Supporting information

Inductive and resonance effects on the acidities of phenol, enols and carbonyl α-hydrogens

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Geometries (computed at the B3LYP/6-31G(d,p) level)of all species described in this paper, as well as their gas phase and solution energies (computed at the B3LYP/6-311+G(3d,2p) level)
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Atom Coordinates 6
CH_4 6
CH_3OH 6
CH_3O^- 6
CH_3CHOH 6
CH_3CHO^- 6
$CH_3C(=O)CH_3$ 7
$CH_3C(=O)CH_2^-$ 7
$(CH_3)_2CHOH$ 7
$(CH_3)_2CHO^-$ 7
CH_3-CH=CH-OH 8
CH_3-$(CH=CH)_2$-OH 8
CH_3-$(CH=CH)_3$-OH 8
CH_3-$(CH=CH)_4$-OH 9
CH_3-$(CH=CH)_5$-OH 9
CH_3-CH=CH-O^- 10
CH_3-$(CH=CH)_2$-O^- 10
CH_3-$(CH=CH)_3$-O^- 10
CH_3-$(CH=CH)_4$-O^- 11
CH_3-$(CH=CH)_5$-O^- 11
C_6H_{11}-OH 12
C_6H_{11}-CH=CH-OH 12
C_6H_{11}-$(CH=CH)_2$-OH 13
C_6H_{11}-$(CH=CH)_3$-OH 13
C_6H_{11}-$(CH=CH)_4$-OH 14
C_6H_{11}-$(CH=CH)_5$-OH 15
C_6H_{11}-O^- 15
C_6H_{11}-CH=CH-O^- 16
C_6H_{11}-$(CH=CH)_2$-O^- 16
C_6H_{11}-$(CH=CH)_3$-O^- 17
C_6H_{11}-$(CH=CH)_4$-O^- 18
C_6H_{11}-$(CH=CH)_5$-O^- 18
Ph-OH 19
Ph-CH=CH-OH 19
Ph-CH=CH-OH (strained) 20
Ph-$(CH=CH)_2$-OH 20
Ph-$(CH=CH)_2$-OH (strained) 21
Ph-$(CH=CH)_3$-OH 21
Ph-$(CH=CH)_3$-OH (strained) 22
Ph-$(CH=CH)_4$-OH 22
Ph-$(CH=CH)_4$-OH (strained) 23
Ph-$(CH=CH)_5$-OH 24
Ph-$(CH=CH)_5$-OH (strained) 24
Ph-O^- 25
Ph-CH=CH-O^- 25
Ph-CH=CH-O^- (strained) 26
Ph-$(CH=CH)_2$-O^- 26
Ph-$(CH=CH)_2$-O^- (strained) 26
Ph-$(CH=CH)_3$-O^- 27

Figure 1: Ph-(CH=CH)$_3$-O$^-$ (strained) 28
Ph-(CH=CH)$_3$-O$^-$ (strained) 28
Ph-(CH=CH)$_4$-O$^-$ 28
Ph-(CH=CH)$_4$-O$^-$ (strained) 29
Ph-(CH=CH)$_5$-O$^-$ 30
Ph-(CH=CH)$_5$-O$^-$ (strained) 30
C_6H_6-OH 31
C_6H_6-CH=CH-OH 31
C_6H_6-CH=CH-OH (strained) 32
C_6H_6-(CH=CH)$_2$-OH 32
C_6H_6-(CH=CH)$_2$-OH (strained) 33
C_6H_6-(CH=CH)$_3$-OH 33
C_6H_6-(CH=CH)$_3$-OH (strained) 34
C_6H_6-(CH=CH)$_4$-OH 34
C_6H_6-(CH=CH)$_4$-OH (strained) 35
C_6H_6-(CH=CH)$_5$-OH 36
C_6H_6-(CH=CH)$_5$-OH (strained) 36
C_6H_6-O$^-$ 37
C_6H_6-CH=CH-O$^-$ 37
C_6H_6-CH=CH-O$^-$ (strained) 38
C_6H_6-(CH=CH)$_2$-O$^-$ 38
C_6H_6-(CH=CH)$_2$-O$^-$ (strained) 39
C_6H_6-(CH=CH)$_3$-O$^-$ 39
C_6H_6-(CH=CH)$_3$-O$^-$ (strained) 40
C_6H_6-(CH=CH)$_4$-O$^-$ 40
C_6H_6-(CH=CH)$_4$-O$^-$ (strained) 41
C_6H_6-(CH=CH)$_5$-O$^-$ 42
C_6H_6-(CH=CH)$_5$-O$^-$ (strained) 42
O=CH-CH$_3$ 43
O=CH-CH$_2^-$ 43
O=CH-CH$_2^-$ (strained, i.e. no resonance) 44
HO-CH=CH$_2$ 44
O=CH-CH=CH-CH$_3$ 44
O=CH-CH=CH-CH$_3$ (strained) 44
O=CH-(CH=CH)$_2$-CH$_3$ 45
O=CH-(CH=CH)$_2$-CH$_3$ (strained) 45
O=CH-(CH=CH)$_3$-CH$_3$ 45
Figure 2: O=CH-(CH=CH)$_3$-CH$_3$ (strained) 46
O=CH-(CH=CH)$_3$-CH$_3$ (strained) 46
O=CH-(CH=CH)$_4$-CH$_3$ 47
O=CH-(CH=CH)$_4$-CH$_3$ (strained) 47
O=CH-(CH=CH)$_5$-CH$_3$ 48
O=CH-(CH=CH)$_5$-CH$_3$ (strained) 48
O=CH-CH=CH-CH$_2^-$ 49
O=CH-CH=CH-CH$_2^-$ (strained) 49
O=CH-(CH=CH)$_2$-CH$_2^-$ 49
O=CH-(CH=CH)$_2$-CH$_2^-$ (strained) 50
O=CH-(CH=CH)$_3$-CH$_2^-$ 50
O=CH-(CH=CH)$_3$-CH$_2^-$ (strained) 50
O=CH-(CH=CH)$_4$-CH$_2^-$ 51

O=CH-(CH=CH)$_4$-CH$_2^-$ (strained) 51
O=CH-(CH=CH)$_5$-CH$_2^-$ 52
O=CH-(CH=CH)$_5$-CH$_2^-$ (strained) 52
H-CH=CH-CH$_3$ 53
H-(CH=CH)$_2$-CH$_3$ 53
H-(CH=CH)$_3$-CH$_3$ 53
H-(CH=CH)$_4$-CH$_3$ 54
H-(CH=CH)$_5$-CH$_3$ 54
H-CH=CH-CH$_2^-$ 55
H-(CH=CH)$_2$-CH$_2^-$ 55
H-(CH=CH)$_3$-CH$_2^-$ 55
H-(CH=CH)$_4$-CH$_2^-$ 56
H-(CH=CH)$_5$-CH$_2^-$ 56
HO-CH=CH-CH=CH$_2$ 57
HO-CH=CH-CH=CH$_2$ (strained) 57
HO-(CH=CH)$_2$-CH=CH$_2$ 57
HO-(CH=CH)$_2$-CH=CH$_2$ (strained) 58
HO-(CH=CH)$_3$-CH=CH$_2$ 58
HO-(CH=CH)$_3$-CH=CH$_2$ (strained) 58
HO-(CH=CH)$_4$-CH=CH$_2$ 59
HO-(CH=CH)$_4$-CH=CH$_2$ (strained) 59
HO-(CH=CH)$_5$-CH=CH$_2$ 60
HO-(CH=CH)$_5$-CH=CH$_2$ (strained) 60
$^-$O-CH=CH-CH=CH$_2$ (strained) 61
$^-$O-(CH=CH)$_2$-CH=CH$_2$ (strained) 61
Figure 3: $^-$O-(CH=CH)$_3$-CH=CH$_2$ (strained) 62
$^-$O-(CH=CH)$_3$-CH=CH$_2$ (strained) 62
$^-$O-(CH=CH)$_4$-CH=CH$_2$ (strained) 62
$^-$O-(CH=CH)$_5$-CH=CH$_2$ (strained) 63
Gas phase energies 64
Raw data used for the elaboration of table 1. 64
Gas phase energies (in hartree) of protonated and deprotonated methanol vinylogues 64
Gas phase energies (in hartree) of protonated and deprotonated cyclohexanol vinylogues 65
Gas phase energies (in hartree) of relaxed protonated and deprotonated 2,4-cyclohexadien-1-ol vinylogues 65
Gas phase energies (in hartree) of strained protonated and deprotonated 2,4-cyclohexadien-1-ol vinylogues 65
Gas phase energies (in hartree) of protonated and deprotonated phenol vinylogues . 65
Gas phase energies (in hartree) of strained protonated and deprotonated phenol vinylogues 66
Gas phase energies (in hartree) of protonated and deprotonated enol vinylogues 66
Gas phase energies (in hartree) of strained protonated and deprotonated enol vinylogues 66
Gas phase energies (in hartree) of protonated and deprotonated methane vinylogues66
Gas phase energies (in hartree) of protonated and deprotonated acetaldehyde vinylogues 67
Gas phase energies (in hartree) of strained protonated and deprotonated acetaldehyde vinylogues 67

Solution energies (kcal.mol^{-1}) of protonated and deprotonated methanol vinylogues 67
Solution energies (kcal.mol^{-1}) of protonated and deprotonated phenol vinylogues ... 67
Solution energies (kcal.mol^{-1}) of strained protonated and deprotonated phenol vinylogues ... 68
Solution energies (kcal.mol^{-1}) of protonated and deprotonated enol vinylogues ... 68
Solution energies (kcal.mol^{-1}) of strained protonated and deprotonated enol vinylogues ... 68
Solution energies (kcal.mol^{-1}) of protonated and deprotonated methane vinylogues 68
Solution energies (kcal.mol^{-1}) of protonated and deprotonated acetaldehyde vinylogues ... 69
Solution energies (kcal.mol^{-1}) of strained protonated and deprotonated acetaldehyde vinylogues ... 69
Dependence of gas phase acidity of 2,4-cyclohexadien-1-ol (n=1) vinylogue (open symbols) and cyclohexanologue (n=1) vinyvinylogues (closed symbols) with the dihedral angle between the ring and the OH group ... 70

Atom Coordinates

CH_4

C	0.000000000	0.000000000	0.000000000
H	0.530433946	-0.951333822	0.076190031
H	0.716547685	0.821859802	0.057506648
H	-0.716547685	0.083844265	0.819591781
H	-0.530433945	0.045629756	-0.953288460

CH_3OH

C	0.725647770	-0.012988537	-0.000003918
H	1.099412996	1.014119021	0.000849213
H	1.125496826	-0.519422522	0.891591911
H	1.125580985	-0.518052556	-0.892345405
O	-0.690372213	0.064014141	-0.000005017
H	-1.033949565	-0.837942266	0.000030563

CH_3O^-

C	-0.622613076	0.000001359	-0.000000758
H	-1.165043020	0.582909688	-0.845795309
H	-1.165053779	-1.023949494	-0.081909694
H	-1.165047251	0.441033302	0.927709742
O	0.687334312	-0.000000610	0.000000270

CH_3CHOH

C	-1.279681975	0.253828800	0.015015471
H	-2.159151836	-0.399173336	-0.001445706
H	-1.314436305	0.862364793	0.923437255
H	-1.351378507	0.927458770	-0.847780684
C	0.008682737	-0.562241315	-0.031783006
H	0.027387497	-1.189186453	-0.937916359
H	0.056274347	-1.240844335	0.826082660
O	1.177801763	0.244186194	0.059338131
H	1.182311594	0.836184545	-0.704467955

CH_3CHO^-

C	1.268502095	0.218379635	0.000000000
H	2.136425733	-0.468826160	0.000000000
H	1.339210672	0.870087965	-0.883606122
H	1.339210672	0.870087965	0.883606122
C	-0.123920115	-0.511386861	0.000000000
H	-0.030942665	-1.247977282	0.889110406
H	-0.030942665	-1.247977282	-0.889110406
O	-1.158189538	0.296986606	0.000000000

$CH_3C(=O)CH_3$

C	0.000005314	-0.100377970	0.000008463
O	-0.000013982	-1.316195316	-0.000001306
C	-1.292563083	0.698797035	0.000088212
H	-1.336755048	1.357060371	0.875510808
H	-1.343107965	1.344434996	-0.884427498
H	-2.146331094	0.020269553	0.007522687
C	1.292575469	0.698776022	-0.000089601
H	2.146338343	0.020249784	-0.007573085
H	1.336712438	1.357042499	-0.875525417
H	1.343154494	1.344432059	0.884428997

$CH_3C(=O)CH_2^-$

C	0.108991768	0.054616465	0.000000000
C	1.220346716	-0.770216956	0.000000000
H	2.223092157	-0.345226608	0.000000000
H	1.133410208	-1.854880868	0.000000000
O	0.054763162	1.325666881	0.000000000
C	-1.271227067	-0.661650351	0.000000000
H	-1.217787062	-1.759163375	0.000000000
H	-1.849884454	-0.340664398	0.878549310
H	-1.849884454	-0.340664398	-0.878549310

$(CH_3)_2CHOH$

C	-1.320360750	0.636971902	-0.113468940
H	-1.441696781	1.657083374	0.266380775
H	-1.343618423	0.667499219	-1.207600536
H	-2.182287615	0.051804779	0.229328429
C	-0.007552188	0.017594458	0.369475506
H	-0.009960799	0.000355405	1.473025363
O	0.150156316	-1.312067030	-0.133504813
H	-0.610975554	-1.829854355	0.160088396
C	1.213860592	0.798654424	-0.099870454
H	1.197858734	1.819723105	0.293534420
H	2.130372315	0.307747214	0.238430882
H	1.235220827	0.845840359	-1.193456020

$(CH_3)_2CHO^-$

C	1.266563757	0.723560851	0.093153320
H	1.314136588	1.749302419	-0.317155374
H	1.299372472	0.784470728	1.191748678
H	2.165268371	0.180587793	-0.227865330
C	0.000305369	-0.106530687	-0.338140773

H	-0.000579633	0.008684425	-1.490003432
O	0.005502055	-1.339421961	0.126312259
C	-1.272306023	0.714461002	0.093160905
H	-1.330023178	1.737480636	-0.322533056
H	-2.166718794	0.161467166	-0.222560278
H	-1.304041209	0.781762175	1.191474846

*** acidity of Phenol **********

CH_3-CH=CH-OH

C	0.559302440	0.411310772	0.000226735
H	0.410806522	1.489318229	0.000523890
C	-0.519129517	-0.372230585	-0.000005650
H	-0.436142255	-1.459195232	-0.000110323
O	-1.794619334	0.136583655	-0.000254394
H	-2.422606277	-0.594001832	0.002526573
C	1.966210502	-0.111283605	-0.000093673
H	2.526067935	0.231613439	0.879575212
H	1.988834258	-1.206236568	0.000696540
H	2.525279158	0.230534536	-0.880691527

CH_3-(CH=CH)$_2$-OH

C	-1.849469322	0.425545047	-0.000238697
H	-1.804037350	1.515177173	-0.001952473
C	-0.697253107	-0.265904878	0.002084748
H	-0.744880328	-1.356610696	0.003571486
C	0.628422464	0.323519284	0.002308895
H	0.715099480	1.408109232	0.003333389
C	1.754122364	-0.406640010	0.000151560
H	1.729257886	-1.495797353	-0.001192136
O	2.992298634	0.173830744	-0.001766827
H	3.665511054	-0.515748954	-0.001938699
C	-3.218932172	-0.184801598	-0.001595929
H	-3.799792855	0.127361979	0.876558902
H	-3.797315958	0.126374214	-0.881732474
H	-3.171670739	-1.278387827	-0.000881537

CH_3-(CH=CH)$_3$-OH

C	-3.111114553	0.410802073	-0.000122577
H	-3.090947130	1.501371731	0.000199782
C	-1.940489475	-0.253109253	0.001123433
H	-1.957804773	-1.344460071	0.000659929
C	-0.634692413	0.371520079	0.002015885
H	-0.610095833	1.461533970	0.001581660
C	0.536312970	-0.307885109	0.001704303
H	0.501606952	-1.398550642	0.001489619
C	1.845524532	0.300017227	0.000150950
H	1.916417617	1.385733988	-0.000867674
C	2.985542566	-0.412806842	-0.000071068

H	2.979057932	-1.502087401	0.000978497
O	4.210815683	0.189828987	-0.001704902
H	4.898092002	-0.485957659	-0.001462841
C	-4.465551428	-0.230166879	-0.002084087
H	-5.052657766	0.069562058	0.876283272
H	-5.050468089	0.070533188	-0.881583921
H	-4.394044079	-1.322189985	-0.002569231

CH_3-$(CH=CH)_4$-OH

C	4.361870019	0.393300213	-0.000099959
H	4.354618908	1.483984224	0.002675425
C	3.182942895	-0.257439342	0.000938818
H	3.186732114	-1.348698618	0.000329747
C	1.887116533	0.383591349	0.000384741
H	1.877089180	1.474025398	0.000108841
C	0.703751899	-0.279540977	0.000654168
H	0.719311754	-1.370452409	0.000850336
C	-0.590855786	0.349085894	0.000283005
H	-0.611219678	1.439157153	-0.000063191
C	-1.768953976	-0.324856184	0.000208194
H	-1.739957686	-1.415557732	0.000443909
C	-3.071644068	0.290843665	-0.000104683
H	-3.136083610	1.376923659	-0.000479912
C	-4.217189452	-0.415340711	-0.000005615
H	-4.217660612	-1.504582738	0.000477797
O	-5.437089457	0.195686240	-0.000770637
H	-6.129958653	-0.474471960	0.001031981
C	5.708433838	-0.263432887	-0.001228841
H	6.297833237	0.033877279	-0.878866809
H	6.297077405	0.028439382	0.878717443
H	5.624325859	-1.354391252	-0.005257012

CH_3-$(CH=CH)_5$-OH

C	3.133508605	-0.382059509	-0.003517278
H	3.131336921	-1.472517074	-0.003300172
C	1.944212170	0.272849179	-0.003418225
H	1.950992140	1.363651006	-0.003046284
C	0.657593876	-0.366827716	-0.002190491
H	0.647954375	-1.457265089	-0.001464195
C	-0.530867122	0.294916901	-0.001866214
H	-0.517089101	1.385745112	-0.002388992
C	-1.820588198	-0.336711685	-0.000832842
H	-1.838204528	-1.426802617	-0.000162128
C	-3.002160939	0.334211017	-0.000419932
H	-2.976297817	1.424931294	-0.001084922
C	-4.301514907	-0.285639583	0.000947137
H	-4.362584713	-1.371894953	0.001633443
C	-5.449925324	0.417038827	0.001329933
H	-5.454123923	1.506245489	0.000601331
O	-6.666881505	-0.198412245	0.002555230

H	−7.362816028	0.468682946	0.002698735
C	4.424062598	0.267688221	−0.002186591
H	4.421128849	1.358822514	−0.004554358
C	5.606757593	−0.377127181	0.002026938
H	5.604122370	−1.467848356	0.004704522
C	6.949863709	0.285473790	0.005596246
H	7.543103335	−0.007398816	−0.870961573
H	6.861221911	1.376066462	0.004128022
H	7.537290412	−0.005683845	0.886596855

CH_3-CH=CH-O^-

C	−0.546854438	−0.458176996	0.000075079
H	−0.461326276	−1.547193045	0.000347691
C	0.612988695	0.299141101	0.000292137
H	0.379516436	1.414764859	−0.000217817
O	1.831253868	−0.046594160	−0.000162654
C	−1.917741236	0.146473983	−0.000105875
H	−2.548671453	−0.113192536	−0.878226133
H	−2.548170509	−0.110322145	0.879273432
H	−1.837900718	1.244998352	−0.001707461

CH_3-$(CH=CH)_2$-O^-

C	−1.859959268	−0.450680429	−0.000563158
H	−1.924469527	−1.540805758	0.000948421
C	−0.631024910	0.143741360	−0.000591051
H	−0.634304838	1.242506214	−0.000365749
C	0.669754017	−0.431058023	−0.000086137
H	0.779136397	−1.516578943	0.000182329
C	1.836106029	0.350448466	−0.000396745
H	1.609239712	1.458430559	−0.001276512
O	3.038048320	−0.009036097	0.000599937
C	−3.161307332	0.298967469	0.000592245
H	−3.797427763	0.086762151	0.880866376
H	−2.983576502	1.382901870	−0.000527400
H	−3.800594996	0.084913966	−0.876908068

