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New 1*H*-Benzimidazole-2-yl hydrazones with combined antiparasitic and antioxidant activity

Maria A. Argirova[a], Miglena K. Georgieva[b], Nadya G. Hristova-Avakumova[c], Dimitar I. Vuchev[d], Galya V. Popova-Daskalova[d], Kameliya K. Anichina[e], Denitsa Y. Yancheva[a*]

[a] *Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Acad. G. Bonchev Str., build. 9, 1113 Sofia, Bulgaria*

[b] *LAQV-REQUIMTE, Department of Chemistry, NOVA School of Science and Technology, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal*

[c] *Department of Medical Physics and Biophysics, Faculty of Medicine, Medical University of Sofia, 2 Zdrave Str., 1431 Sofia, Bulgaria*

[d] *Department of Infectious diseases, Parasitology and Tropical medicine, Medical University, 15-A Vassil Aprilov Boulevard, 4002 Plovdiv, Bulgaria*

[e] *University of Chemical Technology and Metallurgy, 8 Kliment Ohridski Blvd., 1756 Sofia, Bulgaria*

[*] *Corresponding author: denitsa.pantaleeva@orgchm.bas.bg (D. Yancheva)*

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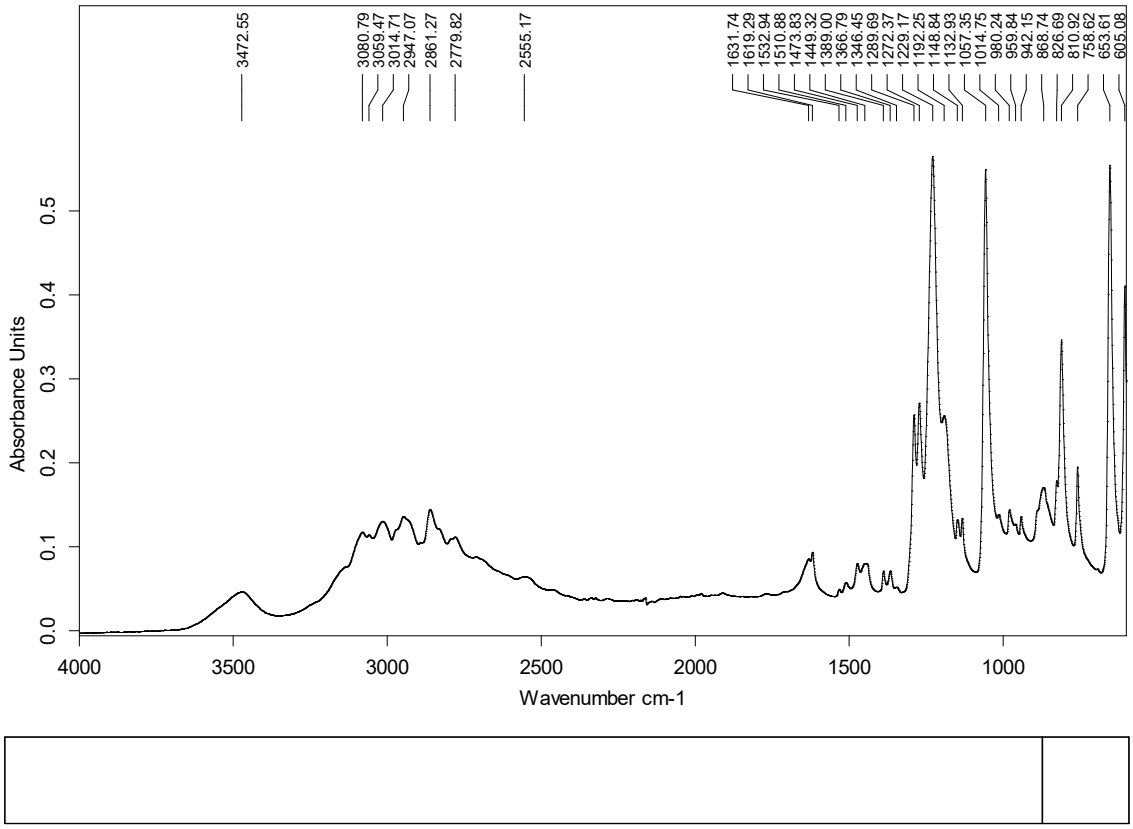

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Fig. S1. IR spectrum of compound **3**

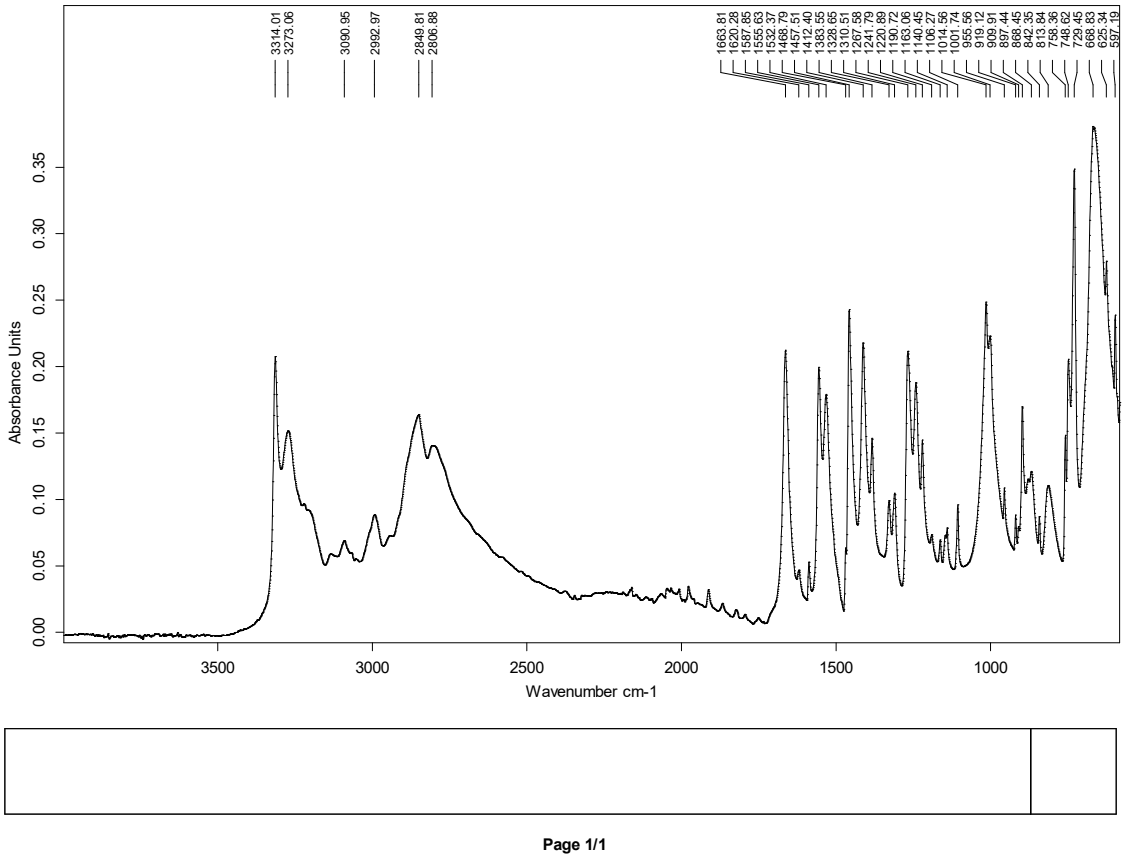

Fig. S2. IR spectrum of compound **4**

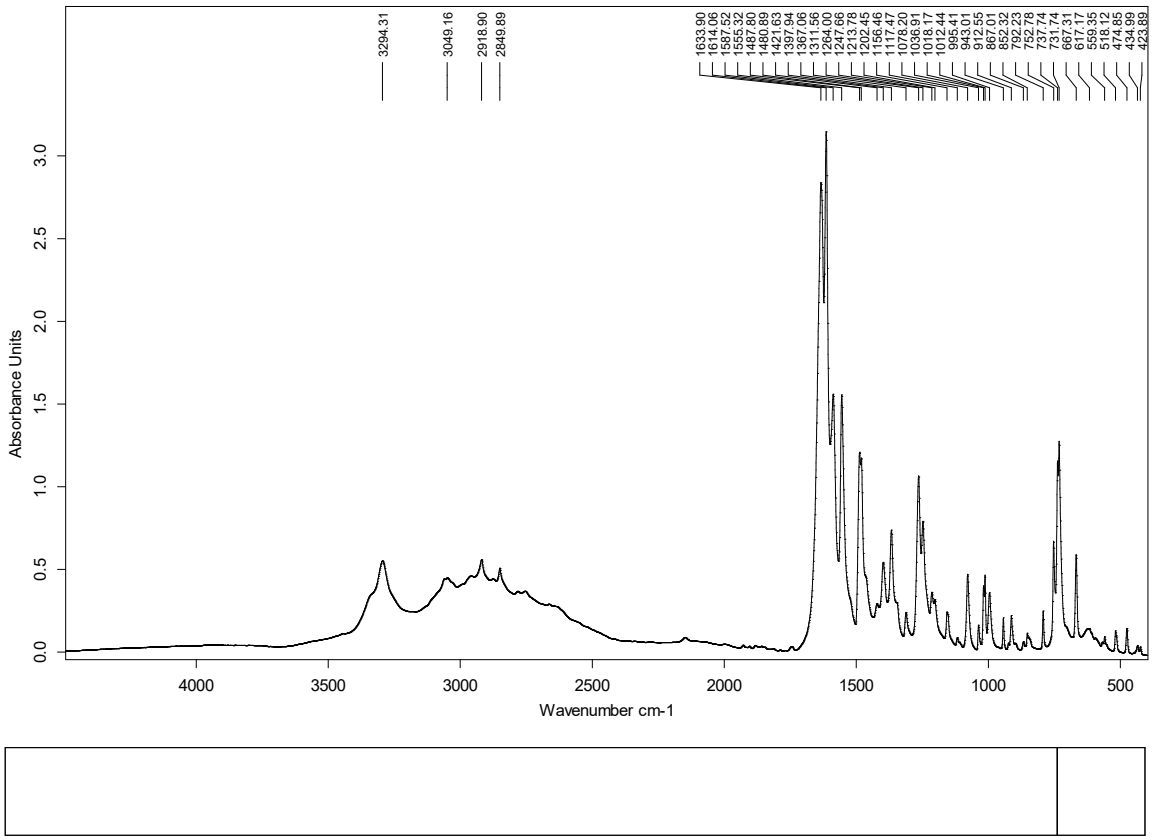

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Fig. S3. IR spectrum of compound **5a**

