C• bond in CH_2=CH—C•(CH=O)CH=O