CH_3-$(CH=CH)_3$-O^-

C	−3.127926834	−0.380040705	0.000084073
H	−3.242039905	−1.465549158	0.000291328
C	−1.875465624	0.150581854	−0.000438412
H	−1.809885658	1.245048067	−0.000592400
C	−0.616537697	−0.527146450	−0.000544712
H	−0.629569776	−1.618633105	−0.000144174
C	0.603792322	0.124495638	−0.000359675
H	0.556553503	1.220410865	−0.000619338
C	1.902324473	−0.410718998	0.000380836
H	2.047067890	−1.491094897	0.001176822
C	3.054013866	0.408842481	0.000092837
H	2.805062175	1.508033101	−0.000152828
O	4.254613449	0.067580276	0.000142550

C	-4.392856964	0.428711392	0.000455068
H	-5.032553701	0.235232226	-0.878335675
H	-5.032029963	0.235150088	0.879602650
H	-4.169370835	1.503026891	0.000440307

CH_3-$(CH{=}CH)_4$-O^-

C	4.377419881	-0.294595285	-0.000855376
H	4.518289655	-1.376682612	-0.002338573
C	3.114001844	0.201116954	0.000294085
H	3.010053344	1.291435683	0.001851328
C	1.881417307	-0.529496147	-0.000290151
H	1.942468365	-1.619116818	-0.001918414
C	0.637721354	0.063449585	0.001055853
H	0.622179289	1.158556527	0.002625211
C	-0.628447539	-0.563604656	0.000486661
H	-0.657784630	-1.654336255	-0.001340969
C	-1.834147828	0.132124439	0.001749276
H	-1.753110618	1.225100513	0.003008024
C	-3.136157190	-0.370742102	0.001370739
H	-3.309139293	-1.446410774	0.001283485
C	-4.272107698	0.480612718	-0.000481703
H	-4.001251976	1.572434467	-0.000959583
O	-5.473700605	0.158705046	-0.001981089
C	5.621932359	0.544776985	-0.000707275
H	6.262647864	0.358696428	0.877062377
H	6.259883578	0.363300048	-0.881478417
H	5.374569695	1.613210583	0.002425835

CH_3-$(CH{=}CH)_5$-O^-

C	-3.134465428	0.497136740	-0.003154079
H	-3.228680381	1.584130814	-0.000474446
C	-1.876942914	-0.056887359	-0.004306454
H	-1.821872631	-1.149873535	-0.006320016
C	-0.633557084	0.622253953	-0.000952583
H	-0.651338513	1.713189910	0.001513580
C	0.596537071	-0.016974596	-0.001159628
H	0.574509556	-1.111279550	-0.003383531
C	1.871567757	0.571825140	0.000579973
H	1.934076152	1.660823724	0.002376905
C	3.062252827	-0.159620248	-0.000175271
H	2.952982947	-1.249479490	-0.002249917
C	4.369012263	0.314714422	0.001177036
H	4.567748426	1.385511097	0.003189876
C	5.489056633	-0.564628873	-0.000060503
H	5.198059035	-1.649654955	-0.002216506
O	6.692616112	-0.261882173	0.002042437
C	-4.347703295	-0.269522166	-0.001999853
H	-4.217331846	-1.356218306	-0.005248774
C	-5.618233190	0.201731244	0.003555595
H	-5.778095839	1.281037052	0.006384307

C	−6.848024106	−0.658500442	0.003496227
H	−7.489651252	−0.478073954	−0.873687497
H	−6.584328429	−1.722580453	−0.001584999
H	−7.485495809	−0.484742709	0.885001095

C_6H_{11}-OH

C	−0.995207963	−0.009842177	−0.330590967
H	−0.962404957	−0.011826686	−1.435491961
C	−0.300305984	1.256823146	0.168342479
H	−0.819300719	2.134797374	−0.231522767
H	−0.409731090	1.293896647	1.260472705
C	1.188012814	1.271908061	−0.212993415
H	1.283561298	1.333528540	−1.306437110
C	−0.277574382	−1.267188956	0.177669605
H	−0.384939417	−1.299146411	1.270167487
H	−0.773159448	−2.165314822	−0.216882020
C	1.210562229	−1.265133019	−0.206777216
H	1.705358225	−2.155483113	0.198161841
H	1.303859103	−1.329075652	−1.300235589
C	1.911142932	0.010895264	0.285156646
H	1.924229385	0.013504144	1.384131595
H	2.958152532	0.018405579	−0.040192691
H	1.667755827	2.171298823	0.189813170
O	−2.349211521	0.048970765	0.115903375
H	−2.794280106	−0.751570053	−0.192245750

C_6H_{11}-CH=CH-OH

C	−2.586817457	−0.000025202	0.410235366
H	−2.520882083	−0.004777495	1.498334405
C	−1.496393886	0.004331560	−0.356779857
H	−1.624434403	0.008051973	−1.438807805
C	−0.090232447	0.001862684	0.181026027
H	−0.140752055	0.001482012	1.281400076
C	0.682663743	−1.265724685	−0.250907460
H	0.149771989	−2.155941985	0.102920882
H	0.682425788	−1.320169561	−1.349458322
C	2.132268283	−1.268119509	0.257953166
H	2.129655109	−1.327716111	1.355939237
C	0.686371745	1.267549723	−0.249776152
H	0.686009110	1.323103221	−1.348272959
H	0.156260462	2.159015982	0.105107085
C	2.136145365	1.265286352	0.258638270
H	2.660614757	2.159876662	−0.098511582
H	2.134149671	1.324616699	1.356636787
C	2.886777145	−0.002455145	−0.173852880
H	2.997213109	−0.002340586	−1.267735600
H	3.901818098	−0.004088435	0.241464591
H	2.654154652	−2.164203210	−0.099227739

O	−3.854675150	−0.002385796	−0.116903430
H	−4.493551428	0.008737891	0.604245946

C_6H_{11}-$(CH=CH)_2$-OH

C	−2.908439950	−0.017025659	−0.306463341
H	−3.013917464	−0.043255597	−1.389019855
C	−4.021295084	0.013470968	0.442814272
H	−3.977156228	0.041000727	1.531031650
C	−1.573425585	−0.013444311	0.261282321
H	−1.509903056	0.011235705	1.350936393
C	−0.430349249	−0.035026818	−0.445709786
H	−0.487390393	−0.060833619	−1.535977687
C	0.953757120	−0.016762823	0.141343047
H	0.861535859	−0.009221846	1.238359696
C	1.762395717	−1.274587236	−0.254753346
H	1.232158424	−2.171886252	0.084963388
H	1.805142311	−1.336092397	−1.352201383
C	3.191279804	−1.249434907	0.308988030
H	3.146910717	−1.302611605	1.406291715
C	1.725861763	1.259062772	−0.271914168
H	1.766960019	1.306697354	−1.370110629
H	1.169410376	2.144982381	0.055328327
C	3.154545949	1.283628652	0.291526976
H	3.678036523	2.183935707	−0.052551621
H	3.109284443	1.351272525	1.387982358
C	3.941211353	0.025382365	−0.103210750
H	4.090030530	0.020086057	−1.192563091
H	4.940802437	0.043208770	0.347573455
H	3.740195409	−2.139508480	−0.021803117
O	−5.269348991	0.013782461	−0.115599283
H	−5.930255018	0.036792192	0.585519314

C_6H_{11}-$(CH=CH)_3$-OH

C	−1.792747244	−0.046569783	−0.398764129
H	−1.839642468	−0.095129655	−1.486916672
C	−2.949293868	−0.004042348	0.304034333
H	−2.891122475	0.045234106	1.392610652
C	−4.271329294	−0.015463520	−0.274977899
H	−4.366351619	−0.064861918	−1.357693525
C	−5.394965690	0.034069589	0.461878167
H	−5.363907062	0.085208299	1.549547564
C	−0.475079114	−0.026994129	0.199990775
H	−0.438919074	0.017494299	1.290024328
C	0.685005961	−0.055425870	−0.482514625
H	0.650513835	−0.099402329	−1.573360088
C	2.055908970	−0.019701514	0.131779056
H	1.941588090	−0.001680969	1.226337568
C	2.881778356	−1.275216400	−0.236034529

H	2.350998730	−2.173482395	0.100061412
H	2.949234952	−1.345544512	−1.331689653
C	4.297756977	−1.233930218	0.358439350
H	4.229559566	−1.277289703	1.454866756
C	2.826331416	1.258003273	−0.279992685
H	2.891166565	1.293663852	−1.377427370
H	2.256607516	2.143038899	0.025818073
C	4.241884465	1.298812187	0.314699041
H	4.765952127	2.199791103	−0.026572187
H	4.171070535	1.376947041	1.409077355
C	5.046818567	0.042810385	−0.049481443
H	5.221061794	0.027882490	−1.134924255
H	6.035449620	0.073065967	0.424169710
H	4.860049205	−2.122807078	0.047736669
O	−6.633383416	0.023387395	−0.112956460
H	−7.305197339	0.066411081	0.576939785

C_6H_{11}-(CH=CH)$_4$-OH

C	0.646414597	−0.047100165	0.433517783
H	0.675560700	−0.090151257	1.522757992
C	1.818072336	−0.014891927	−0.249639181
H	1.783500832	0.029446545	−1.339237275
C	3.123281108	−0.031237022	0.356198550
H	3.162167382	−0.076037496	1.444857851
C	4.289707151	0.006874634	−0.336795982
H	4.242474231	0.052173315	−1.425924936
C	5.602507059	−0.006575322	0.256837018
H	5.684950207	−0.051905838	1.340735444
C	6.736043569	0.035495360	−0.467250595
H	6.718502645	0.081884269	−1.555395764
C	−0.660472028	−0.023432452	−0.184142315
H	−0.682198269	0.019222463	−1.274418667
C	−1.829039229	−0.046572453	0.485551963
H	−1.806159013	−0.087683967	1.576859424
C	−3.193711254	−0.011761884	−0.141374005
H	−3.070717574	0.008800265	−1.234808636
C	−4.017557166	−1.271264428	0.218461549
H	−3.481550343	−2.166819150	−0.116421047
H	−4.091557727	−1.344274205	1.313511076
C	−5.430201777	−1.233398032	−0.384277702
H	−5.355398806	−1.273817306	−1.480355270
C	−3.970651002	1.262526609	0.268741526
H	−4.042450288	1.295538479	1.365797258
H	−3.402695655	2.150423278	−0.031890048
C	−5.383018486	1.299316513	−0.334113776
H	−5.911935267	2.197863875	0.005979028
H	−5.305876671	1.380139566	−1.427874076
C	−6.185404414	0.039776483	0.023004935
H	−6.365435634	0.021786050	1.107466529
H	−7.171570709	0.067909591	−0.455840634

H	−5.990864024	−2.125043407	−0.078800640
O	7.965890986	0.022392063	0.123403205
H	8.647500432	0.058159800	−0.557283249

C_6H_{11}-(CH=CH)$_5$-OH

C	0.518619820	0.003118106	−0.441684372
H	0.498620395	0.026016729	−1.531741277
C	−0.660696017	−0.010321791	0.231253590
H	−0.637964165	−0.032051652	1.321640616
C	−1.956126525	0.004486135	−0.389819970
H	−1.980717465	0.029596868	−1.479758599
C	−3.135881864	−0.009609482	0.287323931
H	−3.108435124	−0.034215192	1.377617161
C	−4.433150571	0.006147975	−0.328292744
H	−4.463444855	0.032229284	−1.417813814
C	−5.607063562	−0.008463882	0.355804437
H	−5.569392944	−0.034296565	1.445879227
C	−6.913022192	0.008042340	−0.249771080
H	−6.985448840	0.034156421	−1.335000562
C	−8.054042760	−0.007137055	0.464662303
H	−8.047087638	−0.033023505	1.553569460
C	1.819599297	−0.007707814	0.186470097
H	1.834245602	−0.024538095	1.277467315
C	2.992272090	0.004663137	−0.477103968
H	2.974542598	0.021069287	−1.569172059
C	4.354468560	−0.000847735	0.155612943
H	4.227237332	−0.009942435	1.248684300
C	5.156095788	−1.265010228	−0.237989672
H	4.604614649	−2.158705056	0.075967221
H	5.226033071	−1.311792910	−1.334645775
C	6.570356147	−1.267656771	0.361739905
H	6.498156027	−1.336441851	1.456619644
C	5.153359508	1.271473968	−0.216755156
H	5.222487489	1.336580540	−1.312603112
H	4.601826110	2.159616548	0.112415874
C	6.567942406	1.265695946	0.381572272
H	7.111770156	2.163525327	0.063859368
H	6.497145731	1.317265204	1.477412279
C	7.346653024	0.002595565	−0.013334365
H	7.523566541	0.010870296	−1.098459411
H	8.334393704	0.000590925	0.463008369
H	7.114550918	−2.160315676	0.030538218
O	−9.277298528	0.008266793	−0.138074251
H	−9.966310875	−0.001996667	0.536088619

C_6H_{11}-O^-

C	1.116813475	−0.000124280	0.297063527
H	0.918615245	−0.000726573	1.439870496

C	0.301699953	1.263439666	-0.190424351
H	0.815614875	2.157823586	0.188684235
H	0.391560426	1.296383857	-1.288480257
C	-1.180987236	1.269970048	0.215722340
H	-1.252970902	1.314034314	1.313865240
C	0.301887633	-1.263469910	-0.191038778
H	0.390473612	-1.295786533	-1.289229595
H	0.815917555	-2.158165461	0.187127853
C	-1.180416512	-1.269855496	0.216342448
H	-1.708795426	-2.162891876	-0.158210439
H	-1.251296823	-1.312467770	1.314635699
C	-1.900655055	-0.000293274	-0.266969291
H	-1.922893593	-0.000642813	-1.368062324
H	-2.951509593	-0.000310227	0.064004815
H	-1.709472524	2.162274250	-0.160448600
O	2.377197607	0.000279957	-0.075900099

C_6H_{11}-CH=CH-O^-

C	-2.680825750	0.000565843	0.350819867
H	-2.415498324	0.006053965	1.457790771
C	-1.543387243	-0.009411203	-0.444800149
H	-1.655411398	-0.012596968	-1.532255751
C	-0.150375496	-0.004651495	0.110457656
H	-0.236223053	-0.002207366	1.212498163
C	0.675808569	-1.263683948	-0.271044628
H	0.131735458	-2.153787200	0.066311483
H	0.718313845	-1.331357444	-1.369865620
C	2.110371199	-1.262575661	0.286673688
H	2.070195873	-1.312669127	1.385810035
C	0.667228093	1.258778745	-0.275530146
H	0.711159813	1.323349707	-1.374430053
H	0.116369365	2.145735971	0.059016259
C	2.100773327	1.269309994	0.284985270
H	2.646639707	2.167164263	-0.042231710
H	2.056847206	1.318890744	1.383982543
C	2.874415667	0.006058617	-0.120796092
H	3.010910088	0.005797883	-1.213087549
H	3.882592605	0.010003067	0.319027600
H	2.662091920	-2.156592569	-0.041345465
O	-3.904681167	0.003717648	0.039835074

C_6H_{11}-$(CH=CH)_2$-O^-

C	-2.976249180	-0.012321672	0.418730549
H	-3.159482769	-0.034056212	1.493631122
C	-4.088130436	0.010113857	-0.441549877
H	-3.787496060	0.032293985	-1.530932601
C	-1.644448150	-0.004896622	-0.069410680
H	-1.570972225	0.019532865	-1.165178090
C	-0.453150829	-0.021608112	0.602351077
H	-0.449685035	-0.046585885	1.695306552

C	0.898138412	-0.007901610	-0.059120044
H	0.741268856	-0.001519579	-1.151129023
C	1.723989201	1.258105261	0.287260267
H	1.152609483	2.145907961	-0.007560031
H	1.833225651	1.313466341	1.381522568
C	3.118631937	1.275309497	-0.360757094
H	3.006485631	1.333800712	-1.454032017
C	1.741561189	-1.266074690	0.270663824
H	1.854176474	-1.333510888	1.363975231
H	1.182676669	-2.158601135	-0.033902169
C	3.136262667	-1.256475997	-0.377956916
H	3.705975123	-2.151112874	-0.088916379
H	3.024632401	-1.302188973	-1.471906955
C	3.920690232	0.012587938	-0.013199123
H	4.130736565	0.005756972	1.066973137
H	4.896011650	0.023228219	-0.519763259
H	3.676277719	2.173697785	-0.059912079
O	-5.309334707	0.008607685	-0.162461030

C_6H_{11}-(CH=CH)$_3$-O^-

C	-1.838430444	0.113773631	0.630569653
H	-1.900696431	0.241466692	1.712629927
C	-3.012454606	0.009340368	-0.096963586
H	-2.889977797	-0.119453215	-1.179279034
C	-4.342011755	0.041939333	0.347863238
H	-4.560704686	0.166235375	1.408329790
C	-5.435550109	-0.084080493	-0.541035105
H	-5.112585854	-0.208080020	-1.613308316
C	-0.539791680	0.056993419	0.042115383
H	-0.532873886	-0.076131851	-1.046100113
C	0.677540237	0.143896692	0.647750468
H	0.727465105	0.272172723	1.731895489
C	1.998810521	0.041870495	-0.065376878
H	1.797321474	-0.022230442	-1.147525797
C	2.894005475	1.284958192	0.161210668
H	2.358028346	2.178650778	-0.179081823
H	3.048314646	1.412568566	1.243697310
C	4.262082392	1.180436463	-0.532861633
H	4.113761429	1.171631955	-1.623067380
C	2.783985753	-1.234835692	0.328075245
H	2.932506081	-1.232160658	1.418761999
H	2.168593090	-2.114026073	0.105406260
C	4.150500059	-1.344674662	-0.367961986
H	4.683629403	-2.244578713	-0.031704509
H	3.995183212	-1.463913252	-1.450701140
C	5.010403208	-0.096239131	-0.122762616
H	5.260190294	-0.038162430	0.947236125
H	5.965104416	-0.172445353	-0.660859944
H	4.873634268	2.066171648	-0.312142761

O	−6.655033673	−0.073575452	−0.280487482

C_6H_{11}-(CH=CH)$_4$-O^-

C	−0.676387362	0.110096997	0.737298529
H	−0.684736513	0.207519690	1.824070734
C	−1.881001257	0.039607547	0.069337377
H	−1.826273581	−0.058677642	−1.020025044
C	−3.182582970	0.075533319	0.613382254
H	−3.281482609	0.171845173	1.695651973
C	−4.342379657	−0.007463888	−0.153913703
H	−4.192311760	−0.103284280	−1.235221636
C	−5.671973783	0.014047692	0.266000485
H	−5.912578041	0.105942022	1.324533098
C	−6.752242209	−0.081565927	−0.651419494
H	−6.413125640	−0.172240763	−1.719922385
C	0.597268854	0.054584613	0.087888811
H	0.559981637	−0.045358312	−1.002157867
C	1.829836469	0.105699965	0.657790308
H	1.909535572	0.201870643	1.743328887
C	3.130766548	0.017437074	−0.093133516
H	2.900223783	−0.057284793	−1.168317441
C	4.013411916	1.274522986	0.102562866
H	3.456738448	2.160186413	−0.225121293
H	4.198009675	1.409081152	1.179361213
C	5.360574309	1.181796663	−0.632492852
H	5.178780651	1.162863443	−1.717343885
C	3.940521288	−1.245225301	0.291190566
H	4.121511233	−1.228702488	1.376788748
H	3.330987468	−2.135238564	0.096929187
C	5.286739859	−1.342993444	−0.444106046
H	5.839950234	−2.233166671	−0.115576927
H	5.101158525	−1.474776641	−1.520472598
C	6.137419655	−0.081658360	−0.235277012
H	6.421856837	−0.011023388	0.824997435
H	7.073643138	−0.150996772	−0.805209738
H	5.965946370	2.077266430	−0.437387271
O	−7.970757697	−0.074867626	−0.404701059

C_6H_{11}-(CH=CH)$_5$-O^-

C	−0.502083538	−0.066078480	0.814371482
H	−0.532337001	−0.144705956	1.902063945
C	0.721486842	−0.019842324	0.187931565
H	0.710484564	0.059003207	−0.903551944
C	2.002596499	−0.061836123	0.787896981
H	2.052955814	−0.140050442	1.874928480
C	3.191039611	−0.008785870	0.074214016
H	3.100101569	0.069903583	−1.013627342