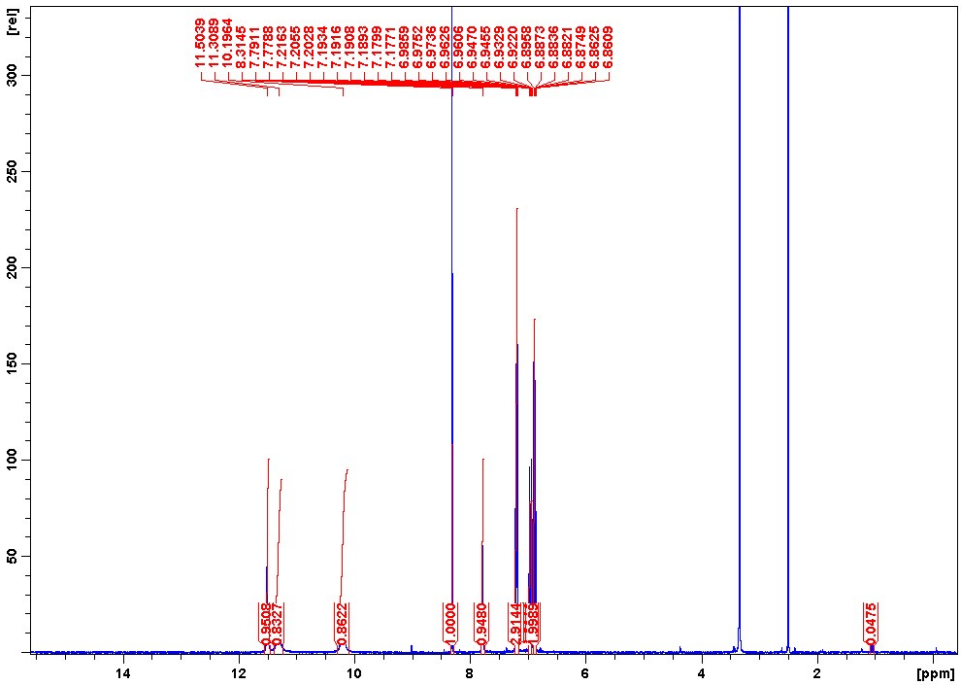

Fig. S4. ^{1}H NMR spectrum of compound **5a**

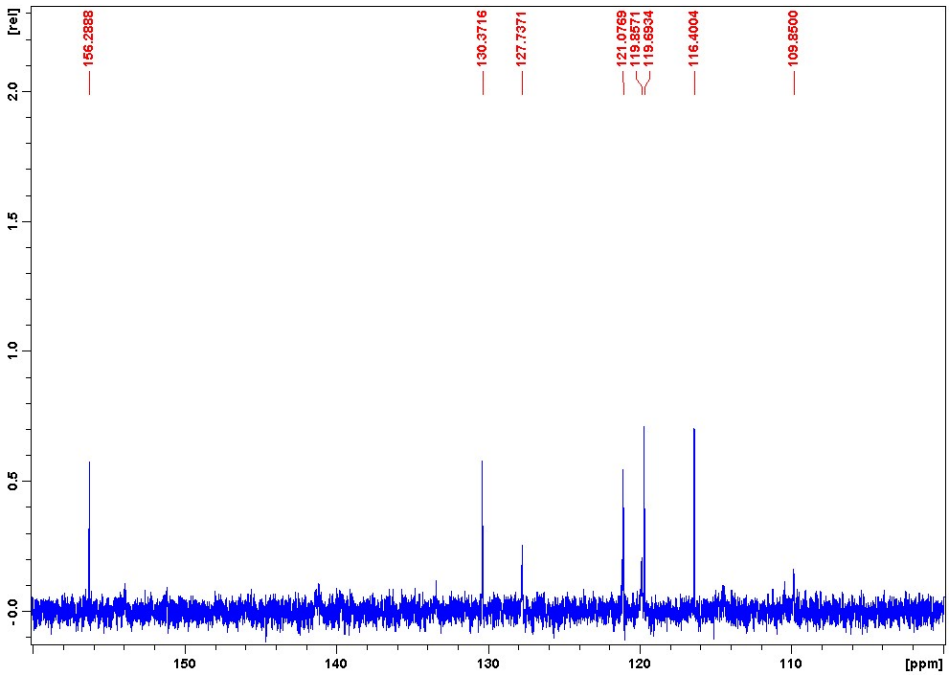

Fig. S5. ^{13}C NMR spectrum of compound **5a**

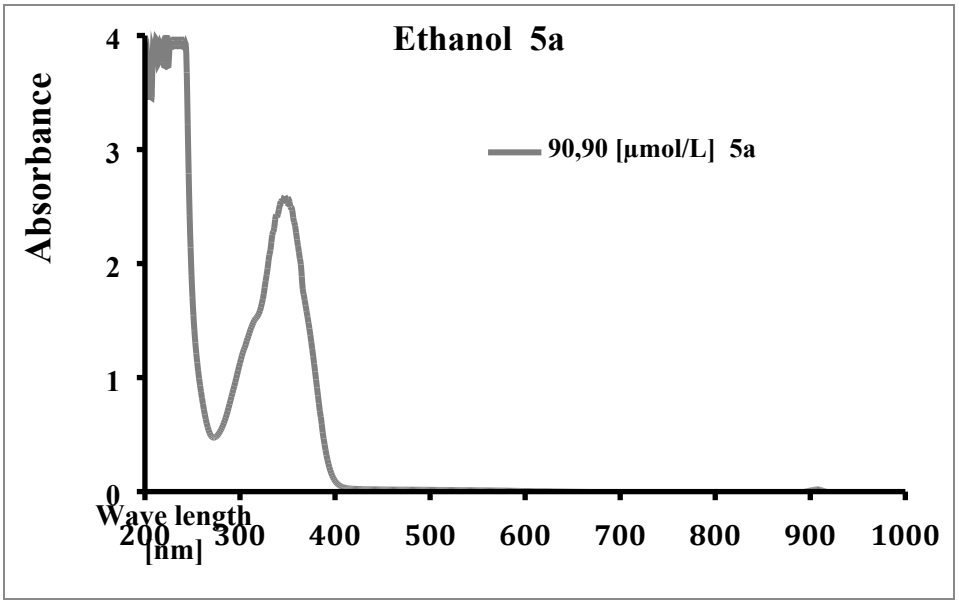

Fig. S6. UV spectrum of compound **5a** in ethanol

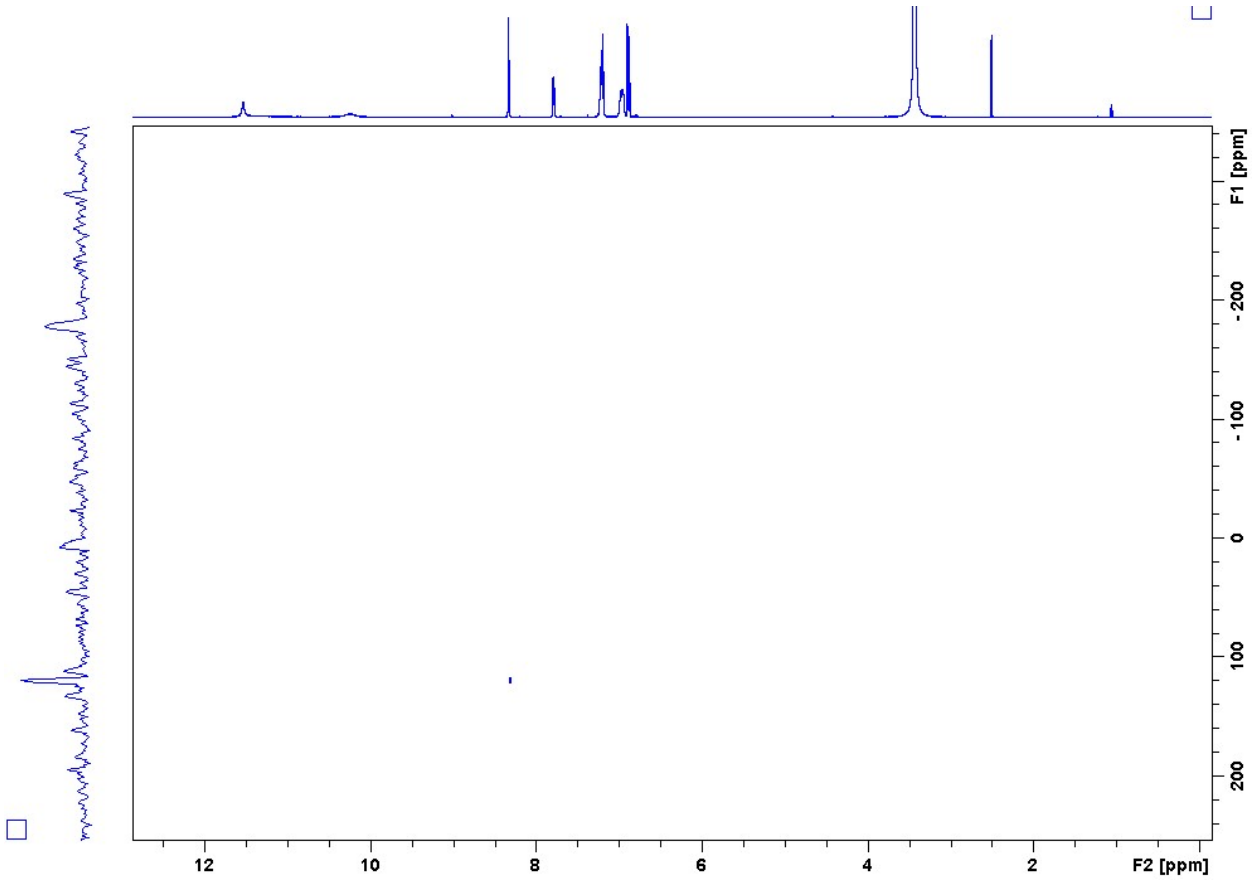

Fig. S7. ^{15}N NMR spectrum of compound **5a**

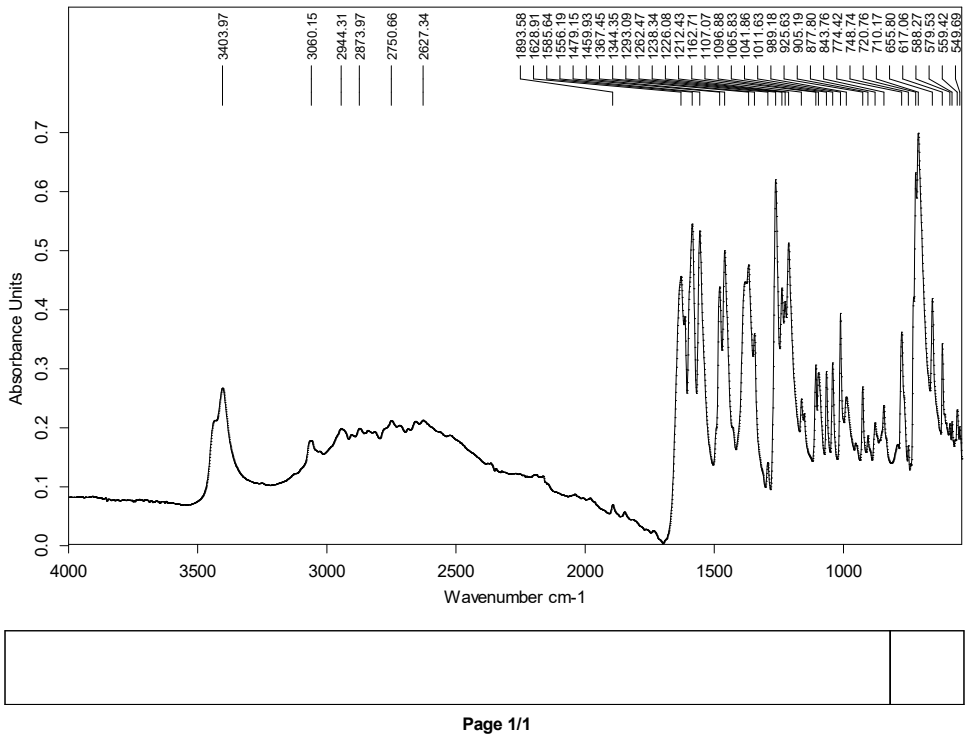

Fig. S8a. IR spectrum of compound **5b**

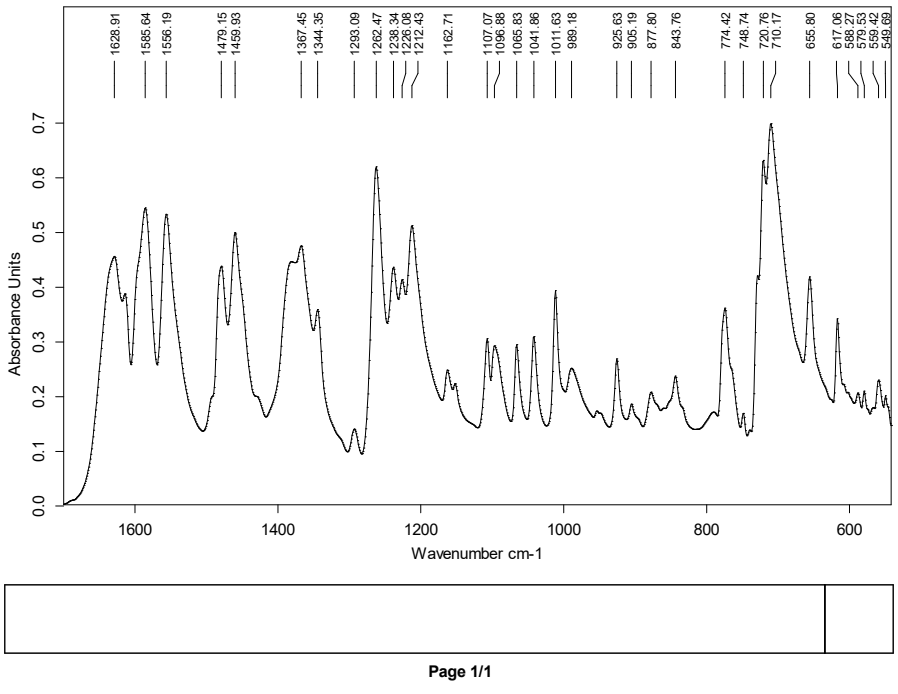

Fig. S8b. IR spectrum of compound **5b**

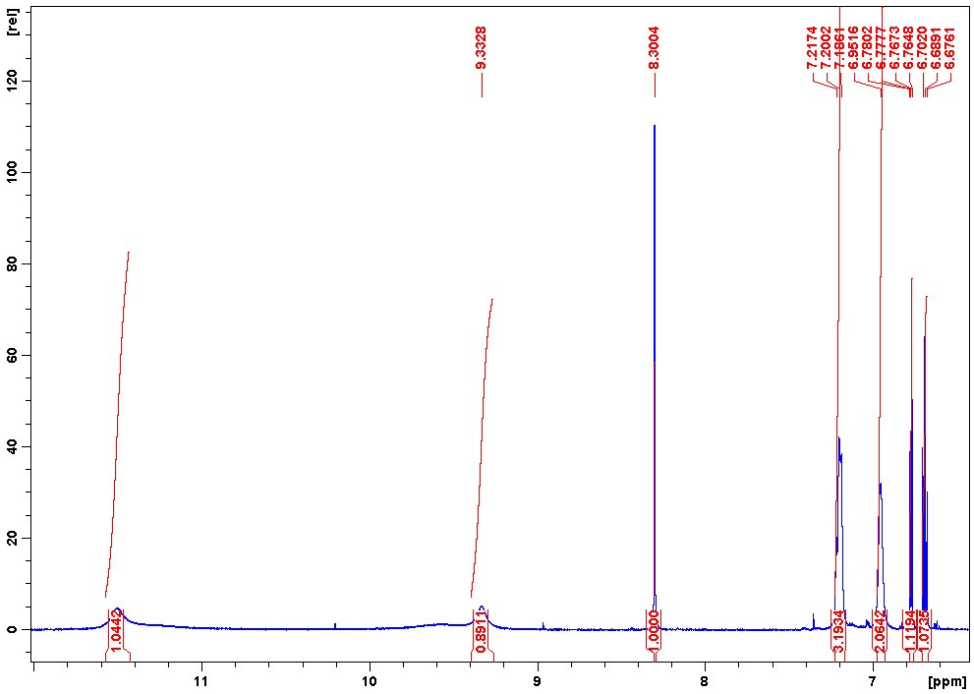

Fig. S9. ^{1}H NMR spectrum of compound **5b**

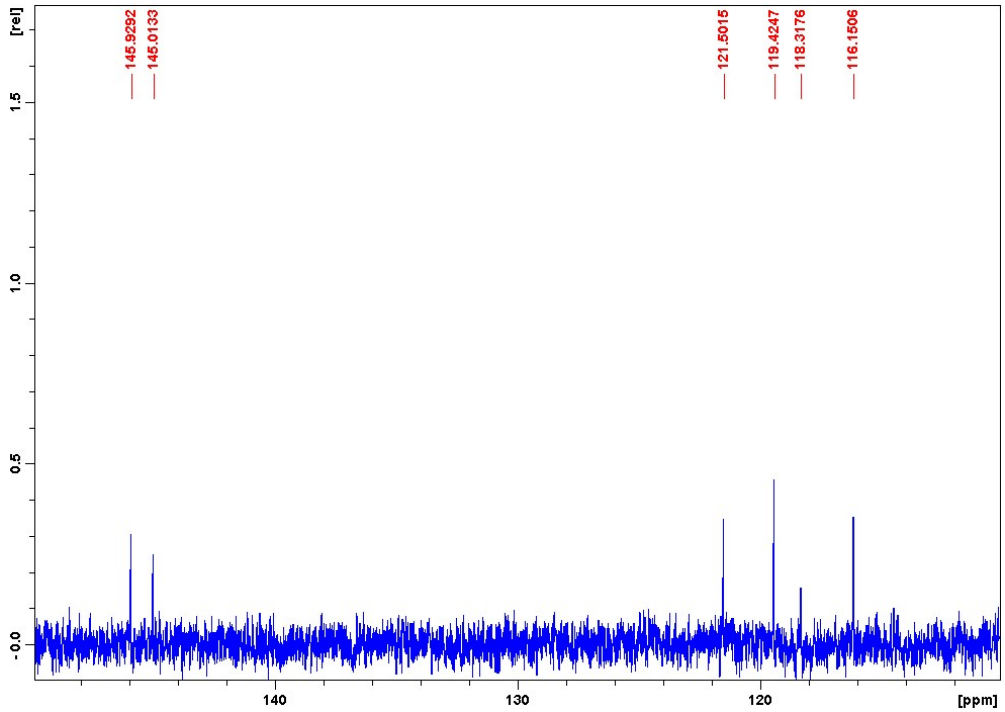

Fig. S10. ^{13}C NMR spectrum of compound **5b**

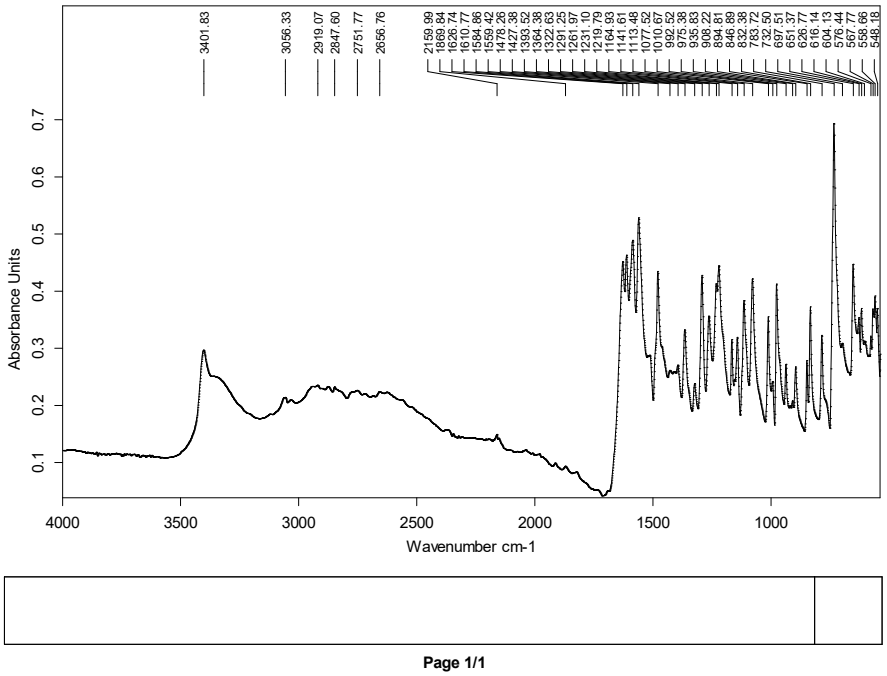

Fig. S11a. IR spectrum of compound **5c**

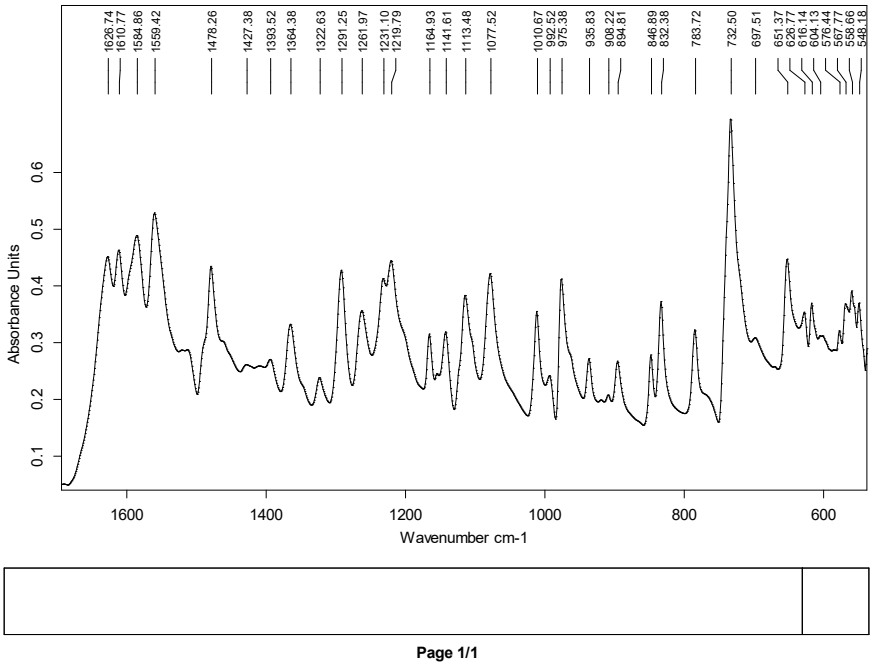

Fig. S11b. IR spectrum of compound **5c**

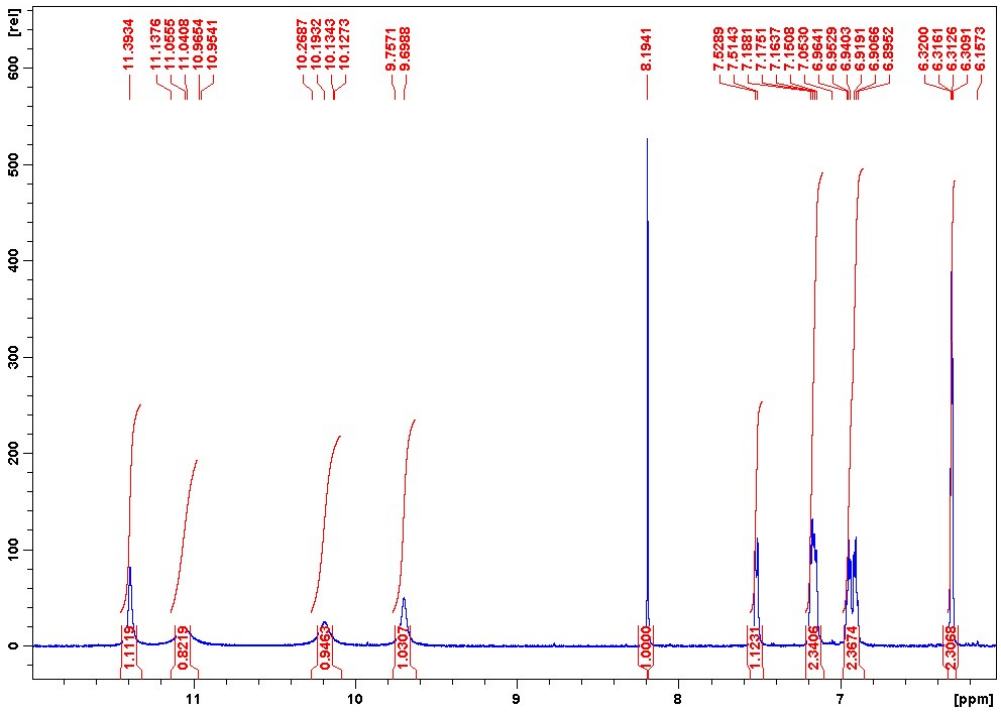

Fig. S12. ^{1}H NMR spectrum of compound **5c**

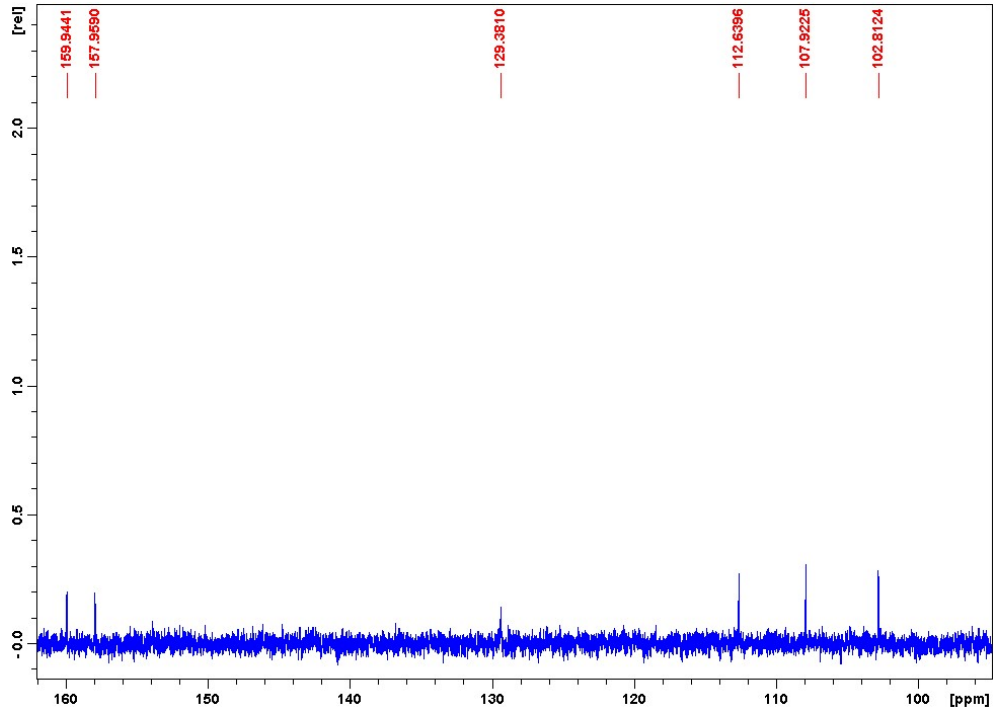

Fig. S13. ^{13}C NMR spectrum of compound **5c**

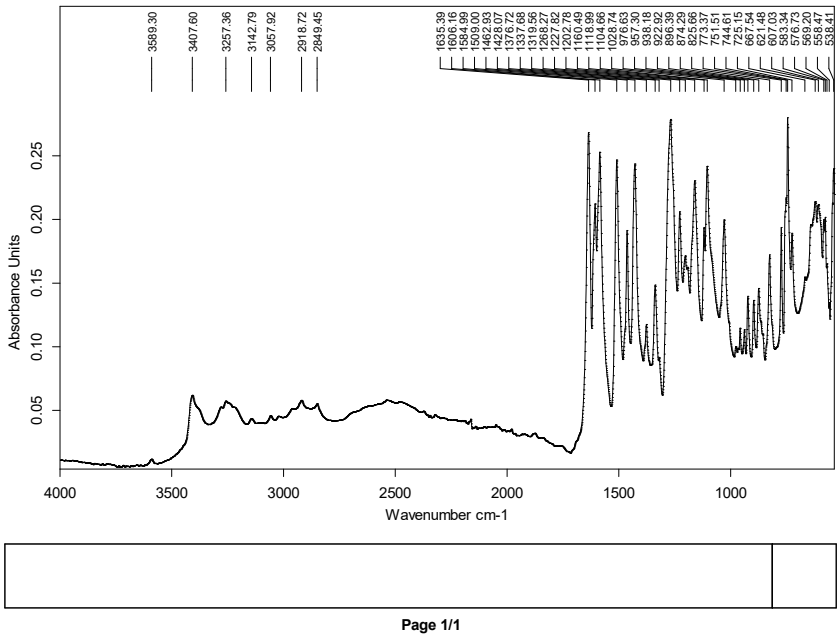

Fig. S14a. IR spectrum of compound **5d**

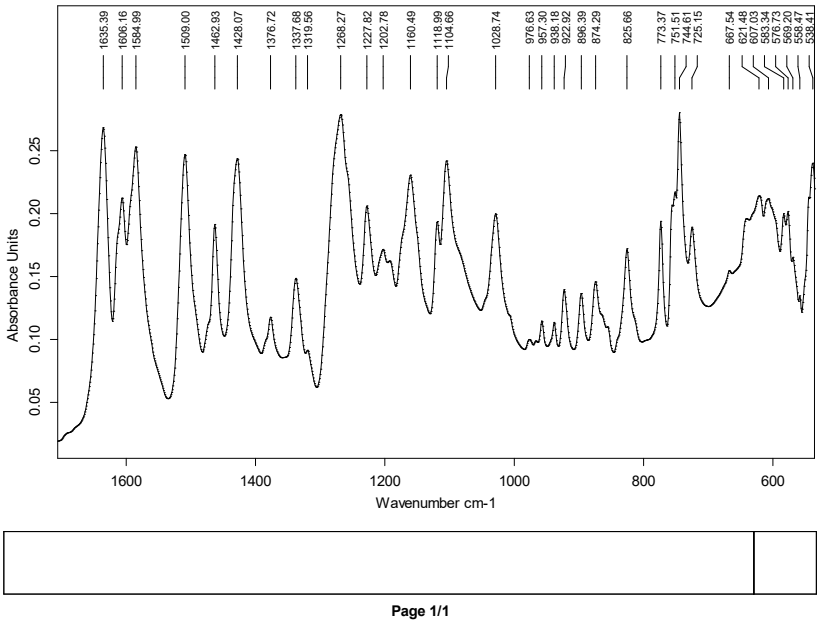

Fig. S14b. IR spectrum of compound **5d**

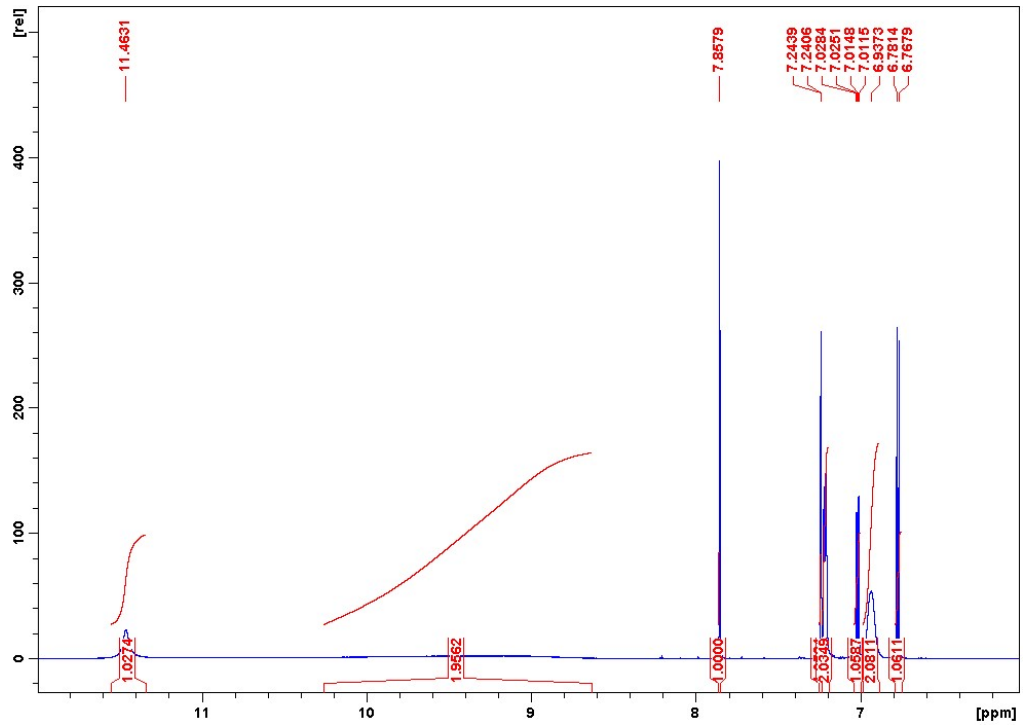

Fig. S15. ^{1}H NMR spectrum of compound **5d**

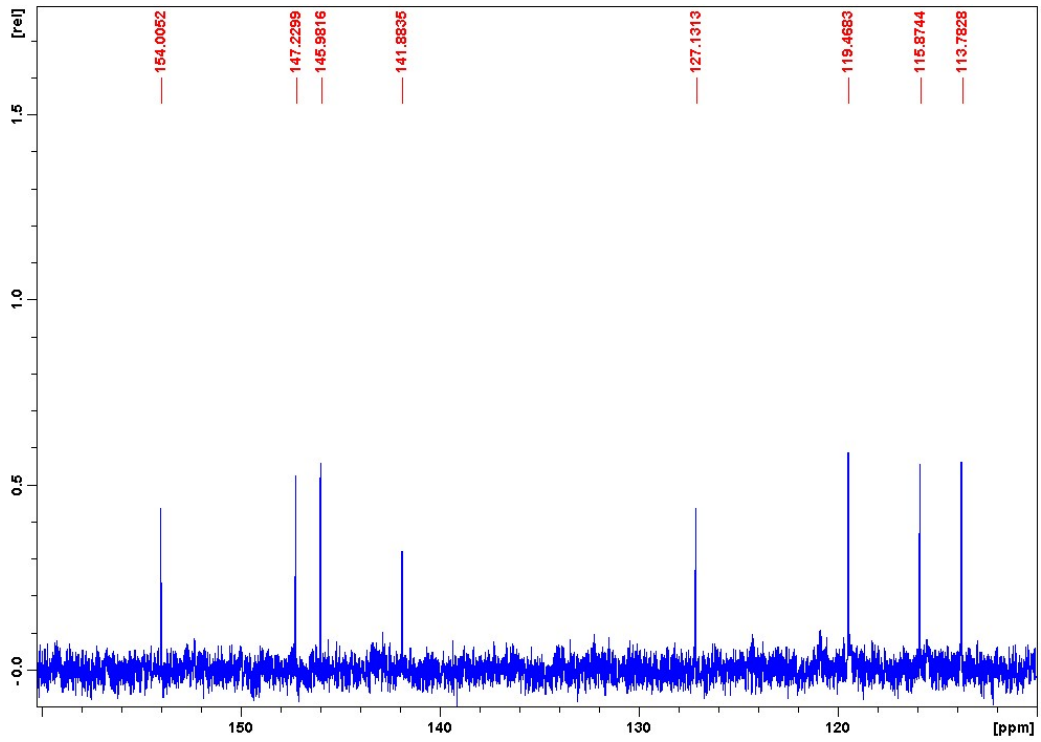

Fig. S16. ^{13}C NMR spectrum of compound **5d**

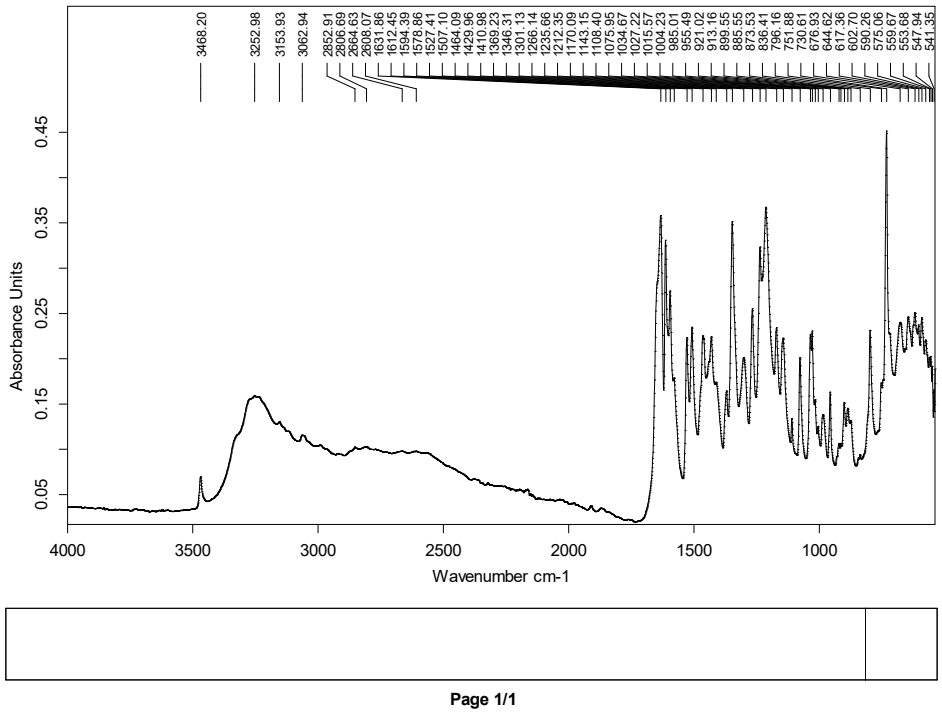

Fig. S17a. IR spectrum of compound **5e**

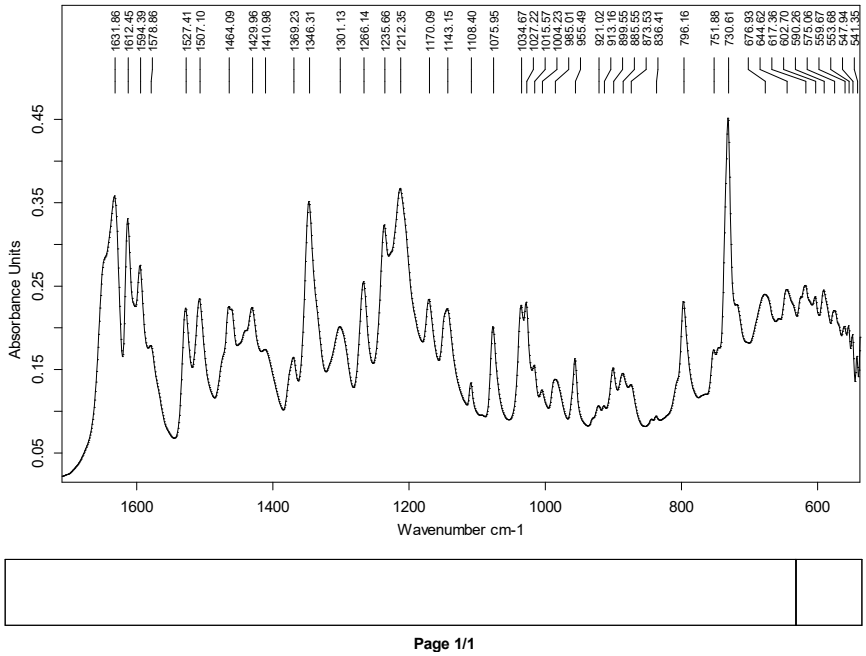

Fig. S17b. IR spectrum of compound **5e**

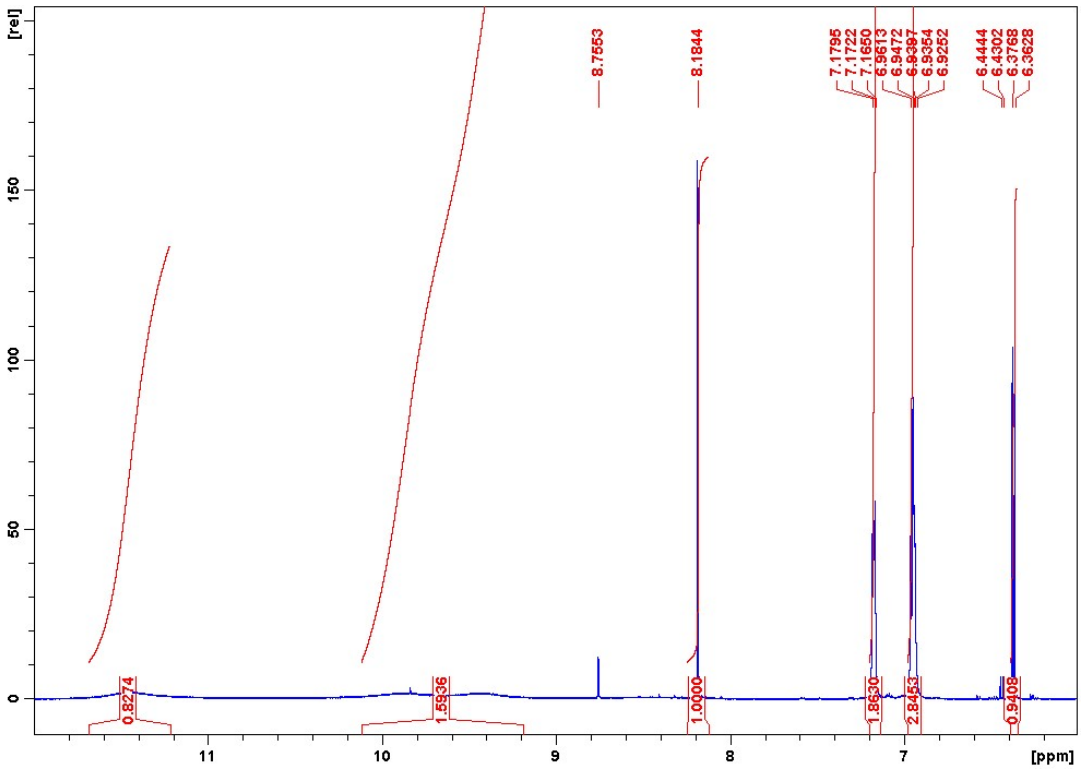

Fig. S18. ^{1}H NMR spectrum of compound **5e**

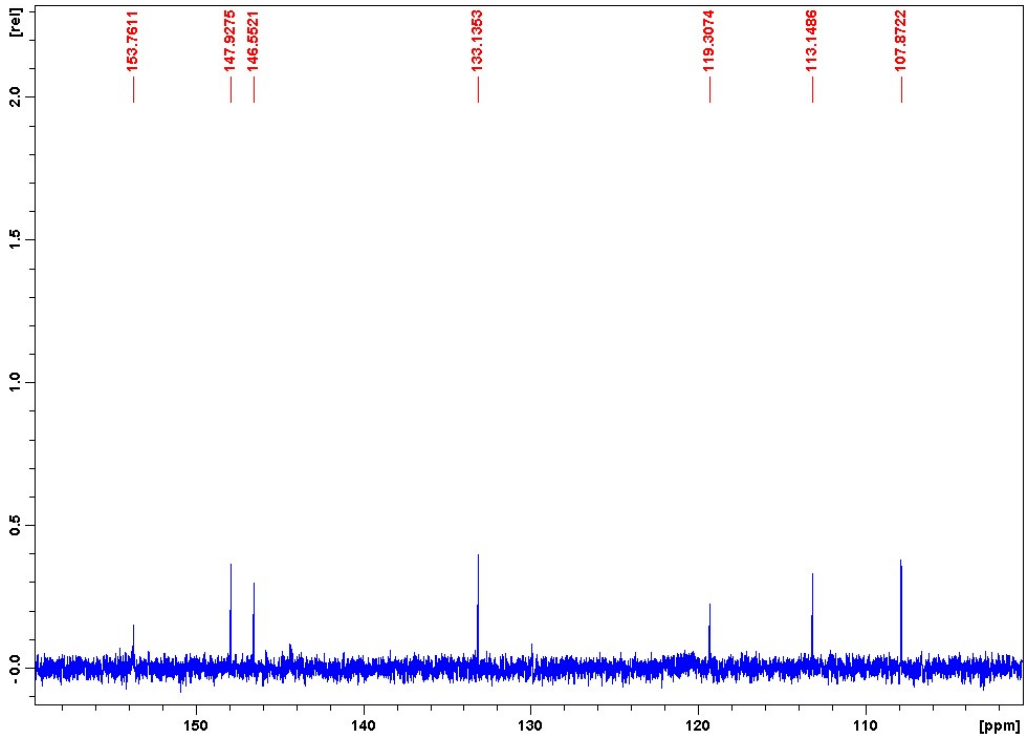

Fig. S19. ^{13}C NMR spectrum of compound **5e**

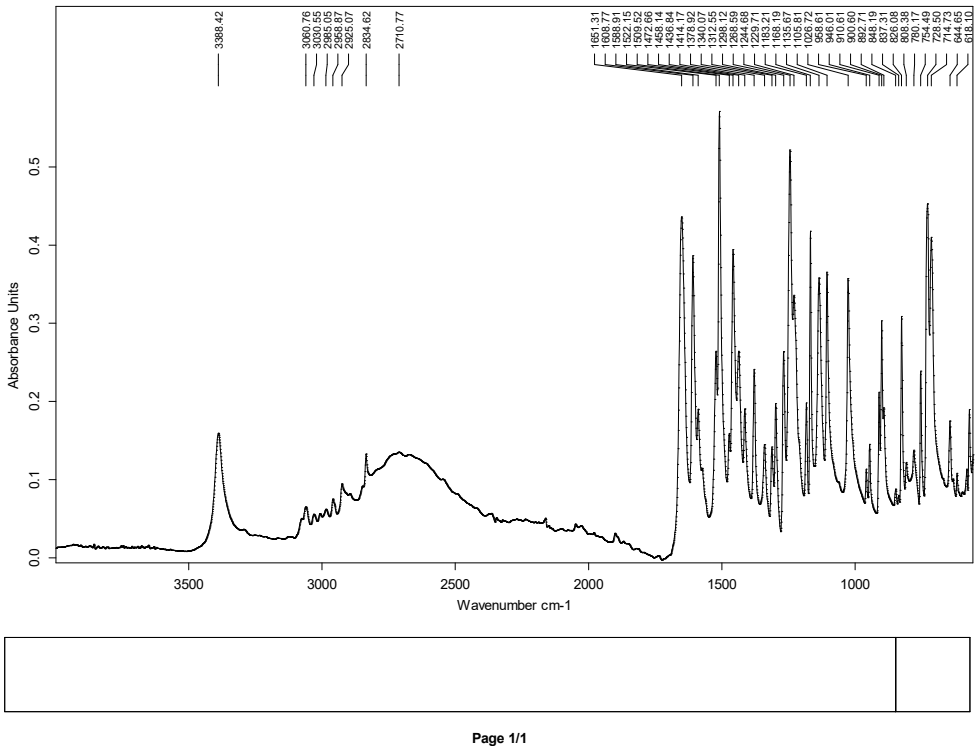

Fig. S20a. IR spectrum of compound **5f**

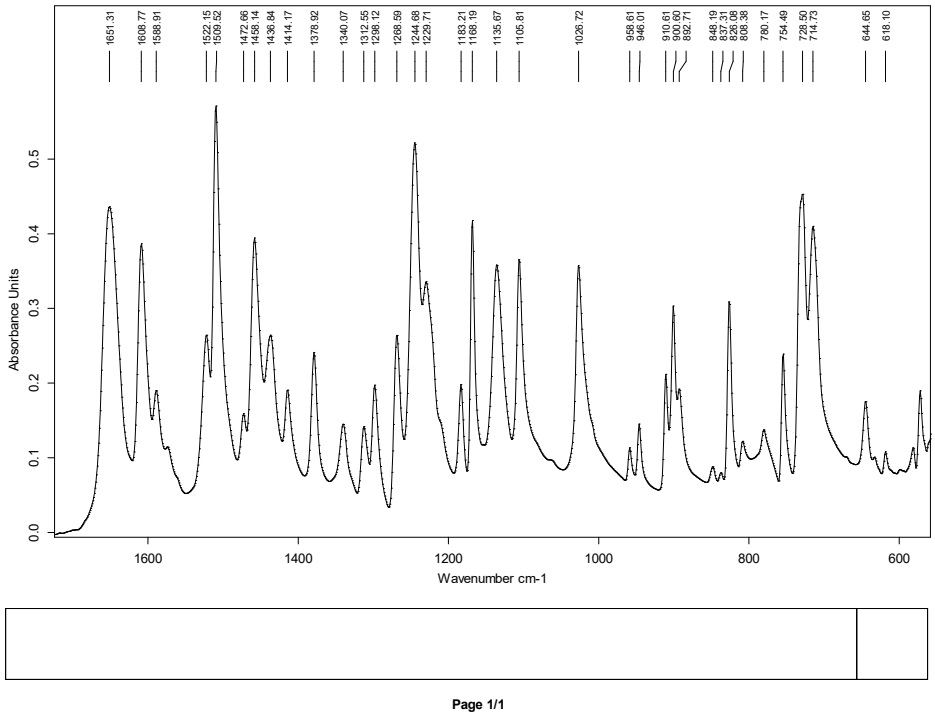

Fig. S20b. IR spectrum of compound **5f**

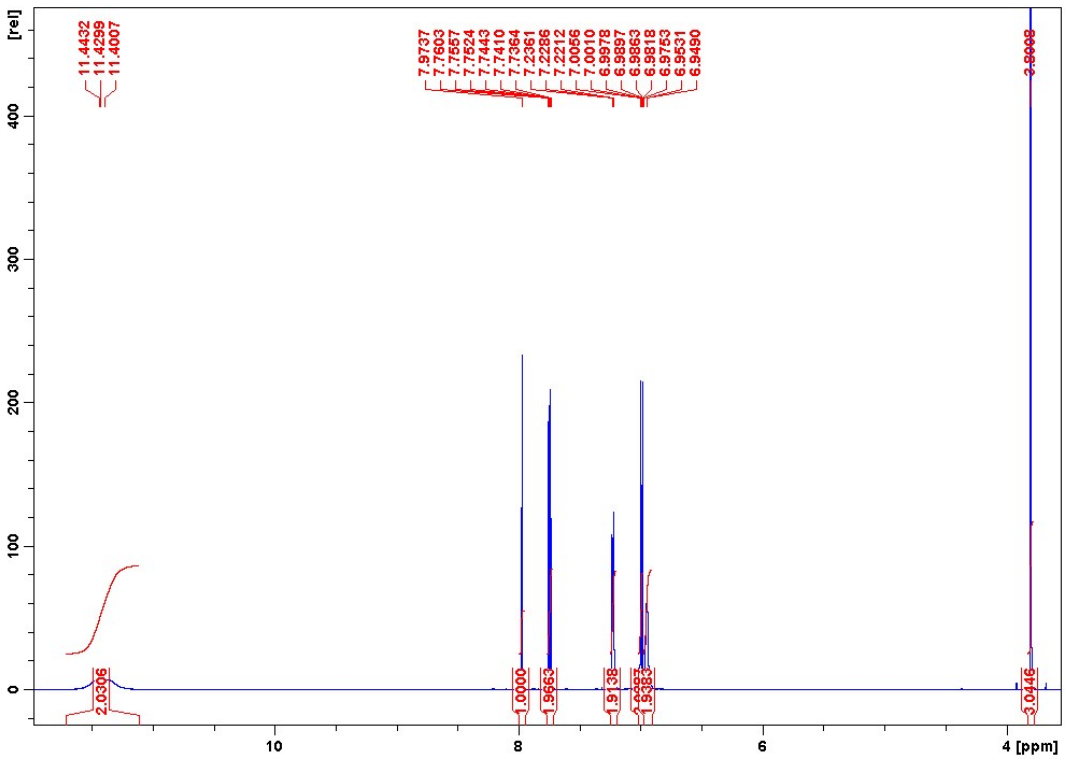

Fig. S21. ^{1}H NMR spectrum of compound **5f**

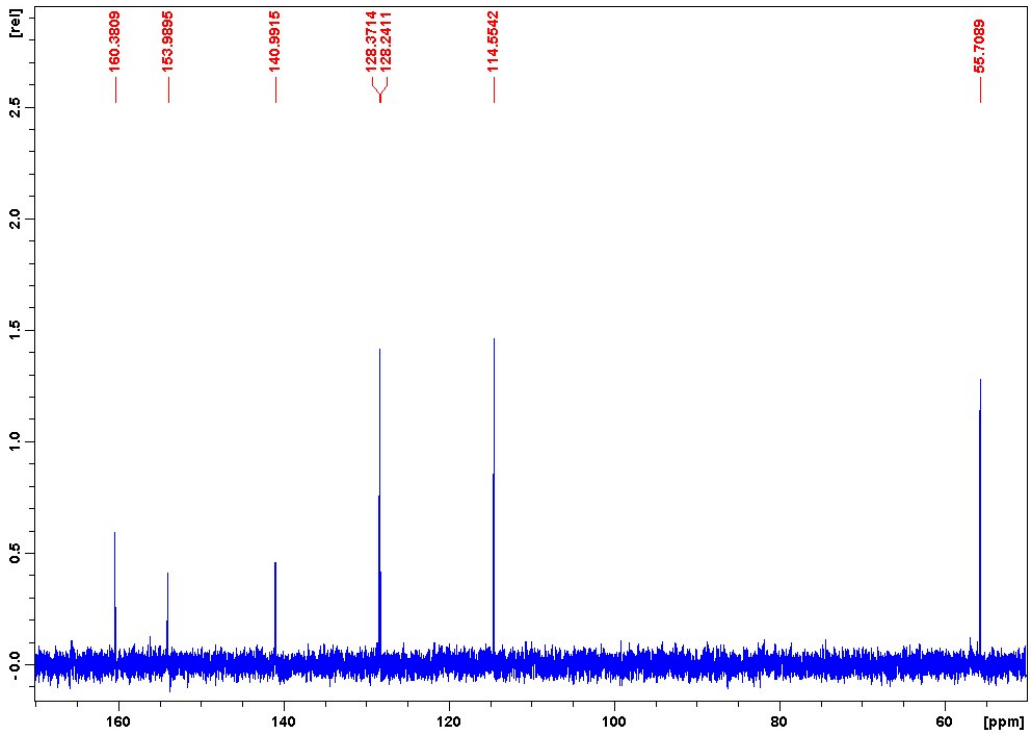

Fig. S22. ^{13}C NMR spectrum of compound **5f**

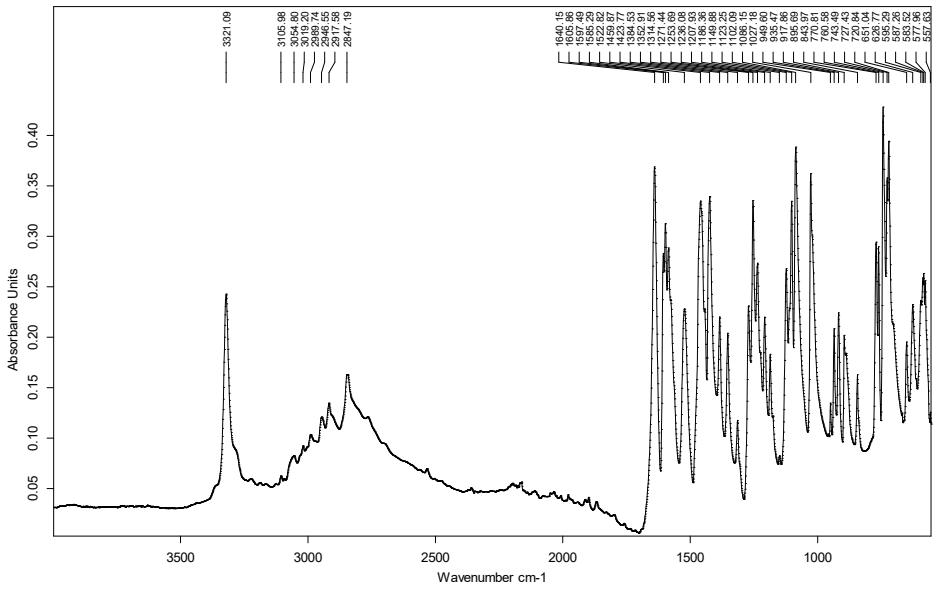

Fig. S23a. IR spectrum of compound **5g**

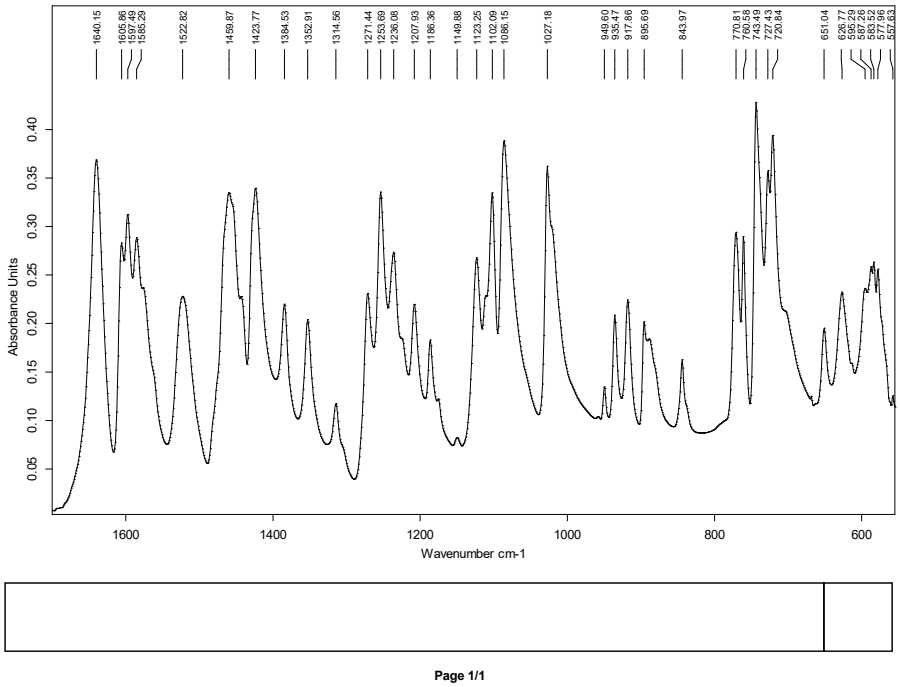

Fig. S23b. IR spectrum of compound **5g**

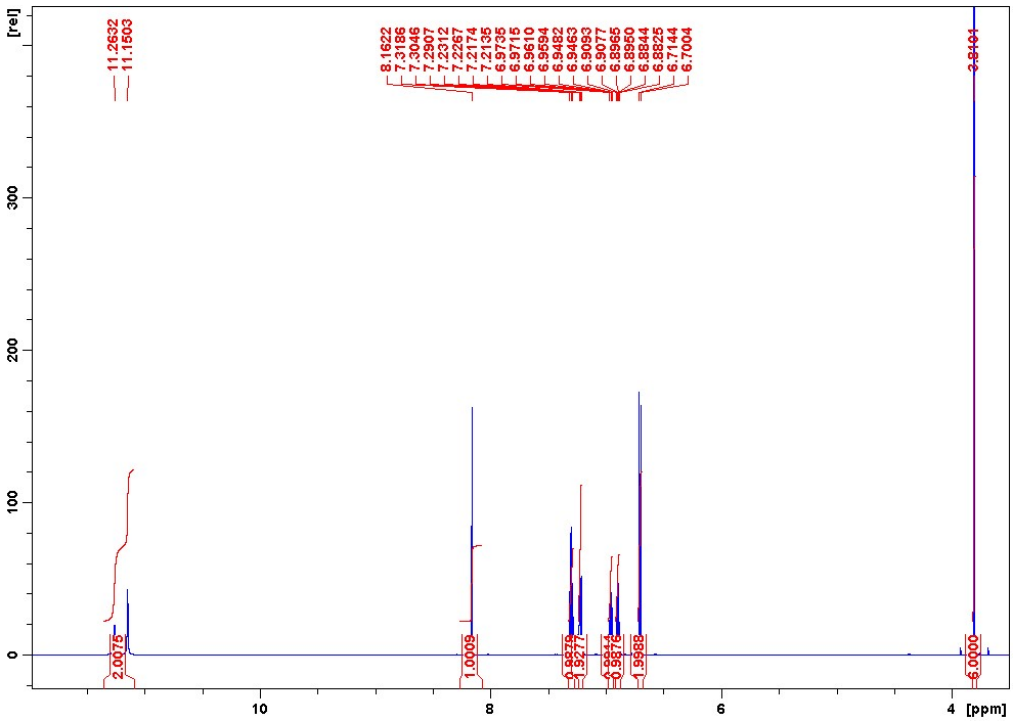

Fig. S24. ^{1}H NMR spectrum of compound **5g**

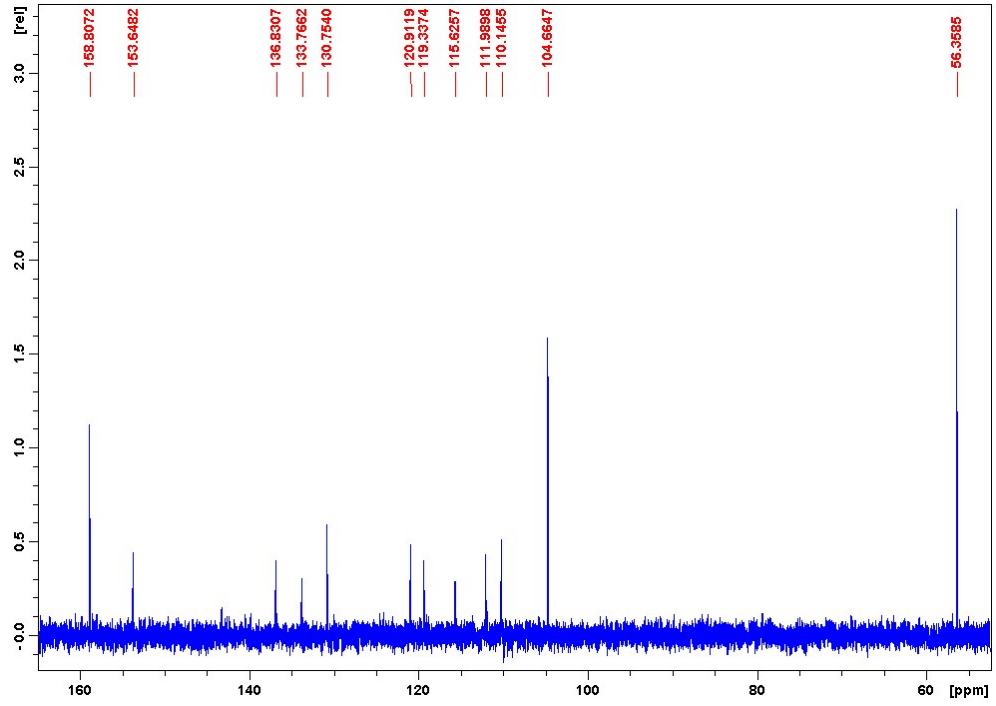

Fig. S25. ^{13}C NMR spectrum of compound **5g**

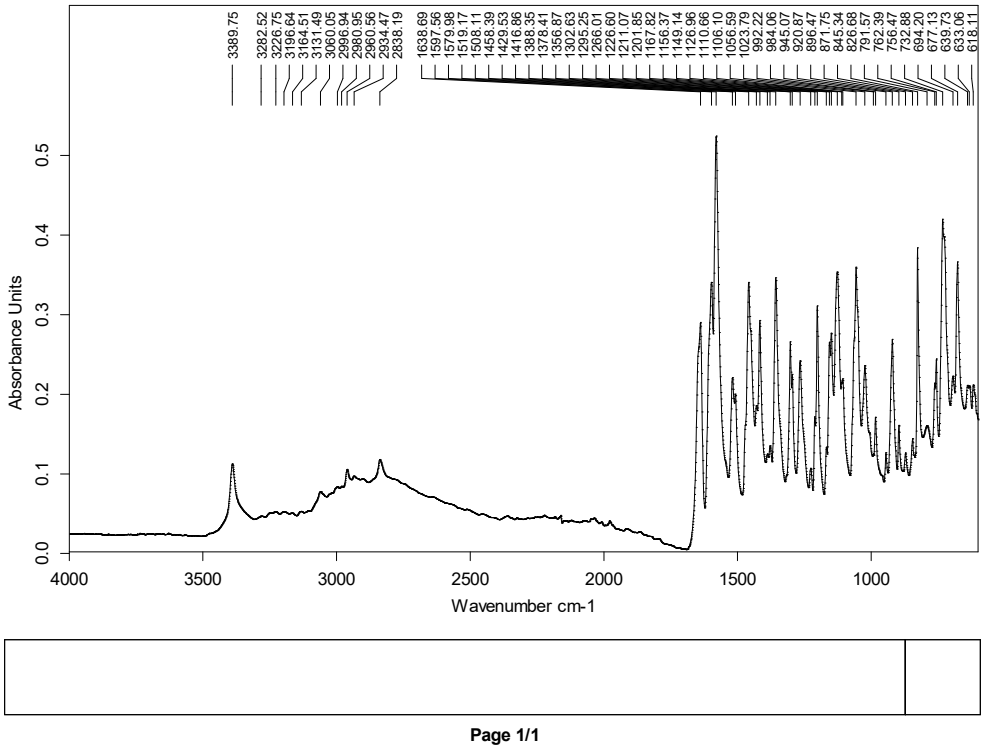

Fig. S26a. IR spectrum of compound **5h**

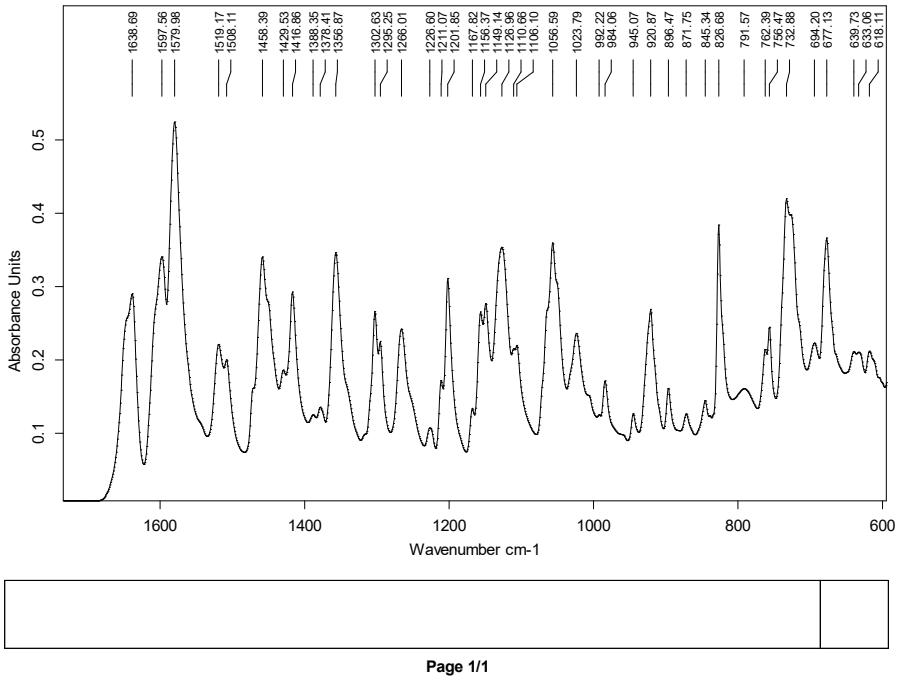

Fig. S26b. IR spectrum of compound **5h**

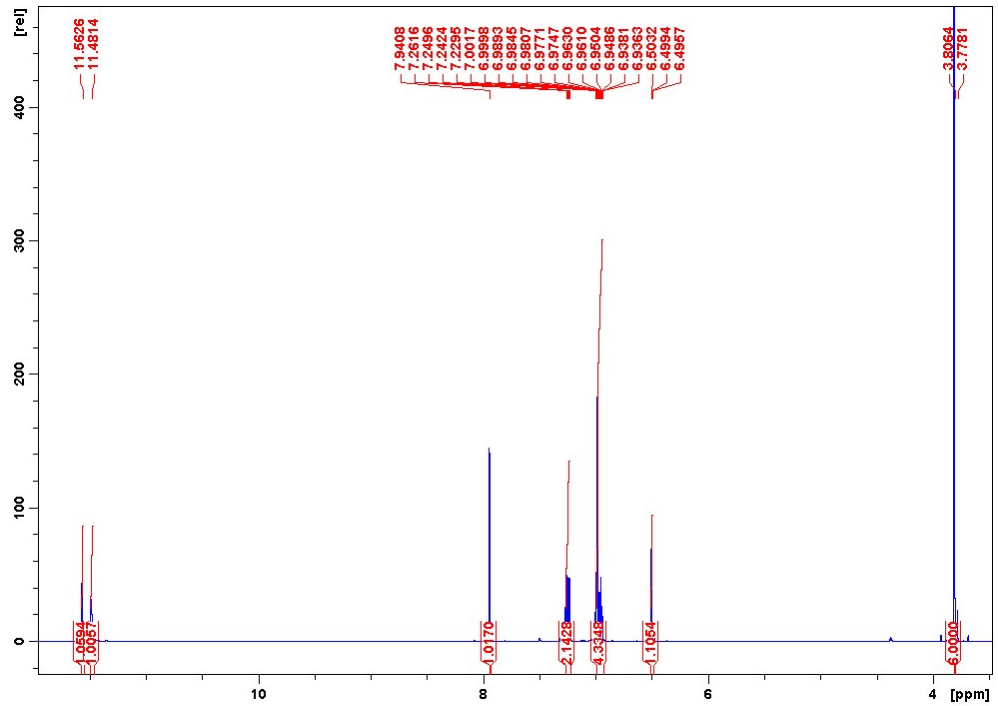

Fig. S27. ^{1}H NMR spectrum of compound **5h**

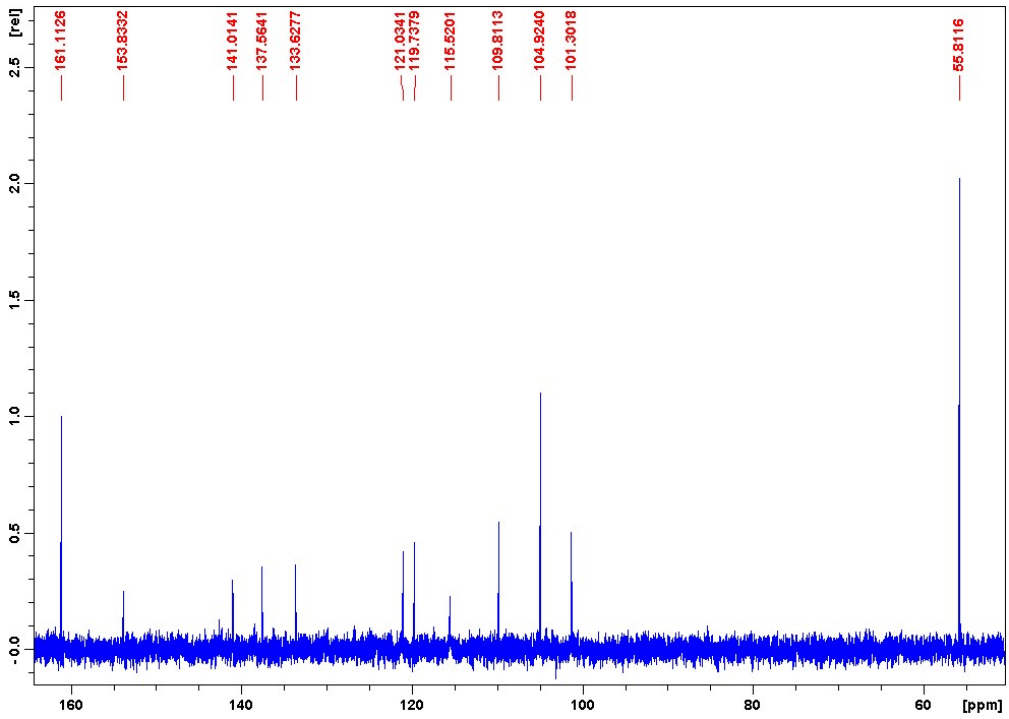

Fig. S28. ^{13}C NMR spectrum of compound **5h**

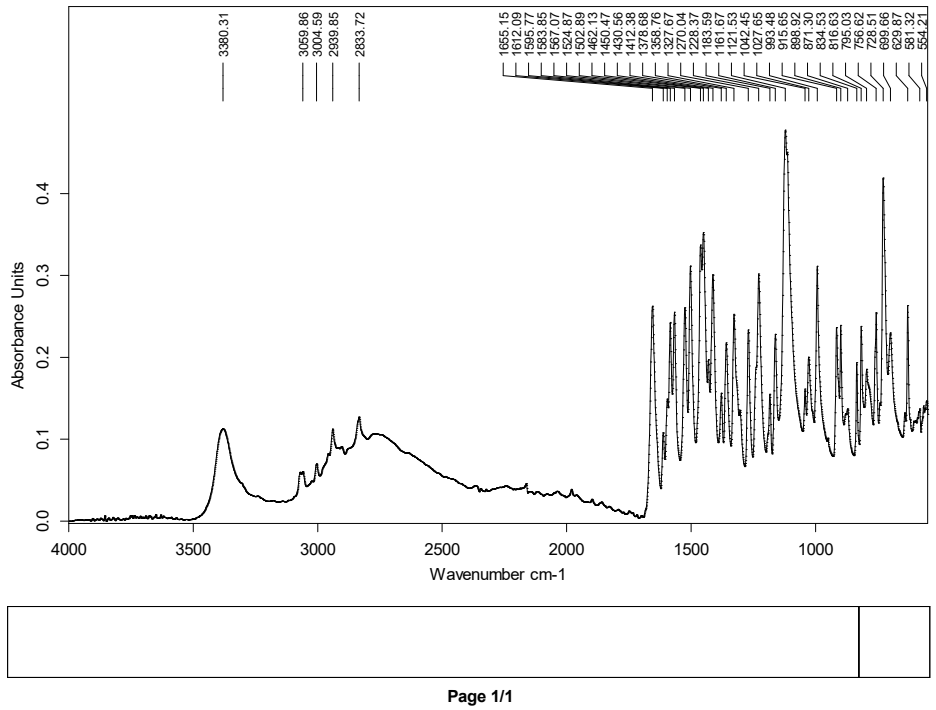

Fig. S29a. IR spectrum of compound **5i**

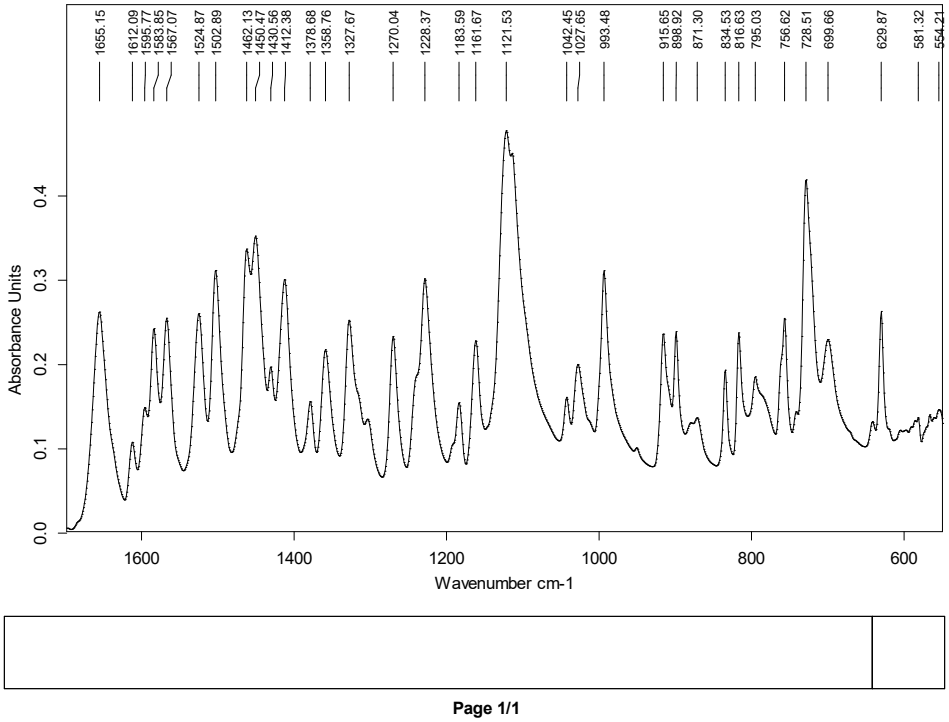

Fig. S29b. IR spectrum of compound **5i**

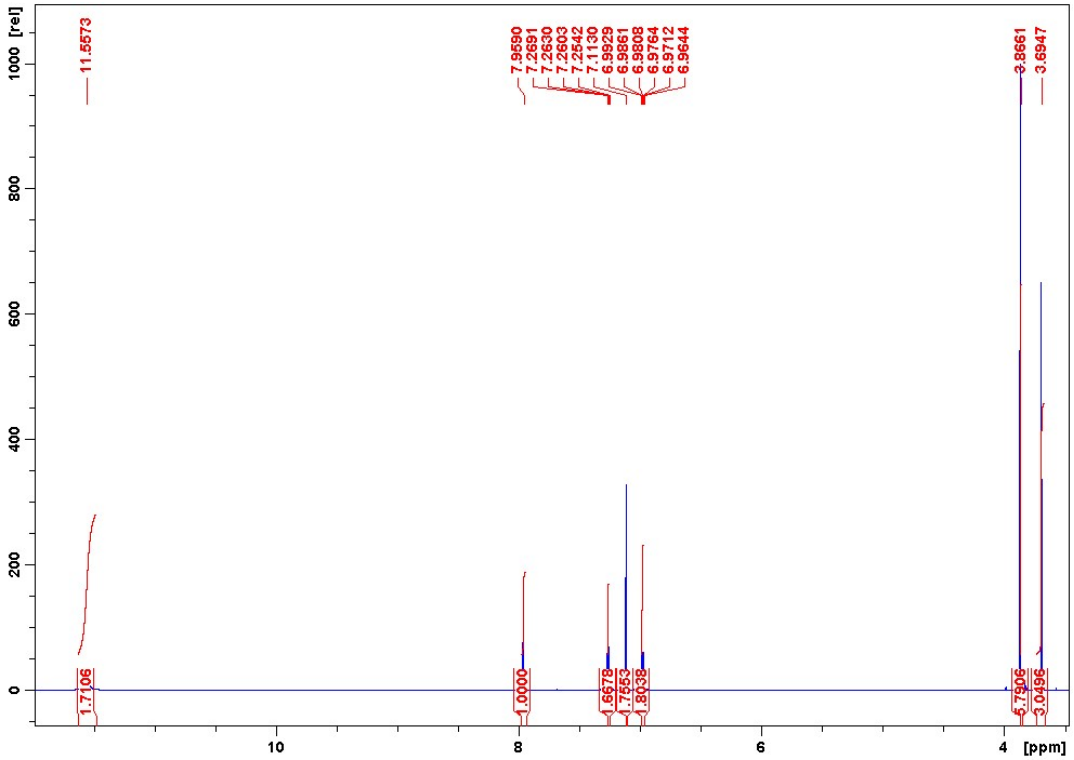

Fig. S30. ^{1}H NMR spectrum of compound **5i**

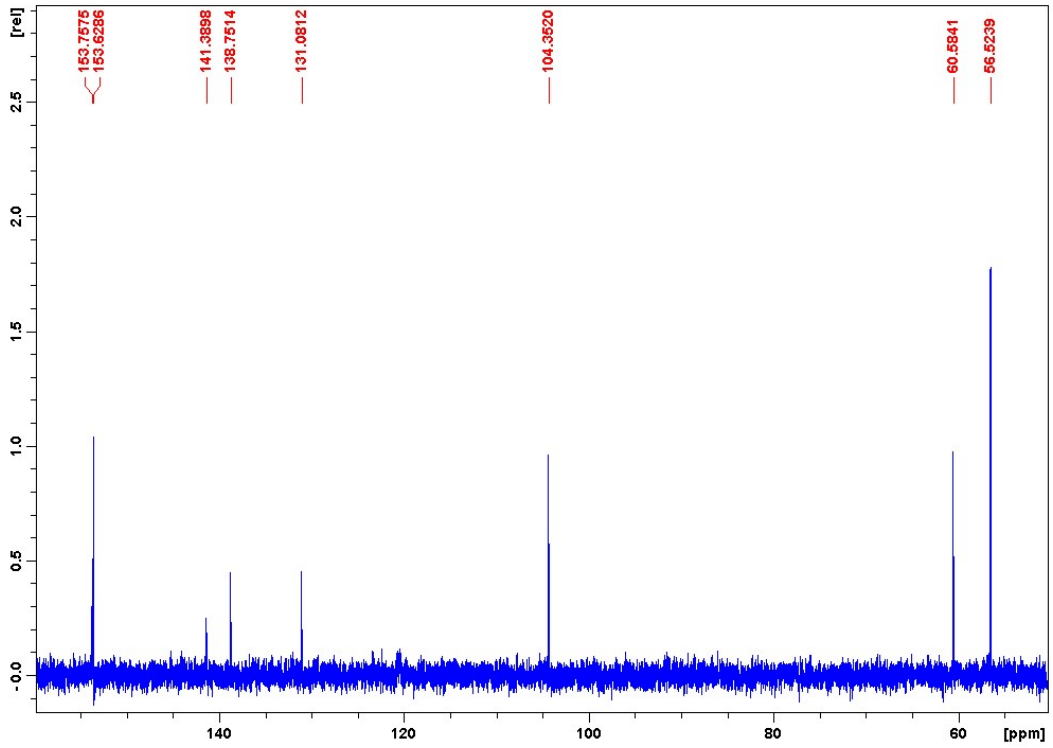

Fig. S31. ^{13}C NMR spectrum of compound **5i**

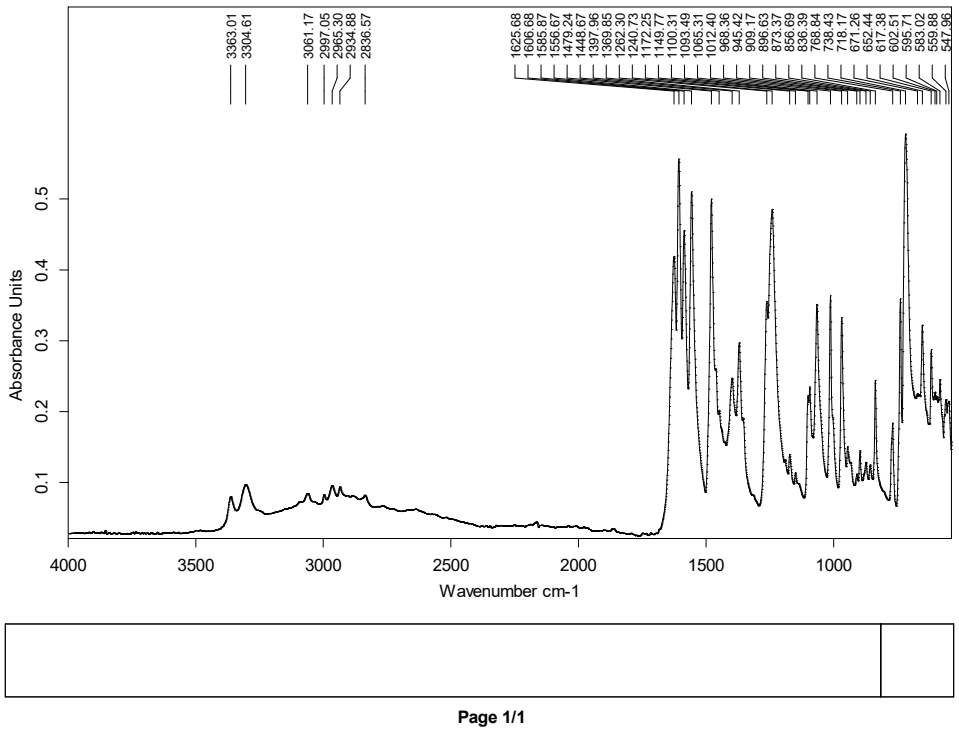

Fig. S32a. IR spectrum of compound **5j**

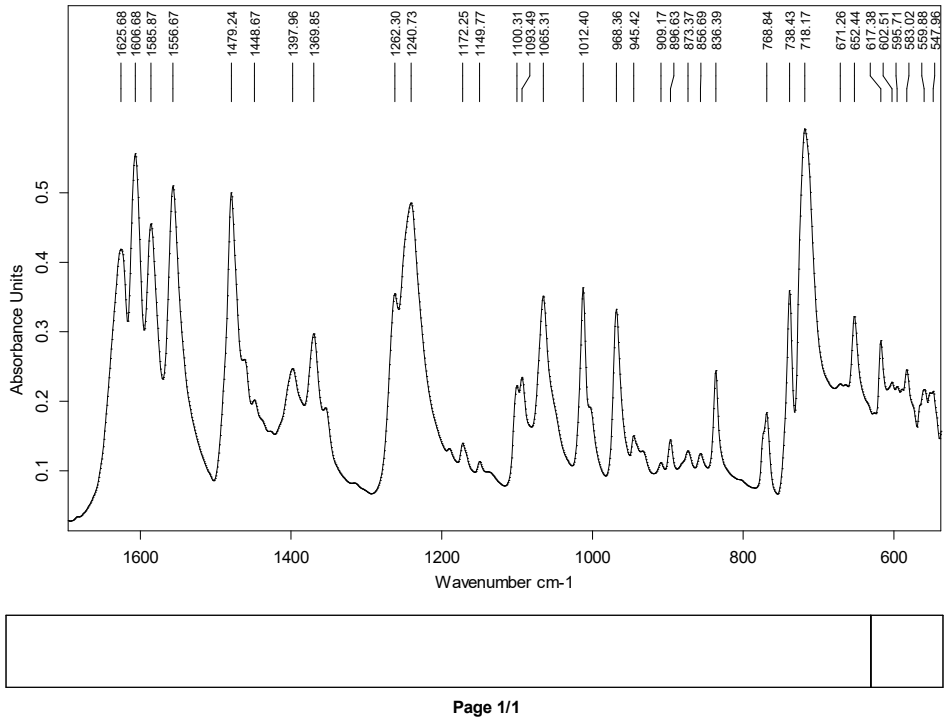

Fig. S32b. IR spectrum of compound **5j**

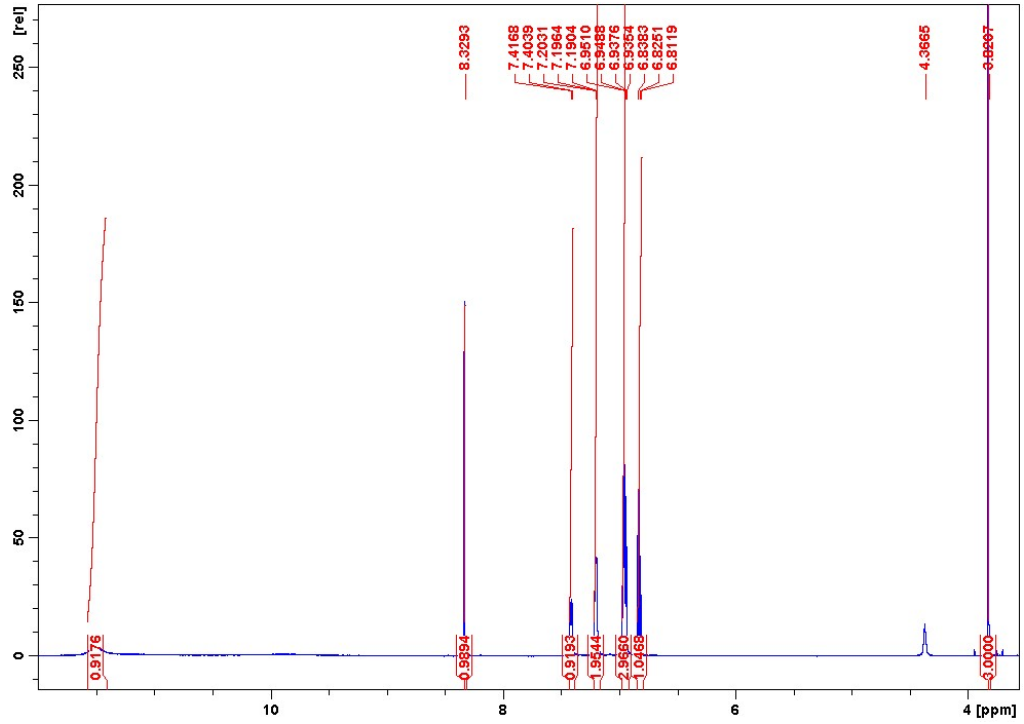

Fig. S33. ^{1}H NMR spectrum of compound **5j**

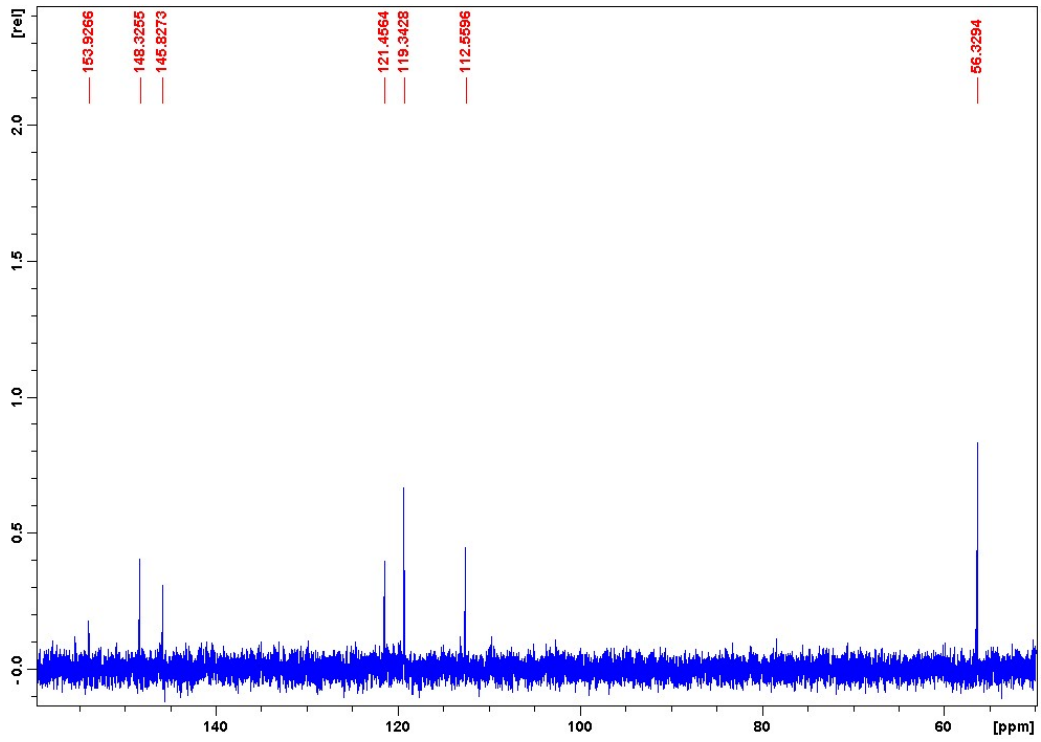

Fig. S34. ^{13}C NMR spectrum of compound **5j**

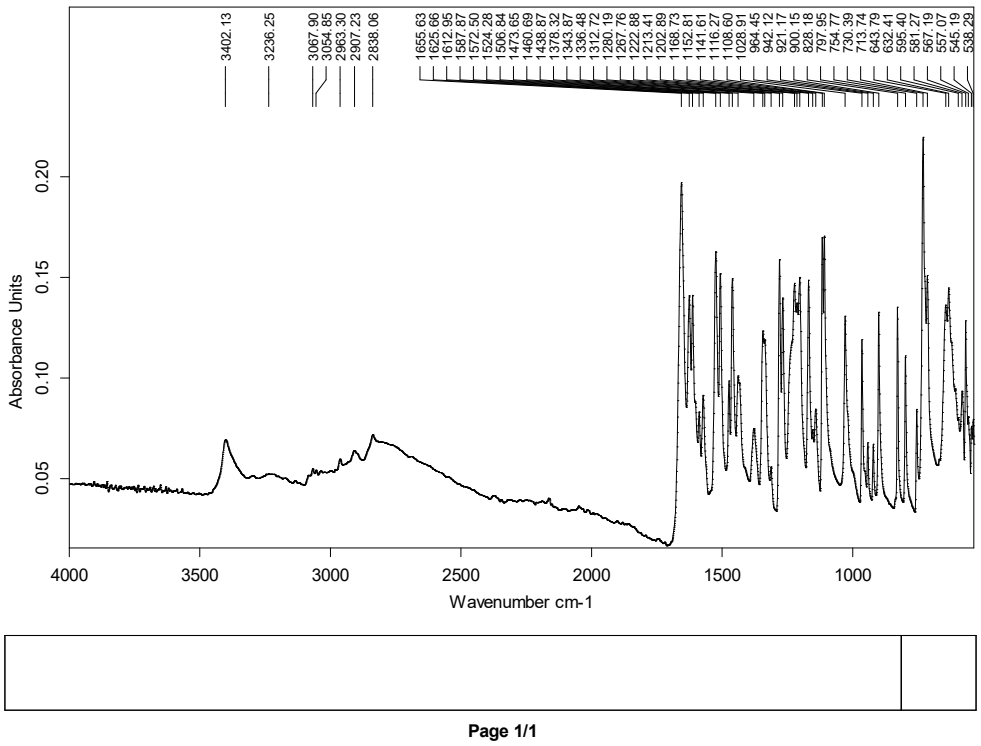

Fig. S35a. IR spectrum of compound **5k**

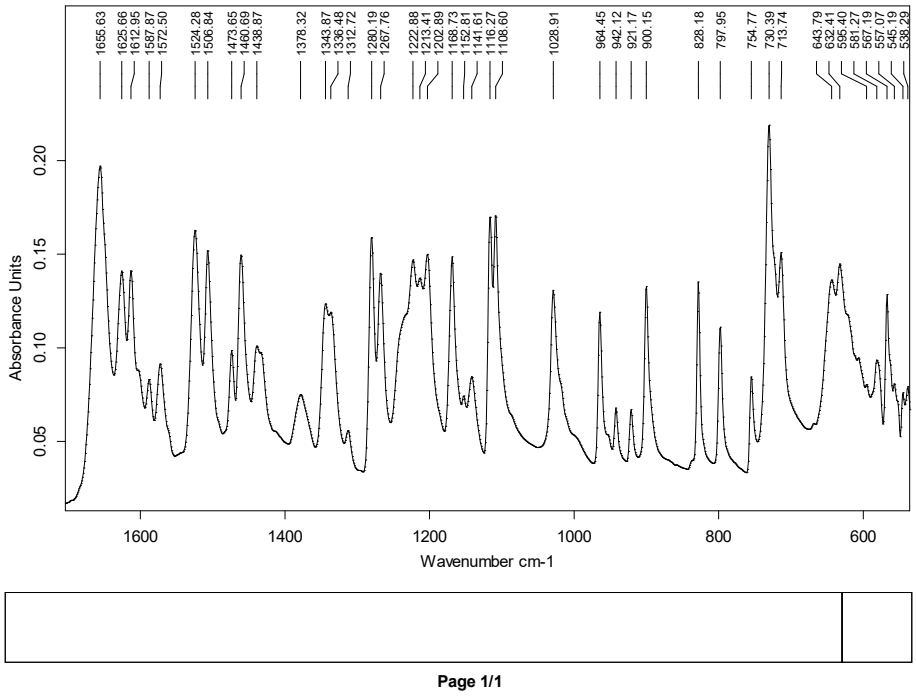

Fig. S35b. IR spectrum of compound **5k**

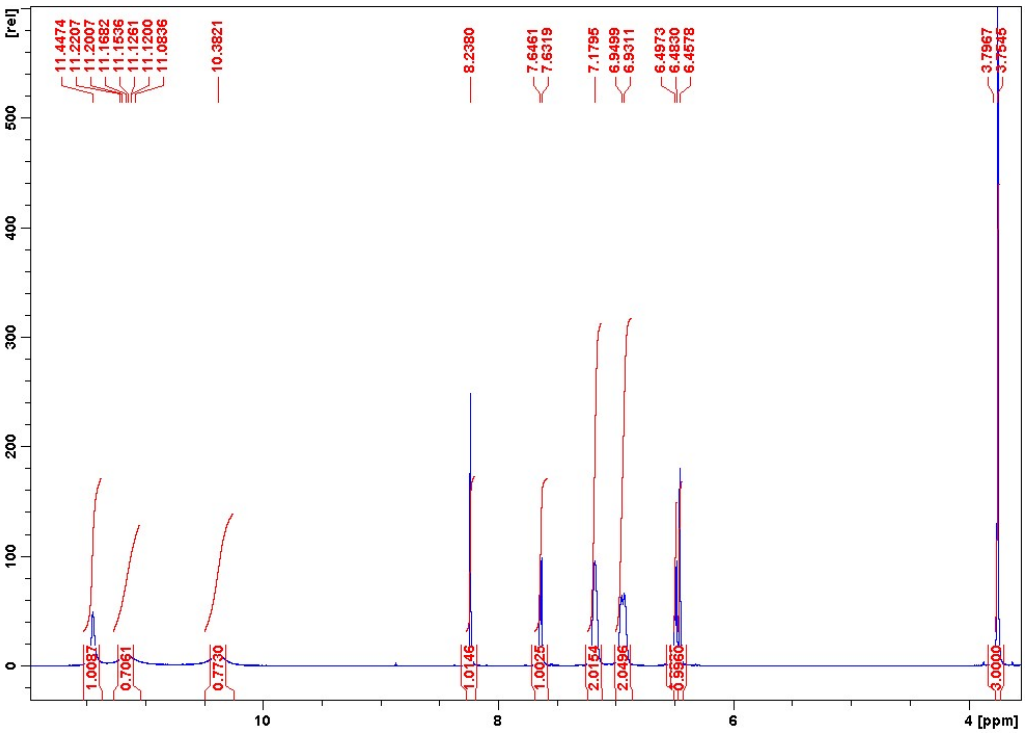

Fig. S36. ^{1}H NMR spectrum of compound **5k**

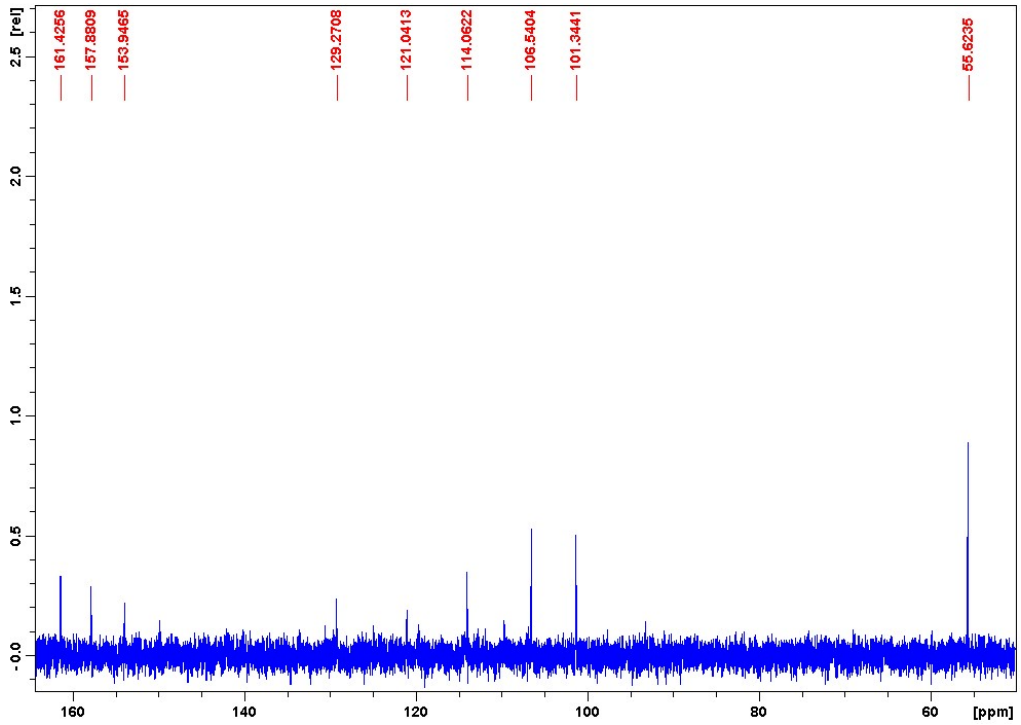

Fig. S37. ^{13}C NMR spectrum of compound **5k**

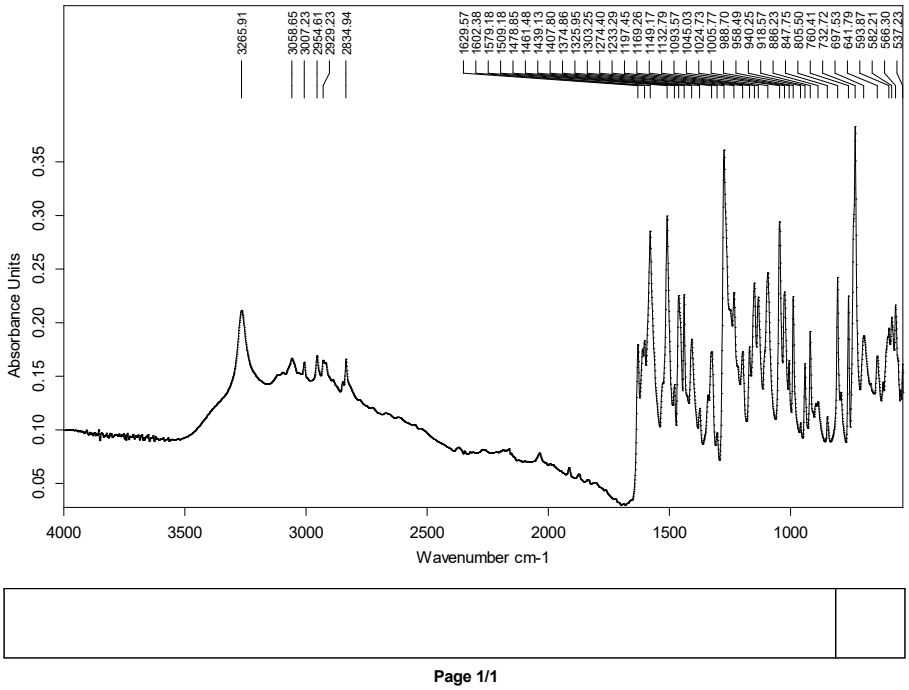

Fig. S38a. IR spectrum of compound **5l**

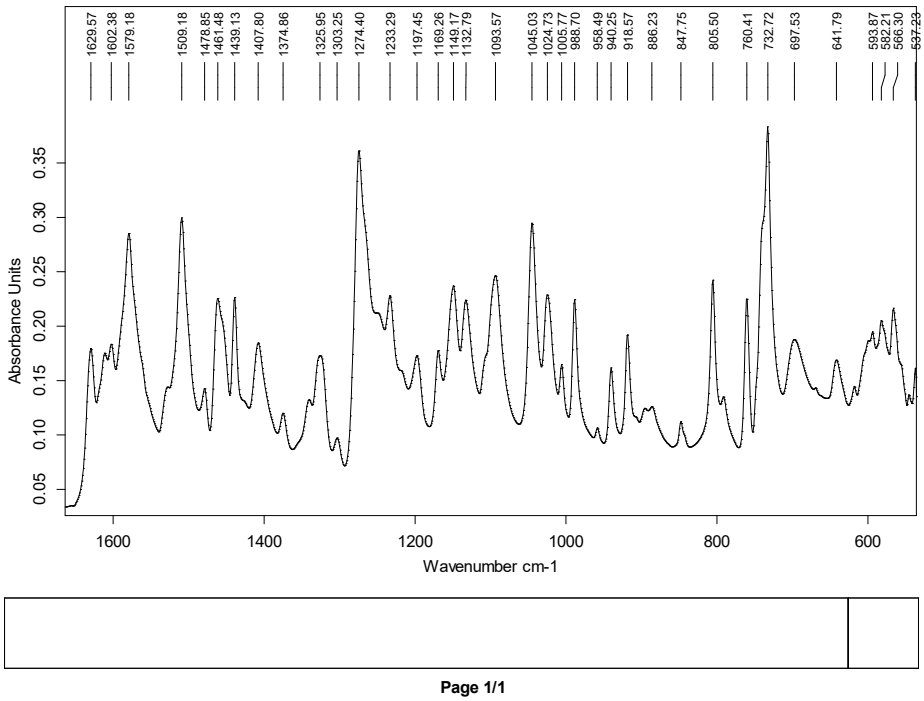

Fig. S38b. IR spectrum of compound **5l**

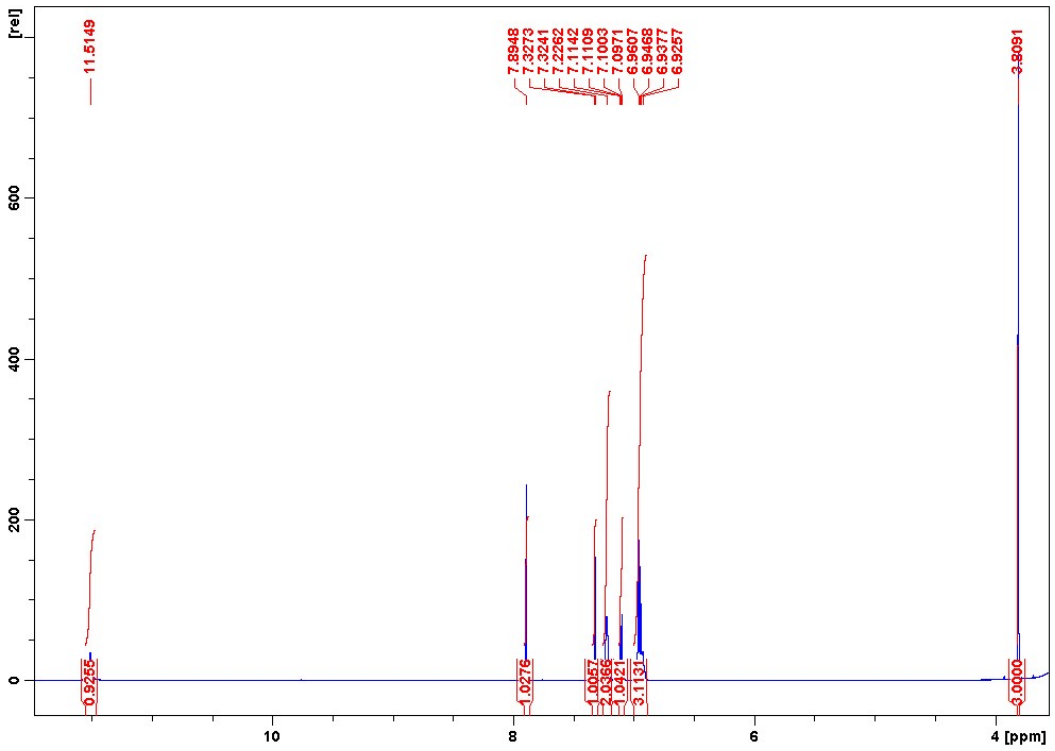

Fig. S39. ^{1}H NMR spectrum of compound **5l**

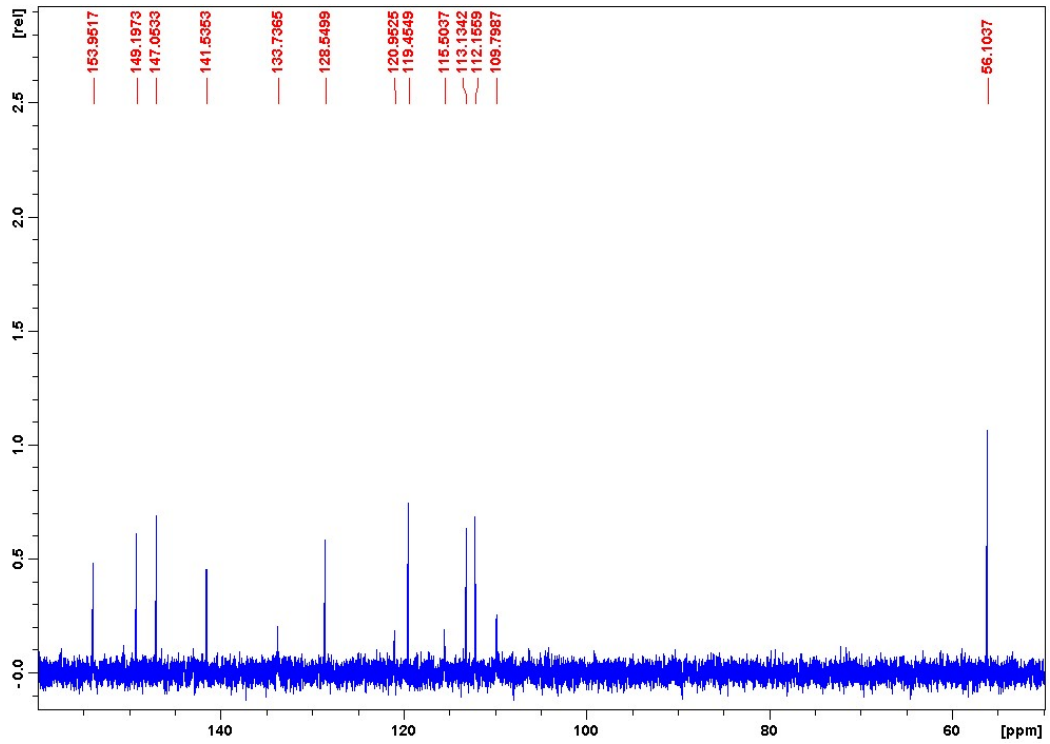

Fig. S40. ^{13}C NMR spectrum of compound **5l**

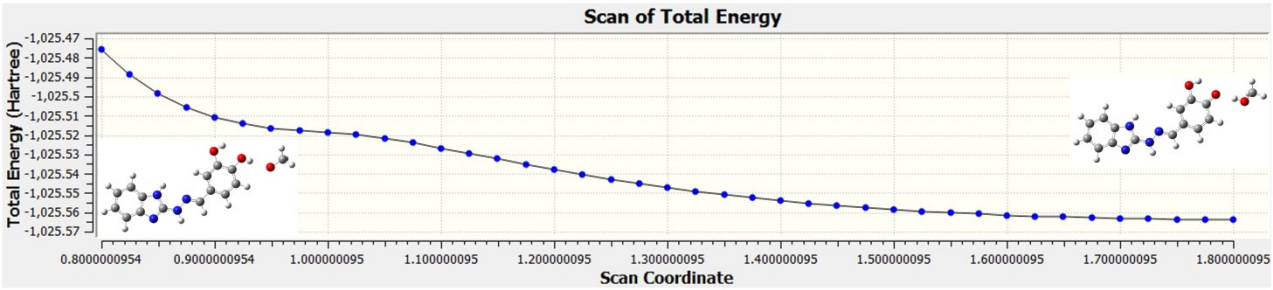

Figure S41. Scan plot of **5d** and $^{\bullet}OCH_3$ changing the distance between O and H from 0.800 to 1.800 Å.

Table S1. Gibbs energies of the reaction for all possible positions for HAT and RAF mechanisms between **5d (imino form)** and the studied radicals.

atom	**ΔGreaction ((U)M06-2X/6-311++G**//(U)B3LYP/6-311++G**)**								
	$^{\bullet}OCH_3$			**$^{\bullet}OOH$**			**$^{\bullet}OOCH_3$**		
	Gas phase	Water	Benzene	Gas phase	Water	Benzene	Gas phase	Water	Benzene
	HAT								
H10	-78.96	-88.03	-82.15	-8.10	-18.00	-11.54	-2.61	-10.40	-4.88
H24	-89.69	-96.33	-92.32	-18.83	-26.30	-21.71	-13.33	-18.70	-15.05
H22	-90.30	-88.23	-91.19	-19.44	-18.21	-20.58	-13.94	-10.60	-13.93
H23	-107.51	-110.39	-109.92	-36.66	-40.36	-39.31	-31.16	-32.76	-32.65
H25	1.63	-6.59	-0.89	72.49	63.44	69.71	77.98	71.04	76.37
	RAF								
C13	-67.62	-63.93	-63.99	-12.33	-13.85	-12.02	1.06	1.31	3.41
C17	-36.14	-24.87	-30.70	29.11	38.08	33.02	39.77	49.22	43.79
C19	-6.16	2.50	-2.20	47.02	53.67	49.82	60.37	67.62	64.15
C6	-4.04	10.32	2.18	61.87	66.34	64.15	70.07	75.60	73.80
C15	-3.10	3.85	0.37	53.22	58.10	56.82	64.16	69.55	69.16
C1	8.35	18.39	13.09	65.63	71.96	68.43	77.87	85.36	82.95