C	4.499551978	-0.043676108	0.579989133
H	4.631449809	-0.122236000	1.659836361
C	5.641392616	0.016638504	-0.224755514
H	5.462152873	0.094977807	-1.302398089
C	6.974989173	-0.009767688	0.163724530
H	7.242580358	-0.086232840	1.216599687
C	8.035935104	0.060903182	-0.784501104
H	7.675125305	0.137892729	-1.845406497
O	9.255950752	0.046515543	-0.560290982
C	-1.755077009	-0.015432271	0.119977217
H	-1.683425756	0.066206110	-0.969157663
C	-3.000412406	-0.055471157	0.656612017
H	-3.108263462	-0.137128250	1.740730436
C	-4.280194897	0.004840717	-0.132166276
H	-4.019403206	0.071766260	-1.200703355
C	-5.141330894	-1.268626097	0.053231766
H	-4.556304282	-2.146677139	-0.243742553
H	-5.359146386	-1.391160250	1.125036251
C	-6.463194778	-1.212728909	-0.728297461
H	-6.244825747	-1.202486176	-1.806316237
C	-5.125600375	1.254299953	0.216046252
H	-5.343425122	1.240683057	1.294716708
H	-4.528992085	2.155739200	0.034681090
C	-6.447089841	1.315756035	-0.565818125
H	-7.028582691	2.197285424	-0.264833910
H	-6.227642740	1.440718720	-1.636428371
C	-7.278785241	0.039194989	-0.372765031
H	-7.598890497	-0.027060408	0.677563795
H	-8.195908826	0.083827167	-0.974826695
H	-7.056710371	-2.117740227	-0.542445394

Ph-OH

C	-0.919927345	0.003367280	0.000000000
C	-0.217712183	1.213111247	0.000000000
C	-0.224052139	-1.210635926	0.000000000
H	-0.760755043	2.156141725	0.000000000
H	-0.788078510	-2.137397363	0.000000000
C	1.177857111	1.204187530	0.000000000
C	1.168429255	-1.205298492	0.000000000
H	1.715274272	2.148140561	0.000000000
H	1.702852911	-2.150984710	0.000000000
C	1.878912160	-0.001536596	0.000000000
H	2.964153104	-0.004582071	0.000000000
O	-2.286459168	-0.056197848	0.000000000
H	-2.640976513	0.842539437	0.000000000

Ph-CH=CH-OH

C	0.035699806	-0.216003922	0.002639707

C	0.957259160	-1.279114173	0.000016417
C	0.552618491	1.094784640	0.003942721
H	0.584529158	-2.300456030	-0.000303162
H	-0.121922513	1.945637547	0.009252739
C	2.331645103	-1.048790179	-0.002475819
C	1.924845194	1.324400886	0.000956482
H	3.016996058	-1.891723544	-0.004424751
H	2.294863068	2.345895533	0.002022407
C	2.825352967	0.255534898	-0.002571954
H	3.895440507	0.439216743	-0.004578757
C	-1.398366760	-0.523504835	0.003892502
H	-1.651088316	-1.584760088	0.014934872
C	-2.409776116	0.359326818	-0.006053267
H	-2.268980273	1.434977401	-0.018838041
O	-3.735964376	0.057562419	-0.000880947
H	-3.839704669	-0.905063019	0.011786823

Ph-CH=CH-OH (strained)

C	0.037378972	-0.001941745	0.273495008
C	0.746528370	-1.205761008	0.143367847
C	0.743508952	1.203935647	0.146519592
H	0.211025271	-2.146155730	0.237078670
H	0.205643926	2.142690782	0.242962886
C	2.119048508	-1.205231440	-0.108110074
C	2.116047006	1.207501918	-0.105126427
H	2.649323843	-2.147963956	-0.209732475
H	2.643953109	2.151824334	-0.204308988
C	2.807980416	0.002178343	-0.232608964
H	3.876256984	0.003744747	-0.429034525
C	-1.426386813	-0.004280835	0.556403987
H	-1.740717458	-0.014697220	1.602343344
C	-2.356429649	0.003243830	-0.404376358
H	-2.102595777	0.011812369	-1.460467039
O	-3.707850366	0.000536243	-0.233343721
H	-3.902665916	-0.005535520	0.714831615

Ph-(CH=CH)$_2$-OH

C	-1.111101187	-0.273122587	0.000000000
C	-2.108388116	-1.267249406	0.000000000
C	-1.531495270	1.072492960	0.000000000
H	-1.808802177	-2.312389053	0.000000000
H	-0.794941263	1.870091364	0.000000000
C	-3.462067836	-0.938395986	0.000000000
C	-2.882964102	1.401182035	0.000000000
H	-4.207915554	-1.728269283	0.000000000
H	-3.179738849	2.446359896	0.000000000
C	-3.858219944	0.399283704	0.000000000
H	-4.912190955	0.660565407	0.000000000
C	0.294127457	-0.682286904	0.000000000

H	0.457296663	-1.760056585	0.000000000
C	1.384193579	0.116629045	0.000000000
H	1.259517629	1.198667114	0.000000000
C	2.747270372	-0.362748184	0.000000000
H	2.903566474	-1.442424229	0.000000000
C	3.816838422	0.455926523	0.000000000
H	3.721864383	1.537987620	0.000000000
O	5.122627958	0.084660274	0.000000000
H	5.177875667	-0.881980524	0.000000000

Ph-(CH=CH)$_2$-OH (strained)

C	1.117182462	0.001520929	-0.360986232
C	1.808499717	1.206091726	-0.159655167
C	1.807173396	-1.204315555	-0.162946917
H	1.286184557	2.146733771	-0.309112595
H	1.283739064	-2.143888198	-0.315127360
C	3.147452192	1.205722813	0.233084509
C	3.146173004	-1.206556446	0.229748735
H	3.663834541	2.148900372	0.388450839
H	3.661537592	-2.150736837	0.382358817
C	3.820657561	-0.001067388	0.428871840
H	4.862889674	-0.002026207	0.734796360
C	-0.309461248	0.003029624	-0.789510196
H	-0.502335772	0.012172951	-1.863771869
C	-1.353475438	-0.004348604	0.058067659
H	-1.154209339	-0.013252354	1.129860527
C	-2.748953693	-0.001030577	-0.339657138
H	-2.970899284	0.005805765	-1.407674122
C	-3.761893790	-0.002877817	0.544616879
H	-3.596478283	-0.008372067	1.618273394
O	-5.090181322	0.002637398	0.260426869
H	-5.207899359	0.008423944	-0.700486479

Ph-(CH=CH)$_3$-OH

C	-2.233698867	-0.277938799	0.000000000
C	-3.267061157	-1.235251413	0.000000000
C	-2.603990726	1.082888492	0.000000000
H	-3.005888990	-2.290557343	0.000000000
H	-1.837798828	1.851864974	0.000000000
C	-4.607397027	-0.856756803	0.000000000
C	-3.942272149	1.460783943	0.000000000
H	-5.382163105	-1.618234288	0.000000000
H	-4.200902630	2.516006806	0.000000000
C	-4.953509558	0.494943114	0.000000000
H	-5.997162588	0.794857683	0.000000000
C	-0.846120168	-0.737410683	0.000000000
H	-0.721440942	-1.820331142	0.000000000
C	0.276498245	0.020148363	0.000000000
H	0.195832132	1.106581107	0.000000000

C	1.612989922	-0.516384344	0.000000000
H	1.708638410	-1.602571812	0.000000000
C	2.739129981	0.240177557	0.000000000
H	2.634309455	1.325643646	0.000000000
C	4.084409409	-0.278656815	0.000000000
H	4.209310508	-1.362435241	0.000000000
C	5.179522508	0.507564607	0.000000000
H	5.117745470	1.591972856	0.000000000
O	6.472412697	0.095841417	0.000000000
H	6.497973178	-0.872090760	0.000000000

Ph-(CH=CH)$_3$-OH (strained)

C	2.242895604	0.003360830	-0.369698782
C	2.922287698	1.206845422	-0.125941477
C	2.918687504	-1.204123059	-0.136022857
H	2.410381036	2.148514757	-0.302295688
H	2.403894531	-2.142654070	-0.320485599
C	4.236471285	1.203549289	0.342927359
C	4.232883011	-1.208766354	0.332880498
H	4.744085397	2.145660427	0.530281964
H	4.737683144	-2.153944307	0.512194330
C	4.896016885	-0.004591013	0.573640241
H	5.918986286	-0.007623365	0.938722960
C	0.843245589	0.007584474	-0.877979987
H	0.710911420	0.019224722	-1.961384009
C	-0.250167281	-0.000440894	-0.091729069
H	-0.115914899	-0.011397591	0.990304247
C	-1.614407449	0.003769947	-0.575963663
H	-1.754060795	0.014767977	-1.657223748
C	-2.703184776	-0.004562425	0.228119981
H	-2.550108260	-0.015638672	1.307855088
C	-4.072890863	-0.000095928	-0.228877123
H	-4.247915177	0.009861178	-1.305582433
C	-5.128808650	-0.004825781	0.607774806
H	-5.015256383	-0.013668073	1.688019920
O	-6.440341410	0.001537210	0.258770660
H	-6.512064859	0.009832382	-0.706739029

Ph-(CH=CH)$_4$-OH

C	3.384682104	0.264794871	-0.000000790
C	4.439225862	1.199105853	0.000015729
C	3.724223546	-1.104257960	-0.000045318
H	4.201565652	2.259901582	0.000051526
H	2.940840565	-1.855638088	-0.000058442
C	5.770538622	0.790602492	-0.000010079
C	5.053641687	-1.511880251	-0.000072057
H	6.562312055	1.534339415	0.000005589
H	5.288701612	-2.572564734	-0.000105170

C	6.086097241	-0.568669783	-0.000054391
H	7.122792260	-0.891770656	-0.000073665
C	2.008633246	0.754934618	0.000026427
H	1.907601533	1.840275899	0.000053045
C	0.867932890	0.022521044	0.000024421
H	0.923005048	-1.065374908	0.000007404
C	-0.452578285	0.591200519	0.000045022
H	-0.522000752	1.679407654	0.000055655
C	-1.601755369	-0.135992429	0.000046335
H	-1.527652330	-1.224265823	0.000047964
C	-2.924913065	0.422848484	0.000013967
H	-3.002493643	1.510479202	0.000028276
C	-4.066136842	-0.313839409	-0.000003232
H	-3.980329676	-1.400939224	-0.000076618
C	-5.400419623	0.229105032	0.000310730
H	-5.506073483	1.314994724	0.000512126
C	-6.510545510	-0.536928755	0.000154886
H	-6.468490944	-1.622299491	0.000671400
O	-7.795054767	-0.101209455	-0.000155489
H	-7.803165497	0.866836931	-0.004029072

Ph-(CH=CH)$_4$-OH (strained)

C	3.394963332	-0.004712338	0.350389366
C	4.065540998	-1.206715957	0.076905794
C	4.060825868	1.204517342	0.098070035
H	3.560871350	-2.149555867	0.267207783
H	3.552381743	2.141822952	0.304911979
C	5.362016334	-1.200172724	-0.438864883
C	5.357336988	1.212143877	-0.417647457
H	5.863063525	-2.140998702	-0.648872372
H	5.854688701	2.158482156	-0.611010588
C	6.012074351	0.009543423	-0.687458187
H	7.021194983	0.015034546	-1.089198129
C	2.014234988	-0.012298101	0.907360712
H	1.919449723	-0.026284944	1.994645032
C	0.893157228	-0.002231582	0.159642447
H	0.988721095	0.011702132	-0.926339774
C	-0.450631216	-0.008904266	0.693427765
H	-0.550569812	-0.022985228	1.779074792
C	-1.572550844	0.001006094	-0.068668145
H	-1.463267512	0.015051494	-1.153939847
C	-2.916593969	-0.005746868	0.445802199
H	-3.030963584	-0.019836315	1.530037459
C	-4.029966220	0.004198146	-0.329825134
H	-3.906185951	0.018271237	-1.413197694
C	-5.383787116	-0.002365623	0.165353236
H	-5.528135000	-0.016461878	1.246604791
C	-6.464655513	0.008090209	-0.640501569
H	-6.382905410	0.022273117	-1.723545484
O	-7.764600481	0.002937330	-0.252638509
H	-7.808543159	-0.009691730	0.714597744

Ph-(CH=CH)$_5$-OH

C	0.723698077	0.631730520	0.019651393
H	0.671456683	1.720561895	0.044083372
C	-0.438737268	-0.076945993	0.002722964
H	-0.382717130	-1.165970099	-0.021997199
C	-1.749006143	0.504277657	0.014156884
H	-1.808087933	1.592775632	0.038123643
C	-2.908035646	-0.210937173	-0.002967578
H	-2.844596021	-1.299695444	-0.027036713
C	-4.223230354	0.361472283	0.008164498
H	-4.290703790	1.449261225	0.032080966
C	-5.373557457	-0.363171510	-0.009231107
H	-5.297407944	-1.451241978	-0.033132559
C	-6.699011143	0.196153688	0.001422875
H	-6.810452929	1.278071990	0.025128527
C	-7.813819940	-0.559386932	-0.016559946
H	-7.767189661	-1.647335794	-0.040396404
O	-9.056908039	-0.001231534	-0.005780016
H	-9.722212644	-0.698793552	-0.021880024
C	2.033586268	0.042163589	0.006416299
H	2.071439495	-1.046183711	-0.016614305
C	3.186246112	0.756791264	0.019402517
H	3.102071046	1.843355857	0.039675940
C	4.553812628	0.245049213	0.007369137
C	4.871626089	-1.129284090	0.021849861
C	5.623163090	1.162240308	-0.019429229
H	4.076352942	-1.867721138	0.044663980
H	5.402444017	2.226632052	-0.030465884
C	6.194178611	-1.558315563	0.008671637
C	6.947467653	0.732258497	-0.032642222
H	6.412241077	-2.622541505	0.020541166
H	7.750969414	1.462999643	-0.053717473
C	7.241385900	-0.631896943	-0.018806026
H	8.272730272	-0.971493575	-0.028677900

Ph-(CH=CH)$_5$-OH (strained)

C	-0.728408730	-0.010843566	0.753600841
H	-0.655748395	-0.030291677	1.841281533
C	0.413745268	0.002534891	0.019789791
H	0.332150780	0.022410560	-1.067784661
C	1.741239581	-0.007560884	0.568957223
H	1.827718431	-0.027702924	1.655661205
C	2.879334601	0.005646675	-0.176172834
H	2.786938817	0.025862697	-1.262982617
C	4.211052620	-0.005548953	0.360285878
H	4.308420498	-0.026008986	1.445864938
C	5.339912079	0.007472409	-0.396140237
H	5.233244450	0.027992390	-1.481744246

C	6.681286152	-0.003755941	0.125293077
H	6.823543410	-0.024296570	1.203649555
C	7.773581730	0.010084931	-0.662070189
H	7.695409444	0.030875215	-1.748301020
O	9.032535353	-0.001091115	-0.140379279
H	9.677112113	0.012861952	-0.857172673
C	-2.057471905	-0.001020376	0.186341581
H	-2.126200836	0.018792404	-0.901569137
C	-3.196717736	-0.015295466	0.906776882
H	-3.127676767	-0.035129113	1.995917904
C	-4.563956113	-0.005865662	0.317721049
C	-5.227532711	-1.207040719	0.024195754
C	-5.224387616	1.204213736	0.055717526
H	-4.726521431	-2.150366451	0.221549805
H	-4.720968307	2.140817494	0.277386964
C	-6.512290654	-1.198797492	-0.520160944
C	-6.509209747	1.213371028	-0.488551538
H	-7.007496916	-2.139115279	-0.745721188
H	-7.002107038	2.160448361	-0.689563628
C	-7.157219530	0.011701023	-0.777948103
H	-8.156979350	0.018553464	-1.202450391

Ph-O$^-$

C	1.036120731	-0.000000011	0.000000000
C	0.238036514	1.212808207	0.000000000
C	0.238036496	-1.212808220	0.000000000
H	0.783009243	2.156656866	0.000000000
H	0.783009212	-2.156656886	0.000000000
C	-1.150090923	1.200732654	0.000000000
C	-1.150090946	-1.200732649	0.000000000
H	-1.689472705	2.151505348	0.000000000
H	-1.689472737	-2.151505337	0.000000000
C	-1.879176821	0.000000011	0.000000000
H	-2.967283644	0.000000068	0.000000000
O	2.302207089	0.000000000	0.000000000

Ph-CH=CH-O$^-$

C	-0.031794859	0.240825148	0.000000000
C	0.951850709	1.280052721	0.000000000
C	0.507349183	-1.086133446	0.000000000
H	0.602487195	2.311572908	0.000000000
H	-0.174812336	-1.931220182	0.000000000
C	2.316275430	1.024924380	0.000000000
C	1.874130948	-1.329952630	0.000000000
H	3.011478453	1.865074868	0.000000000
H	2.221656755	-2.363611658	0.000000000
C	2.810941035	-0.286431733	0.000000000
H	3.879353656	-0.487380887	0.000000000

C	−1.421356417	0.568536561	0.000000000
H	−1.676340838	1.628925712	0.000000000
C	−2.508594420	−0.322785269	0.000000000
H	−2.223246363	−1.409185882	0.000000000
O	−3.730582626	−0.042487552	0.000000000

Ph-CH=CH-O⁻ (strained)

C	0.015049350	−0.000348132	−0.308578209
C	−0.722413644	−1.195757199	−0.157420410
C	−0.721896176	1.195455870	−0.157905382
H	−0.182302741	−2.133589142	−0.261218178
H	−0.181356691	2.132981014	−0.262218802
C	−2.091196063	−1.203114279	0.122061273
C	−2.090704006	1.203490041	0.121671858
H	−2.618033566	−2.149963365	0.234905004
H	−2.617236063	2.150554552	0.234090745
C	−2.786338184	0.000365955	0.262641666
H	−3.852311524	0.000727842	0.482388594
C	1.468784877	−0.000641578	−0.608268623
H	1.765365599	−0.001804233	−1.658518497
C	2.456180953	0.000393905	0.372429957
H	2.020649791	0.001764192	1.417578269
O	3.712427908	0.000074332	0.253327088

Ph-(CH=CH)$_2$-O⁻

C	1.055520524	0.324611171	0.000000000
C	2.134763610	1.255033255	0.000000000
C	1.436883799	−1.049319679	0.000000000
H	1.896320060	2.317243816	0.000000000
H	0.665020260	−1.813690782	0.000000000
C	3.464717164	0.854493512	0.000000000
C	2.768900895	−1.442355865	0.000000000
H	4.247791537	1.611940770	0.000000000
H	3.004531731	−2.506023415	0.000000000
C	3.808826267	−0.502903499	0.000000000
H	4.848838348	−0.818427104	0.000000000
C	−0.300986333	0.796661679	0.000000000
H	−0.419958147	1.880990153	0.000000000
C	−1.454800136	0.029960685	0.000000000
H	−1.332840616	−1.057510224	0.000000000
C	−2.786095239	0.464266227	0.000000000
H	−3.013975102	1.529967859	0.000000000
C	−3.873208077	−0.444457938	0.000000000
H	−3.542611733	−1.520558899	0.000000000
O	−5.092688809	−0.190864719	0.000000000

Ph-(CH=CH)$_2$-O⁻ (strained)

C	−1.075128208	−0.004031267	−0.412693223
C	−1.778869229	−1.199749093	−0.165416776

C	−1.773601722	1.196851527	−0.175841439
H	−1.260967922	−2.140012230	−0.335397728
H	−1.251751104	2.133368143	−0.354055167
C	−3.098066141	−1.200685140	0.292878585
C	−3.092724538	1.207315244	0.282686999
H	−3.606846198	−2.144901659	0.478353458
H	−3.597543329	2.155223273	0.460040519
C	−3.763814946	0.005789711	0.519139087
H	−4.790753262	0.009681379	0.877806221
C	0.326373641	−0.009324654	−0.912782392
H	0.453163466	−0.020007521	−1.996684556
C	1.429758399	−0.000983557	−0.099168179
H	1.228096195	0.009763759	0.978806651
C	2.805010085	−0.004471969	−0.434704503
H	3.107980299	−0.015188685	−1.482232482
C	3.812986496	0.004935587	0.547593050
H	3.392499562	0.015553584	1.595772649
O	5.056142120	0.003046972	0.404851019

Ph-(CH=CH)$_3$-O$^-$

C	−2.183331833	−0.319952563	0.000000000
C	−3.307209636	−1.190458347	0.000000000
C	−2.480790176	1.071250867	0.000000000
H	−3.127552583	−2.263833029	0.000000000
H	−1.665818921	1.789197674	0.000000000
C	−4.613271558	−0.715806583	0.000000000
C	−3.788513806	1.539942591	0.000000000
H	−5.438220563	−1.426455204	0.000000000
H	−3.964747003	2.614391053	0.000000000
C	−4.877051705	0.658487226	0.000000000
H	−5.897466242	1.031898301	0.000000000
C	−0.850958418	−0.868964356	0.000000000
H	−0.794182271	−1.958154275	0.000000000
C	0.340318638	−0.173578591	0.000000000
H	0.292238376	0.918188757	0.000000000
C	1.641709944	−0.714288030	0.000000000
H	1.744655911	−1.800365750	0.000000000
C	2.800623450	0.061823362	0.000000000
H	2.648421933	1.146736773	0.000000000
C	4.128189020	−0.358309377	0.000000000
H	4.369915779	−1.420353320	0.000000000
C	5.209371676	0.565591346	0.000000000
H	4.871858766	1.637634483	0.000000000
O	6.426190501	0.316360637	0.000000000