C2	11.46	20.70	15.20	65.99	69.59	67.10	78.75	82.35	79.17
C8	20.02	32.07	26.16	78.94	87.15	83.78	91.24	100.10	96.33
C14	33.40	37.86	36.27	87.48	89.98	89.04	100.11	104.06	102.04
C16	6.14	8.05	7.23	69.24	69.37	70.53	80.14	80.46	81.49

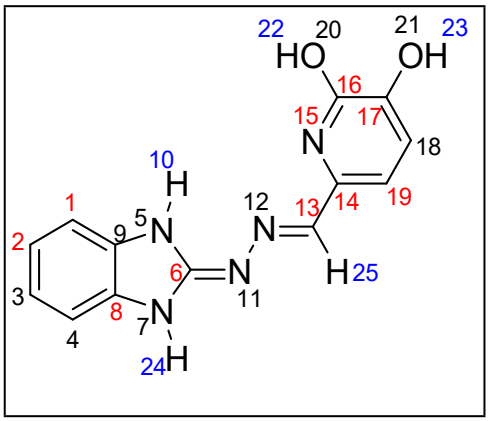

Table S2. Activation energies ($\Delta G^{\ddagger}$) of all possible calculated transition states for the HAT and RAF mechanisms between **5d (imino form)** and the studied radicals.

atom	**$\Delta G^{\ddagger}$ ((U)M06-2X/6-311++G**//(U)B3LYP/6-311++G**)**								
	$^{\bullet}OCH_3$			**$^{\bullet}OOH$**			**$^{\bullet}OOCH_3$**		
	Gas phase	Water	Benzene	Gas phase	Water	Benzene	Gas phase	Water	Benzene
	HAT								
H10	44.05	21.60	-	66.72	66.54	66.45	75.99	65.49	68.61
H24	44.07	-	-	71.77	69.37	71.94	76.58	68.64	74.65
H22	-	-	-	72.38	67.97	71.14	75.96	62.54	74.16
H23	-	-	-	65.09	72.49	62.46	67.06	67.22	66.39
H25	66.38	74.05	72.36	112.97	109.46	110.67	120.41	120.11	120.88
	RAF								
C1	70.73	75.96	72.61	103.34	106.73	105.24	116.35	119.88	119.22
C2	72.03	74.27	73.16	102.74	102.32	103.17	115.48	116.16	116.48
C6	80.30	83.09	83.66	113.44	108.86	113.33	124.79	123.02	125.14
C8	67.78	73.85	71.73	101.14	102.94	104.08	113.54	117.15	117.34
C13	54.80	52.47	55.38	72.35	68.79	71.77	80.92	78.43	81.24
C14	85.26	82.42	85.19	113.97	110.52	113.02	127.72	126.87	127.83
C15	65.61	69.67	71.12	99.73	100.11	102.93	109.84	111.36	113.60
C16	67.93	69.81	68.29	105.54	100.31	105.81	117.57	113.07	118.17
C17	42.80	56.86	49.21	79.32	87.19	82.33	91.06	100.00	95.45
C19	65.53	69.26	67.71	92.05	95.74	93.38	104.34	108.39	106.85

Structural parameters of the isomers of the molecules **5a-l** in amino form

5a_1, optimization in gas phase
B3LYP/6-311++G**, E= -835.161269457 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.196234 a.u.
Sum of electronic and thermal Free Energies= -834.965036 a.u.

0; 1			
6	5.829335000	0.185591000	0.145649000
6	4.993560000	-0.928247000	0.126841000
6	5.315522000	1.489738000	0.068498000
1	5.388697000	-1.935194000	0.186353000
6	3.617574000	-0.715327000	0.027973000
6	3.943658000	1.722979000	-0.030101000
1	3.548067000	2.730429000	-0.089453000
6	3.118861000	0.605506000	-0.048962000
6	1.495703000	-0.893824000	-0.104533000
7	2.571484000	-1.630985000	-0.007484000
7	1.735314000	0.455795000	-0.136346000
1	1.041650000	1.181925000	-0.199771000
7	0.231382000	-1.424921000	-0.199346000
7	-0.874277000	-0.646646000	-0.115975000
6	-2.028667000	-1.223915000	-0.062154000
1	-2.097864000	-2.316283000	-0.065521000
1	0.165974000	-2.431127000	-0.082850000
1	5.996332000	2.332779000	0.085489000
6	-3.279583000	-0.490211000	0.001553000
6	-3.335711000	0.925493000	0.000251000
6	-4.489243000	-1.206958000	0.065481000
6	-4.569847000	1.575438000	0.061463000
6	-5.712393000	-0.558441000	0.126485000
6	-5.746119000	0.839807000	0.124231000
1	6.901562000	0.045017000	0.221083000
1	-6.631246000	-1.129648000	0.175328000
1	-4.580326000	2.658663000	0.058680000
1	-6.696695000	1.358893000	0.171752000
8	-2.217696000	1.684003000	-0.060149000
1	-1.449900000	1.079847000	-0.097201000
1	-4.451307000	-2.291695000	0.065981000

5a_2, optimization in gas phase
B3LYP/6-311++G**, E= -835.163197407 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.197920 a.u.
Sum of electronic and thermal Free Energies= -834.965277 a.u.

0; 1			
6	-5.443576000	0.625822000	-0.673877000
6	-4.625955000	-0.439200000	-1.038643000
6	-5.026367000	1.581832000	0.270361000
1	-4.946319000	-1.175018000	-1.766710000
6	-3.368374000	-0.535879000	-0.435750000
6	-3.774650000	1.506227000	0.876820000
1	-3.453450000	2.243926000	1.602618000
6	-2.964913000	0.434815000	0.508816000
6	-1.398684000	-1.099900000	0.190165000
7	-2.358408000	-1.474129000	-0.619588000
7	-1.687601000	0.048615000	0.891052000
1	-1.164789000	0.408921000	1.675095000
7	-0.238631000	-1.837949000	0.414694000
7	1.054064000	-1.380277000	0.243642000
6	1.328462000	-0.134031000	0.070424000
1	0.554889000	0.630573000	0.004162000
1	-0.318481000	-2.791422000	0.088849000
1	-5.692896000	2.395628000	0.531417000
6	2.706990000	0.320684000	-0.060219000
6	3.812557000	-0.562675000	0.019341000
6	2.955856000	1.688780000	-0.271227000
6	5.112039000	-0.063833000	-0.105988000
6	4.247264000	2.179423000	-0.399527000
6	5.326206000	1.293402000	-0.314589000
1	-6.424165000	0.723942000	-1.125245000
1	4.416244000	3.236680000	-0.563263000
1	5.940437000	-0.759232000	-0.039953000
1	6.340712000	1.663095000	-0.412325000
8	3.655112000	-1.891703000	0.216593000
1	2.689424000	-2.076342000	0.282643000
1	2.110396000	2.366253000	-0.335272000

5a_3, optimization in gas phase
B3LYP/6-311++G**, E= -835.160243698 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.198214 a.u.
Sum of electronic and thermal Free Energies= -834.962030 a.u.

0; 1			
6	-5.495864000	-0.940033000	-0.393232000
6	-4.249273000	-1.475479000	-0.709626000
6	-5.619765000	0.321290000	0.214201000
1	-4.154945000	-2.447743000	-1.178921000
6	-3.114356000	-0.720898000	-0.403906000
6	-4.498348000	1.089261000	0.526800000
1	-4.593532000	2.061327000	0.996007000
6	-3.258081000	0.545804000	0.209374000
6	-1.140139000	0.043616000	-0.139820000
7	-1.766222000	-1.004191000	-0.611219000
7	-1.957416000	1.008781000	0.373270000

1	-1.646460000	1.904010000	0.719180000
7	0.247408000	0.159075000	-0.084086000
7	0.728353000	1.463664000	0.029879000
6	2.002866000	1.624358000	0.012877000
1	2.304272000	2.668998000	0.038664000
1	0.705679000	-0.428271000	-0.781556000
1	-6.606299000	0.705715000	0.445932000
6	3.095848000	0.638963000	-0.067155000
6	3.140208000	-0.568863000	0.667556000