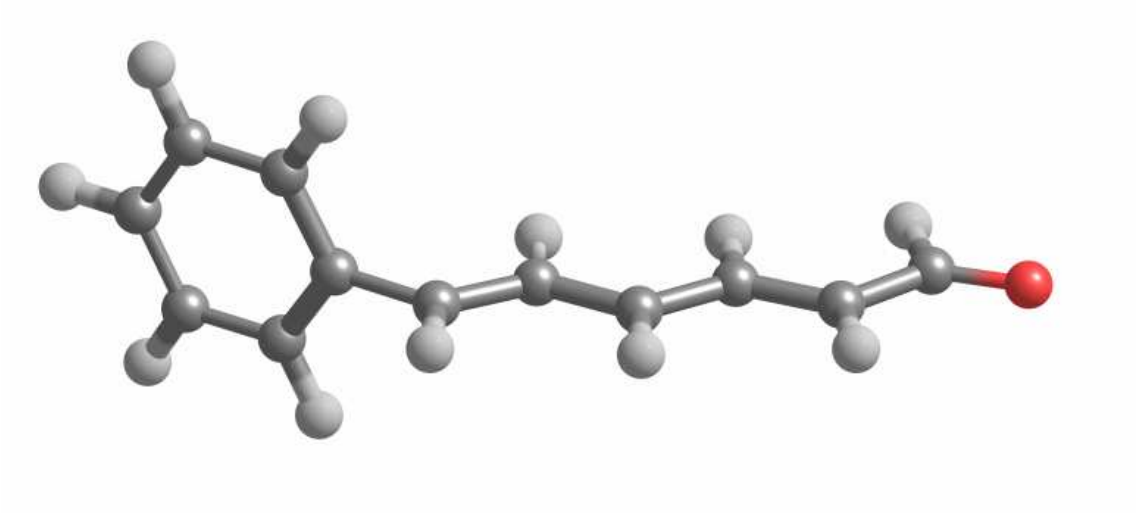

Figure 1: Ph-(CH=CH)$_3$-O$^-$ (strained)

Ph-(CH=CH)$_3$-O$^-$ (strained)

C	−2.204299822	−0.008102752	−0.411109081
C	−2.882134881	−1.201802856	−0.099384418
C	−2.874963767	1.197629305	−0.131848448
H	−2.381652985	−2.144832769	−0.301882624
H	−2.368656089	2.131678426	−0.359835278
C	−4.160264083	−1.195017661	0.462720797
C	−4.153023346	1.213720024	0.430145740
H	−4.653767368	−2.136014231	0.696643918
H	−4.641007707	2.163553932	0.638527836
C	−4.803372220	0.015111701	0.729730357
H	−5.798110813	0.024057564	1.168992777
C	−0.846762037	−0.020010859	−1.021475341
H	−0.803393117	−0.038479088	−2.111662229
C	0.315006387	−0.006985748	−0.304058027
H	0.215461032	0.011540617	0.786013094
C	1.654019053	−0.014589654	−0.789010749
H	1.803160335	−0.032651061	−1.869829017
C	2.765763122	−0.000063939	0.039597924
H	2.555906269	0.017765117	1.115725910
C	4.124574475	−0.004969097	−0.298388306
H	4.429352404	−0.022450040	−1.344534613
C	5.143448193	0.011910426	0.685253047
H	4.736219556	0.029319704	1.735073815
O	6.378569112	0.009661689	0.521383703

Ph-(CH=CH)$_4$-O$^-$

C	3.335082610	0.282609197	0.000000000
C	4.488854493	1.109163932	0.000000000
C	3.572677215	−1.117829965	0.000000000
H	4.351298441	2.188535185	0.000000000

H	2.728801544	-1.801346591	0.000000000
C	5.775530827	0.582808559	0.000000000
C	4.860533376	-1.639306052	0.000000000
H	6.628595270	1.258754196	0.000000000
H	4.994575401	-2.719400811	0.000000000
C	5.981706998	-0.800560608	0.000000000
H	6.986234970	-1.214496041	0.000000000
C	2.022453540	0.885553576	0.000000000
H	2.010382152	1.975984412	0.000000000
C	0.807578487	0.240705971	0.000000000
H	0.805313326	-0.851549829	0.000000000
C	-0.469735519	0.846161877	0.000000000
H	-0.515926539	1.936181618	0.000000000
C	-1.662783099	0.135249557	0.000000000
H	-1.577844079	-0.955679496	0.000000000
C	-2.965517224	0.651628063	0.000000000
H	-3.089427506	1.735158974	0.000000000
C	-4.115142461	-0.146732382	0.000000000
H	-3.945618755	-1.228574811	0.000000000
C	-5.442930870	0.256796540	0.000000000
H	-5.699394751	1.315100157	0.000000000
C	-6.514582565	-0.684067109	0.000000000
H	-6.165558114	-1.751261905	0.000000000
O	-7.730891765	-0.444685080	0.000000000

Ph-(CH=CH)$_4$-O$^-$ (strained)

C	-3.354611130	0.360550528	0.047646518
C	-4.012043131	0.196580714	-1.185142892
C	-4.006615598	-0.127978695	1.194409210
H	-3.524641511	0.565136750	-2.083577043
H	-3.514994864	-0.013140998	2.156529756
C	-5.257769155	-0.427751628	-1.271499766
C	-5.252317897	-0.753455282	1.115894916
H	-5.738523460	-0.543976393	-2.240225655
H	-5.728843243	-1.125132313	2.020243899
C	-5.884630812	-0.905852489	-0.119360684
H	-6.854376654	-1.393187868	-0.183608510
C	-2.030546532	1.034979666	0.136462150
H	-2.041590768	2.116709722	0.279127343
C	-0.835346292	0.387644517	0.051510285
H	-0.868257101	-0.696307721	-0.091522141
C	0.472146333	0.956918442	0.126709207
H	0.546451243	2.036112754	0.268901573
C	1.634591809	0.218087209	0.029211245
H	1.512649349	-0.860682897	-0.112948252
C	2.964727392	0.679013794	0.089685291
H	3.130627140	1.747975592	0.230428865
C	4.075848786	-0.156438875	-0.020643674
H	3.858898223	-1.221244205	-0.160819860
C	5.426976064	0.178925233	0.023135298
H	5.733505636	1.215282546	0.159516326

C	6.449018906	-0.800920202	-0.106111807
H	6.044942994	-1.841155323	-0.242893184
O	7.679271630	-0.629570177	-0.083902320

Ph-(CH=CH)$_5$-O$^-$

C	0.717799481	0.919161923	0.007050377
H	0.713574802	2.009944753	0.020733065
C	-0.497729757	0.255687108	-0.001526957
H	-0.459381877	-0.837277230	-0.014625308
C	-1.779987968	0.831283177	0.006724121
H	-1.852048668	1.919575039	0.020235730
C	-2.962183604	0.093252230	-0.001236461
H	-2.855050633	-0.995226876	-0.014691758
C	-4.268766060	0.586308043	0.005750387
H	-4.412945324	1.667040988	0.019101594
C	-5.407271721	-0.233653342	-0.003372907
H	-5.220424060	-1.312172685	-0.016963473
C	-6.736784977	0.151852024	0.002641957
H	-7.009680031	1.205736174	0.015970846
C	-7.797466604	-0.805753348	-0.008333199
H	-7.436684244	-1.867984688	-0.021967874
O	-9.013966614	-0.577729541	-0.004100732
C	1.974621018	0.265402363	0.000707866
H	1.933422072	-0.825590120	-0.012627700
C	3.206576593	0.870232159	0.007374016
H	3.229643987	1.960339062	0.012614524
C	4.502023895	0.225297587	0.002952633
C	4.692322646	-1.180566324	0.014322241
C	5.678159087	1.016573677	-0.011017505
H	3.827118503	-1.836461429	0.031166900
H	5.573761839	2.099444755	-0.019079819
C	5.963180466	-1.742855902	0.007654332
C	6.948197539	0.450166322	-0.016226462
H	6.063935190	-2.826222015	0.017092650
H	7.822203444	1.098167762	-0.027617222
C	7.108789666	-0.938641247	-0.007798591
H	8.099649585	-1.384127209	-0.011722889

Ph-(CH=CH)$_5$-O$^-$ (strained)

C	0.721777157	-1.051161034	-0.014720331
H	0.701549641	-2.141713936	-0.030254597
C	-0.472468151	-0.365728339	-0.004988716
H	-0.410313229	0.726594280	0.010230203
C	-1.777022811	-0.908666678	-0.013205041
H	-1.876673354	-1.994903314	-0.028431599
C	-2.933914338	-0.140470255	-0.002632527
H	-2.795300625	0.944924811	0.012536354
C	-4.261111861	-0.590840075	-0.008646740
H	-4.439697109	-1.666627411	-0.023453625

C	−5.368428731	0.264831050	0.003578655
H	−5.143418887	1.336481437	0.018481020
C	−6.715669619	−0.068729507	−0.000602841
H	−7.027875379	−1.111899057	−0.015148068
C	−7.736631652	0.926405057	0.013745141
H	−7.332530358	1.974036404	0.028168074
O	−8.963991586	0.750996185	0.011548658
C	2.002838372	−0.413818880	−0.005800679
H	1.987007635	0.679208813	0.009032323
C	3.220546459	−1.017897653	−0.013886811
H	3.272805449	−2.107714680	−0.028560045
C	4.518241731	−0.288196828	−0.004009301
C	5.162460833	0.039356675	1.202101731
C	5.154853471	0.085924038	−1.200541157
H	4.683635085	−0.237139608	2.137347628
H	4.670183528	−0.154330197	−2.142748477
C	6.386234174	0.710947314	1.214701031
C	6.378593405	0.757753758	−1.194738811
H	6.858113492	0.956335945	2.163247200
H	6.844572430	1.039706038	−2.136012404
C	7.000668218	1.072654656	0.014575282
H	7.952414947	1.597810501	0.021729667

C_6H_6-OH

C	0.941817037	0.002248464	0.365974855
C	0.193785495	−1.259907360	−0.014557744
C	0.226682145	1.248068900	−0.160763556
H	0.768151315	−2.177589857	−0.125702128
C	−1.144375829	−1.255857644	−0.115753312
C	−1.269880072	1.175293499	0.032546230
H	−1.688538236	−2.174043598	−0.321930219
H	−1.829182602	2.105328779	0.088393762
C	−1.902079719	−0.009161080	0.043976170
H	−2.983833242	−0.062516941	0.131204393
O	2.272559312	0.040961767	−0.149675648
H	2.768030101	−0.683440276	0.254192086
H	0.651658838	2.138603977	0.311871389
H	0.449544979	1.331908711	−1.237247313
H	0.970392332	0.054185768	1.471715068

C_6H_6-CH=CH-OH

C	0.012256421	−0.001594464	−0.231421085
C	−0.780517168	1.263087366	0.065136466
C	−0.765023686	−1.248323731	0.254637165
H	−0.225964982	2.188497140	0.198145286
C	−2.123363986	1.250583101	0.078354132
C	−2.237547318	−1.179879009	−0.076572843
H	−2.682004173	2.170356370	0.233201823
H	−2.788048096	−2.109676098	−0.196996319

C	−2.865764458	0.005210852	−0.138106040
H	−3.934768995	0.060036730	−0.326873712
C	1.406166032	0.035933521	0.339208352
H	1.508405160	0.110445900	1.420639592
C	2.509955894	−0.022755362	−0.406547191
H	2.461993435	−0.094803436	−1.493172983
H	−0.304868435	−2.147747744	−0.167467567
H	−0.654280368	−1.337747981	1.348981800
H	0.097346613	−0.069392403	−1.330951337
O	3.766540074	0.003295175	0.141962027
H	4.419235183	−0.039884689	−0.565557533

C_6H_6-CH=CH-OH (strained)

C	−0.057338209	0.101346250	−0.669710223
C	−0.773155662	1.293804792	−0.045698051
C	−0.585405831	−1.213661171	−0.058409690
H	−0.236942344	2.236835311	0.018993887
C	−2.052820738	1.192943595	0.349048646
C	−2.094093806	−1.223486010	0.034197546
H	−2.578449442	2.056544754	0.748843805
H	−2.610925260	−2.179295937	0.002373243
C	−2.769349785	−0.081211309	0.241026748
H	−3.849632151	−0.086772653	0.360649577
C	1.453708702	0.235884981	−0.640827767
H	1.903472616	0.772711410	−1.478048663
C	2.257033057	−0.185239378	0.340095226
H	1.900876494	−0.714601366	1.218034126
O	3.613311849	−0.040173175	0.397033521
H	3.907417754	0.441611304	−0.389346501
H	−0.217789665	−2.060181734	−0.647001124
H	−0.182708391	−1.351687151	0.958612397
H	−0.354701011	0.089048407	−1.732941219

C_6H_6-(CH=CH)$_2$-OH

C	−1.138068332	−0.310540476	0.582632597
C	−2.032284139	−1.304837790	−0.145660633
C	−1.445568228	1.125527790	0.124230051
H	−1.659433732	−2.314302578	−0.301404206
C	−3.277525113	−0.963347129	−0.513208505
C	−2.932805259	1.383687191	0.045456705
H	−3.935154278	−1.690470064	−0.982802942
H	−3.291327404	2.400509449	0.183758613
C	−3.780365390	0.392522351	−0.274753248
H	−4.844478591	0.583712529	−0.385924601
C	0.318428838	−0.700179594	0.511302865
H	0.526433734	−1.731758492	0.801939968
C	1.351712641	0.078519719	0.150963534
H	1.168970277	1.111514016	−0.141098776
C	2.737957384	−0.353774576	0.117966088
H	2.952564913	−1.384089545	0.405732506

C	3.751500460	0.450834116	-0.245405350
H	3.596669144	1.484610439	-0.541182839
O	5.070657347	0.124815143	-0.301375339
H	5.178093648	-0.800129024	-0.036925228
H	-0.961573509	1.841372449	0.796993909
H	-1.008821873	1.294945726	-0.874623776
H	-1.433402381	-0.376542723	1.649230392

C_6H_6-(CH=CH)$_2$-OH (strained)

C	-1.170699297	0.219892183	-0.762057625
C	-1.824331372	1.289139558	0.107504340
C	-1.559036105	-1.185919787	-0.257479288
H	-1.320022150	2.246400004	0.208763593
C	-3.023017639	1.072922891	0.673035099
C	-3.033508381	-1.284791137	0.058115267
H	-3.509369516	1.854154374	1.251914955
H	-3.518276337	-2.254629177	-0.021008378
C	-3.705237150	-0.213995236	0.511530341
H	-4.752769744	-0.290734649	0.791001914
C	0.322000409	0.434346108	-0.917017204
H	0.615545273	1.098425912	-1.730912092
C	1.290151804	-0.055099746	-0.124177906
H	1.025276662	-0.707183272	0.707440381
C	2.707200934	0.212868297	-0.290744062
H	3.004604034	0.864794464	-1.113590222
C	3.653125834	-0.301093876	0.514521655
H	3.415775331	-0.956551140	1.347665598
O	4.994692299	-0.097704967	0.427404302
H	5.176770631	0.488272070	-0.321304792
H	-1.261829601	-1.932414462	-1.000985991
H	-0.998488295	-1.429477338	0.659838233
H	-1.617391630	0.327901711	-1.766158057

C_6H_6-(CH=CH)$_3$-OH

C	2.264516301	-0.345855051	-0.558811168
C	3.171218923	-1.255410947	0.259620407
C	2.492935266	1.127292984	-0.177939092
H	2.835514610	-2.269449752	0.462608599
C	4.385929571	-0.837951900	0.649876146
C	3.963735397	1.455040337	-0.059622454
H	5.054954354	-1.506575341	1.185588436
H	4.284012784	2.477241085	-0.244340967
C	4.839568128	0.522658696	0.348706331
H	5.889461336	0.767465055	0.486593835
C	0.825290244	-0.795625504	-0.516489279
H	0.674543250	-1.854794751	-0.734096796
C	-0.259359630	-0.041412138	-0.262703041
H	-0.139661876	1.018831658	-0.043971505
C	-1.618444965	-0.542745416	-0.257300323
H	-1.752353425	-1.603487152	-0.471938877

C	-2.709770327	0.217262316	-0.006817753
H	-2.566424540	1.277065644	0.207359734
C	-4.071982856	-0.263640206	0.001087427
H	-4.235749520	-1.321521588	-0.209788207
C	-5.133360286	0.526190025	0.253389383
H	-5.032306181	1.586015803	0.468791058
O	-6.437956076	0.148872001	0.279240681
H	-6.497732173	-0.797532070	0.084220800
H	2.007492717	1.779959188	-0.911134552
H	2.007981634	1.335708792	0.790709048
H	2.601335248	-0.463091358	-1.608777922

C_6H_6-(CH=CH)$_3$-OH (strained)

C	-2.309665394	0.354974590	-0.708741545
C	-2.910715993	1.217747751	0.396911057
C	-2.626739596	-1.133707548	-0.453775665
H	-2.419416181	2.155977578	0.639958254
C	-4.054341355	0.855890609	1.000383039
C	-4.068342266	-1.342134789	-0.051145208
H	-4.506804846	1.495332265	1.754281222
H	-4.538671476	-2.295629424	-0.277890134
C	-4.722053171	-0.400220655	0.647989046
H	-5.741936353	-0.564162728	0.986050265
C	-0.839944180	0.650900189	-0.926812755
H	-0.626786052	1.472476961	-1.611829603
C	0.202754533	0.057997937	-0.316527877
H	0.025342372	-0.755286330	0.386720994
C	1.587660826	0.423120561	-0.529373459
H	1.779887632	1.235599451	-1.230961256
C	2.635949281	-0.173101832	0.085147816
H	2.434028712	-0.983896990	0.786124687
C	4.022613349	0.181178236	-0.109493861
H	4.244907381	0.989354484	-0.807963823
C	5.038852243	-0.435302345	0.524173113
H	4.879043145	-1.246129375	1.229044900
O	6.362330748	-0.159428605	0.394943606
H	6.474674303	0.565796964	-0.236515200
H	-2.377555105	-1.715148196	-1.347230377
H	-1.987145064	-1.525789444	0.353579619
H	-2.836152230	0.637616216	-1.637327148

C_6H_6-(CH=CH)$_4$-OH

C	-3.415139866	-0.354509015	0.525610524
C	-4.325083850	-1.196693989	-0.358943600
C	-3.593266690	1.141321346	0.212670171
H	-4.012643934	-2.208993142	-0.603398941
C	-5.516678093	-0.725160909	-0.758690929
C	-5.051156056	1.516498215	0.076453107
H	-6.189901958	-1.347649957	-1.342560825
H	-5.348985753	2.535899014	0.308075302

C	-5.940835447	0.631234239	-0.401033895
H	-6.979819915	0.912219734	-0.551854841
C	-1.988433993	-0.842106189	0.493643565
H	-1.871277652	-1.915118674	0.657174383
C	-0.876558682	-0.106251513	0.308041691
H	-0.960375561	0.967140866	0.144302666
C	0.465129953	-0.647448649	0.309560806
H	0.562825524	-1.721612963	0.470217058
C	1.588649349	0.089994934	0.127622361
H	1.485819561	1.164286601	-0.031956423
C	2.927571524	-0.438616935	0.127410107
H	3.034218020	-1.512382073	0.284950283
C	4.044950600	0.309048634	-0.054939461
H	3.930281379	1.382120635	-0.211993453
C	5.392590489	-0.203987580	-0.058849203
H	5.526950903	-1.275640155	0.095942233
C	6.479218333	0.572059695	-0.243672557
H	6.408932671	1.644272248	-0.402259734
O	7.773523264	0.163159577	-0.260962253
H	7.805834020	-0.794000698	-0.118926493
H	-3.107331854	1.743600556	0.987412599
H	-3.080644614	1.382187730	-0.733906366
H	-3.780712995	-0.514100320	1.560255813

C_6H_6-(CH=CH)$_4$-OH (strained)