6	4.218000000	0.984436000	-0.847659000
6	4.265782000	-1.396700000	0.576224000
6	5.325030000	0.157028000	-0.940991000
6	5.344126000	-1.041705000	-0.220084000
1	-6.391654000	-1.506898000	-0.620032000
1	6.167788000	0.441359000	-1.559061000
1	4.271494000	-2.313662000	1.153154000
1	6.206384000	-1.696367000	-0.274618000
8	2.171610000	-0.959587000	1.538665000
1	1.303725000	-0.593681000	1.279057000
1	4.199599000	1.924144000	-1.389390000

5b_1, optimization in gas phase B3LYP/6-311++G**, E= -910.410123175 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.199044 a.u. Sum of electronic and thermal Free Energies= -910.211079 a.u.			
0; 1			
6	6.022182000	0.440970000	0.178274000
6	5.212811000	-0.684677000	0.308862000
6	5.506007000	1.667836000	-0.268032000
1	5.609859000	-1.632374000	0.652063000
6	3.860995000	-0.562769000	-0.016718000
6	4.158591000	1.808875000	-0.600334000
1	3.761871000	2.756568000	-0.946038000
6	3.359397000	0.680819000	-0.464465000
6	1.782110000	-0.866539000	-0.388169000
7	2.844909000	-1.512012000	0.014982000
7	2.004325000	0.450438000	-0.700514000
1	1.308512000	1.120362000	-0.982368000
7	0.535851000	-1.444382000	-0.456243000
7	-0.483189000	-0.852083000	-1.127407000
6	-1.593222000	-1.500866000	-1.252837000
1	-1.696807000	-2.505098000	-0.831278000
1	0.502994000	-2.436677000	-0.245407000
1	6.165753000	2.522997000	-0.356895000
6	-2.747965000	-0.956621000	-1.944367000
6	-3.936050000	-1.711161000	-2.014187000
6	-2.717516000	0.309142000	-2.557783000
6	-5.050958000	-1.213031000	-2.669933000
6	-3.847749000	0.805031000	-3.221805000
6	-5.009945000	0.045938000	-3.275108000
1	7.075093000	0.370918000	0.426280000
1	-5.960392000	-1.799459000	-2.716577000
8	-1.621326000	1.117243000	-2.553515000

5b_2, optimization in gas phase B3LYP/6-311++G**, E= -910.392359664 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.198864 a.u. Sum of electronic and thermal Free Energies= -910.193496 a.u.			
0; 1			
6	6.175568000	1.078792000	0.107714000
6	4.906291000	1.436725000	-0.340692000
6	6.440963000	-0.207595000	0.601392000
1	4.700461000	2.430273000	-0.720455000
6	3.895907000	0.476498000	-0.286453000
6	5.443333000	-1.180719000	0.661796000
1	5.651283000	-2.174234000	1.042146000
6	4.180973000	-0.812371000	0.212994000
6	2.049980000	-0.614247000	-0.401591000
7	2.557206000	0.567865000	-0.660422000
7	2.975437000	-1.501482000	0.122070000
1	2.798963000	-2.440560000	0.440251000
7	0.751957000	-1.031873000	-0.579458000
7	-0.300525000	-0.405457000	-1.185941000
6	-0.220843000	0.837765000	-1.508623000
1	0.688497000	1.395451000	-1.304662000
1	0.561063000	-2.010356000	-0.438527000
1	7.440191000	-0.451858000	0.942339000
6	-1.354070000	1.518733000	-2.136544000
6	-2.635944000	0.941284000	-2.208725000
6	-1.171805000	2.799233000	-2.680046000
6	-3.688966000	1.628378000	-2.790094000
6	-2.241052000	3.491817000	-3.268529000
6	-3.498046000	2.907344000	-3.321245000
1	6.976700000	1.808112000	0.076396000
1	-4.672409000	1.175199000	-2.832332000
8	0.020488000	3.489466000	-2.693775000

1	-0.907655000	0.645183000	-2.076519000	1	0.763683000	2.919481000	-2.470780000
1	-3.967526000	-2.688315000	-1.545256000	1	-2.778648000	-0.046272000	-1.790170000
1	-5.870974000	0.451051000	-3.792758000	1	-4.309747000	3.458346000	-3.780538000
8	-3.806019000	2.030204000	-3.814261000	8	-2.045963000	4.735370000	-3.793013000
1	-2.922963000	2.400574000	-3.681757000	1	-1.112268000	4.962386000	-3.690222000

5b_3, optimization in gas phase
B3LYP/6-311++G**, E= -910.397275917 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.199377 a.u.
Sum of electronic and thermal Free Energies= -910.197899 a.u.

0; 1

6	5.861743000	0.739188000	0.783742000
6	5.110108000	-0.428470000	0.889955000
6	5.400335000	1.843874000	0.050377000
1	5.464721000	-1.281766000	1.455521000
6	3.874094000	-0.475885000	0.243323000
6	4.168149000	1.816125000	-0.602963000
1	3.813814000	2.669761000	-1.169410000
6	3.425174000	0.647163000	-0.491435000
6	1.970057000	-1.011702000	-0.548608000
7	2.934289000	-1.500197000	0.185919000
7	2.184825000	0.264981000	-0.995402000
1	1.537318000	0.792626000	-1.558584000
7	0.829815000	-1.709236000	-0.880150000
7	-0.167750000	-1.076285000	-1.524832000
6	-1.282279000	-1.684984000	-1.749210000
1	-2.018460000	-1.072592000	-2.265327000
1	0.706339000	-2.621293000	-0.450641000
1	6.012459000	2.736190000	-0.010868000
6	-1.650428000	-3.077154000	-1.412251000
6	-0.841699000	-4.178132000	-1.750917000
6	-2.880038000	-3.321639000	-0.789431000
6	-1.265619000	-5.473211000	-1.478034000
6	-3.305092000	-4.628085000	-0.512695000
6	-2.494079000	-5.702236000	-0.859063000
1	6.824806000	0.799051000	1.277788000
1	-0.640685000	-6.313966000	-1.753928000
8	-3.755307000	-2.331262000	-0.406107000
1	-3.308917000	-1.477470000	-0.375469000
1	0.096434000	-4.011915000	-2.266689000
8	-4.499922000	-4.849930000	0.098464000
1	-4.905722000	-3.995656000	0.297768000
1	-2.835741000	-6.704984000	-0.633270000

5c_1, optimization in gas phase
B3LYP/6-311++G**, E= -910.410390840 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.199252 a.u.
Sum of electronic and thermal Free Energies= -910.211139 a.u.

0; 1

6	6.122703000	0.269062000	-0.079849000
6	5.239175000	-0.750444000	0.266461000
6	5.668514000	1.477860000	-0.630200000
1	5.588666000	-1.683979000	0.690768000
6	3.876047000	-0.539859000	0.052231000

5c_2, optimization in gas phase
B3LYP/6-311++G**, E= -910.392380569 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.198543 a.u.
Sum of electronic and thermal Free Energies= -910.193838 a.u.

0; 1

6	6.133813000	1.082272000	0.093242000
6	4.916454000	1.372311000	-0.519183000
6	6.341356000	-0.128918000	0.770248000
1	4.755752000	2.307004000	-1.042920000
6	3.899401000	0.420865000	-0.442508000

6	4.310474000	1.706151000	-0.854284000	6	5.335004000	-1.091345000	0.858335000
1	3.960881000	2.639372000	-1.280859000	1	5.497240000	-2.025517000	1.383792000
6	3.437572000	0.684121000	-0.503682000	6	4.125650000	-0.791798000	0.243569000
6	1.751596000	-0.684664000	-0.087434000	1	6.939390000	1.805870000	0.046104000
7	2.792596000	-1.376826000	0.296911000	6	2.067232000	-0.688698000	-0.601864000
7	2.051444000	0.558369000	-0.583845000	7	2.606705000	0.453170000	-0.959911000
1	1.388441000	1.248003000	-0.896062000	7	2.926285000	-1.488950000	0.134155000
7	0.459357000	-1.137717000	0.036263000	1	2.744915000	-2.421500000	0.468118000
7	-0.558687000	-0.539963000	-0.641923000	7	0.804903000	-1.149755000	-0.884945000
6	-1.726457000	-1.091255000	-0.599269000	7	-0.260667000	-0.511949000	-1.464323000
1	-1.877443000	-2.017959000	-0.036572000	6	-0.102776000	0.634142000	-2.030370000
1	0.366964000	-2.099962000	0.345617000	1	0.878574000	1.100226000	-2.038067000
1	6.384944000	2.249464000	-0.886895000	1	0.515349000	-2.000961000	-0.432237000
6	-2.883802000	-0.540264000	-1.272895000	6	-1.223307000	1.311045000	-2.676346000
6	-4.130452000	-1.183639000	-1.154605000	6	-2.463412000	0.676560000	-2.882025000
6	-2.818691000	0.633751000	-2.064506000	6	-1.089349000	2.638149000	-3.133173000
6	-5.268337000	-0.703846000	-1.774499000	6	-3.517440000	1.305432000	-3.515084000
6	-3.961847000	1.124029000	-2.693900000	6	-2.145642000	3.283770000	-3.778088000
6	-5.177002000	0.460237000	-2.548605000	6	-3.351816000	2.620545000	-3.968845000
1	7.185884000	0.128277000	0.078304000	1	7.301062000	-0.322312000	1.235035000
1	-6.223105000	-1.203525000	-1.677084000	1	-2.001380000	4.305816000	-4.111733000
1	-3.876960000	2.024622000	-3.292672000	1	-4.464098000	0.805095000	-3.674102000
8	-1.664157000	1.311139000	-2.238370000	8	0.048696000	3.378918000	-2.986174000
1	-0.962707000	0.833443000	-1.748260000	1	0.698281000	2.910861000	-2.450671000
8	-6.321259000	0.901561000	-3.143188000	8	-4.416098000	3.205929000	-4.593286000
1	-6.142939000	1.700960000	-3.650251000	1	-4.184145000	4.100155000	-4.865586000
1	-4.194802000	-2.085030000	-0.553816000	1	-2.572946000	-0.342727000	-2.533058000

5c_3, optimization in gas phase
B3LYP/6-311++G**, E= -910.399978377 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.201367 a.u.
Sum of electronic and thermal Free Energies= -910.198612 a.u.

0; 1

6	6.029973000	0.700011000	0.188797000
6	5.464972000	-0.183422000	-0.726683000
6	5.234737000	1.454000000	1.067558000
1	6.076420000	-0.764891000	-1.406140000
6	4.074543000	-0.303625000	-0.750005000
6	3.844950000	1.346636000	1.060909000
1	3.233180000	1.927467000	1.741537000
6	3.289263000	0.461308000	0.144068000
6	2.048369000	-0.810941000	-1.159863000
7	3.257770000	-1.091836000	-1.557028000
7	1.976417000	0.096809000	-0.140122000
1	1.117122000	0.492161000	0.208364000
7	0.899725000	-1.426034000	-1.665383000
7	-0.283321000	-0.709664000	-1.462523000
6	-1.353624000	-1.185811000	-1.992723000
1	-2.218681000	-0.540674000	-1.853252000
1	1.052474000	-1.764469000	-2.616411000
1	5.710283000	2.132114000	1.766624000
6	-1.587180000	-2.412197000	-2.766250000
6	-2.537617000	-2.349360000	-3.808356000
6	-1.024670000	-3.678467000	-2.472092000
6	-2.887343000	-3.447775000	-4.566072000
6	-1.380270000	-4.796373000	-3.234247000
6	-2.296930000	-4.684526000	-4.271404000

1	7.107635000	0.811036000	0.226326000
1	-3.607769000	-3.378826000	-5.370578000
1	-0.930904000	-5.749546000	-2.977055000
8	-0.194769000	-3.916376000	-1.429919000
1	0.286910000	-3.103859000	-1.174350000
8	-2.670867000	-5.748782000	-5.034491000
1	-2.209949000	-6.543161000	-4.743257000
1	-3.001581000	-1.392200000	-4.022230000

5d_1, optimization in gas phase
B3LYP/6-311++G**, E= -910.403405101 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.197038 a.u.
Sum of electronic and thermal Free Energies= -910.206367 a.u.

0; 1

6	6.312687000	0.556319000	0.003950000
6	5.597824000	-0.639485000	0.003620000
6	5.661582000	1.799660000	0.001771000
1	6.099692000	-1.599674000	0.005308000
6	4.203689000	-0.573191000	0.001031000
6	4.268864000	1.887166000	-0.000842000
1	3.766876000	2.847995000	-0.002551000
6	3.564700000	0.689844000	-0.001154000
6	2.109324000	-0.971348000	-0.002346000
7	3.259986000	-1.594942000	0.000242000
7	2.203609000	0.395362000	-0.003476000
1	1.418348000	1.026041000	-0.004516000
7	0.894013000	-1.607351000	-0.004566000
7	-0.254019000	-0.897350000	-0.003076000
6	-1.365820000	-1.540536000	-0.001300000
1	-1.377667000	-2.636315000	-0.000582000
1	0.903827000	-2.622507000	-0.000815000
1	6.249877000	2.709953000	0.002095000
6	-2.664517000	-0.873581000	-0.000269000
6	-3.827526000	-1.654206000	0.002026000
6	-2.783005000	0.526629000	-0.001537000
1	-3.754186000	-2.735823000	0.002984000
1	-1.900337000	1.152424000	-0.003363000
6	-5.085204000	-1.052852000	0.003074000
6	-4.029418000	1.127074000	-0.000519000
6	-5.188740000	0.330365000	0.001818000
1	7.396452000	0.528350000	0.005923000
8	-4.126572000	2.485550000	-0.001820000
1	-5.061589000	2.728461000	-0.000557000
8	-6.374082000	1.026761000	0.002696000
1	-7.124332000	0.424044000	0.004389000
1	-5.983490000	-1.662631000	0.004864000

5d_2, optimization in gas phase
B3LYP/6-311++G**, E= -910.394144785 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.197767 a.u.
Sum of electronic and thermal Free Energies= -910.196378 a.u.