C	3.464097221	0.503718281	0.564945092
C	4.046114150	1.024125596	-0.745856404
C	3.720473717	-1.012340398	0.697205431
H	3.577564364	1.888539984	-1.208432706
C	5.149923827	0.468569072	-1.271403011
C	5.134685498	-1.381476650	0.313892050
H	5.589963139	0.871106785	-2.180410871
H	5.582305905	-2.263252710	0.765417439
C	5.789108068	-0.682190191	-0.627435475
H	6.787138140	-0.973182706	-0.944426347
C	2.015006104	0.905597680	0.747210155
H	1.855091938	1.882224109	1.205552759
C	0.930091094	0.215747362	0.346315188
H	1.054218930	-0.756119115	-0.130351346
C	-0.432162208	0.672306234	0.510151847
H	-0.573334670	1.642412982	0.987830017
C	-1.524902823	-0.024003706	0.108806488
H	-1.376889121	-0.993720814	-0.368494019
C	-2.885512481	0.419083623	0.263265953
H	-3.038729483	1.387223919	0.741073128
C	-3.969623235	-0.287122873	-0.145549666
H	-3.807770556	-1.254258900	-0.622728582
C	-5.339077614	0.140087158	-0.000246959
H	-5.520957880	1.104852129	0.475608088
C	-6.390154782	-0.591295084	-0.421795152
H	-6.271272000	-1.558312514	-0.901878587

O	-7.701976478	-0.257753670	-0.321482186
H	-7.777977798	0.606339278	0.108610630
H	3.492242045	-1.330232121	1.719592329
H	3.033598643	-1.572897903	0.042694872
H	4.038444111	0.994889437	1.370063077

C_6H_6-(CH=CH)$_5$-OH

C	-4.582782566	-0.349413654	0.488870309
C	-5.489731228	-1.134788632	-0.449735986
C	-4.727448001	1.161851659	0.240642219
H	-5.189961717	-2.140476497	-0.733954131
C	-6.664714599	-0.623962284	-0.850162674
C	-6.175030438	1.570179433	0.090892718
H	-7.336573557	-1.206978709	-1.474895660
H	-6.458366082	2.584620736	0.359493688
C	-7.071073757	0.723533070	-0.441564867
H	-8.101245539	1.031121591	-0.600609124
C	-3.165381482	-0.862616079	0.463675546
H	-3.070998519	-1.943348359	0.585655140
C	-2.036486931	-0.141229670	0.327340950
H	-2.097088598	0.939272382	0.206332054
C	-0.706749800	-0.708808498	0.329417885
H	-0.632373916	-1.790159019	0.448767139
C	0.435117686	0.012777415	0.194638845
H	0.356672180	1.094312739	0.076322680
C	1.759835819	-0.544161054	0.194492207
H	1.841301122	-1.625362500	0.311042943
C	2.900420538	0.184046416	0.058461716
H	2.815116849	1.265283888	-0.057865238
C	4.227707823	-0.365056773	0.054751747
H	4.315822867	-1.445874605	0.169774584
C	5.360535926	0.371592542	-0.083012906
H	5.264791474	1.451761806	-0.198131009
O	9.087119582	0.171449111	-0.252091048
H	9.102065163	-0.791263496	-0.149994463
H	-4.249066875	1.718974723	1.053011664
H	-4.189040614	1.436500343	-0.682109908
H	-4.972864537	-0.548838738	1.507582019
C	6.698394022	-0.163203288	-0.091380747
H	6.813550869	-1.242224856	0.022181345
C	7.800217885	0.601467846	-0.232789537
H	7.749531876	1.680205727	-0.348743600

C_6H_6-(CH=CH)$_5$-OH (strained)

C	4.630647355	-0.550195678	-0.447078516
C	5.197839510	-0.824061659	0.942588075
C	4.851270883	0.928019517	-0.829723634
H	4.742375761	-1.611389983	1.537000983
C	6.275724764	-0.155781438	1.384138720
C	6.249171664	1.394054770	-0.495671011

H	6.706642920	-0.385543811	2.355437603
H	6.685619875	2.195756769	-1.085956701
C	6.900475635	0.884586759	0.562612150
H	7.885163888	1.251414655	0.840218482
C	3.196320177	-1.018194401	-0.579398559
H	3.070234772	-2.063392235	-0.864207714
C	2.086019780	-0.301219027	-0.318283923
H	2.175543555	0.741201186	-0.014351759
C	0.740893358	-0.819176503	-0.421537116
H	0.634937678	-1.860744221	-0.726586249
C	-0.379221264	-0.096056081	-0.164686814
H	-0.267418218	0.945407817	0.139736298
C	-1.720987081	-0.600076338	-0.264743803
H	-1.837252440	-1.640806487	-0.568884689
C	-2.837706807	0.132959332	-0.008380043
H	-2.716737287	1.173661454	0.295199144
C	-4.183070886	-0.359917770	-0.108082815
H	-4.307603249	-1.399994575	-0.411095416
C	-5.290879177	0.383280433	0.148014779
H	-5.158558814	1.422734999	0.449948155
O	-9.024234634	0.301071503	0.243113277
H	-9.073221305	-0.627064622	-0.028249906
H	4.632447851	1.064180128	-1.893649314
H	4.139675576	1.570524000	-0.286491555
H	5.232713307	-1.154937025	-1.147893907
C	-6.646938269	-0.093820862	0.051372442
H	-6.798735871	-1.131528534	-0.249241007
C	-7.722347614	0.677023113	0.312434592
H	-7.634026392	1.716209375	0.615762152

C_6H_6-O^-

C	-1.091119479	0.031499743	-0.370618419
C	-0.255121872	-1.246322435	-0.156557143
C	-0.209523964	1.318724465	-0.041174457
H	-0.860336867	-2.153763214	-0.142191756
C	1.069782373	-1.293075242	0.085492930
C	1.291174862	1.150589199	0.015477445
H	1.582966404	-2.234479909	0.296807424
H	1.917373906	2.043962722	0.097392621
C	1.867304251	-0.062611872	0.092897769
H	2.950828766	-0.148665602	0.195883032
O	-2.214861467	-0.009618643	0.335431013
H	-0.475549311	2.122154067	-0.743106246
H	-0.572819808	1.653442044	0.946225427
H	-1.211968422	0.074929873	-1.515651058

C_6H_6-CH=CH-O^-

C	-0.077015021	-0.010107101	-0.276197837
C	0.760094946	-1.258955261	-0.057259644

C	0.725683313	1.272235182	0.111352925
H	0.200381681	-2.192326814	-0.024583069
C	2.100703842	-1.256214647	0.078310933
C	2.229420353	1.182487648	-0.035425345
H	2.649663563	-2.184901055	0.231028860
H	2.808322230	2.106654168	-0.065260339
C	2.857817429	-0.005025600	-0.011903499
H	3.945847842	-0.057021851	-0.051646478
C	-1.422962030	-0.077342631	0.395151541
H	-1.438753283	-0.218414824	1.477248009
C	-2.619337346	0.036497278	-0.301489706
H	-2.440498876	0.186623821	-1.415208972
H	0.325521994	2.118044517	-0.460192370
H	0.496104597	1.512952015	1.164306503
H	-0.273023986	0.027721999	-1.365577230
O	-3.812182890	0.005476888	0.105246137

C_6H_6-CH=CH-O^- (strained)

C	-0.015293194	0.139359001	-0.837898768
C	-0.770714063	1.309833386	-0.215459890
C	-0.568014385	-1.236846549	-0.356378289
H	-0.279838060	2.277103209	-0.302864401
C	-1.950011111	1.190897586	0.424780461
C	-2.005215228	-1.235348314	0.112274967
H	-2.433766167	2.055307094	0.878911796
H	-2.508049978	-2.197320602	0.218585011
C	-2.620696109	-0.108226491	0.508686182
H	-3.633200165	-0.145907521	0.910755368
C	1.487196549	0.303546028	-0.673253569
H	2.006388844	0.820705084	-1.481514189
C	2.256944813	-0.154056582	0.387803250
H	1.651117872	-0.654333244	1.201664584
O	3.506736314	-0.080061357	0.562177200
H	-0.430921146	-1.967551786	-1.163537879
H	0.054176349	-1.610892896	0.469127308
H	-0.240705782	0.203112837	-1.920447001

C_6H_6-(CH=CH $)_2$-O^-

C	1.107915628	-0.381662263	-0.581845497
C	2.073586909	-1.279718022	0.182570117
C	1.338921190	1.086773880	-0.175460552
H	1.757550013	-2.303712786	0.372052149
C	3.294408144	-0.856852837	0.554246888
C	2.806125480	1.441437168	-0.095028130
H	3.992342517	-1.523773673	1.058114546
H	3.108596809	2.472455741	-0.272584257
C	3.712708123	0.520289371	0.273295491
H	4.763123613	0.784723288	0.384778964
C	-0.326287342	-0.849885736	-0.476908190
H	-0.468780828	-1.908005076	-0.709341068

C	-1.422391426	-0.090933696	-0.177957645
H	-1.250941080	0.969032914	0.039031523
C	-2.788171820	-0.471070473	-0.100940763
H	-3.074201173	-1.503928285	-0.302915250
C	-3.802380180	0.445873056	0.225052860
H	-3.397765172	1.484494116	0.414170542
O	-5.037381733	0.262204540	0.325238597
H	0.813544816	1.746306810	-0.873840361
H	0.877736235	1.265245083	0.810526630
H	1.450967986	-0.455817963	-1.640810041

C_6H_6-(CH=CH)$_2$-O^- (strained)

C	1.141810777	-0.345463850	-0.757903988
C	1.843647158	-1.269889820	0.237143712
C	1.470750333	1.126860138	-0.419163670
H	1.379000346	-2.235906425	0.421911812
C	3.005526392	-0.935420841	0.826246168
C	2.921545358	1.339889611	-0.050145402
H	3.510282905	-1.621428613	1.505164973
H	3.367337571	2.319786626	-0.216453447
C	3.623472187	0.366976591	0.555453102
H	4.651998848	0.535803898	0.871162797
C	-0.336351043	-0.631849248	-0.946224006
H	-0.569742933	-1.379277502	-1.705670385
C	-1.363390545	-0.084643180	-0.227222521
H	-1.095878319	0.652207694	0.539746411
C	-2.758418422	-0.321369109	-0.322094397
H	-3.135516250	-1.043991503	-1.046805252
C	-3.689266898	0.348327595	0.492014453
H	-3.194338211	1.072077185	1.205001482
O	-4.936747939	0.244273268	0.521241404
H	1.177466318	1.758081478	-1.264524787
H	0.850610016	1.460033602	0.428340926
H	1.642547146	-0.553075777	-1.724604128

C_6H_6-(CH=CH)$_3$-O^-

C	2.242063607	-0.425759313	-0.546304286
C	3.214214890	-1.176614402	0.355953386
C	2.351653315	1.087667268	-0.282332082
H	2.954796731	-2.195608155	0.635522381
C	4.382171314	-0.633630438	0.739264700
C	3.786793713	1.548690305	-0.168322604
H	5.091273588	-1.196978613	1.343080641
H	4.029847816	2.575607300	-0.435281297
C	4.727745612	0.733461666	0.337099250
H	5.750885102	1.078971691	0.473139427
C	0.837688295	-0.980752566	-0.474438366
H	0.772981679	-2.061466205	-0.618960431
C	-0.315573913	-0.282237974	-0.286781873
H	-0.238348589	0.800109318	-0.151847142

C	-1.650726059	-0.786976087	-0.241831290
H	-1.791617222	-1.860871064	-0.375481626
C	-2.763628167	0.012291710	-0.040861460
H	-2.563065038	1.082865913	0.088481748
C	-4.117989264	-0.346415439	0.020501018
H	-4.413362920	-1.388477024	-0.100722608
C	-5.139357594	0.608546268	0.236911680
H	-4.739054620	1.655763731	0.349148613
O	-6.370630095	0.426615443	0.312557207
H	1.826677472	1.636566364	-1.070862968
H	1.828235317	1.330378912	0.657610240
H	2.640490019	-0.586599542	-1.573348458

C_6H_6-(CH=CH)$_3$-O^- (strained)

C	2.288959810	-0.576798718	-0.571790364
C	2.940063843	-1.021394008	0.736769333
C	2.499155021	0.941298313	-0.769372891
H	2.512684201	-1.888661822	1.234525451
C	4.027927636	-0.404581583	1.230073268
C	3.900612925	1.387514233	-0.419714506
H	4.506203542	-0.756524207	2.142521442
H	4.305600144	2.273333317	-0.906228399
C	4.599223419	0.755632379	0.538433845
H	5.587320276	1.106649077	0.830709981
C	0.852649534	-1.037327343	-0.735103158
H	0.728784972	-2.025473230	-1.179608959
C	-0.262184985	-0.363101700	-0.335460923
H	-0.122849337	0.620478213	0.123810730
C	-1.624160206	-0.773258585	-0.444209881
H	-1.825311791	-1.750014419	-0.887645828
C	-2.693058758	0.000573938	-0.021945196
H	-2.433533017	0.972518487	0.414860342
C	-4.066025719	-0.277119635	-0.071933444
H	-4.418904636	-1.219976110	-0.489373404
C	-5.035892011	0.636080345	0.406358891
H	-4.579708736	1.579814873	0.818892958
O	-6.276655335	0.515147695	0.418909240
H	2.242230876	1.204726197	-1.800560918
H	1.794304590	1.501723455	-0.134491912
H	2.882987959	-1.072817188	-1.363725600

C_6H_6-(CH=CH)$_4$-O^-

C	3.391308167	-0.412195356	-0.497373609
C	4.368734575	-1.047696113	0.483685989
C	3.419375901	1.119693052	-0.345651623
H	4.149747667	-2.054135148	0.833808311
C	5.498552824	-0.420614912	0.851661555
C	4.827397037	1.657405698	-0.230851468
H	6.215478192	-0.902303434	1.513579493
H	5.028564326	2.672911667	-0.566266050

C	5.791261071	0.927546322	0.355195959
H	6.792762109	1.331386713	0.489177468
C	2.014196573	-1.031076896	-0.424192320
H	2.005587177	-2.120812760	-0.493752486
C	0.826795063	-0.382343528	-0.309056476
H	0.840726723	0.708188162	-0.245957620
C	-0.479199528	-0.967094581	-0.261342491
H	-0.548324799	-2.054246266	-0.323159163
C	-1.641570578	-0.234187874	-0.144011611
H	-1.525243268	0.853210042	-0.085217937
C	-2.969768167	-0.707520655	-0.091467187
H	-3.131634072	-1.784947992	-0.147626540
C	-4.080686677	0.125088319	0.026689180
H	-3.867732752	1.198728890	0.080015939
C	-5.430079074	-0.220486404	0.086104305
H	-5.733217623	-1.265799395	0.039392740
C	-6.452547557	0.758421371	0.207447049
H	-6.052232701	1.808525249	0.248532660
O	-7.681190619	0.579383972	0.269273752
H	2.892193273	1.582245616	-1.186388042
H	2.859372842	1.406203706	0.560288163
H	3.821098596	-0.631461548	-1.499356927

C_6H_6-(CH=CH)$_4$-O^- (strained)

C	-3.444741596	-0.634755627	0.388332355
C	-4.056791039	-0.699010159	-1.008989653
C	-3.578397107	0.797190407	0.951824747
H	-3.654813548	-1.438087827	-1.697767839
C	-5.088840922	0.087050293	-1.360648136
C	-4.938876609	1.400574459	0.688157339
H	-5.543998174	0.004179440	-2.345787960
H	-5.315877548	2.160299260	1.370330912
C	-5.629287075	1.069682031	-0.415949491
H	-6.584491704	1.541220229	-0.638436036
C	-2.042985767	-1.208827589	0.468327114
H	-1.989471611	-2.283089953	0.648168718
C	-0.880080008	-0.529697922	0.283281365
H	-0.938169922	0.544130616	0.085795205
C	0.448344279	-1.057960530	0.324011028
H	0.560685635	-2.126929411	0.512204366
C	1.583029518	-0.294695715	0.139832129
H	1.424502035	0.772775076	-0.046090729
C	2.928581913	-0.716589103	0.160528736
H	3.131029914	-1.772884482	0.343409304
C	4.009040377	0.140908849	-0.038901842
H	3.756126686	1.191688763	-0.219518136
C	5.370855815	-0.156130112	-0.040151714
H	5.711365407	-1.176553914	0.131308373
C	6.357757712	0.841944848	-0.261702477
H	5.918938177	1.863482187	-0.429615773
O	7.592821803	0.705243327	-0.287038670

H	-3.350182367	0.782217192	2.022568222
H	-2.820824644	1.453347643	0.494049897
H	-4.094727550	-1.274198421	1.015371292

C_6H_6-(CH=CH)$_5$-O^-

C	-4.551382044	-0.357694891	0.460451243
C	-5.539943808	-0.921368085	-0.552223143
C	-4.524014162	1.178990473	0.368983436
H	-5.353913373	-1.920852564	-0.939150552
C	-6.643321310	-0.240410458	-0.903453697
C	-5.911755683	1.768942261	0.265902938
H	-7.370794458	-0.670856024	-1.588429207
H	-6.080795735	2.776002664	0.641402487
C	-6.894454041	1.096130374	-0.355689668
H	-7.880485488	1.538418958	-0.481099698
C	-3.196459603	-1.021427243	0.373884705
H	-3.226082822	-2.112718385	0.393888231
C	-1.987112934	-0.412843175	0.302876801
H	-1.955535018	0.678458830	0.290397683
C	-0.705987416	-1.055091123	0.242785798
H	-0.689206196	-2.145811158	0.254167606
C	0.487858523	-0.375562409	0.176033911
H	0.430591657	0.717308973	0.168318676
C	1.791237693	-0.923656933	0.118125848
H	1.886441257	-2.010469022	0.123901248
C	2.948309886	-0.160519474	0.057573369
H	2.813296022	0.925569691	0.054038971
C	4.274590689	-0.614725312	0.001112338
H	4.449794874	-1.691247403	0.003184460
C	5.382189769	0.237019678	-0.055734457
H	5.160069513	1.309494277	-0.056131685
O	8.976776278	0.715764697	-0.215819053
H	-3.988247209	1.589777209	1.230952694
H	-3.946607667	1.480515006	-0.521023135
H	-4.991713203	-0.602596498	1.451062814
C	6.728764740	-0.099570095	-0.110798052
H	7.037808914	-1.143814954	-0.113650694
C	7.750069474	0.892455910	-0.165350759
H	7.347572812	1.941043929	-0.159478054

C_6H_6-(CH=CH)$_5$-O^- *(strained)*

C	4.608988862	-0.580763267	-0.307062424
C	5.189892326	-0.481761414	1.101138182
C	4.699416714	0.792392447	-1.008487419
H	4.800137573	-1.162422293	1.853962207
C	6.184765887	0.374469533	1.388908143
C	6.032785035	1.467909033	-0.784873469
H	6.619994360	0.409285189	2.385597598
H	6.397410034	2.166731403	-1.535134392
C	6.711805328	1.274166721	0.358046282

H	7.645888711	1.798998194	0.547366389
C	3.230975262	-1.213134193	-0.345402792
H	3.220765956	-2.301911317	-0.406664166
C	2.040967030	-0.568424530	-0.247613930
H	2.045963797	0.521325439	-0.167632543
C	0.739892202	-1.168886338	-0.244768836
H	0.689263346	-2.256392962	-0.316522195
C	-0.434507113	-0.457548230	-0.155900259
H	-0.345879920	0.630914581	-0.085830003
C	-1.752505343	-0.970895963	-0.144019240
H	-1.876672626	-2.052671139	-0.212359056
C	-2.890201730	-0.181559168	-0.052611252
H	-2.727739422	0.898635797	0.014623133
C	-4.227511444	-0.604508564	-0.036968916
H	-4.428771829	-1.674476131	-0.102323622
C	-5.315088359	0.269921253	0.056091075
H	-5.067424485	1.334911441	0.118851393
O	-8.898903016	0.825041460	0.203476572
H	4.492120680	0.663819855	-2.075814065
H	3.910164330	1.460932124	-0.628636656
H	5.291878892	-1.254416749	-0.857923570
C	-6.669430616	-0.036736209	0.078899044
H	-7.002684340	-1.071946839	0.021949604
C	-7.668118383	0.975238430	0.175589274
H	-7.241281112	2.012694642	0.229859077

*** acidity of carbonyl α-hydrogens **********

O=CH-CH$_3$

C	-0.128944695	-0.400892415	0.120345688
H	-0.173107864	-1.465400693	0.446988333
O	-1.145648299	0.219943409	-0.095633193
C	1.263194772	0.159795209	-0.018437173
H	1.832410890	-0.436225792	-0.742355177
H	1.225315078	1.202087265	-0.339356047
H	1.792325318	0.079581836	0.939083414