0; 1

6	6.349472000	1.246015000	-0.020434000
6	4.997893000	1.581519000	-0.065892000
6	6.769091000	-0.091236000	0.044208000
1	4.671706000	2.613411000	-0.116177000
6	4.062518000	0.546862000	-0.046036000
6	5.847868000	-1.139144000	0.067440000
1	6.174802000	-2.171489000	0.119147000
6	4.503065000	-0.793167000	0.021291000
6	2.281463000	-0.648178000	-0.041415000
7	2.672363000	0.601790000	-0.085415000
7	3.334540000	-1.547967000	0.030661000
1	3.272713000	-2.553029000	0.031104000
7	0.996202000	-1.131630000	-0.070245000
7	-0.203308000	-0.476816000	-0.046097000
6	-0.262951000	0.805657000	-0.118722000
1	0.628043000	1.422742000	-0.191097000
1	0.873288000	-2.123664000	0.046598000
1	7.828618000	-0.316724000	0.077890000
6	-1.563360000	1.482296000	-0.103127000
6	-1.592224000	2.879850000	-0.183750000
6	-2.775528000	0.778265000	-0.012013000
1	-0.663847000	3.434815000	-0.254330000
1	-2.774641000	-0.302187000	0.050895000
6	-2.806073000	3.565663000	-0.174139000
6	-3.982346000	1.455155000	-0.002208000
6	-3.996170000	2.858491000	-0.084371000
1	7.094529000	2.033179000	-0.035567000
8	-5.152226000	0.759062000	0.086999000
1	-5.884157000	1.389192000	0.084838000
8	-5.247032000	3.433619000	-0.067299000
1	-5.178960000	4.392077000	-0.118305000
1	-2.824483000	4.649630000	-0.236671000

5d_3, optimization in gas phase
B3LYP/6-311++G**, E= -910.397957707 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.199333 a.u.
Sum of electronic and thermal Free Energies= -910.198624 a.u.

0; 1

6	6.323502000	1.054679000	-0.283743000
6	5.666936000	-0.058791000	-0.802924000
6	5.662650000	1.975176000	0.544876000
1	6.176048000	-0.770003000	-1.442326000
6	4.322060000	-0.241217000	-0.477079000
6	4.319144000	1.810069000	0.883074000

5d_4, optimization in gas phase
B3LYP/6-311++G**, E= -910.383153498 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.199665 a.u.
Sum of electronic and thermal Free Energies= -910.183488 a.u.

0; 1

6	6.695076000	0.322393000	-1.121629000
6	5.839306000	-0.772887000	-1.203234000
6	6.267185000	1.550404000	-0.591287000
1	6.168000000	-1.720136000	-1.613676000
6	4.531120000	-0.621958000	-0.738209000
6	4.964007000	1.721911000	-0.125076000

1	3.810153000	2.520967000	1.523985000	1	4.633754000	2.671253000	0.281265000
6	3.672338000	0.696713000	0.360847000	6	4.118607000	0.621903000	-0.208367000
6	2.315508000	-0.927837000	-0.266778000	6	2.483700000	-0.872489000	-0.173369000
7	3.439473000	-1.248363000	-0.853331000	7	3.482080000	-1.530209000	-0.708970000
7	2.371253000	0.217818000	0.481145000	7	2.785776000	0.429068000	0.144868000
1	1.584163000	0.622092000	0.962941000	1	2.185480000	1.083872000	0.618241000
7	1.162971000	-1.679964000	-0.344933000	7	1.247423000	-1.468183000	0.067498000
7	0.010927000	-1.131908000	0.115177000	7	0.047760000	-0.727484000	-0.030414000
6	-1.120324000	-1.716021000	-0.075974000	6	-0.262969000	0.085944000	0.912547000
1	-1.965372000	-1.148285000	0.304745000	1	-1.193838000	0.612795000	0.703493000
1	1.161834000	-2.405190000	-1.055217000	1	1.170718000	-2.273194000	-0.542911000
1	6.205348000	2.830276000	0.930975000	1	6.961395000	2.381421000	-0.543677000
6	-1.447199000	-2.983993000	-0.750287000	6	0.332083000	0.421699000	2.218665000
6	-2.686603000	-3.077447000	-1.401014000	6	-0.137747000	1.585392000	2.848905000
6	-0.608717000	-4.113515000	-0.735337000	6	1.259586000	-0.390307000	2.898175000
1	-3.355158000	-2.224506000	-1.407890000	1	-0.870686000	2.209023000	2.349911000
1	0.325014000	-4.123804000	-0.187469000	1	1.632731000	-1.302256000	2.454514000
6	-3.066227000	-4.249576000	-2.048085000	6	0.320157000	1.947279000	4.112064000
6	-0.989220000	-5.288044000	-1.370441000	6	1.698901000	-0.045115000	4.166447000
6	-2.220735000	-5.351423000	-2.039550000	6	1.234434000	1.135679000	4.771446000
1	7.368350000	1.216255000	-0.523663000	1	7.715520000	0.227996000	-1.475407000
8	-0.165687000	-6.369343000	-1.328246000	8	2.580627000	-0.852311000	4.812761000
1	-0.578260000	-7.093442000	-1.817104000	1	2.791447000	-0.462661000	5.671277000
8	-2.497721000	-6.554523000	-2.641102000	8	1.744929000	1.390933000	6.017202000
1	-3.353184000	-6.529132000	-3.081428000	1	1.400599000	2.218320000	6.368920000
1	-4.023210000	-4.307228000	-2.557747000	1	-0.041854000	2.853134000	4.588338000

5e_1, optimization in gas phase B3LYP/6-311++G**, E= -985.660156013 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.202114 a.u. Sum of electronic and thermal Free Energies= -985.458042 a.u.				**5e_2,** optimization in gas phase B3LYP/6-311++G**, E= -985.641882418 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.201854 a.u. Sum of electronic and thermal Free Energies= -985.440028 a.u.			
0; 1				0; 1			
6	6.019117000	0.446634000	0.118497000	6	6.142521000	1.064799000	0.103802000
6	5.224564000	-0.693495000	0.210736000	6	4.931754000	1.347873000	-0.524664000
6	5.477341000	1.691227000	-0.239092000	6	6.338396000	-0.133209000	0.807232000
1	5.641647000	-1.654853000	0.485377000	1	4.780597000	2.272286000	-1.069124000
6	3.861454000	-0.568263000	-0.062085000	6	3.909245000	0.403220000	-0.436896000
6	4.118138000	1.835884000	-0.518433000	6	5.326641000	-1.088738000	0.906608000
1	3.701512000	2.797304000	-0.796271000	1	5.479818000	-2.012641000	1.452488000
6	3.333951000	0.693467000	-0.420937000	6	4.123905000	-0.796087000	0.275728000
6	1.773782000	-0.873693000	-0.382265000	1	6.952093000	1.783323000	0.048507000
7	2.856021000	-1.529297000	-0.053087000	6	2.072936000	-0.700972000	-0.588410000
7	1.974408000	0.461501000	-0.626840000	7	2.620932000	0.430924000	-0.965716000
1	1.260299000	1.139629000	-0.833317000	7	2.922200000	-1.489699000	0.170537000
7	0.527818000	-1.453837000	-0.432932000	1	2.733442000	-2.414256000	0.522258000
7	-0.496375000	-0.851310000	-1.100012000	7	0.810141000	-1.162123000	-0.870676000
6	-1.606484000	-1.501250000	-1.225146000	7	-0.248561000	-0.529862000	-1.467547000
1	-1.707910000	-2.507908000	-0.808461000	6	-0.076686000	0.597175000	-2.066054000
1	0.517059000	-2.459145000	-0.293961000	1	0.909745000	1.051491000	-2.088780000
1	6.125888000	2.557352000	-0.300192000	1	0.511923000	-1.999071000	-0.397272000
6	-2.759145000	-0.956250000	-1.910644000	6	-1.187862000	1.272930000	-2.728367000

6	-3.955620000	-1.695111000	-1.983028000	6	-2.447881000	0.671037000	-2.905147000
6	-2.724695000	0.312030000	-2.529264000	6	-1.013108000	2.575763000	-3.228632000
6	-5.075052000	-1.203402000	-2.633316000	6	-3.482394000	1.321785000	-3.554768000
6	-3.847227000	0.805155000	-3.185645000	6	-2.051702000	3.234669000	-3.883624000
6	-5.023600000	0.054659000	-3.239372000	6	-3.287570000	2.613315000	-4.050794000
1	7.080387000	0.373889000	0.327100000	1	7.293230000	-0.321567000	1.283927000
1	-5.994805000	-1.771360000	-2.686222000	1	-4.447336000	0.850485000	-3.693126000
8	-1.626749000	1.114564000	-2.533080000	8	0.143540000	3.315499000	-3.136209000
1	-0.912830000	0.637515000	-2.057363000	1	0.782376000	2.900910000	-2.546734000
1	-3.996626000	-2.671912000	-1.514177000	1	-2.590847000	-0.331717000	-2.524177000
8	-3.848596000	2.030305000	-3.799587000	8	-1.909193000	4.507043000	-4.378623000
1	-2.973452000	2.427770000	-3.700762000	1	-1.022669000	4.824043000	-4.162945000
8	-6.117010000	0.542030000	-3.879129000	8	-4.301264000	3.258834000	-4.688321000
1	-5.902365000	1.413145000	-4.239469000	1	-3.987188000	4.132664000	-4.956587000

5e_3, optimization in gas phase
B3LYP/6-311++G**, E= -985.651233033 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.204949 a.u.
Sum of electronic and thermal Free Energies= -985.446284 a.u.

0; 1

6	5.750717000	0.429868000	1.120077000
6	4.996925000	-0.717397000	0.889945000
6	5.364685000	1.677368000	0.602260000
1	5.291740000	-1.680153000	1.289710000
6	3.836507000	-0.596740000	0.123569000
6	4.210917000	1.817787000	-0.166917000
1	3.916306000	2.780958000	-0.567303000
6	3.464785000	0.666405000	-0.393105000
6	2.026416000	-0.906396000	-0.952044000
7	2.904900000	-1.563287000	-0.248425000
7	2.289884000	0.426255000	-1.099772000
1	1.658130000	1.085359000	-1.527337000
7	0.928976000	-1.505561000	-1.582770000
7	-0.104638000	-0.616028000	-1.910643000
6	-1.172421000	-1.125923000	-2.413791000
1	-1.959483000	-0.392121000	-2.574522000
1	0.632049000	-2.339696000	-1.073480000
1	5.976787000	2.549028000	0.802685000
6	-1.503720000	-2.510794000	-2.767951000
6	-2.835157000	-2.940027000	-2.583333000
6	-0.600977000	-3.413710000	-3.370362000
6	-3.252217000	-4.213051000	-2.928360000
6	-1.026993000	-4.695539000	-3.724900000
6	-2.341553000	-5.102843000	-3.503903000
1	6.655827000	0.362378000	1.712726000
1	-4.273297000	-4.536318000	-2.771598000
8	0.683273000	-3.130793000	-3.730338000
1	1.070270000	-2.462724000	-3.121727000
1	-3.545909000	-2.248638000	-2.145078000
8	-0.179745000	-5.588419000	-4.321493000
1	0.688925000	-5.170107000	-4.404577000
8	-2.743508000	-6.349218000	-3.857955000
1	-1.992864000	-6.817080000	-4.248687000

5f_1, optimization in gas phase
B3LYP/6-311++G**, E= -874.464309704 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.220632 a.u.
Sum of electronic and thermal Free Energies= -874.243677 a.u.

0; 1			
6	6.539314000	0.504350000	0.008459000
6	5.789084000	-0.669725000	0.008605000
6	5.925676000	1.766456000	0.002845000
1	6.262185000	-1.644403000	0.012950000
6	4.397570000	-0.562260000	0.002942000
6	4.536022000	1.895132000	-0.002854000
1	4.063011000	2.870600000	-0.007212000
6	3.796526000	0.719389000	-0.002693000
6	2.291998000	-0.898304000	-0.004108000
7	3.424108000	-1.555527000	0.002025000
7	2.427311000	0.465282000	-0.007514000
1	1.660673000	1.118204000	-0.010449000
7	1.058579000	-1.496371000	-0.008402000
7	-0.068961000	-0.750657000	-0.006375000
6	-1.198295000	-1.363288000	-0.003000000
1	-1.237331000	-2.458894000	-0.001160000
1	1.036608000	-2.511204000	-0.000930000
1	6.540794000	2.658854000	0.002884000
6	-2.478668000	-0.665145000	-0.001674000
6	-2.578737000	0.740381000	-0.004358000
6	-3.664331000	-1.406881000	0.002434000
6	-3.810242000	1.364130000	-0.002891000
6	-4.914940000	-0.789466000	0.003954000
6	-4.992287000	0.604757000	0.001351000
1	7.621767000	0.444037000	0.012748000
8	-6.151695000	1.317259000	0.002347000
6	-7.386909000	0.611723000	0.006439000
1	-7.491471000	-0.013218000	-0.886759000
1	-7.487532000	-0.009625000	0.902584000
1	-8.163967000	1.373962000	0.006661000
1	-3.616390000	-2.491246000	0.004465000
1	-5.807571000	-1.400108000	0.007192000
1	-3.892049000	2.444435000	-0.004959000
1	-1.673102000	1.333950000	-0.007639000

5f_2, optimization in gas phase
B3LYP/6-311++G**, E= -874.454699232 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.221598 a.u.
Sum of electronic and thermal Free Energies= -874.233101 a.u.

0; 1			
6	5.490924000	1.935359000	0.043088000
6	4.100176000	1.871839000	-0.013876000
6	6.274622000	0.772827000	0.095226000
1	3.493283000	2.768356000	-0.054489000
6	3.499207000	0.613009000	-0.018310000
6	5.690960000	-0.494802000	0.092970000
1	6.298597000	-1.391657000	0.134687000
6	4.303833000	-0.546316000	0.035329000
1	5.980148000	2.902639000	0.046962000
6	2.133366000	-1.040925000	-0.048692000
7	2.151601000	0.269202000	-0.071816000
7	3.399611000	-1.603445000	0.020283000
1	3.627325000	-2.584261000	0.019265000
7	1.040017000	-1.870403000	-0.099355000
7	-0.298253000	-1.586283000	-0.051648000
6	-0.719684000	-0.371414000	-0.090067000
1	-0.038037000	0.472444000	-0.150137000
1	1.206526000	-2.857961000	-0.000831000
6	-2.155939000	-0.085948000	-0.050829000
6	-2.583282000	1.252209000	-0.091408000
6	-3.133840000	-1.085848000	0.024113000
6	-3.929218000	1.580238000	-0.059258000
6	-4.488128000	-0.771271000	0.056810000
6	-4.893636000	0.569086000	0.015062000
1	7.354127000	0.858761000	0.138610000
8	-6.192437000	0.984015000	0.041516000
6	-7.220989000	0.005593000	0.113766000
1	-7.200914000	-0.660808000	-0.755279000
1	-7.144612000	-0.588114000	1.031062000
1	-8.157977000	0.560027000	0.120788000
1	-1.844102000	2.044535000	-0.149022000
1	-2.822467000	-2.122790000	0.056439000
1	-5.215116000	-1.570423000	0.114781000
1	-4.258345000	2.611815000	-0.090766000

5f_3, optimization in gas phase
B3LYP/6-311++G**, E= -874.459471874 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.222925 a.u.
Sum of electronic and thermal Free Energies= -874.236547 a.u.

0; 1			
6	5.999618000	1.405267000	-0.315425000
6	4.683382000	1.856549000	-0.383777000
6	6.300762000	0.062772000	-0.037169000
1	4.450038000	2.892405000	-0.599394000
6	3.658836000	0.933802000	-0.166859000
6	5.291290000	-0.874645000	0.183755000
1	5.525039000	-1.911023000	0.399368000
6	3.981717000	-0.415705000	0.113588000
6	1.799968000	-0.079640000	0.080857000
7	2.278837000	1.109479000	-0.179807000
7	2.751081000	-1.044912000	0.275332000
1	2.547255000	-2.018087000	0.438573000

7	0.455633000	-0.361389000	0.199086000
7	0.081630000	-1.668481000	0.230618000
6	-1.162911000	-1.992822000	0.168725000
1	-1.322328000	-3.068288000	0.159630000
1	-0.168538000	0.354673000	-0.159236000
1	7.336646000	-0.253038000	0.007696000
6	-2.373454000	-1.162752000	0.071878000
6	-3.491319000	-1.702575000	-0.595987000
6	-2.515986000	0.107970000	0.648072000
6	-4.673433000	-0.997099000	-0.716294000
6	-3.707159000	0.825390000	0.544755000
6	-4.790446000	0.280886000	-0.150278000
1	6.811380000	2.104504000	-0.481236000
8	-5.988395000	0.898325000	-0.323043000
6	-6.178390000	2.195686000	0.232464000
1	-6.081728000	2.179552000	1.322971000
1	-5.469988000	2.916094000	-0.189201000
1	-7.192338000	2.486238000	-0.035789000
1	-1.711951000	0.537675000	1.232657000
1	-3.776517000	1.797212000	1.014225000
1	-3.419256000	-2.693402000	-1.032142000
1	-5.525680000	-1.412494000	-1.240203000

5g_1, optimization in gas phase B3LYP/6-311++G**, E= -989.009465483 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.250102 a.u. Sum of electronic and thermal Free Energies= -988.759364 a.u.			
0; 1			
6	-6.425200000	-0.226913000	-0.240968000
6	-5.519400000	-1.238661000	0.070599000
6	-5.995289000	1.075816000	-0.537558000
1	-5.850157000	-2.244841000	0.298865000
6	-4.159501000	-0.924748000	0.081819000
6	-4.640489000	1.410307000	-0.529729000
1	-4.309537000	2.416793000	-0.759206000
6	-3.744453000	0.395513000	-0.217937000
6	-2.033044000	-0.928569000	0.219231000
7	-3.058503000	-1.730687000	0.352460000
7	-2.356896000	0.360587000	-0.113215000
1	-1.680932000	1.082496000	-0.310301000
7	-0.725136000	-1.305878000	0.397641000
7	0.258230000	-0.402306000	0.193812000
6	1.471720000	-0.829333000	0.207252000
1	1.680343000	-1.890004000	0.356057000
1	-0.536901000	-2.299079000	0.501132000
1	-6.728036000	1.837712000	-0.777149000
6	2.641998000	0.020171000	0.000792000
6	2.623661000	1.429413000	-0.091697000
6	3.902034000	-0.622919000	-0.148105000
6	3.786844000	2.152634000	-0.351585000
6	5.064295000	0.104829000	-0.396169000
6	4.997929000	1.492614000	-0.504446000
1	-7.486338000	-0.448619000	-0.255975000

5g_2, optimization in gas phase B3LYP/6-311++G**, E= -988.997738835 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.249625 a.u. Sum of electronic and thermal Free Energies= -988.748114 a.u.			
0; 1			
6	-5.346031000	1.600144000	-0.666262000
6	-3.955680000	1.627040000	-0.578620000
6	-6.075075000	0.438230000	-0.371106000
1	-3.390413000	2.522574000	-0.807063000
6	-3.298613000	0.460600000	-0.186645000
6	-5.435116000	-0.737985000	0.021952000
1	-6.000708000	-1.634815000	0.248216000
6	-4.048810000	-0.699722000	0.106261000
1	-5.878134000	2.494751000	-0.968962000
6	-1.860474000	-1.034719000	0.354851000
7	-1.938974000	0.218215000	-0.017777000
7	-3.098410000	-1.654411000	0.451824000
1	-3.279214000	-2.608220000	0.718929000
7	-0.732735000	-1.757511000	0.663485000
7	0.594681000	-1.463113000	0.492524000
6	0.959478000	-0.276061000	0.157939000
1	0.246255000	0.529968000	0.030692000
1	-0.861151000	-2.735496000	0.863603000
6	2.377335000	0.049979000	-0.046320000
6	2.775623000	1.397998000	0.150318000
6	3.358944000	-0.858396000	-0.487756000
6	4.090229000	1.806636000	-0.070833000
6	4.673271000	-0.446267000	-0.718743000
6	5.033590000	0.876061000	-0.504936000
1	-7.155930000	0.452136000	-0.449940000

8	3.885933000	-1.985184000	-0.044231000	8	3.027554000	-2.155312000	-0.795523000
6	5.104843000	-2.705754000	-0.183657000	6	3.284250000	-3.116875000	0.229403000
1	5.543379000	-2.557483000	-1.175629000	1	4.343497000	-3.117301000	0.511259000
1	5.828286000	-2.417427000	0.585661000	1	2.662171000	-2.919023000	1.106116000
1	4.842728000	-3.754910000	-0.058097000	1	3.023208000	-4.087723000	-0.192168000
8	1.454865000	2.142477000	0.025521000	1	5.388163000	-1.172316000	-1.086391000
6	1.046039000	2.421589000	1.368474000	1	6.053733000	1.195950000	-0.684923000
1	0.822714000	1.502402000	1.916200000	1	4.385383000	2.834025000	0.089297000
1	1.819347000	2.990458000	1.896055000	8	1.791883000	2.239687000	0.579265000
1	0.142285000	3.026188000	1.295024000	6	2.086376000	3.619526000	0.748216000
1	3.714649000	3.229999000	-0.434020000	1	2.845471000	3.773633000	1.522524000
1	5.901498000	2.055918000	-0.707017000	1	2.421947000	4.074485000	-0.189674000
1	6.014515000	-0.395886000	-0.514687000	1	1.152504000	4.082968000	1.061843000

5g_3, optimization in gas phase
B3LYP/6-311++G**, E= -989.014836737 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.252891 a.u.
Sum of electronic and thermal Free Energies= -988.761946 a.u.

0; 1

6	6.224507000	0.396937000	-0.528892000
6	5.036613000	1.074793000	-0.795717000
6	6.224921000	-0.871737000	0.071322000
1	5.035783000	2.054437000	-1.258850000
6	3.832882000	0.458341000	-0.450049000
6	5.032397000	-1.505685000	0.423273000
1	5.033838000	-2.486507000	0.885219000
6	3.852969000	-0.822810000	0.153409000
6	1.793445000	-0.064385000	-0.104147000
7	2.524618000	0.905778000	-0.595616000
7	2.513304000	-1.134983000	0.357120000
1	2.104448000	-1.935594000	0.812228000
7	0.418522000	-0.055893000	-0.072822000
7	-0.197476000	-0.994508000	0.687739000
6	-1.477354000	-1.011099000	0.825732000
1	-1.828999000	-1.867973000	1.389851000
1	-0.020087000	0.850373000	-0.210659000
1	7.167755000	-1.370470000	0.264349000
6	-2.550131000	-0.152146000	0.280379000
6	-3.737165000	-0.800985000	-0.141707000
6	-2.529273000	1.256050000	0.223836000
6	-4.831449000	-0.080054000	-0.622459000
6	-3.619766000	1.985210000	-0.258996000
6	-4.757495000	1.307981000	-0.678243000
1	7.170612000	0.857788000	-0.789794000
8	-1.390843000	1.855145000	0.689114000
6	-1.330525000	3.279177000	0.788482000
1	-1.412032000	3.750413000	-0.195177000
1	-2.115651000	3.655051000	1.450197000
1	-0.353666000	3.499211000	1.214362000
8	-3.719845000	-2.159212000	-0.051846000
6	-4.880180000	-2.893729000	-0.425773000
1	-5.743842000	-2.613972000	0.185945000
1	-5.116361000	-2.750118000	-1.484854000
1	-4.634375000	-3.939427000	-0.249818000
1	-3.590147000	3.064351000	-0.299638000
1	-5.603912000	1.871481000	-1.053665000
1	-5.727023000	-0.584422000	-0.955491000

5h_1, optimization in gas phase B3LYP/6-311++G**, E= -989.019600506 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.249427 a.u. Sum of electronic and thermal Free Energies= -988.770173 a.u.			
0; 1			
6	6.814565000	0.031703000	0.005426000
6	5.982488000	-1.085556000	0.004449000
6	6.292554000	1.334543000	0.003170000
1	6.384209000	-2.091719000	0.006146000
6	4.602273000	-0.878167000	0.001157000
6	4.915917000	1.562830000	-0.000174000
1	4.514410000	2.569815000	-0.001976000
6	4.094157000	0.442934000	-0.001063000
6	2.478493000	-1.063203000	-0.003454000
7	3.560120000	-1.799361000	-0.000337000
7	2.710069000	0.287081000	-0.004438000
1	1.992042000	0.992925000	-0.004690000
7	1.205233000	-1.574028000	-0.006534000
7	0.132863000	-0.755323000	-0.004328000
6	-1.035616000	-1.288942000	-0.002850000
1	-1.148783000	-2.378819000	-0.002862000
1	1.114155000	-2.585290000	-0.002830000
1	6.970138000	2.180457000	0.003985000
6	-2.268494000	-0.502827000	-0.001201000
6	-2.248288000	0.899185000	-0.001154000
6	-3.486285000	-1.197110000	0.000272000
1	-1.296921000	1.408999000	-0.002275000
1	-3.480337000	-2.278657000	0.000158000
6	-3.456647000	1.595716000	0.000425000
6	-4.688232000	-0.479998000	0.001856000
6	-4.674993000	0.911772000	0.001929000
8	-5.924011000	-1.057270000	0.003390000
6	-6.018239000	-2.475525000	0.003158000
1	-5.558632000	-2.907690000	-0.892289000
1	-5.556445000	-2.908131000	0.897267000
1	-7.083304000	-2.701032000	0.004401000
8	-3.555819000	2.955816000	0.000598000
6	-2.361986000	3.727569000	-0.001009000
1	-1.759776000	3.533399000	0.892976000
1	-1.761964000	3.533086000	-0.896393000
1	-2.682391000	4.768058000	-0.000780000
1	7.889918000	-0.105583000	0.007962000
1	-5.605687000	1.463677000	0.003128000

5h_2, optimization in gas phase B3LYP/6-311++G**, E= -989.010797000 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.250257 a.u. Sum of electronic and thermal Free Energies= -988.760540 a.u.			
0; 1			
6	5.767137000	1.748168000	0.089544000
6	4.375215000	1.718276000	0.039105000
6	6.524224000	0.566829000	0.100443000
1	3.788991000	2.629289000	0.030451000
6	3.745659000	0.474098000	-0.001067000
6	5.911963000	-0.686346000	0.062132000
1	6.499085000	-1.597622000	0.071918000
6	4.523587000	-0.704293000	0.011375000
1	6.278642000	2.703307000	0.120976000
6	2.342671000	-1.146294000	-0.075107000
7	2.390114000	0.162760000	-0.057093000
7	3.595284000	-1.739563000	-0.031636000
1	3.800560000	-2.724834000	-0.064499000
7	1.229419000	-1.949562000	-0.143351000
7	-0.099230000	-1.636404000	-0.087674000
6	-0.494374000	-0.412711000	-0.088004000
1	0.204075000	0.418212000	-0.121760000
1	1.374098000	-2.943569000	-0.080744000
6	-1.928691000	-0.101155000	-0.040187000
6	-2.297864000	1.250237000	-0.043476000
6	-2.904830000	-1.105861000	0.005773000
1	-1.526458000	2.007344000	-0.078811000
1	-2.587189000	-2.137732000	0.006875000
6	-3.653813000	1.593938000	-0.001448000
6	-4.250622000	-0.743660000	0.047047000
6	-4.628745000	0.601472000	0.043531000
8	-5.282640000	-1.637114000	0.093480000
6	-4.978199000	-3.025129000	0.098731000
1	-4.445403000	-3.321401000	-0.811213000
1	-4.381666000	-3.300637000	0.975026000
1	-5.937690000	-3.538561000	0.138895000
8	-4.118125000	2.878486000	-0.001155000
6	-3.177142000	3.942658000	-0.040511000
1	-2.516826000	3.926401000	0.833260000
1	-2.573737000	3.911015000	-0.954149000
1	-3.765639000	4.858753000	-0.029779000
1	7.605597000	0.626862000	0.139866000
1	-5.676491000	0.870216000	0.076079000

5h_3, optimization in gas phase B3LYP/6-311++G**, E= -989.015196258 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.251465 a.u. Sum of electronic and thermal Free Energies= -988.763731 a.u.			
0; 1			
6	-6.403580000	0.823464000	0.522595000
6	-5.136452000	1.367919000	0.718635000
6	-6.575377000	-0.444158000	-0.055482000
1	-5.002773000	2.345902000	1.165359000
6	-4.028870000	0.616359000	0.322914000
6	-5.481342000	-1.210419000	-0.458441000
1	-5.615427000	-2.188910000	-0.905353000
6	-4.221462000	-0.659448000	-0.259254000