O=CH-CH$_2^-$

C	-0.000413841	0.364688613	0.000000000
C	-1.248446697	-0.229229451	0.000000000
H	-1.364989334	-1.313530360	0.000000000
H	-2.150498609	0.382158780	0.000000000
H	-0.080178021	1.501696345	0.000000000
O	1.163503171	-0.137562356	0.0000000001

O=CH-CH_2^- (strained, i.e. no resonance)

C	-0.033409617	0.370417871	-0.000000041
C	1.285889874	-0.217460183	0.000000055
H	1.786183268	-0.440390330	-0.938578430
H	1.786183194	-0.440390115	0.938578631
H	-0.137279898	1.530657827	-0.000000169
O	-1.156100860	-0.155702966	-0.000000012

HO-CH=CH_2

C	-0.094678378	0.425855900	0.000000000
C	-1.249049206	-0.242277225	0.000000000
H	-1.291434818	-1.328359317	0.000000000
H	-2.188238210	0.296099926	0.000000000
H	-0.047904767	1.511101582	0.000000000
O	1.161435076	-0.100712015	0.000000000
H	1.094299694	-1.066309744	0.0000000001

O=CH-CH=CH-CH_3

C	1.414107105	0.468004368	0.002043410
H	2.043552271	1.384632346	0.009628641
O	1.933169108	-0.634680068	-0.001660207
C	-0.042784605	0.714367537	-0.001876097
H	-0.372698239	1.751841846	-0.006828340
C	-0.925375489	-0.296895334	0.001989206
H	-0.516687675	-1.307214974	0.006115482
C	-2.412230883	-0.157980613	-0.000441121
H	-2.847837579	-0.649990042	0.878436430
H	-2.729585761	0.888211576	-0.004718643
H	-2.845325797	-0.656820092	-0.876709830

O=CH-CH=CH-CH_3 (strained)

C	1.373886291	-0.332465132	0.282551553
H	1.679460936	-0.966606312	1.146275899
O	2.169461802	0.421769777	-0.234452102
C	-0.046077135	-0.494877538	-0.171624885
H	-0.216135650	-1.255633499	-0.934985979
C	-1.059466388	0.234464659	0.299131657
H	-0.854757966	0.987037716	1.061561332
C	-2.488482888	0.112151693	-0.141204325
H	-2.853786170	1.061893440	-0.550457444
H	-2.610055190	-0.658891054	-0.907256592

H	-3.140821343	-0.137664905	0.704588225

O=CH-(CH=CH)$_2$-CH$_3$

C	-2.629816219	-0.321367905	-0.001073519
H	-3.419338340	-1.104102630	-0.002432496
O	-2.935333278	0.861023272	-0.000205182
C	-1.251147280	-0.832008969	-0.000431017
H	-1.115711455	-1.911778976	-0.001409236
C	-0.189151687	0.005189693	0.001414255
H	-0.401083618	1.074000350	0.002140742
C	1.195652498	-0.404698363	0.001804313
H	1.402152056	-1.474886440	0.003723122
C	2.222660364	0.466691296	0.001061738
H	1.994927166	1.533068086	-0.001266504
C	3.670936170	0.094487945	-0.001844268
H	4.185086558	0.510717158	0.873923648
H	3.811954629	-0.989843961	0.000636546
H	4.179559643	0.505843219	-0.883150682

O=CH-(CH=CH)$_2$-CH$_3$ (strained)

C	2.594038617	0.155230335	-0.341766868
H	2.965789662	0.429699028	-1.355767760
O	3.295735039	-0.480685942	0.415050447
C	1.210732717	0.623589082	-0.008909658
H	1.137846236	1.606273340	0.458132924
C	0.107336936	-0.105898294	-0.238748650
H	0.208247922	-1.087838538	-0.701887773
C	-1.244968771	0.317014119	0.089385000
H	-1.352938475	1.294700789	0.559791662
C	-2.339824982	-0.422320262	-0.152266632
H	-2.213855839	-1.398870568	-0.621554192
C	-3.744258219	-0.017890870	0.173910266
H	-4.213943936	-0.736904011	0.857309340
H	-3.782630033	0.970409433	0.641052458
H	-4.369244243	0.005892296	-0.728040891

O=CH-(CH=CH)$_3$-CH$_3$

C	-3.833983919	0.196469822	0.000030900
H	-4.685595975	0.911202922	0.000133941
O	-4.041280890	-1.008025312	-0.000034670
C	-2.504597575	0.818816829	-0.000007001
H	-2.458009573	1.906006586	-0.000046841
C	-1.374104982	0.070715974	0.000014314
H	-1.500064167	-1.011654575	0.000055336

C	-0.034238107	0.588313313	-0.000010190
H	0.089437733	1.670900655	-0.000051887
C	1.068172692	-0.203856284	0.000014940
H	0.930938520	-1.285394334	0.000056856
C	2.428645921	0.279728897	-0.000010503
H	2.570072442	1.360719259	-0.000052640
C	3.509575291	-0.524363958	0.000014894
H	3.352211931	-1.603561298	0.000056892
C	4.931294685	-0.059215243	-0.000009839
H	5.000668245	1.032264278	-0.000051556
H	5.469841478	-0.436472952	0.878913614
H	5.469832623	-0.436539550	-0.878910144

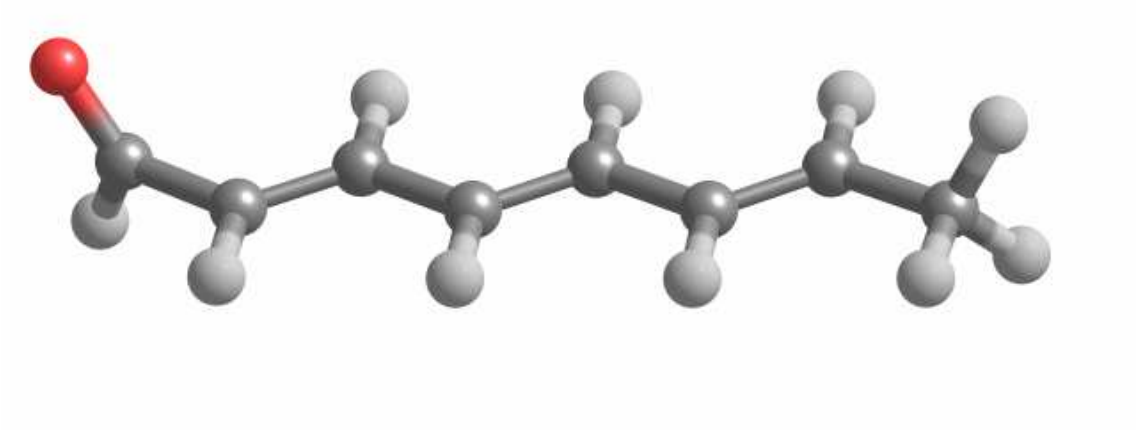

Figure 2: O=CH-(CH=CH)$_3$-CH$_3$ (strained)

O=CH-(CH=CH)$_3$-CH$_3$ (strained)

C	-3.812561966	-0.046921079	-0.326659077
H	-4.204303850	-0.183150371	-1.361002191
O	-4.478478354	0.526792292	0.508406190
C	-2.452928041	-0.618227066	-0.067423843
H	-2.427558266	-1.650891758	0.281855867
C	-1.311908871	0.073574993	-0.236113507
H	-1.366489552	1.104646631	-0.586662530
C	0.013387780	-0.450690869	0.018807667
H	0.077839325	-1.479510782	0.372689310
C	1.151514817	0.259259647	-0.156100595
H	1.077992121	1.288389703	-0.509247520
C	2.483552746	-0.248516812	0.094009574
H	2.558649536	-1.277338492	0.447798864
C	3.610419348	0.465568057	-0.082211869
H	3.523904557	1.493751057	-0.435814754
C	4.998133491	-0.036615744	0.169534030
H	4.995884026	-1.072514243	0.520817734
H	5.609558127	0.013684157	-0.740856763
H	5.511899072	0.577044852	0.920927457

O=CH-(CH=CH)$_4$-CH$_3$

C	-5.042202778	0.094476650	0.000030954
H	-5.925355574	0.769884795	0.000136680
O	-5.195143695	-1.118626670	-0.000039541
C	-3.743534850	0.776111191	-0.000003950
H	-3.746161670	1.864290813	-0.000039216
C	-2.578660727	0.079835334	0.000014340
H	-2.655974542	-1.007122777	0.000050734
C	-1.266318180	0.656708354	-0.000007772
H	-1.190722569	1.743688458	-0.000044894
C	-0.125590131	-0.086128671	0.000014155
H	-0.216275571	-1.172633177	0.000051548
C	1.203857798	0.454534701	-0.000009157
H	1.301114140	1.540034388	-0.000046780
C	2.328931955	-0.306474510	0.000012892
H	2.224341618	-1.391813600	0.000050366
C	3.673950546	0.217367532	-0.000009907
H	3.781160334	1.302464880	-0.000047463
C	4.781513856	-0.550092404	0.000012269
H	4.660903120	-1.634041913	0.000049820
C	6.186901338	-0.036934271	-0.000010525
H	6.218851981	1.056375734	-0.000047763
H	6.738749055	-0.394717871	0.878925318
H	6.738742265	-0.394777529	-0.878926357

O=CH-(CH=CH)$_4$-CH$_3$ (strained)

C	5.034728683	0.028105743	0.301619360
H	5.439884534	-0.038941751	1.337634957
O	5.676147254	0.572865995	-0.571182911
C	3.690032367	-0.595005579	0.088956943
H	3.691035698	-1.645784320	-0.202237431
C	2.530228341	0.073055295	0.230889179
H	2.558767075	1.123159841	0.523199938
C	1.220277513	-0.500899085	0.018984442
H	1.181064691	-1.548986741	-0.277123993
C	0.061007586	0.186949203	0.166002374
H	0.110484633	1.235594994	0.461285537
C	-1.251117648	-0.367366085	-0.041760243
H	-1.304411936	-1.415166010	-0.337927698
C	-2.404955191	0.329575650	0.106966391
H	-2.348962597	1.377675344	0.402736777
C	-3.726058067	-0.218838963	-0.100217523
H	-3.781557650	-1.267094239	-0.396208874
C	-4.868778889	0.477933048	0.048501199
H	-4.803434657	1.525700596	0.344351913
C	-6.246072300	-0.070134138	-0.160585466
H	-6.221739128	-1.123544809	-0.454351434

H	−6.850469119	0.015505478	0.751967571
H	−6.782087892	0.488405496	−0.939089305

O=CH-(CH=CH)$_5$-CH$_3$

C	−6.255359296	0.007595371	0.000030660
H	−7.157738266	0.657125586	0.000139018
O	−6.373318643	−1.209703938	−0.000044214
C	−4.977649569	0.726427663	−0.000001931
H	−5.011865684	1.814074145	−0.000034160
C	−3.792136498	0.064294145	0.000014544
H	−3.837909555	−1.024453462	0.000048012
C	−2.498409839	0.678648196	−0.000005909
H	−2.454007589	1.767345024	−0.000040104
C	−1.334850474	−0.031240545	0.000014158
H	−1.394695166	−1.119907914	0.000048569
C	−0.024692913	0.546590044	−0.000007584
H	0.042459753	1.634323926	−0.000042308
C	1.125545386	−0.183358013	0.000012549
H	1.049639930	−1.271135008	0.000047263
C	2.446812242	0.374856656	−0.000008768
H	2.527748769	1.461861026	−0.000043667
C	3.585142231	−0.367096111	0.000011621
H	3.499509194	−1.454120087	0.000046548
C	4.920431349	0.180555732	−0.000009859
H	5.007251405	1.267592213	−0.000044987
C	6.043236018	−0.564687172	0.000010588
H	5.944554271	−1.650862902	0.000045783
C	7.438074715	−0.022992414	−0.000011195
H	7.447316589	1.070806461	−0.000046084
H	7.997605168	−0.368754056	0.878955416
H	7.997599345	−0.368810044	−0.878959497

O=CH-(CH=CH)$_5$-CH$_3$ (strained)

C	−6.259633238	−0.087521859	0.276913340
H	−6.672246699	−0.065246863	1.312017426
O	−6.885834446	−0.611240693	−0.619370402
C	−4.925074537	0.566657460	0.096371462
H	−4.942912249	1.627117229	−0.156524689
C	−3.753961614	−0.085627917	0.222275777
H	−3.765427619	−1.145976589	0.476317641
C	−2.454032659	0.518279465	0.040402089
H	−2.431650291	1.576896956	−0.217417311
C	−1.282343644	−0.154475960	0.170505380
H	−1.315386918	−1.213760969	0.427687609
C	0.018359359	0.428802403	−0.008385919
H	0.055854980	1.487171028	−0.266751924

C	1.186740952	−0.254355189	0.122981064
H	1.145315953	−1.313067001	0.381074954
C	2.491489643	0.320039368	−0.055647217
H	2.534583263	1.378311718	−0.314309658
C	3.654588555	−0.367544746	0.076221229
H	3.610459660	−1.425985150	0.334754867
C	4.968577148	0.204958685	−0.102811091
H	5.011065186	1.263710696	−0.361506727
C	6.120644528	−0.480691162	0.028849340
H	6.067572099	−1.538923507	0.287573429
C	7.491059237	0.093460620	−0.152001303
H	7.453318576	1.156124699	−0.409016875
H	8.091586108	−0.014713615	0.760782588
H	8.040151550	−0.429197538	−0.946235912

O=CH-CH=CH-CH$_2^-$

C	1.330871643	−0.462564176	−0.000219557
H	1.956522571	−1.403501376	0.000755760
O	1.931534595	0.641710540	−0.000340513
C	−0.048219327	−0.732784843	0.000242365
H	−0.357193634	−1.779795997	0.001319566
C	−1.041012462	0.289032540	0.000892045
H	−0.614903150	1.296171359	0.002461876
C	−2.399715510	0.185528519	−0.000578123
H	−2.904397361	−0.780592930	−0.003329723
H	−3.039038322	1.065608639	0.000187322

O=CH-CH=CH-CH$_2^-$ (strained)

C	−1.309075662	0.251794282	0.326600608
H	−1.641873070	0.636676409	1.344614342
O	−2.168764048	−0.388770456	−0.273373087
C	0.059934683	0.571862754	−0.097703421
H	0.175243412	1.504211734	−0.654847541
C	1.164219659	−0.245415325	0.181122581
H	0.909607511	−1.149490578	0.753683898
C	2.508383262	−0.128359690	−0.123842677
H	2.899348595	0.708161384	−0.702063724
H	3.221776895	−0.886159587	0.189779462

O=CH-(CH=CH)$_2$-CH$_2^-$

C	2.566734134	−0.295929563	0.000018350
H	3.373114764	−1.082107413	0.000081133
O	2.912882911	0.905391935	−0.000015524
C	1.261793759	−0.844308897	−0.000004111
H	1.176307015	−1.931685926	−0.000021922
C	0.097197162	−0.055730891	−0.000000745
H	0.286745199	1.020966054	0.000016526
C	−1.224029977	−0.460076275	−0.000006813
H	−1.450284448	−1.528915694	−0.000026477

C	−2.329446992	0.447013486	0.000016498
H	−2.049086661	1.505334398	0.000029395
C	−3.658862171	0.164103335	−0.000013657
H	−4.024432728	−0.861019614	−0.000021917
H	−4.408764769	0.949993508	0.000076251

O=CH-(CH=CH)$_2$-CH$_2^-$ (strained)

C	2.528718277	−0.046760763	0.365787725
H	2.898210972	−0.185604400	1.424397388
O	3.320188492	0.479062215	−0.407473558
C	1.217950883	−0.640961774	0.040217140
H	1.259008326	−1.667787550	−0.327772391
C	0.010602463	0.017963485	0.176672231
H	0.074780230	1.042851591	0.564027795
C	−1.295228015	−0.413915831	−0.105781011
H	−1.435063439	−1.419764403	−0.508135019
C	−2.444281189	0.393727600	0.094615557
H	−2.225215456	1.391715475	0.495928954
C	−3.766089665	0.120597699	−0.129487253
H	−4.094672351	−0.838877324	−0.525472253
H	−4.540143722	0.853551747	0.080816117

O=CH-(CH=CH)$_3$-CH$_2^-$

C	3.776908225	0.136832031	0.000061469
H	4.654992960	0.838204870	0.000155068
O	3.996750047	−1.089458648	−0.000063821
C	2.523443862	0.808528911	0.000099201
H	2.541347416	1.898631369	0.000246728
C	1.298898242	0.135164196	−0.000042169
H	1.378792438	−0.954410267	−0.000161253
C	0.018592863	0.677417596	−0.000023192
H	−0.087734028	1.764116667	0.000087121
C	−1.162176540	−0.098735750	−0.000139542
H	−1.014333629	−1.183305814	−0.000393144
C	−2.467649328	0.342453314	−0.000023723
H	−2.659380209	1.416894038	0.000047232
C	−3.602624998	−0.531177407	0.000179238
H	−3.361798213	−1.598522806	0.000791355
C	−4.916213110	−0.193134582	−0.000052934
H	−5.237401248	0.846266802	−0.000871797
H	−5.698084221	−0.946547907	0.000416806

O=CH-(CH=CH)$_3$-CH$_2^-$ (strained)

C	−3.743646227	0.069631408	−0.357219898
H	−4.111458859	0.021227805	−1.420498006
O	−4.455313668	0.658199089	0.442828462
C	−2.474544319	−0.636271302	−0.071394372
H	−2.577324895	−1.679685201	0.230615670
C	−1.236027326	−0.050982967	−0.168902896
H	−1.221779115	0.999659877	−0.479779195

C	0.037861282	−0.614442475	0.072362272
H	0.084958624	−1.656607347	0.393434411
C	1.236375295	0.093813495	−0.078105191
H	1.127013478	1.136865523	−0.398700742
C	2.541521911	−0.337665643	0.119039988
H	2.709768747	−1.367850127	0.439200198
C	3.685485565	0.491264376	−0.075122550
H	3.456164463	1.513425007	−0.396829775
C	5.003214889	0.184603071	0.081304376
H	5.326176878	−0.805158356	0.397965973
H	5.783166408	0.918087345	−0.101495779

O=CH-(CH=CH)$_4$-CH$_2^-$

C	−4.983846258	−0.010915711	0.000028943
H	−5.901378581	0.635064713	0.000114756
O	−5.124651895	−1.245781604	−0.000025964
C	−3.766698820	0.733708682	0.000005452
H	−3.846877933	1.820657829	−0.000006312
C	−2.512012782	0.131303243	0.000002950
H	−2.525649719	−0.960646955	0.000016179
C	−1.263073112	0.754412869	−0.000008289
H	−1.227213879	1.845369937	−0.000023311
C	−0.043857399	0.056941192	−0.000000709
H	−0.116767093	−1.034537662	0.000014870
C	1.235240319	0.591858908	−0.000011273
H	1.343151369	1.677639349	−0.000027088
C	2.417531288	−0.187388583	−0.000003064
H	2.272754794	−1.271987180	0.000011548
C	3.717123631	0.261124455	−0.000004492
H	3.902422633	1.336337173	−0.000020002
C	4.859780182	−0.605782521	0.000023694
H	4.630533363	−1.675043695	0.000023776
C	6.165985243	−0.247885677	−0.000014654
H	6.470205102	0.796359688	−0.000026746
H	6.959505902	−0.988633865	0.000113402

O=CH-(CH=CH)$_4$-CH$_2^-$ (strained)

C	−4.955585985	0.205765023	−0.351029995
H	−5.321985368	0.223164586	−1.413339413
O	−5.625742115	0.795097110	0.481087170
C	−3.717208177	−0.570786989	−0.101880467
H	−3.863818947	−1.621986600	0.150048613
C	−2.459216802	−0.038177581	−0.174112127
H	−2.390457312	1.023339749	−0.432840626
C	−1.214561227	−0.685882635	0.038796032
H	−1.229936489	−1.743540711	0.306457815
C	0.014760995	−0.044696258	−0.076322251
H	−0.023305789	1.016757003	−0.344733669
C	1.294016723	−0.579332498	0.103128529
H	1.379353383	−1.633933360	0.370890814

C	2.481470996	0.163431564	-0.044123551
H	2.348801100	1.217266917	-0.312362184
C	3.786282621	-0.265958544	0.104913106
H	3.968155788	-1.308522071	0.371822415
C	4.925735539	0.580017860	-0.070779314
H	4.691283537	1.615974455	-0.335774077
C	6.239472613	0.257231104	0.050711655
H	6.557276385	-0.749757018	0.312322689
H	7.023056791	0.991982192	-0.107826288

O=CH-(CH=CH)$_5$-CH$_2^-$

C	-6.190936721	-0.152508892	0.000126660
H	-7.134453325	0.452632539	0.000296316
O	-6.274950868	-1.390331564	-0.000060409
C	-5.001817959	0.642698821	0.000162365
H	-5.125403945	1.725307156	0.000292031
C	-3.728642496	0.090425778	0.000044733
H	-3.696246718	-1.000796935	-0.000081471
C	-2.504494235	0.768738787	0.000073937
H	-2.517566123	1.859935162	0.000195331
C	-1.261419924	0.126263856	-0.000044645
H	-1.282620547	-0.966990344	-0.000163665
C	-0.004865276	0.724385546	-0.000035562
H	0.047626578	1.814106908	0.000084161
C	1.207017302	0.007841178	-0.000173417
H	1.121793458	-1.082521156	-0.000270139
C	2.487511572	0.530518499	-0.000177740
H	2.605409022	1.615027625	-0.000051914
C	3.665678055	-0.259477449	-0.000318534
H	3.514898814	-1.342805176	-0.000433196
C	4.963694226	0.186106529	-0.000250273
H	5.151159191	1.260748287	-0.000294068
C	6.106735614	-0.682950554	0.000221311
H	5.879461548	-1.752143842	-0.000075100
C	7.409485422	-0.318304833	0.000389707
H	7.707439253	0.727589053	0.000365716
H	8.207134920	-1.054359352	0.000873959

O=CH-(CH=CH)$_5$-CH$_2^-$ (strained)

C	6.167197033	-0.341861766	-0.343995882
H	6.530998983	-0.409484948	-1.403546788
O	6.811223657	-0.920637731	0.514068645
C	4.952239711	0.483265738	-0.125722174
H	5.130518157	1.538125290	0.086699543
C	3.681778345	-0.011301118	-0.179647375
H	3.574182865	-1.077924996	-0.398084361
C	2.460826243	0.694543198	0.009885528
H	2.520677107	1.759664877	0.237581808
C	1.211604702	0.101950733	-0.080826328
H	1.199089032	-0.968607896	-0.309445178

C	−0.044446302	0.707240462	0.081813423
H	−0.073736529	1.773672525	0.310867335
C	−1.260233352	0.023958117	−0.034767932
H	−1.189958002	−1.044136186	−0.264142790
C	−2.545002053	0.538205910	0.104443034
H	−2.655177605	1.599684373	0.332119982
C	−3.721524874	−0.232137509	−0.032346926
H	−3.571142186	−1.292282205	−0.260065217
C	−5.027057963	0.190669794	0.086698494
H	−5.220365206	1.240367942	0.313548018
C	−6.161040065	−0.670392061	−0.070767343
H	−5.921589990	−1.713530507	−0.297333047
C	−7.472593992	−0.341158643	0.027227861
H	−7.789635410	0.675225542	0.249593161
H	−8.256708504	−1.078890171	−0.112355299

H-CH=CH-CH$_3$

C	1.257497177	0.226797404	−0.000027728
H	1.281965340	1.314173209	0.000102067
C	0.106623457	−0.445377403	0.000092469
H	0.134311395	−1.535561070	−0.000271367
C	−1.259613521	0.176901145	−0.000020564
H	−1.837370872	−0.135459556	0.879068319
H	−1.203353218	1.269503604	0.000443382
H	−1.836816345	−0.134739455	−0.879731828
H	2.216915374	−0.281653735	−0.000136573

H-(CH=CH)$_2$-CH$_3$

C	2.498776710	−0.263524303	0.000939697
H	2.543634997	−1.349657477	0.001114965
C	1.328132954	0.389662408	−0.000400642
H	1.327616670	1.479829020	−0.000465460
C	0.022126115	−0.253157594	−0.001311754
H	0.015435647	−1.343951015	−0.003489775
C	−1.146223788	0.408816781	−0.000456513
H	−1.125510931	1.499543192	0.002023477
C	−2.501623818	−0.229612995	0.000809404
H	−3.087206873	0.077641719	−0.875476722
H	−2.433467098	−1.321458263	−0.002397138
H	−3.082751460	0.072653303	0.881805771
H	3.446735865	0.264050032	0.001883478

H-(CH=CH)$_3$-CH$_3$

C	3.737487173	−0.275191267	0.000000674
H	3.791851817	−1.360758925	0.000001378
C	2.559008120	0.368429688	−0.000000651
H	2.550660096	1.458551874	−0.000000797
C	1.264041662	−0.282475309	−0.000000373

H	1.262337674	-1.372841791	-0.000000943
C	0.082329572	0.375247219	0.000000120
H	0.089600193	1.465883929	0.000000749
C	-1.215790421	-0.266404689	-0.000000285
H	-1.222361847	-1.357209686	-0.000000968
C	-2.389363547	0.391610951	0.000000213
H	-2.373632503	1.482260308	0.000000742
C	-3.740454885	-0.254470535	0.000000160
H	-3.665895687	-1.345935038	-0.000000035
H	-4.326064928	0.046447031	0.878649066
H	-4.326065081	0.046447320	-0.878648548
H	4.680173958	0.261489351	0.000001047

H-(CH=CH)$_4$-CH$_3$

C	-4.975241644	0.277703931	-0.000000133
H	-5.035693368	1.362902111	-0.000000346
C	-3.792339312	-0.359615091	0.000000064
H	-3.778311494	-1.449660231	0.000000263
C	-2.502935785	0.297735093	0.000000027
H	-2.505990586	1.388007154	-0.000000156
C	-1.315003715	-0.355255962	0.000000161
H	-1.318971521	-1.445913512	0.000000306
C	-0.026861802	0.288818941	0.000000040
H	-0.020725929	1.379203257	-0.000000113
C	1.158399528	-0.369705671	0.000000064
H	1.151616176	-1.460202041	0.000000225
C	2.453070907	0.273701388	-0.000000200
H	2.457526038	1.364564109	-0.000000523
C	3.629478720	-0.381371395	-0.000000229
H	3.616810166	-1.472009810	-0.000000396
C	4.978238938	0.268973620	-0.000000213
H	4.900185963	1.360198733	-0.000011161
H	5.564973091	-0.029943572	0.878650474
H	5.564987026	-0.029965815	-0.878633529
H	-5.914709854	-0.264497154	-0.000000034

H-(CH=CH)$_5$-CH$_3$

C	6.212465747	-0.276092855	0.000001079
H	6.277147392	-1.361024284	0.000002293
C	5.026697565	0.356760507	-0.000000622
H	5.008589008	1.446731203	-0.000001218
C	3.740764020	-0.305374102	-0.000000203
H	3.747657128	-1.395592060	-0.000000376
C	2.549092845	0.343615783	-0.000000024
H	2.549556786	1.434271176	0.000000282
C	1.265962111	-0.304203046	-0.000000398
H	1.262385327	-1.394515276	-0.000000668
C	0.075223616	0.351926460	-0.000000256
H	0.080916958	1.442441399	0.000000071
C	-1.209973861	-0.291217334	-0.000000392

H	−1.216162661	−1.381660299	−0.000000855
C	−2.397358749	0.366566823	0.000000010
H	−2.391539815	1.457024882	0.000000572
C	−3.690116838	−0.278398535	−0.000000108
H	−3.693046313	−1.369280273	−0.000000805
C	−4.868157602	0.374760027	0.000000483
H	−4.857406840	1.465396466	0.000001239
C	−6.215523227	−0.278170561	0.000000238
H	−6.135346247	−1.369243749	−0.000000212
H	−6.802907150	0.019552111	0.878652099
H	−6.802907149	0.019552805	−0.878651394
H	7.149723670	0.269874311	0.000001269

H-CH=CH-CH$_2^-$

C	−1.281079529	0.178967355	0.000017943
H	−1.450736468	1.256555654	0.001346397
C	0.000027684	−0.368841200	0.000107103
H	0.000328184	−1.472510413	0.000306629
C	1.281052831	0.179006528	−0.000078367
H	1.450336300	1.256684120	−0.000962325
H	2.165338605	−0.455572780	0.000489281
H	−2.165278369	−0.455761284	−0.001735767

H-(CH=CH)$_2$-CH$_2^-$

C	2.530054099	−0.158419302	0.000001386
H	2.739822308	−1.227196274	0.000005754
C	1.245577209	0.329123916	−0.000003990
H	1.159233355	1.424865259	−0.000010119
C	−0.000019608	−0.339606260	0.000001547
H	−0.000084999	−1.432900687	0.000005997
C	−1.245601301	0.329219997	0.000005338
H	−1.159582974	1.424993047	0.000000081
C	−2.529996979	−0.158451069	−0.000008897
H	−2.739307298	−1.227339014	0.000005919
H	−3.389258086	0.507454029	0.000047149
H	3.389017904	0.507890245	0.000000188

H-(CH=CH)$_3$-CH$_2^-$

C	3.768676920	0.094783534	0.000047548
H	4.002495662	1.157816049	0.000195901
C	2.480279636	−0.357408652	−0.000055029
H	2.349922289	−1.446367817	−0.000189427
C	1.262050561	0.377089649	0.000006065
H	1.325241277	1.467544607	0.000128171
C	0.000029214	−0.216952769	−0.000086713
H	−0.000041440	−1.314510173	−0.000314477
C	−1.262218491	0.376840827	0.000031382
H	−1.325763386	1.467263239	0.000151251

C	−2.480228222	−0.357726324	0.000111077
H	−2.350441612	−1.446761116	0.000481458
C	−3.768537748	0.094951043	−0.000062115
H	−4.001262944	1.158280909	−0.000558683
H	−4.611878762	−0.589899157	0.000212762
H	4.611111315	−0.591215575	−0.000014264

$H\text{-}(CH{=}CH)_4\text{-}CH_2^-$

C	−5.001592297	0.011921055	0.000005480
H	−5.253343859	1.070433310	0.000012403
C	−3.709716767	−0.415222693	−0.000002524
H	−3.549528795	−1.498789330	−0.000009083
C	−2.512810490	0.362573152	−0.000000470
H	−2.615841067	1.449439836	0.000004058
C	−1.239177232	−0.183846052	−0.000003414
H	−1.189079070	−1.278795035	−0.000007726
C	0.000067760	0.476731011	−0.000001586
H	0.000235478	1.568434108	0.000002533
C	1.239114148	−0.184006206	−0.000005209
H	1.189081147	−1.278955762	−0.000010996
C	2.512912140	0.362231942	0.000001859
H	2.616195492	1.449068736	0.000008017
C	3.709686679	−0.415503386	0.000010466
H	3.550082718	−1.499164284	−0.000001784
C	5.001465325	0.012205277	−0.000010103
H	5.252028530	1.071051876	−0.000002336
H	5.832486638	−0.686911324	0.000065725
H	−5.831713140	−0.688297875	0.000004680

$H\text{-}(CH{=}CH)_5\text{-}CH_2^-$

C	6.230936999	−0.082033556	−0.000123239
H	6.497030192	0.972705350	−0.000242612
C	4.936050661	−0.489677510	−0.000030761
H	4.753541357	−1.568789060	0.000087609
C	3.756244120	0.319588291	−0.000070543
H	3.888153143	1.402955795	−0.000183733
C	2.474192930	−0.192380580	0.000025781
H	2.388609246	−1.284187124	0.000136936
C	1.254508325	0.514751489	0.000004957
H	1.296941067	1.605329376	−0.000106941
C	0.000033571	−0.096055664	0.000119920
H	0.000078132	−1.191180274	0.000218000
C	−1.254609152	0.514564497	0.000105101
H	−1.297390305	1.605132684	−0.000011726
C	−2.474129401	−0.192672245	0.000218822
H	−2.388581178	−1.284478518	0.000332650
C	−3.756294280	0.319185591	0.000175862
H	−3.888356710	1.402531451	0.000156560

C	-4.936061107	-0.489910303	-0.000097352
H	-4.754195762	-1.569138286	0.000144055
C	-6.230822980	-0.081599587	-0.000284690
H	-6.495619941	0.973511360	-0.000375734
H	-7.051902419	-0.791957165	-0.000596005
H	7.051101574	-0.793483471	-0.000081272

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HO-CH=CH-CH=CH$_2$

C	1.251005492	-0.575228504	0.000010372
H	1.924172610	-1.429802921	0.001387500
O	1.841107097	0.658680980	-0.000368586
C	-0.082764156	-0.735258710	0.000132791
H	-0.454684923	-1.756227032	-0.000525916
C	-1.050605430	0.347430838	0.000385051
H	-0.643661951	1.356283644	0.002059788
C	-2.381262030	0.175221142	-0.000271099
H	-2.828181811	-0.815900389	-0.001612487
H	-3.063629489	1.018616763	0.000410704
H	2.798896691	0.553906969	0.001068729

HO-CH=CH-CH=CH$_2$ (strained)

C	-1.229629219	0.468121614	-0.187820012
H	-2.034807840	1.104045601	-0.552401481
O	-1.567741377	-0.826260162	0.100840235
C	0.007920899	0.945082618	-0.030081224
H	0.162590861	1.991350025	-0.285353346
C	1.167854750	0.160295607	0.460339885
H	1.336595220	0.156233353	1.539255190
C	2.002864582	-0.527222248	-0.319668652
H	1.875086698	-0.563002566	-1.398069974
H	2.841010958	-1.080018859	0.095394280
H	-2.505829946	-0.953110971	-0.079667554

HO-(CH=CH)$_2$-CH=CH$_2$

C	2.492565966	-0.439099744	0.000007879
H	3.314918561	-1.150860045	0.000040929
O	2.835486278	0.883682442	-0.000001520
C	1.210228104	-0.848358307	-0.000002724
H	1.040180027	-1.921573647	-0.000006842
C	0.061662438	0.027038037	-0.000004711
H	0.261936560	1.096873245	-0.000001591
C	-1.223673338	-0.397900288	-0.000002755
H	-1.429386686	-1.468876882	-0.000005861
C	-2.369998755	0.487594190	0.000008913
H	-2.151494408	1.555778410	0.000010943
C	-3.651569017	0.085095395	-0.000005209

H	−3.915686315	−0.969351658	−0.000010638
H	−4.472199594	0.794521629	0.000026458
H	3.795625797	0.965230304	−0.000045875

HO-(CH=CH)$_2$-CH=CH$_2$ (strained)

C	−2.449079789	0.308004277	−0.170632758
H	−3.330232802	0.902039961	−0.402945278
O	−2.666648155	−1.011969699	0.114646699
C	−1.220327043	0.851280663	−0.166362548
H	−1.151204878	1.909081576	−0.405469563
C	0.005237799	0.133329199	0.131597931
H	−0.092398479	−0.924458096	0.365999570
C	1.228213388	0.693986597	0.132850038
H	1.320308892	1.755613974	−0.106931207
C	2.485678839	−0.031357764	0.440471456
H	2.798871296	−0.049024252	1.487197888
C	3.246427119	−0.653138742	−0.462206381
H	2.979748018	−0.670248551	−1.515479658
H	4.159966629	−1.167204559	−0.176721648
H	−3.610126538	−1.199043188	0.057426804

HO-(CH=CH)$_3$-CH=CH$_2$

C	3.707273158	0.329093538	0.000035743
H	4.579341155	0.978870647	0.000083558
O	3.951655156	−1.014755438	−0.000021999
C	2.457075575	0.831171482	0.000045380
H	2.366602274	1.914040130	0.000122469
C	1.249702943	0.043520691	−0.000034220
H	1.369606076	−1.038156940	−0.000095431
C	−0.003800867	0.564173920	−0.000023231
H	−0.124179018	1.648079556	0.000035388
C	−1.207219018	−0.225145736	−0.000076918
H	−1.081885162	−1.308701915	−0.000234851
C	−2.465416400	0.280942833	0.000031943
H	−2.599224082	1.363010549	0.000121780
C	−3.666116466	−0.526474447	0.000129246
H	−3.520131214	−1.606958261	0.000500477
C	−4.918552725	−0.038915732	−0.000078360
H	−5.111112026	1.030802523	−0.000518897
H	−5.784737911	−0.691876651	0.000132100
H	4.903142161	−1.167363973	−0.000149692

HO-(CH=CH)$_3$-CH=CH$_2$ (strained)

C	−3.663697516	−0.202448468	0.145909336
H	−4.570166295	−0.777213877	0.321317079
O	−3.830408324	1.128344434	−0.116946501
C	−2.448014947	−0.779043167	0.187512052
H	−2.420132782	−1.843559466	0.404113161
C	−1.197023553	−0.091998194	−0.031989101

H	−1.254806583	0.973533768	−0.246078234
C	0.018949499	−0.686093588	0.012261365
H	0.079782708	−1.753785119	0.226453230
C	1.269699063	0.007911747	−0.208641558
H	1.205658865	1.075101109	−0.421770567
C	2.484517367	−0.572869463	−0.167171192
H	2.546382715	−1.641192465	0.050253256
C	3.765943623	0.137845861	−0.397635173
H	4.127709574	0.175037907	−1.428095057
C	4.493100076	0.724686414	0.554766398
H	4.178220830	0.720484300	1.594755636
H	5.427034180	1.229798057	0.324831152
H	−4.769931921	1.342044929	−0.101047457

HO-(CH=CH)$_4$-CH=CH$_2$

C	−4.922606426	0.243745686	0.000013852
H	−5.818246827	0.860565193	0.000058297
O	−5.116101878	−1.107958973	−0.000002715
C	−3.691445412	0.792254943	0.000001630
H	−3.641694832	1.877770330	−0.000000080
C	−2.456555850	0.050747429	−0.000003511
H	−2.535421463	−1.034671072	−0.000000908
C	−1.222064922	0.618780656	−0.000005737
H	−1.143708542	1.706579635	−0.000009050
C	0.007891773	−0.122356624	−0.000002856
H	−0.074031054	−1.209928015	0.000001232
C	1.248789798	0.434692512	−0.000005284
H	1.334475528	1.521675333	−0.000009585
C	2.473951130	−0.316177255	−0.000002982
H	2.383451960	−1.403229091	−0.000000249
C	3.716654475	0.229605935	−0.000000272
H	3.815882740	1.315344156	−0.000002071
C	4.941599464	−0.539078418	0.000013668
H	4.830466739	−1.623658768	0.000010063
C	6.177967099	−0.011293387	−0.000005806
H	6.335950186	1.064042693	−0.000014664
H	7.064640159	−0.636115062	0.000040893
H	−6.061138207	−1.296662888	−0.000062949

HO-(CH=CH)$_4$-CH=CH$_2$ (strained)

C	−4.883067354	0.126649990	−0.124872540
H	−5.800701999	0.692440584	−0.267837611
O	−5.025060242	−1.210601881	0.115443900
C	−3.675344115	0.720894560	−0.183188210
H	−3.667495376	1.789685516	−0.379557695
C	−2.412473914	0.048743671	−0.006296681
H	−2.448951025	−1.021313848	0.188658663
C	−1.203592538	0.663291910	−0.068154278
H	−1.167506777	1.735680963	−0.263405086

C	0.056195351	-0.009382097	0.108086839
H	0.016034364	-1.081781315	0.302784615
C	1.270034209	0.593554760	0.049012977
H	1.316730762	1.665481916	-0.145272223
C	2.529039641	-0.094106540	0.227790395
H	2.479137806	-1.165750318	0.421382072
C	3.738570107	0.498141929	0.170255136
H	3.786360876	1.570887372	-0.027786349
C	5.030089295	-0.205827872	0.358144070
H	5.415036640	-0.259597203	1.379442969
C	5.740186284	-0.768017103	-0.621622421
H	5.401957901	-0.746644591	-1.653991692
H	6.683350379	-1.268930209	-0.422325196
H	-5.961570705	-1.437706167	0.117402000

HO-(CH=CH)$_5$-CH=CH$_2$

C	6.141463796	-0.174585256	0.000088167
H	7.050660862	-0.771196819	0.000161494
O	6.304283625	1.180897070	0.000050488
C	4.922582726	-0.750611061	0.000071119
H	4.897260343	-1.836970863	0.000109174
C	3.671982478	-0.037201569	0.000014632
H	3.726113996	1.049710701	-0.000022831
C	2.449873160	-0.633288938	0.000008254
H	2.396589105	-1.722608256	0.000045066
C	1.204773484	0.079077553	-0.000043809
H	1.261219537	1.168222485	-0.000079160
C	-0.024689927	-0.507054773	-0.000057403
H	-0.084072745	-1.595841073	-0.000020570
C	-1.264118878	0.213001981	-0.000121658
H	-1.201344160	1.301875744	-0.000143913
C	-2.496788617	-0.365264312	-0.000139286
H	-2.563626239	-1.453517898	-0.000100380
C	-3.733416868	0.364346201	-0.000179728
H	-3.661867198	1.452777867	-0.000225140
C	-4.966950289	-0.203226628	-0.000138691
H	-5.047057305	-1.290520930	-0.000157214
C	-6.204723728	0.543863250	0.000115788
H	-6.112772612	1.630204132	-0.000072649
C	-7.431654900	-0.005888531	0.000291138
H	-7.570541339	-1.083842821	0.000342656
H	-8.329218189	0.603155756	0.000548985
H	7.244769644	1.391250480	-0.000097597