6	-2.081885000	-0.136840000	-0.107970000
7	-2.671902000	0.913150000	0.402379000
7	-2.936235000	-1.119054000	-0.531703000
1	-2.642194000	-2.003684000	-0.913964000
7	-0.717426000	-0.256229000	-0.256461000
7	-0.212217000	-1.461485000	-0.616639000
6	1.059057000	-1.664229000	-0.624512000
1	1.330576000	-2.682709000	-0.889401000
1	-0.155525000	0.425074000	0.244563000
1	-7.576488000	-0.836341000	-0.192343000
6	2.175639000	-0.756385000	-0.297927000
6	3.310807000	-1.328762000	0.293701000
6	2.150616000	0.615223000	-0.597000000
1	3.315815000	-2.389368000	0.504280000
1	1.310288000	1.039301000	-1.125625000
6	4.407211000	-0.521348000	0.611695000
6	3.264363000	1.405355000	-0.285701000
6	4.383072000	0.842953000	0.325965000
8	3.348601000	2.738013000	-0.548141000
6	2.238208000	3.394520000	-1.151309000
1	2.025932000	2.988792000	-2.145829000
1	1.342615000	3.322929000	-0.525620000
1	2.529489000	4.439093000	-1.244278000
8	5.547502000	-0.976672000	1.200731000
6	5.650846000	-2.359623000	1.517856000
1	4.877283000	-2.664982000	2.230242000
1	5.587927000	-2.981147000	0.618418000
1	6.630970000	-2.485223000	1.974425000
1	-7.278333000	1.389210000	0.822680000
1	5.236042000	1.462710000	0.569390000

5i_1, optimization in gas phase B3LYP/6-311++G**, E= -1103.56432825 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.277122 a.u. Sum of electronic and thermal Free Energies= -1103.287206 a.u.			
0; 1			
6	7.396811000	0.284968000	0.038055000
6	6.628397000	-0.876387000	0.080238000
6	6.803036000	1.555246000	-0.020596000
1	7.086020000	-1.857363000	0.125473000
6	5.238807000	-0.747469000	0.062835000
6	5.415707000	1.705245000	-0.038679000
1	4.958359000	2.687118000	-0.084138000
6	4.657860000	0.541972000	0.003847000
6	3.128450000	-1.051330000	0.057289000
7	4.249876000	-1.724950000	0.095009000
7	3.284750000	0.308844000	0.002409000
1	2.528510000	0.972398000	-0.036473000
7	1.885904000	-1.631110000	0.073079000
7	0.769425000	-0.872913000	0.015970000
6	-0.367300000	-1.471443000	0.009726000
1	-0.419516000	-2.565522000	0.046033000
1	1.850393000	-2.645454000	0.095694000

5i_2, optimization in gas phase B3LYP/6-311++G**, E= -1103.55554379 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.278079 a.u. Sum of electronic and thermal Free Energies= -1103.277465 a.u.			
0; 1			
6	6.294264000	1.884143000	0.147135000
6	4.905737000	1.803145000	0.065903000
6	7.092824000	0.731306000	0.190376000
1	4.287481000	2.692150000	0.032028000
6	4.322255000	0.536632000	0.027827000
6	6.526831000	-0.543669000	0.154788000
1	7.145934000	-1.432902000	0.189840000
6	5.141610000	-0.612555000	0.073142000
1	6.770185000	2.857556000	0.177309000
6	2.980210000	-1.134543000	-0.056106000
7	2.980420000	0.175770000	-0.054272000
7	4.252284000	-1.681291000	0.024231000
1	4.493959000	-2.658503000	-0.000215000
7	1.899036000	-1.978349000	-0.139527000
7	0.557612000	-1.712635000	-0.114313000
6	0.120260000	-0.503578000	-0.146568000
1	0.790695000	0.350144000	-0.182377000

1	7.432150000	2.437225000	-0.052620000	1	2.077738000	-2.964758000	-0.050631000
6	-1.641117000	-0.758814000	-0.045249000	6	-1.322523000	-0.239809000	-0.134165000
6	-1.704917000	0.640165000	-0.084962000	6	-1.741860000	1.094947000	-0.169544000
6	-2.819888000	-1.515445000	-0.056343000	6	-2.268360000	-1.272006000	-0.089784000
1	-0.784895000	1.204986000	-0.071051000	1	-0.997621000	1.879213000	-0.199826000
1	-2.757362000	-2.595021000	-0.025818000	1	-1.919207000	-2.293679000	-0.064232000
6	-2.943126000	1.276813000	-0.135886000	6	-3.105098000	1.404262000	-0.161118000
6	-4.061563000	-0.877695000	-0.112931000	6	-3.626160000	-0.965026000	-0.086488000
6	-4.134095000	0.523359000	-0.155970000	6	-4.058759000	0.375428000	-0.125116000
8	-5.259148000	-1.526488000	-0.131981000	8	-4.623814000	-1.893696000	-0.047988000
6	-5.264148000	-2.948038000	-0.156319000	6	-4.265639000	-3.269163000	-0.059035000
1	-4.745832000	-3.333551000	-1.040566000	1	-3.704130000	-3.527196000	-0.962970000
1	-4.808909000	-3.367196000	0.747630000	1	-3.675778000	-3.536831000	0.824265000
1	-6.312540000	-3.238387000	-0.198776000	1	-5.205491000	-3.819010000	-0.047461000
8	-3.110742000	2.625611000	-0.168103000	8	-3.605167000	2.670872000	-0.185133000
6	-1.954281000	3.451516000	-0.197996000	6	-2.692675000	3.756757000	-0.269094000
1	-1.346436000	3.322828000	0.704216000	1	-2.030371000	3.794298000	0.602833000
1	-1.342661000	3.248773000	-1.083507000	1	-2.090249000	3.703857000	-1.182274000
1	-2.324271000	4.474488000	-0.241347000	1	-3.306402000	4.655847000	-0.294312000
1	8.478127000	0.208227000	0.050431000	1	8.170182000	0.830885000	0.253056000
8	-5.333644000	1.158509000	-0.295551000	8	-5.388798000	0.678382000	-0.205302000
6	-6.094360000	1.319485000	0.907534000	6	-6.102002000	0.657480000	1.035411000
1	-6.345539000	0.348785000	1.343658000	1	-6.069584000	-0.337343000	1.488513000
1	-5.544080000	1.926819000	1.633370000	1	-5.692482000	1.399400000	1.728878000
1	-7.008577000	1.837800000	0.620042000	1	-7.133590000	0.915438000	0.796722000

5i_3, optimization in gas phase
B3LYP/6-311++G**, E= -1103.56001438 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.279067 a.u.
Sum of electronic and thermal Free Energies= -1103.280948 a.u.

0; 1

6	-6.841838000	0.895722000	0.935960000
6	-5.539918000	1.368613000	1.084232000
6	-7.112553000	-0.309040000	0.268386000
1	-5.330089000	2.297998000	1.600114000
6	-4.498630000	0.609541000	0.547917000
6	-6.085860000	-1.081804000	-0.275131000
1	-6.296261000	-2.011651000	-0.791185000
6	-4.790682000	-0.602598000	-0.122438000
6	-2.623279000	-0.183553000	-0.083511000
7	-3.126941000	0.842211000	0.553518000
7	-3.550327000	-1.089241000	-0.524638000
1	-3.324563000	-1.950830000	-0.995686000
7	-1.279624000	-0.345849000	-0.340966000
7	-0.857654000	-1.547107000	-0.813641000
6	0.400312000	-1.800798000	-0.917352000
1	0.607778000	-2.809469000	-1.265334000
1	-0.655240000	0.261320000	0.181062000
1	-8.138036000	-0.646412000	0.171897000
6	1.574581000	-0.965470000	-0.606797000
6	2.722031000	-1.619752000	-0.138097000
6	1.598350000	0.423446000	-0.804278000
1	2.697981000	-2.692761000	-0.004685000
1	0.744585000	0.922546000	-1.237632000
6	3.875553000	-0.892605000	0.158822000
6	2.758223000	1.151901000	-0.519838000
6	3.903339000	0.500766000	-0.029075000

8	2.876259000	2.493308000	-0.687795000
6	1.765172000	3.219394000	-1.202800000
1	1.495196000	2.876594000	-2.206909000
1	0.895069000	3.144122000	-0.542184000
1	2.091348000	4.256581000	-1.252526000
8	5.027824000	-1.438907000	0.632089000
6	5.097260000	-2.850453000	0.796576000
1	4.364288000	-3.204627000	1.529159000
1	4.946425000	-3.370111000	-0.155262000
1	6.101728000	-3.054802000	1.162928000
1	-7.666140000	1.469016000	1.344854000
8	5.049554000	1.210470000	0.174072000
6	5.339865000	1.545316000	1.537075000
1	4.551597000	2.180435000	1.953620000
1	5.456681000	0.643880000	2.144506000
1	6.278803000	2.097357000	1.518516000

5j_1, optimization in gas phase B3LYP/6-311++G**, E= -949.710403419 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.224555 a.u. Sum of electronic and thermal Free Energies= -949.485848 a.u.			
0; 1			
6	5.990430000	0.478279000	0.526707000
6	5.206071000	-0.672378000	0.540896000
6	5.505015000	1.690725000	0.011909000
1	5.579218000	-1.608508000	0.938433000
6	3.911644000	-0.591284000	0.025019000
6	4.214674000	1.791531000	-0.508655000
1	3.840966000	2.728308000	-0.905891000
6	3.440726000	0.638207000	-0.490370000
6	1.914274000	-0.954370000	-0.630553000
7	2.927808000	-1.568635000	-0.078023000
7	2.139755000	0.368126000	-0.914192000
1	1.473532000	1.015257000	-1.301351000
7	0.729638000	-1.585750000	-0.926318000
7	-0.346802000	-0.902689000	-1.383189000
6	-1.480431000	-1.518102000	-1.454869000
1	-1.563606000	-2.557089000	-1.121413000
1	0.629604000	-2.529625000	-0.566649000
1	6.143701000	2.566247000	0.017887000
6	-2.690030000	-0.900857000	-1.970081000
6	-3.889065000	-1.637719000	-1.944071000
6	-2.702402000	0.417057000	-2.484476000
1	-3.874645000	-2.647106000	-1.547007000
6	-5.071710000	-1.088518000	-2.409842000
6	-3.903453000	0.961249000	-2.975848000
6	-5.072604000	0.209171000	-2.926158000
8	-3.970718000	2.252985000	-3.427841000
6	-3.231679000	2.557554000	-4.619018000
1	-2.159330000	2.427432000	-4.465565000
1	-3.570598000	1.928026000	-5.449051000
1	-3.448271000	3.601061000	-4.844325000
1	6.999144000	0.439515000	0.921801000

5j_2, optimization in gas phase B3LYP/6-311++G**, E= -949.704775850 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.225366 a.u. Sum of electronic and thermal Free Energies= -949.479410 a.u.			
0; 1			
6	6.221118000	1.026463000	0.045679000
6	4.947351000	1.428836000	-0.349001000
6	6.468034000	-0.277599000	0.501460000
1	4.754612000	2.434981000	-0.701165000
6	3.913299000	0.495339000	-0.278408000
6	5.446699000	-1.224792000	0.576744000
1	5.640614000	-2.231957000	0.927538000
6	4.180071000	-0.812209000	0.181685000
6	2.037334000	-0.539427000	-0.352213000
7	2.565373000	0.632164000	-0.600883000
7	2.952897000	-1.466256000	0.118136000
1	2.764096000	-2.411224000	0.410676000
7	0.719336000	-0.911578000	-0.484020000
7	-0.317179000	-0.243470000	-1.079268000
6	-0.216993000	0.991777000	-1.448816000
1	0.706403000	1.547581000	-1.318424000
1	0.500190000	-1.884916000	-0.351367000
1	7.471616000	-0.556502000	0.800572000
6	-1.348211000	1.675079000	-2.062967000
6	-1.173974000	3.008492000	-2.476817000
6	-2.598217000	1.045027000	-2.274511000
1	-0.211118000	3.480727000	-2.315220000
6	-2.203812000	3.707593000	-3.084337000
6	-3.646431000	1.768623000	-2.875380000
6	-3.438043000	3.083114000	-3.278020000
8	-4.854848000	1.181726000	-3.154857000
6	-5.640103000	0.759693000	-2.032397000
1	-5.141256000	-0.034155000	-1.474474000
1	-5.847803000	1.608345000	-1.370949000
1	-6.576439000	0.387719000	-2.447355000
1	7.040916000	1.734042000	0.000758000

1	-5.983278000	0.666305000	-3.294794000
1	-5.990831000	-1.660599000	-2.378953000
8	-1.588082000	1.184235000	-2.512814000
1	-0.856529000	0.653318000	-2.136722000
1	-4.262155000	3.602361000	-3.753181000
1	-2.057344000	4.731828000	-3.404998000
8	-2.823201000	-0.241253000	-1.927550000
1	-1.992360000	-0.591886000	-1.534572000

5j_3, optimization in gas phase
B3LYP/6-311++G**, E= -949.699803121 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.226318 a.u.
Sum of electronic and thermal Free Energies= -949.473486 a.u.

0; 1

6	6.140301000	0.691340000	0.256899000
6	5.534263000	-0.493199000	-0.152166000
6	5.400486000	1.873326000	0.426113000
1	6.102695000	-1.406263000	-0.281871000
6	4.159502000	-0.477362000	-0.393064000
6	4.027413000	1.909764000	0.188870000
1	3.458884000	2.823503000	0.317976000
6	3.430625000	0.722451000	-0.220217000
6	2.135568000	-0.942014000	-0.860125000
7	3.309456000	-1.504892000	-0.795357000
7	2.118970000	0.387973000	-0.545174000
1	1.281410000	0.942035000	-0.458061000
7	0.980213000	-1.603557000	-1.283074000
7	-0.217055000	-1.008221000	-0.896470000
6	-1.303037000	-1.644084000	-1.154456000
1	-2.192220000	-1.147779000	-0.772728000
1	1.051189000	-2.611029000	-1.135597000
1	5.906748000	2.776718000	0.745822000
6	-1.523602000	-2.931139000	-1.838566000
6	-2.535809000	-3.764107000	-1.321619000
6	-0.864925000	-3.309341000	-3.030780000
1	-3.055885000	-3.452584000	-0.422427000
6	-2.865041000	-4.958254000	-1.937915000
6	-1.201741000	-4.535388000	-3.648240000
6	-2.192829000	-5.339898000	-3.100377000
8	-0.648394000	-4.917072000	-4.839305000
6	0.768443000	-5.145467000	-4.866824000
1	1.323915000	-4.221159000	-4.706024000
1	1.048211000	-5.889793000	-4.113544000
1	0.983917000	-5.537969000	-5.859669000
1	7.206760000	0.704772000	0.450558000
1	-2.436635000	-6.261962000	-3.614573000
1	-3.640299000	-5.592150000	-1.525036000
8	0.022294000	-2.519380000	-3.686681000
1	0.479202000	-1.920138000	-3.065526000

5k_1, optimization in gas phase
B3LYP/6-311++G**, E= -949.719728712 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.225195 a.u.
Sum of electronic and thermal Free Energies= -949.494533 a.u.

0; 1

6	5.952933000	0.506927000	0.449092000
6	5.158687000	-0.634953000	0.523408000
6	5.481397000	1.691396000	-0.138088000

5k_2, optimization in gas phase
B3LYP/6-311++G**, E= -949.713760678 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.226188 a.u.
Sum of electronic and thermal Free Energies= -949.487572 a.u.

0; 1

6	6.178841000	1.016412000	0.322708000
6	4.972942000	1.386491000	-0.268919000
6	6.354901000	-0.253836000	0.891894000

1	5.521421000	-1.549465000	0.977051000	1	4.835099000	2.366999000	-0.708477000
6	3.868811000	-0.574305000	-0.006411000	6	3.935230000	0.454637000	-0.282905000
6	4.195120000	1.771821000	-0.672870000	6	5.327287000	-1.197742000	0.889203000
1	3.831915000	2.687007000	-1.126351000	1	5.465323000	-2.178002000	1.331040000
6	3.411820000	0.627439000	-0.595195000	6	4.129635000	-0.818246000	0.296050000
6	1.873795000	-0.960292000	-0.658726000	6	2.083413000	-0.593053000	-0.551371000
7	2.878135000	-1.548342000	-0.060870000	7	2.648653000	0.560729000	-0.805064000
7	2.111967000	0.343413000	-1.012100000	7	2.915764000	-1.475806000	0.118592000
1	1.462769000	0.963053000	-1.466890000	1	2.711680000	-2.429683000	0.368638000
7	0.693001000	-1.601102000	-0.945105000	7	0.815669000	-1.001230000	-0.891418000
7	-0.399137000	-0.913764000	-1.375052000	7	-0.234294000	-0.263293000	-1.380321000
6	-1.527631000	-1.541291000	-1.437528000	6	-0.074340000	0.942887000	-1.822816000
1	-1.591401000	-2.588211000	-1.123683000	1	0.897516000	1.426841000	-1.803179000
1	0.587896000	-2.524425000	-0.536976000	1	0.497030000	-1.873491000	-0.503331000
1	6.127278000	2.560761000	-0.178231000	1	7.306528000	-0.508486000	1.343606000
6	-2.748753000	-0.930371000	-1.917405000	6	-1.200903000	1.687537000	-2.355304000
6	-3.942697000	-1.680100000	-1.939176000	6	-0.995723000	3.001050000	-2.823103000
6	-2.804959000	0.405421000	-2.379523000	6	-2.512087000	1.160561000	-2.433427000
1	-3.918340000	-2.707104000	-1.589290000	1	0.004468000	3.418050000	-2.768632000
6	-5.132244000	-1.149344000	-2.390375000	6	-2.020364000	3.764071000	-3.343058000
6	-4.003846000	0.953982000	-2.839810000	6	-3.558562000	1.924601000	-2.959207000
6	-5.163500000	0.180941000	-2.845499000	6	-3.314341000	3.219268000	-3.411489000
1	6.958532000	0.482771000	0.853322000	1	7.000151000	1.723397000	0.344749000
1	-6.045348000	-1.729856000	-2.404916000	1	-1.855526000	4.772252000	-3.700251000
8	-1.709979000	1.196698000	-2.395833000	8	-2.806574000	-0.086619000	-2.011204000
1	-0.960057000	0.670641000	-2.048986000	1	-1.975615000	-0.491554000	-1.673662000
8	-6.372354000	0.627121000	-3.273054000	8	-4.268703000	4.033581000	-3.937334000
6	-6.483727000	1.964163000	-3.750647000	6	-5.602019000	3.548411000	-4.042917000
1	-6.227514000	2.687175000	-2.969668000	1	-5.654335000	2.665825000	-4.688773000
1	-5.846841000	2.127149000	-4.625909000	1	-6.016896000	3.306583000	-3.058924000
1	-7.527189000	2.090532000	-4.033136000	1	-6.177061000	4.358063000	-4.488954000
1	-3.988585000	1.979146000	-3.181643000	1	-4.539629000	1.472537000	-2.996188000

5k_3, optimization in gas phase
B3LYP/6-311++G**, E= -949.709454608 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.227251 a.u.
Sum of electronic and thermal Free Energies= -949.482203 a.u.

0; 1

6	5.726152000	0.422755000	1.265309000
6	5.010749000	-0.730646000	0.955670000
6	5.311043000	1.686447000	0.814009000
1	5.328216000	-1.706179000	1.303876000
6	3.859593000	-0.599809000	0.177265000
6	4.165460000	1.837529000	0.034192000
1	3.848473000	2.813442000	-0.315155000
6	3.457744000	0.680313000	-0.271205000
6	2.076333000	-0.899633000	-0.945891000
7	2.963926000	-1.569817000	-0.265420000
7	2.301764000	0.447346000	-1.010380000
1	1.658374000	1.111716000	-1.411371000
7	1.008568000	-1.489086000	-1.626916000
7	-0.055459000	-0.626503000	-1.903930000
6	-1.106871000	-1.145666000	-2.432307000
1	-1.917257000	-0.429621000	-2.553552000
1	0.754124000	-2.384881000	-1.208395000
1	5.893422000	2.562500000	1.074948000
6	-1.396894000	-2.520784000	-2.856139000

6	-2.718608000	-2.990760000	-2.678971000
6	-0.494091000	-3.368966000	-3.537321000
1	-3.433564000	-2.339356000	-2.187326000
6	-3.123937000	-4.238772000	-3.094505000
6	-0.900211000	-4.639136000	-3.968519000
6	-2.201429000	-5.076249000	-3.748006000
1	6.623459000	0.346985000	1.868808000
1	-4.135903000	-4.589793000	-2.939715000
8	0.765326000	-3.011481000	-3.885830000
1	1.109833000	-2.317789000	-3.288874000
8	-2.676021000	-6.286959000	-4.134743000
6	-1.801572000	-7.182892000	-4.815041000
1	-1.446561000	-6.751283000	-5.756169000
1	-0.945874000	-7.453717000	-4.188548000
1	-2.394203000	-8.071472000	-5.023942000
1	-0.166840000	-5.241102000	-4.485803000

5l_1, optimization in gas phase B3LYP/6-311++G**, E= -949.703436941 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.222663 a.u. Sum of electronic and thermal Free Energies= -949.480774 a.u.			
0; 1			
6	-6.860538000	0.447491000	0.080473000
6	-6.088604000	-0.711019000	0.131648000
6	-6.271259000	1.717312000	-0.020713000
1	-6.542585000	-1.691618000	0.209820000
6	-4.700097000	-0.579501000	0.079487000
6	-4.885257000	1.869851000	-0.073919000
1	-4.431352000	2.851191000	-0.152233000
6	-4.123736000	0.709243000	-0.022175000
6	-2.590006000	-0.878672000	0.034044000
7	-3.708005000	-1.553923000	0.112392000
7	-2.750402000	0.479157000	-0.049523000
1	-1.997106000	1.144297000	-0.115285000
7	-1.345764000	-1.457160000	0.031195000
7	-0.233121000	-0.697365000	-0.033090000
6	0.907376000	-1.288411000	-0.018443000
1	0.966803000	-2.381123000	0.045639000
1	-1.307820000	-2.469271000	0.102661000
1	-6.903174000	2.597043000	-0.058593000
6	2.173134000	-0.563484000	-0.084166000
6	2.245303000	0.834152000	-0.175324000
6	3.369576000	-1.295438000	-0.058075000
6	3.480429000	1.463402000	-0.225149000
6	4.608601000	-0.664568000	-0.123682000
6	4.673173000	0.737743000	-0.193086000
1	-7.941106000	0.369032000	0.119124000
8	5.854513000	1.415535000	-0.316473000
6	6.788593000	1.303098000	0.767362000
1	6.333144000	1.656205000	1.698775000
1	7.137096000	0.276466000	0.887940000

5l_2, optimization in gas phase B3LYP/6-311++G**, E= -949.695588644 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.223745 a.u. Sum of electronic and thermal Free Energies= -949.471843 a.u.			
0; 1			
6	-5.818621000	1.891459000	-0.053219000
6	-4.426080000	1.859640000	-0.027114000
6	-6.577749000	0.711511000	-0.035914000
1	-3.838103000	2.769442000	-0.040547000
6	-3.798171000	0.614807000	0.017409000
6	-5.967044000	-0.542309000	0.007105000
1	-6.555821000	-1.452500000	0.019025000
6	-4.578028000	-0.562229000	0.033341000
1	-6.328969000	2.847106000	-0.087726000
6	-2.396595000	-1.007005000	0.086185000
7	-2.442369000	0.301649000	0.053167000
7	-3.650670000	-1.598738000	0.072461000
1	-3.856943000	-2.583081000	0.121973000
7	-1.282835000	-1.810272000	0.144324000
7	0.044883000	-1.496853000	0.057912000
6	0.439142000	-0.272400000	0.037899000
1	-0.257257000	0.559970000	0.078704000
1	-1.428487000	-2.804674000	0.092492000
6	1.868953000	0.037710000	-0.044555000
6	2.272212000	1.377864000	-0.054147000
6	2.851947000	-0.961179000	-0.118263000
6	3.623629000	1.705226000	-0.121912000
6	4.197767000	-0.635725000	-0.199748000
6	4.600132000	0.716260000	-0.188378000
1	-7.659554000	0.773110000	-0.057065000
8	5.910092000	1.089555000	-0.328428000
6	6.809217000	0.701880000	0.719507000
1	6.488196000	1.132118000	1.674533000
1	6.878109000	-0.383782000	0.803967000

1	7.625195000	1.949275000	0.505041000	1	7.780134000	1.112841000	0.445273000
1	3.334345000	-2.380775000	-0.001410000	1	1.527420000	2.164104000	-0.004057000
1	3.552968000	2.542282000	-0.297331000	1	2.544320000	-2.002208000	-0.125553000
1	1.333422000	1.415853000	-0.201569000	1	3.949113000	2.738710000	-0.132594000
8	5.787509000	-1.362217000	-0.137649000	8	5.177569000	-1.588844000	-0.308132000
1	5.604898000	-2.307549000	-0.126112000	1	4.769217000	-2.460391000	-0.340174000

5l_3, optimization in gas phase
B3LYP/6-311++G**, E= -949.699113007 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.225043 a.u.
Sum of electronic and thermal Free Energies= -949.474070 a.u.

0; 1

6	6.208978000	-1.382127000	0.394726000
6	4.888477000	-1.791731000	0.564259000
6	6.523586000	-0.090923000	-0.057436000
1	4.644571000	-2.787668000	0.914256000
6	3.873696000	-0.879388000	0.271074000
6	5.523918000	0.834900000	-0.357068000
1	5.768366000	1.831441000	-0.706790000
6	4.209755000	0.417779000	-0.184776000
6	2.025564000	0.137560000	-0.034091000
7	2.491931000	-1.021113000	0.353489000
7	2.985085000	1.049975000	-0.380341000
1	2.794125000	2.001556000	-0.651234000
7	0.681249000	0.429131000	-0.138136000
7	0.323236000	1.727221000	-0.326033000
6	-0.915739000	2.073006000	-0.274174000
1	-1.069002000	3.142264000	-0.394226000
1	0.063543000	-0.217155000	0.343461000
1	7.562567000	0.193638000	-0.176873000
6	-2.128775000	1.269114000	-0.048171000
6	-3.212387000	1.874995000	0.603310000
6	-2.279792000	-0.055158000	-0.495939000
6	-4.391298000	1.172141000	0.817284000
6	-3.460775000	-0.760390000	-0.281118000
6	-4.539241000	-0.143498000	0.381381000
1	7.013591000	-2.073815000	0.617086000
8	-5.695254000	-0.803065000	0.685174000
6	-6.478314000	-1.310791000	-0.406964000
1	-6.752663000	-0.497010000	-1.086430000
1	-5.944517000	-2.089490000	-0.952409000
1	-7.378358000	-1.724649000	0.045194000
1	-1.487888000	-0.537917000	-1.059222000
1	-3.127159000	2.900010000	0.945798000
1	-5.227840000	1.628610000	1.332825000
8	-3.619168000	-2.056816000	-0.686463000
1	-2.800382000	-2.380199000	-1.077762000

Structural parameters of the isomers of the molecules **5a-l** in imino form

5a_1, optimization in gas phase
B3LYP/6-311++G**, E= -835.174806842 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.196831 a.u.
Sum of electronic and thermal Free Energies= -834.977976 a.u.

0; 1			
6	-5.226797000	1.547770000	-0.070724000
6	-3.838451000	1.726721000	-0.077439000
6	-5.793030000	0.270897000	-0.018726000
1	-3.398332000	2.715640000	-0.117566000
6	-3.049785000	0.587446000	-0.030863000
6	-4.994837000	-0.877868000	0.028221000
1	-5.435058000	-1.866733000	0.067560000
6	-3.619212000	-0.698142000	0.021476000
6	-1.356827000	-0.929890000	0.028066000
7	-1.666381000	0.409565000	-0.022370000
7	-2.558930000	-1.598562000	0.057157000
1	-6.871280000	0.164583000	-0.014815000
1	-0.969864000	1.133630000	-0.076164000
1	-2.617359000	-2.603491000	0.100875000
7	-0.205508000	-1.543671000	0.045196000
7	0.867447000	-0.681038000	0.029361000
6	2.028746000	-1.250608000	-0.011691000
1	2.089386000	-2.340341000	-0.041351000
6	3.272415000	-0.499144000	-0.016945000
6	3.302655000	0.916323000	0.054677000
6	4.497038000	-1.188348000	-0.089955000
6	4.523705000	1.593830000	0.050587000
6	5.709707000	-0.513324000	-0.095300000
6	5.717148000	0.883711000	-0.024743000
1	-5.871700000	2.417617000	-0.106592000
1	4.516827000	2.676141000	0.106429000
1	6.640661000	-1.064222000	-0.153425000
1	6.658123000	1.422336000	-0.028032000
8	2.159611000	1.638244000	0.129793000
1	1.411628000	0.990610000	0.122847000
1	4.478839000	-2.272033000	-0.143365000

5a_2, optimization in gas phase
B3LYP/6-311++G**, E= -835.174806732 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.196863 a.u.
Sum of electronic and thermal Free Energies= -834.977943 a.u.