HO-(CH=CH)$_5$-CH=CH$_2$ (strained)

C	-6.106232009	0.067644515	-0.107073971
H	-7.030586350	0.627525129	-0.228098276
O	-6.232822692	-1.274201794	0.112983476
C	-4.904110099	0.673725283	-0.171972650
H	-4.908493508	1.745635405	-0.350620707

C	−3.634147530	0.010535041	−0.023470191
H	−3.657919763	−1.062835163	0.154268746
C	−2.430487441	0.637853312	−0.091468527
H	−2.407784912	1.713619453	−0.269406295
C	−1.164823193	−0.024061765	0.056530224
H	−1.190466765	−1.099809262	0.234051817
C	0.045306371	0.594047611	−0.009334756
H	0.074127672	1.669552800	−0.186524254
C	1.307227336	−0.076342319	0.139684670
H	1.274379765	−1.152099503	0.316525440
C	2.518997944	0.532842031	0.075981354
H	2.558692861	1.608061206	−0.100513291
C	3.782002120	−0.152265130	0.227516368
H	3.739263433	−1.227206164	0.403518456
C	4.988354867	0.446786271	0.165043586
H	5.028631728	1.522911270	−0.015427165
C	6.285112894	−0.254126439	0.325235475
H	6.682562269	−0.323127607	1.340785066
C	6.985409885	−0.796555838	−0.672531241
H	6.634434680	−0.759452401	−1.700174191
H	7.933165010	−1.296299870	−0.493230453
H	−7.167081762	−1.510292785	0.124032072

$^{-}$O-CH=CH-CH=CH$_2$ (strained)

C	−1.283414304	−0.358530666	0.172505732
H	−2.020475859	−1.119223751	0.581119597
O	−1.714911817	0.797688448	−0.095421068
C	−0.013507987	−0.909521991	0.047121970
H	0.121073316	−1.955628921	0.329641913
C	1.173781488	−0.177901451	−0.442731244
H	1.395721158	−0.185243024	−1.526740284
C	2.046379898	0.518494673	0.298434490
H	1.919733519	0.606567156	1.376161671
H	2.901156752	1.036738207	−0.142734428

$^{-}$O-(CH=CH)$_2$-CH=CH$_2$ (strained)

C	−2.502259986	0.172032431	−0.144043019
H	−3.370921486	0.846166788	−0.399307423
O	−2.748527583	−1.028790941	0.125183649
C	−1.266597877	0.844775794	−0.179469379
H	−1.275728036	1.904595385	−0.439486770
C	−0.029902228	0.206049828	0.106076584
H	−0.131702240	−0.854271772	0.350331841
C	1.231763056	0.733544788	0.115400265
H	1.372931567	1.790377524	−0.127044640
C	2.459375107	−0.031225415	0.436345514
H	2.790629469	−0.072794373	1.486840201
C	3.226838669	−0.693155526	−0.438033421

H	2.976164841	-0.719240219	-1.496331395
H	4.119761398	-1.236652866	-0.126739204

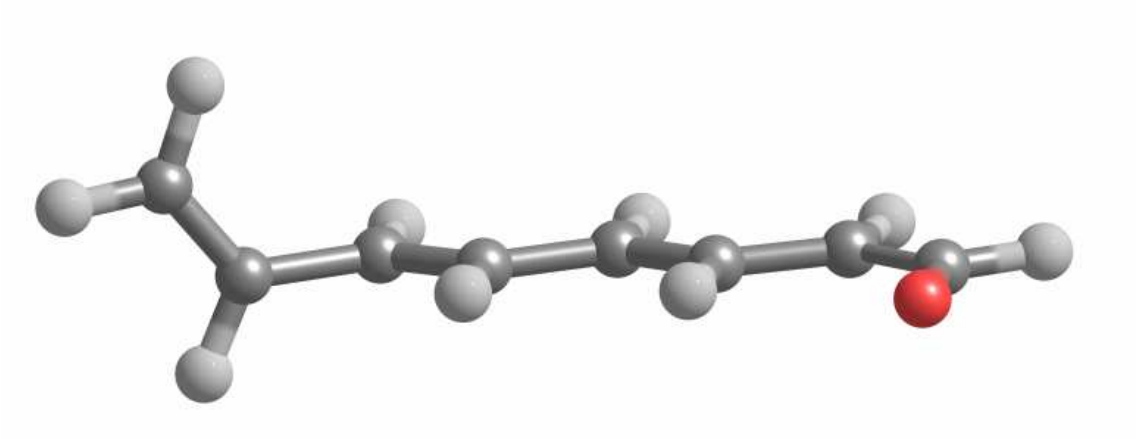

Figure 3: $^{-}$O-(CH=CH)$_3$-CH=CH$_2$ (strained)

$^{-}$O-(CH=CH)$_3$-CH=CH$_2$ (strained)

C	3.713861677	-0.017026280	-0.108592456
H	4.629657613	-0.643748197	-0.296781884
O	3.868966120	1.197565867	0.138067147
C	2.509107050	-0.758377094	-0.191120013
H	2.591277833	-1.821619320	-0.419552898
C	1.242151066	-0.185717177	0.006658973
H	1.263337626	0.884224231	0.229041839
C	0.000946179	-0.794458778	-0.042365087
H	-0.054610810	-1.863115545	-0.261658262
C	-1.227468911	-0.103045813	0.179074376
H	-1.128539795	0.965272196	0.393176741
C	-2.493640548	-0.609767878	0.156540334
H	-2.636671292	-1.671134007	-0.057899384
C	-3.719014172	0.185094946	0.405855951
H	-4.082739136	0.261904352	1.440889090
C	-4.436080847	0.828200414	-0.522154520
H	-4.143898213	0.811788798	-1.569578105
H	-5.330332690	1.395792125	-0.266450453

$^{-}$O-(CH=CH)$_4$-CH=CH$_2$ (strained)

C	-4.925088311	-0.123857786	-0.077134627
H	-5.868275201	0.468366961	-0.224656339
O	-5.019436540	-1.345404775	0.145154632
C	-3.745018883	0.665540420	-0.175649804
H	-3.872203502	1.729337642	-0.377256061
C	-2.461826377	0.136143573	-0.026052675
H	-2.431736543	-0.937445639	0.173441447
C	-1.242700282	0.802997749	-0.099599266
H	-1.246879189	1.876687568	-0.297594980
C	0.007554172	0.170164583	0.068539791

H	−0.029026039	−0.905885242	0.264552400
C	1.260716183	0.744321922	0.016836277
H	1.339118438	1.815616338	−0.176095786
C	2.477051313	0.016195125	0.202339426
H	2.360538491	−1.054322710	0.392707331
C	3.747603953	0.502852984	0.169048663
H	3.901946413	1.566584426	−0.023292030
C	4.964626556	−0.316902474	0.378190068
H	5.340813471	−0.420719576	1.404710066
C	5.652053179	−0.947275420	−0.579525711
H	5.341111568	−0.899768425	−1.620359702
H	6.541346679	−1.534325972	−0.355231553

˙O-(CH=CH)$_5$-CH=CH$_2$ (strained)

C	6.136794708	−0.257335343	0.049627040
H	7.098718816	0.307641198	0.168365342
O	6.186012579	−1.482782536	−0.149148181
C	4.976862758	0.568589494	0.152338483
H	5.136280084	1.632010281	0.329844583
C	3.683224041	0.071092182	0.035609202
H	3.617138754	−1.004455490	−0.140991456
C	2.483047569	0.780448041	0.117161959
H	2.527632719	1.856777650	0.292845503
C	1.217561659	0.188016005	−0.015176702
H	1.209189004	−0.891632450	−0.190361721
C	−0.018443656	0.814955014	0.050125660
H	−0.044447404	1.891933797	0.223188289
C	−1.253840673	0.141585331	−0.095933018
H	−1.191649480	−0.937083225	−0.267720094
C	−2.515580251	0.688498004	−0.047948041
H	−2.616170733	1.761576429	0.121653634
C	−3.719718699	−0.069746307	−0.208819614
H	−3.585982221	−1.141555948	−0.376267733
C	−4.994147661	0.400312025	−0.175617009
H	−5.159599597	1.466034248	−0.005414914
C	−6.202348857	−0.439475826	−0.356577093
H	−6.582455497	−0.568619942	−1.377644427
C	−6.871546738	−1.056083102	0.622125286
H	−6.552172482	−0.980313620	1.658575720
H	−7.754812420	−1.659167775	0.419847592

Gas phase energies

Raw data used for the elaboration of table 1. H^+ contribution for enthalpy is 1.48 kcal.mol^{-1}

	6-311+G(3d,2p) gas phase energy (in Hartree)	in solvent (kcal.mol-1)	ZPVE and thermal contribution to ΔH (kcal.mol^{-1})	Gas phase enthalpy (kcal.mol^{-1})
$CH_3C(=O)CH_3$	-193.2306269	-121255.8	55.547	-121198.60
$CH_3C(=O)CH_2^-$	-192.6318107	-120940.15	46.774	-120831.61
Phenol	-307.576983	-193009.44	68.506	-192939.13
Phenoxide	-307.0110884	-192710.23	59.699	-192592.83
Ethanol	-155.1054459	-97330.73	52.628	-97277.59
Ethoxide	-154.4901225	-97011.25	42.329	-96901.77
methanol	-115.7732592	-72650.36	34.298	-72614.58
methoxide	-115.1518605	-72331.23	23.719	-72235.22
isopropanol	-194.4374574	-122010.5	70.642	-121940.81
isopropanoxide	-193.8257662	-121690.43	60.381	-121567.23
Acetaldehyde	-153.891863	-96570.81	37.244	-96531.44
Acetaldehyde enol	-153.8757651	-96559.24	37.742	-96520.84
Acetaldehyde enolate	-153.298365	-96260.35	28.537	-96167.72
Methane	-40.5372885		30.104	-25407.45
CH_3^+	-39.8566143		19.528	-24990.90
H_2O	-76.464347126		15.504	-47966.64
HO^-	-75.831186357		7.022	-47577.81

Gas phase energies (in hartree) of protonated and deprotonated methanol vinylogues

n	$CH_3-(CH=CH)_n-OH$	$CH_3-(CH=CH)_n-O^-$	Diff (kcal.mol^{-1})
0	-115.7732592	-115.1518605	389.9
1	-193.2033712	-192.6236726	363.8
2	-270.6340498	-270.0744557	351.2
3	-348.0659263	-347.5194334	342.9
4	-425.4981842	-424.9610436	337.1
5	-502.9306187	-502.4005520	332.6

Gas phase energies (in hartree) of protonated and deprotonated cyclohexanol vinylogues

n	$C_6H_{11}-(CH=CH)_n-OH$	$C_6H_{11}-(CH=CH)_n-O^-$	Diff (kcal.mol^{-1})
0	-311.2080645	-310.5973787	383.2
1	-388.6285742	-388.0538599	360.6
2	-466.0589996	-465.5021263	349.4
3	-543.4908522	-542.9461008	341.8
4	-620.9231195	-620.3871279	336.3
5	-698.3555547	-697.8262389	332.2

Gas phase energies (in hartree) of relaxed protonated and deprotonated 2,4-cyclohexadien-1-ol vinylogues

n	$C_6H_6-(CH=CH)_n-OH$	$C_6H_6-(CH=CH)_n-O^-$	Diff (kcal.mol^{-1})
0	-308.74289514	-308.13894233	379.0
1	-386.16616223	-385.59641048	357.5
2	-463.59580074	-463.03965132	349.0
3	-541.02752929	-540.48310659	341.6
4	-618.45970793	-617.92384504	336.3
5	-695.89210626	-695.36278658	332.2

Gas phase energies (in hartree) of <u>strained</u> protonated and deprotonated 2,4-cyclohexadien-1-ol vinylogues

n	$C_6H_6-(CH=CH)_n-OH$	$C_6H_6-(CH=CH)_n-O^-$	Diff (kcal.mol^{-1})
1	-386.16350027	-385.58892667	360.6
2	-463.59405197	-463.03889036	348.4
3	-541.02577150	-540.48208892	341.2
4	-618.45796549	-617.92274724	335.9
5	-695.89023742	-695.36153552	331.8

Gas phase energies (in hartree) of protonated and deprotonated phenol vinylogues

n	$Ph-(CH=CH)_n-OH$	$Ph-(CH=CH)_n-O^-$	Diff (kcal.mol^{-1})
1	-385.0010274	-384.4480672	347.0
2	-462.4330458	-461.8924057	339.3
3	-539.8651915	-539.3323749	334.3
4	-617.2975357	-616.7707858	330.5
5	-694.7286513	-694.2080948	326.7

Gas phase energies (in hartree) of <u>strained</u> protonated and deprotonated phenol vinylogues

n	Ph-(CH=CH)$_n$-OH	Ph-(CH=CH)$_n$-O$^-$	Diff (kcal.mol^{-1})
1	-384.9954605	-384.4260645	357.3
2	-462.4252832	-461.8727241	346.7
3	-539.8568366	-539.3154070	339.8
4	-617.2889318	-616.7555964	334.7
5	-694.7199189	-694.1941735	329.9

Gas phase energies (in hartree) of protonated and deprotonated enol vinylogues

n	CH_2=CH - (CH=CH)$_n$-OH	CH_2=CH - (CH=CH)$_n$-O$^-$	Diff (kcal.mol^{-1})
0	-153.8757651	-153.2983650	362.3
1	-231.3027053	-230.7453670	349.7
2	-308.7344032	-308.1889182	342.3
3	-386.1665298	-385.6296085	336.9
4	-463.5988809	-463.0684968	332.8
5	-541.0313443	-540.5061387	329.6

Gas phase energies (in hartree) of <u>strained</u> protonated and deprotonated enol vinylogues

n	CH_2=CH - (CH=CH)$_n$-OH	CH_2=CH - (CH=CH)$_n$-O$^-$	Diff (kcal.mol^{-1})
1	-231.2909606	-230.7199525	358.3
2	-308.7211341	-308.1652073	348.8
3	-386.1529604	-385.6080730	341.9
4	-463.5851228	-463.0484140	336.8
5	-541.0174903	-540.4871241	332.8

Gas phase energies (in hartree) of protonated and deprotonated methane vinylogues

n	H-(CH=CH)$_n$-CH_3	H-(CH=CH)$_n$-CH_2^-	Diff (kcal.mol^{-1})
0	-40.5372885	-39.8566143	427.1
1	-117.9532840	-117.3215946	396.4
2	-195.3828791	-194.7780419	379.5
3	-272.8142536	-272.2267988	368.6
4	-350.2462601	-349.6712419	360.8
5	-427.6785462	-427.1129345	354.9

Gas phase energies (in hartree) of protonated and deprotonated acetaldehyde vinylogues

n	$HCO-(CH=CH)_n-CH_3$	$HCO-(CH=CH)_n-CH_2^-$	Diff (kcal.mol^{-1})
0	-153.8918630	-153.2983650	372.4
1	-231.3172574	-230.7453670	358.9
2	-308.7489857	-308.1889182	351.4
3	-386.1811176	-385.6296085	346.1
4	-463.6134660	-463.0684968	342.0
5	-541.0459317	-540.5061387	338.7

Gas phase energies (in hartree) of <u>strained</u> protonated and deprotonated acetaldehyde vinylogues

n	$HCO-(CH=CH)_n-CH_3$	$HCO-(CH=CH)_n-CH_2^-$	Diff (kcal.mol^{-1})
0	-153.8918630	-153.2315259	414.4
1	-231.3053220	-230.6926489	384.5
2	-308.7348126	-308.1447995	370.2
3	-386.1661454	-385.5906483	361.1
4	-463.5981328	-463.0331203	354.6
5	-541.0303978	-540.4733784	349.5

Solution energies (kcal.mol^{1}) of protonated and deprotonated methanol vinylogues

n	$CH_3-(CH=CH)_n-OH$	$CH_3-(CH=CH)_n-O^-$	Diff (kcal.mol^{-1})
0	-72650.36	-72331.23	319.13
1	-121237.78	-120935.17	302.61
2	-169825.96	-169528.59	297.37
3	-218414.71	-218120.03	294.68
4	-267003.56	-266710.77	292.79
5	-315592.73	-315300.76	291.97

Solution energies (kcal.mol^{1}) of protonated and deprotonated phenol vinylogues

n	$Ph-(CH=CH)_n-OH$	$Ph-(CH=CH)_n-O^-$	Diff (kcal.mol^{-1})
1	-241593.11	-241296.65	296.46
2	-290181.91	-289888.12	293.79
3	-338770.88	-338478.22	292.66
4	-387359.74	-387068.01	291.73
5	-435948.53	-435657.61	290.92

Solution energies (kcal.mol^{-1}) of <u>strained</u> protonated and deprotonated phenol vinylogues

n	Ph–(CH=CH)$_n$–OH	Ph–(CH=CH)$_n$–O$^-$	Diff (kcal.mol^{-1})
1	–241588.76	–241287.10	301.66
2	–290176.53	–289879.21	297.32
3	–338764.91	–338470.05	294.86
4	–387353.48	–387060.45	293.03
5	–435942.74	–435650.41	292.33

Solution energies (kcal.mol^{-1}) of protonated and deprotonated enol vinylogues

n	CH_2=CH –(CH=CH)$_n$–OH	CH_2=CH –(CH=CH)$_n$–O$^-$	Diff (kcal.mol^{-1})
0	–96559.24	–96260.35	298.89
1	–145145.87	–144850.64	295.23
2	–193734.36	–193440.78	293.58
3	–242323.15	–242030.67	292.48
4	–290912.19	–290620.23	291.96
5	–339501.17	–339209.58	291.59

Solution energies (kcal.mol^{-1}) of <u>strained</u> protonated and deprotonated enol vinylogues

n	CH_2=CH –(CH=CH)$_n$–OH	CH_2=CH –(CH=CH)$_n$–O$^-$	Diff (kcal.mol^{-1})
1	–145138.45	–144838.23	300.22
2	–193725.83	–193429.25	296.58
3	–242315.29	–242019.92	295.37
4	–290903.18	–290609.91	293.27
5	–339492.34	–339199.58	292.76

Solution energies (kcal.mol^{-1}) of protonated and deprotonated methane vinylogues

n	H–(CH=CH)$_n$–CH_3	H–(CH=CH)$_n$–CH_2^-	Diff (kcal.mol^{-1})
0	–25435.35	–25079.54	355.81
1	–74014.38	–73677.27	337.11
2	–122601.39	–122274.33	327.06
3	–171189.69	–170868.50	321.19
4	–219778.30	–219461.17	317.13
5	–268367.33	–268052.86	314.47

Solution energies (kcal.mol^{1}) of protonated and deprotonated acetaldehyde vinylogues

n	HCO–(CH=CH)$_n$–CH$_3$	HCO–(CH=CH)$_n$–CH$_2^-$	Diff (kcal.mol^{-1})
0	–96570.81	–96260.35	310.46
1	–145155.13	–144850.64	304.49
2	–193744.02	–193440.78	303.24
3	–242332.96	–242030.67	302.29
4	–290922.08	–290620.23	301.85
5	–339510.83	–339209.58	301.25

Solution energies (kcal.mol^{1}) of <u>strained</u> protonated and deprotonated acetaldehyde vinylogues

n	HCO–(CH=CH)$_n$–CH$_3$	HCO–(CH=CH)$_n$–CH$_2^-$	Diff (kcal.mol^{-1})
0	–96570.81	–96213.83	356.98
1	–145147.62	–144814.21	333.41
2	–193734.64	–193410.08	324.56
3	–242322.67	–242003.74	318.93
4	–290911.66	–290595.79	315.87
5	–339500.44	–339186.96	313.48

Dependence of gas phase acidity of 2,4-cyclohexadien-1-ol (n=1) vinylogue (open symbols) and cyclohexanologue (n=1) vinyvinylogues (closed symbols) with the dihedral angle between the ring and the OH group, computed at the B3LYP/6-31G(d,p) level. All energy values in kcal.mol^{-1}, dihedral angles in degrees.