0; 1			
6	-5.226791000	1.547799000	-0.072018000
6	-3.838446000	1.726669000	-0.079150000
6	-5.793103000	0.271012000	-0.018650000
1	-3.398274000	2.715523000	-0.120261000
6	-3.049828000	0.587392000	-0.031681000
6	-4.994970000	-0.877747000	0.029188000
1	-5.435197000	-1.866567000	0.069580000
6	-3.619343000	-0.698104000	0.021940000
6	-1.357002000	-0.929968000	0.028417000
7	-1.666432000	0.409426000	-0.022927000
7	-2.559076000	-1.598590000	0.058132000
1	-6.871360000	0.164795000	-0.014379000
1	-0.969792000	1.133171000	-0.079450000
1	-2.617584000	-2.603428000	0.103768000
7	-0.205610000	-1.543734000	0.045788000
7	0.867182000	-0.680930000	0.029620000
6	2.028506000	-1.250324000	-0.012105000
1	2.089310000	-2.340044000	-0.042266000
6	3.272254000	-0.498953000	-0.017297000
6	3.302993000	0.916451000	0.055738000
6	4.496655000	-1.188398000	-0.091597000
6	4.524232000	1.593568000	0.051711000
6	5.709560000	-0.513721000	-0.096912000
6	5.717482000	0.883176000	-0.024958000
1	-5.871653000	2.417647000	-0.108596000
1	4.517716000	2.675814000	0.108689000
1	6.640265000	-1.064939000	-0.156069000
1	6.658566000	1.421616000	-0.028192000
8	2.160272000	1.638797000	0.132236000
1	1.411983000	0.991739000	0.125299000
1	4.478194000	-2.272026000	-0.146053000

5a_3, optimization in gas phase
B3LYP/6-311++G**, E= -835.171240770 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.197548 a.u.
Sum of electronic and thermal Free Energies= -834.973693 a.u.

0; 1			
6	5.659794000	-0.545073000	-0.071844000
6	4.499952000	-1.318940000	0.043850000
6	5.595531000	0.845330000	-0.205918000
1	4.549150000	-2.395877000	0.147465000
6	3.284965000	-0.650570000	0.020873000
6	4.368843000	1.517610000	-0.229178000
1	4.318249000	2.594491000	-0.332347000
6	3.220809000	0.748096000	-0.113945000
6	1.103754000	-0.043106000	0.036987000
7	1.968253000	-1.100155000	0.108933000
7	1.867791000	1.086027000	-0.098925000

1	6.512059000	1.416308000	-0.293648000
1	1.634337000	-2.045224000	0.221557000
1	1.477543000	2.011856000	-0.180442000
7	-0.205709000	-0.054380000	0.076144000
7	-0.704941000	-1.331873000	0.246609000
6	-1.984131000	-1.497060000	0.229374000
1	-2.265638000	-2.542679000	0.338152000
6	-3.146059000	-0.604614000	0.053175000
6	-3.204125000	0.806146000	0.220909000
6	-4.348828000	-1.269843000	-0.273769000
6	-4.426758000	1.471807000	0.039856000
6	-5.550229000	-0.604202000	-0.455597000
6	-5.583658000	0.784021000	-0.293703000
1	6.625517000	-1.035921000	-0.057113000
1	-4.437438000	2.546822000	0.177285000
1	-6.447547000	-1.154367000	-0.711862000
1	-6.512582000	1.328492000	-0.422971000
8	-2.156527000	1.566655000	0.592242000
1	-1.300221000	1.056825000	0.425896000
1	-4.318129000	-2.348897000	-0.385657000

5b_1, optimization in gas phase B3LYP/6-311++G**, E= -910.413957329 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.199741 a.u. Sum of electronic and thermal Free Energies= -910.214216 a.u.			
0; 1			
6	-5.346038000	1.797055000	0.100833000
6	-4.104231000	1.775604000	0.746972000
6	-5.839585000	0.667868000	-0.554762000
1	-3.723075000	2.652036000	1.257241000
6	-3.384164000	0.592600000	0.708644000
6	-5.110674000	-0.526475000	-0.592896000
1	-5.495443000	-1.401162000	-1.103466000
6	-3.880288000	-0.545182000	0.045398000
6	-1.842940000	-1.073246000	0.919455000
7	-2.144726000	0.234575000	1.240461000
7	-2.918681000	-1.540272000	0.193369000
1	-6.804622000	0.713387000	-1.044944000
1	-1.492534000	0.838774000	1.710597000
1	-2.956826000	-2.484823000	-0.152117000
7	-0.800361000	-1.799112000	1.185795000
7	0.125003000	-1.143417000	1.969177000
6	1.244980000	-1.769824000	2.133504000
1	1.395317000	-2.731471000	1.639728000
6	2.315990000	-1.244267000	2.961400000
6	3.537305000	-1.939090000	3.064560000
6	2.161893000	-0.046207000	3.684180000
6	4.564191000	-1.449170000	3.856959000
6	3.202149000	0.440947000	4.486729000
6	4.399603000	-0.257536000	4.570087000
1	-5.932234000	2.707964000	0.112686000
1	5.500465000	-1.989431000	3.928436000
8	1.018864000	0.690524000	3.653914000

5b_2, optimization in gas phase B3LYP/6-311++G**, E= -910.400106076 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.198530 a.u. Sum of electronic and thermal Free Energies= -910.201576 a.u.			
0; 1			
6	-4.579995000	1.081139000	-2.437096000
6	-3.585463000	1.349521000	-1.489123000
6	-5.525088000	0.075081000	-2.229423000
1	-2.852833000	2.130865000	-1.651883000
6	-3.574393000	0.579449000	-0.336932000
6	-5.513760000	-0.702425000	-1.065380000
1	-6.248524000	-1.482650000	-0.906219000
6	-4.528665000	-0.435524000	-0.127573000
6	-3.142725000	-0.385926000	1.676480000
7	-2.745354000	0.581319000	0.781839000
7	-4.236723000	-1.003157000	1.110479000
1	-6.282907000	-0.110335000	-2.981107000
1	-1.957768000	1.176287000	0.983320000
1	-4.717807000	-1.761613000	1.564558000
7	-2.643835000	-0.709474000	2.833644000
7	-1.550886000	0.073646000	3.136148000
6	-1.019147000	-0.172152000	4.280744000
1	-1.468909000	-0.958521000	4.896052000
6	0.166490000	0.528937000	4.769168000
6	0.985867000	1.293795000	3.915764000
6	0.531380000	0.438872000	6.121193000
6	2.119440000	1.927527000	4.398697000
6	1.679781000	1.079991000	6.607479000
6	2.474784000	1.823008000	5.746188000
1	-4.614006000	1.667006000	-3.347747000
1	2.743426000	2.504944000	3.726562000
8	-0.172495000	-0.261653000	7.079555000

1	0.388389000	0.201469000	3.065752000	1	-1.060780000	-0.468041000	6.773368000
1	3.662773000	-2.863780000	2.512398000	1	0.716277000	1.358996000	2.870168000
1	5.190535000	0.139100000	5.195301000	1	3.356823000	2.312000000	6.141350000
8	3.034229000	1.601100000	5.184099000	8	2.013388000	0.981855000	7.926322000
1	2.141489000	1.926714000	5.006067000	1	1.332185000	0.460000000	8.370692000

5b_3, optimization in gas phase
B3LYP/6-311++G**, E= -910.412291587 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.200962 a.u.
Sum of electronic and thermal Free Energies= -910.197662 a.u.

0; 1			
6	-5.023253000	2.149028000	-0.489416000
6	-3.762274000	2.028387000	0.104752000
6	-5.833377000	1.032111000	-0.704327000
1	-3.134746000	2.895693000	0.270259000
6	-3.348611000	0.757552000	0.472225000
6	-5.415122000	-0.250370000	-0.332797000
1	-6.045522000	-1.115552000	-0.499464000
6	-4.165880000	-0.367309000	0.255549000
6	-2.240418000	-1.069276000	1.231966000
7	-2.179149000	0.289244000	1.068659000
7	-3.457518000	-1.470146000	0.735464000
1	-6.804923000	1.157521000	-1.166758000
1	-1.369625000	0.803271000	1.381297000
1	-3.750644000	-2.433034000	0.717553000
7	-1.344037000	-1.864711000	1.744745000
7	-0.230303000	-1.161198000	2.177742000
6	0.779397000	-1.826050000	2.624597000
1	1.603222000	-1.174003000	2.908416000
6	1.091903000	-3.254408000	2.803177000
6	2.462641000	-3.538223000	3.013607000
6	0.190118000	-4.339046000	2.820026000
6	2.922678000	-4.828446000	3.208078000
6	0.671497000	-5.648654000	3.024253000
6	2.020932000	-5.896085000	3.214461000
1	-5.375014000	3.129276000	-0.787579000
1	3.979318000	-5.012959000	3.360261000
8	-1.154675000	-4.258794000	2.690887000
1	-1.394419000	-3.359412000	2.295667000
1	3.163995000	-2.711231000	3.015357000
1	2.349208000	-6.916629000	3.371281000
8	-0.221507000	-6.678332000	3.041143000
1	-1.095607000	-6.292197000	2.883085000

5c_1, optimization in gas phase
B3LYP/6-311++G**, E= -910.413748482 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.199466 a.u.
Sum of electronic and thermal Free Energies= -910.214283 a.u.

0; 1			
6	-5.480322000	1.684057000	0.312699000
6	-4.243032000	1.662382000	0.968305000
6	-5.885790000	0.624946000	-0.500588000
1	-3.928453000	2.485751000	1.598349000
6	-3.438713000	0.550187000	0.780413000

5c_2, optimization in gas phase
B3LYP/6-311++G**, E= -910.399917606 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.198079 a.u.
Sum of electronic and thermal Free Energies= -910.201838 a.u.

0; 1			
6	-4.702021000	1.363774000	-2.196475000
6	-3.721157000	1.600139000	-1.225393000
6	-5.533646000	0.245356000	-2.127041000
1	-3.076390000	2.469059000	-1.280922000
6	-3.606946000	0.682920000	-0.192925000

6	-5.071800000	-0.498456000	-0.689635000	6	-5.417911000	-0.681496000	-1.083779000
1	-5.389386000	-1.319827000	-1.320838000	1	-6.064553000	-1.549376000	-1.032068000
6	-3.848138000	-0.518988000	-0.038823000	6	-4.447001000	-0.446310000	-0.123086000
6	-1.789242000	-1.023698000	0.800595000	6	-3.037095000	-0.502950000	1.664009000
7	-2.176885000	0.215402000	1.271204000	7	-2.759613000	0.616021000	0.909674000
7	-2.822450000	-1.458476000	-0.005794000	7	-4.072762000	-1.147725000	1.020132000
1	-6.848009000	0.669244000	-0.996477000	1	-6.283484000	0.087755000	-2.892993000
1	-1.624298000	0.739286000	1.928093000	1	-2.037249000	1.259296000	1.190299000
1	-2.786413000	-2.342412000	-0.485411000	1	-4.467694000	-2.005370000	1.368085000
7	-0.714802000	-1.717697000	1.011869000	7	-2.486677000	-0.927359000	2.761005000
7	0.194037000	-1.066620000	1.822546000	7	-1.472821000	-0.081614000	3.168826000
6	1.234026000	-1.765508000	2.146382000	6	-0.906969000	-0.427537000	4.270772000
1	1.314163000	-2.794386000	1.789473000	1	-1.278988000	-1.331589000	4.766052000
6	2.307378000	-1.238088000	2.963494000	6	0.206417000	0.305576000	4.861516000
6	3.392566000	-2.059819000	3.319274000	6	0.918112000	1.282798000	4.138378000
6	2.315439000	0.103481000	3.424246000	6	0.631457000	0.046300000	6.180981000
6	4.441228000	-1.600998000	4.095670000	6	1.991852000	1.966426000	4.675538000
6	3.369611000	0.575055000	4.206486000	6	1.718385000	0.723635000	6.734275000
6	4.422426000	-0.272995000	4.539392000	6	2.395402000	1.678878000	5.985247000
1	-6.131456000	2.540290000	0.441035000	1	-4.814444000	2.063966000	-3.015525000
1	5.271536000	-2.239947000	4.366554000	1	2.534639000	2.708853000	4.104505000
1	3.346408000	1.606515000	4.542433000	1	2.007295000	0.493741000	7.754306000
8	1.314099000	0.952911000	3.118702000	8	0.024606000	-0.862441000	7.003092000
1	0.676072000	0.444465000	2.556573000	1	-0.773145000	-1.207771000	6.589840000
8	5.474850000	0.143422000	5.304039000	8	3.464644000	2.371723000	6.478933000
1	5.357269000	1.068451000	5.544957000	1	3.649683000	2.088182000	7.380508000
1	3.399500000	-3.087370000	2.970615000	1	0.606479000	1.482737000	3.121034000

5c_3, optimization in gas phase
B3LYP/6-311++G**, E= -910.410803693 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.199836 a.u.
Sum of electronic and thermal Free Energies= -910.210968 a.u.

0; 1

6	-5.403948000	2.083729000	0.168036000
6	-4.177493000	1.903219000	0.817774000
6	-5.961393000	1.075293000	-0.620145000
1	-3.746237000	2.686402000	1.429441000
6	-3.537596000	0.685618000	0.648729000
6	-5.314559000	-0.154146000	-0.790572000
1	-5.748782000	-0.935426000	-1.402835000
6	-4.100238000	-0.330721000	-0.146637000
6	-2.129282000	-1.092999000	0.686236000
7	-2.334963000	0.184078000	1.141769000
7	-3.211987000	-1.405876000	-0.103253000
1	-6.912311000	1.244211000	-1.110870000
1	-1.654619000	0.625096000	1.741463000
1	-3.314655000	-2.296263000	-0.561511000
7	-1.127183000	-1.885988000	0.928976000
7	-0.187187000	-1.284998000	1.753692000
6	0.848961000	-1.969572000	2.103764000
1	1.502855000	-1.394181000	2.756911000
6	1.360557000	-3.325067000	1.857791000
6	2.528844000	-3.643733000	2.588881000
6	0.857925000	-4.335512000	0.986568000
6	3.180715000	-4.857395000	2.507002000
6	1.519839000	-5.568252000	0.901836000
6	2.660824000	-5.830493000	1.646761000

1	-5.928182000	3.025025000	0.280966000
1	4.072189000	-5.067333000	3.083241000
1	1.107311000	-6.312154000	0.227989000
8	-0.220140000	-4.203507000	0.203972000
1	-0.675101000	-3.323956000	0.393040000
8	3.319116000	-7.024528000	1.576379000
1	2.870846000	-7.605570000	0.952483000
1	2.931031000	-2.885118000	3.252288000

5d_1, optimization in gas phase B3LYP/6-311++G**, E= -910.402835344 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.197873 a.u. Sum of electronic and thermal Free Energies= -910.204963 a.u.			
0; 1			
6	5.557733000	1.861264000	0.000165000
6	4.157552000	1.887856000	0.000018000
6	6.258088000	0.654272000	0.000247000
1	3.615323000	2.825844000	-0.000032000
6	3.492834000	0.671879000	-0.000047000
6	5.586212000	-0.574460000	0.000155000
1	6.132098000	-1.510481000	0.000185000
6	4.200618000	-0.546959000	0.000020000
6	1.973629000	-1.022876000	-0.000137000
7	2.139975000	0.345245000	-0.000101000
7	3.245143000	-1.559439000	-0.000251000
1	7.341474000	0.664153000	0.000367000
1	1.341702000	0.959466000	-0.000430000
1	3.405799000	-2.552771000	0.000728000
7	0.886128000	-1.731669000	-0.000089000
7	-0.233358000	-0.920837000	-0.000065000
6	-1.349898000	-1.555688000	0.000035000
1	-1.349517000	-2.648999000	0.000105000
6	-2.646590000	-0.881798000	0.000055000
6	-3.814414000	-1.656225000	0.000215000
6	-2.762801000	0.518980000	-0.000100000
6	-5.070034000	-1.050509000	0.000259000
6	-4.006731000	1.124513000	-0.000084000
6	-5.168403000	0.333278000	0.000104000
1	6.104092000	2.796846000	0.000222000
1	-3.742929000	-2.737896000	0.000328000
1	-1.875872000	1.138571000	-0.000259000
8	-6.354509000	1.033463000	0.000181000
1	-7.103382000	0.429373000	-0.000746000
1	-5.971258000	-1.656505000	0.000434000
8	-4.100299000	2.486064000	-0.000252000
1	-5.035204000	2.728553000	-0.000413000

5d_2, optimization in gas phase B3LYP/6-311++G**, E= -910.402842889 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.197931 a.u. Sum of electronic and thermal Free Energies= -910.204912 a.u.			
0; 1			
6	6.169712000	0.955572000	-1.810068000
6	4.850098000	1.356520000	-1.566693000
6	6.740402000	-0.112664000	-1.117008000
1	4.408447000	2.185807000	-2.106180000
6	4.131728000	0.653875000	-0.612374000
6	6.014309000	-0.822776000	-0.152702000
1	6.459368000	-1.651989000	0.384350000
6	4.708624000	-0.425033000	0.087444000
6	2.570816000	-0.164449000	0.827846000
7	2.830241000	0.784775000	-0.137084000
7	3.731079000	-0.900430000	0.957055000
1	7.763671000	-0.400840000	-1.326071000
1	2.123018000	1.449299000	-0.406790000
1	3.807493000	-1.668259000	1.602904000
7	1.491205000	-0.384127000	1.514329000
7	0.494309000	0.509906000	1.170683000
6	-0.607046000	0.348908000	1.811708000
1	-0.686761000	-0.448410000	2.555538000
6	-1.782936000	1.189313000	1.596381000
6	-2.941716000	0.938512000	2.343423000
6	-1.792398000	2.241572000	0.664418000
6	-4.084495000	1.717069000	2.166897000
6	-2.924223000	3.016993000	0.485930000
6	-4.078351000	2.752117000	1.243070000
1	6.755369000	1.486764000	-2.550779000
1	-2.951854000	0.130601000	3.066124000
1	-0.910099000	2.455002000	0.075777000
8	-5.148946000	3.580688000	0.989688000
1	-5.897332000	3.345153000	1.546688000
1	-4.979443000	1.517436000	2.748790000
8	-2.914855000	4.034723000	-0.423258000
1	-3.779931000	4.464033000	-0.410724000

5d_3, optimization in gas phase B3LYP/6-311++G**, E= -910.398292322 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.198560 a.u. Sum of electronic and thermal Free Energies= -910.199732 a.u.			
0; 1			
6	5.514655000	2.234879000	0.000091000
6	4.121265000	2.098310000	-0.000042000

5d_4, optimization in gas phase B3LYP/6-311++G**, E= -910.398259561 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.198555 a.u. Sum of electronic and thermal Free Energies= -910.199704 a.u.			
0; 1			
6	6.089720000	0.921565000	-3.572154000
6	4.914834000	1.399275000	-2.979149000

6	6.351303000	1.117583000	0.000238000	6	6.890408000	-0.025613000	-2.931690000
1	3.473270000	2.966588000	-0.000156000	1	4.294720000	2.134645000	-3.477601000
6	3.602665000	0.812786000	-0.000016000	6	4.575356000	0.897013000	-1.732561000
6	5.827693000	-0.180938000	0.000251000	6	6.547747000	-0.532898000	-1.672503000
1	6.478988000	-1.046902000	0.000354000	1	7.170586000	-1.268130000	-1.176964000
6	4.448276000	-0.314774000	0.000129000	6	5.384427000	-0.059350000	-1.086655000
6	2.293870000	-1.046161000	-0.000003000	6	3.609159000	0.392369000	0.262526000
7	2.298106000	0.329623000	-0.000110000	7	3.503766000	1.148778000	-0.881828000
7	3.617067000	-1.431945000	0.000060000	7	4.765969000	-0.344715000	0.127798000
1	7.426115000	1.253860000	0.000338000	1	7.794310000	-0.376738000	-3.414846000
1	1.427350000	0.837733000	-0.000197000	1	2.720818000	1.771815000	-1.005148000
1	3.894102000	-2.399487000	0.000451000	1	5.078567000	-0.987005000	0.836762000
7	1.289459000	-1.872555000	0.000029000	7	2.819079000	0.335089000	1.294243000
7	0.098760000	-1.170493000	-0.000054000	7	1.751053000	1.195055000	1.120294000
6	-1.004580000	-1.838983000	-0.000037000	6	0.862744000	1.262869000	2.053298000
1	-1.885635000	-1.198693000	-0.000088000	1	0.063895000	1.966895000	1.824514000
6	-1.308399000	-3.274307000	0.000051000	6	0.713172000	0.589184000	3.347957000
6	-2.670035000	-3.627678000	0.000096000	6	-0.417301000	0.937258000	4.109339000
6	-0.349697000	-4.305306000	0.000086000	6	1.605067000	-0.365341000	3.872964000
6	-3.066607000	-4.960297000	0.000157000	6	-0.654437000	0.357322000	5.350558000
6	-0.744028000	-5.634723000	0.000163000	6	1.369488000	-0.944522000	5.110693000
6	-2.106321000	-5.964655000	0.000195000	6	0.236671000	-0.583066000	5.852858000
1	5.948287000	3.227746000	0.000078000	1	6.379967000	1.296181000	-4.546459000
1	-3.425044000	-2.849669000	0.000067000	1	-1.117166000	1.670226000	3.724159000
1	0.701241000	-4.063461000	0.000068000	1	2.479916000	-0.652068000	3.311309000
8	-2.389542000	-7.312291000	0.000231000	8	0.096935000	-1.216431000	7.067719000
1	-3.340857000	-7.456605000	0.000906000	1	-0.706396000	-0.923915000	7.509216000
1	-4.121190000	-5.220094000	0.000165000	1	-1.530863000	0.634876000	5.928909000
8	0.204116000	-6.618371000	0.000206000	8	2.248844000	-1.868461000	5.600119000
1	-0.243759000	-7.473901000	0.000416000	1	1.931404000	-2.164419000	6.462777000

5e_1, optimization in gas phase B3LYP/6-311++G**, E= -985.663792068 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.202173 a.u. Sum of electronic and thermal Free Energies= -985.461619 a.u.				**5e_2,** optimization in gas phase B3LYP/6-311++G**, E= -985.649312324 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.201155 a.u. Sum of electronic and thermal Free Energies= -985.448157 a.u.			
0; 1				0; 1			
6	-6.223717000	1.539138000	0.000304000	6	-4.579769000	1.072262000	-2.475295000
6	-4.843138000	1.773556000	0.000146000	6	-3.610043000	1.362411000	-1.507757000
6	-6.736340000	0.241110000	0.000341000	6	-5.495921000	0.035404000	-2.292858000
1	-4.446414000	2.781759000	0.000113000	1	-2.899709000	2.167823000	-1.651076000
6	-4.007115000	0.669015000	0.000042000	6	-3.593794000	0.582402000	-0.362463000
6	-5.890084000	-0.874124000	0.000222000	6	-5.479455000	-0.752416000	-1.135452000
1	-6.290474000	-1.880853000	0.000244000	1	-6.191751000	-1.556908000	-0.995992000
6	-4.523696000	-0.640389000	0.000079000	6	-4.519417000	-0.463912000	-0.178395000
6	-2.247476000	-0.782324000	-0.000126000	6	-3.165270000	-0.388650000	1.650140000
7	-2.617249000	0.548359000	-0.000141000	7	-2.783869000	0.599509000	0.769853000
7	-3.428395000	-1.498153000	-0.000089000	7	-4.231127000	-1.033950000	1.059081000
1	-7.809124000	0.090001000	0.000460000	1	-6.234816000	-0.166716000	-3.058972000
1	-1.947439000	1.297755000	0.000014000	1	-2.018349000	1.216263000	0.989228000
1	-3.438792000	-2.504477000	0.000121000	1	-4.695587000	-1.811795000	1.497094000
7	-1.080465000	-1.346547000	-0.000147000	7	-2.675288000	-0.707173000	2.810662000
7	-0.037422000	-0.442841000	-0.000234000	7	-1.610094000	0.107576000	3.140178000
6	1.142578000	-0.977007000	-0.000146000	6	-1.089314000	-0.140099000	4.289672000

1	1.233208000	-2.064716000	0.000016000	1	-1.530146000	-0.949419000	4.882628000
6	2.354300000	-0.184680000	-0.000269000	6	0.063078000	0.581818000	4.815722000
6	3.619443000	-0.802224000	-0.000212000	6	0.850674000	1.429379000	4.012899000
6	2.307238000	1.226446000	-0.000497000	6	0.442213000	0.436434000	6.162566000
6	4.790199000	-0.061129000	-0.000381000	6	1.957582000	2.093582000	4.513667000
6	3.481744000	1.971413000	-0.000679000	6	1.556296000	1.099772000	6.671662000
6	4.723543000	1.334907000	-0.000623000	6	2.318992000	1.930017000	5.852613000
1	-6.903160000	2.382897000	0.000396000	1	-4.616737000	1.665572000	-3.381024000
1	5.762528000	-0.536808000	-0.000343000	1	2.561332000	2.736885000	3.885846000
8	1.140980000	1.922482000	-0.000542000	8	-0.216366000	-0.340601000	7.090753000
1	0.417941000	1.240333000	-0.000327000	1	-1.076932000	-0.615281000	6.759269000
1	3.671131000	-1.885241000	-0.000044000	1	0.575978000	1.542496000	2.972685000
8	3.467199000	3.344213000	-0.000913000	8	1.940738000	0.976679000	7.983821000
1	2.546480000	3.637230000	-0.000904000	1	1.305089000	0.410019000	8.439512000
8	5.868836000	2.068182000	-0.000791000	8	3.404941000	2.581478000	6.351509000
1	5.632548000	3.005411000	-0.000975000	1	3.496811000	2.352765000	7.285999000

5e_3, optimization in gas phase
B3LYP/6-311++G**, E= -985.663058722 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.203031 a.u.
Sum of electronic and thermal Free Energies= -985.460028 a.u.

0; 1

6	-6.151693000	1.810876000	-1.029061000
6	-4.752951000	1.820670000	-1.069936000
6	-6.850040000	0.805990000	-0.356819000
1	-4.212384000	2.600911000	-1.591905000
6	-4.087579000	0.795028000	-0.417069000
6	-6.177447000	-0.229282000	0.302194000
1	-6.721261000	-1.007889000	0.823595000
6	-4.792467000	-0.217172000	0.260707000
6	-2.570675000	-0.633593000	0.479234000
7	-2.732891000	0.506892000	-0.262958000
7	-3.833057000	-1.076099000	0.799359000
1	-7.933066000	0.825123000	-0.342841000
1	-1.927489000	1.009430000	-0.603667000
1	-4.001534000	-1.907138000	1.341619000
7	-1.460325000	-1.215148000	0.831526000
7	-0.351449000	-0.524225000	0.360886000
6	0.821572000	-1.000948000	0.608394000
1	1.606040000	-0.380539000	0.178996000
6	1.355318000	-2.174197000	1.310706000
6	2.758004000	-2.335641000	1.212119000
6	0.652668000	-3.140476000	2.073946000
6	3.445701000	-3.376574000	1.808043000
6	1.353781000	-4.190207000	2.674772000
6	2.733446000	-4.319854000	2.551225000
1	-6.700363000	2.599537000	-1.529592000
1	4.519370000	-3.476336000	1.714351000
8	-0.675930000	-3.165855000	2.314314000
1	-1.129430000	-2.435144000	1.772128000
1	3.314562000	-1.603654000	0.637661000
8	0.691595000	-5.134143000	3.419474000
1	-0.248733000	-4.905248000	3.398366000
8	3.383556000	-5.352386000	3.150481000
1	2.730772000	-5.891346000	3.617511000

5f_1, optimization in gas phase B3LYP/6-311++G**, E= -874.463507275 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.221680 a.u. Sum of electronic and thermal Free Energies= -874.241827 a.u.			
0; 1			
6	5.828602000	1.827739000	0.000152000
6	4.429663000	1.897399000	-0.000018000
6	6.491000000	0.599724000	0.000242000
1	3.916923000	2.851872000	-0.000113000
6	3.727330000	0.702826000	-0.000057000
6	5.781063000	-0.607654000	0.000181000
1	6.297743000	-1.560106000	0.000258000
6	4.397021000	-0.537570000	0.000039000
6	2.155758000	-0.944625000	-0.000132000
7	2.365125000	0.418327000	-0.000336000
7	3.410971000	-1.519917000	0.000006000
1	7.574172000	0.575722000	0.000364000
1	1.585982000	1.056333000	0.000101000
1	3.541179000	-2.517668000	-0.000129000
7	1.047347000	-1.618388000	-0.000052000
7	-0.048834000	-0.773417000	-0.000099000
6	-1.182443000	-1.378321000	-0.000002000
1	-1.208341000	-2.471654000	0.000198000
6	-2.461222000	-0.674111000	-0.000098000
6	-2.560174000	0.731657000	-0.000239000
6	-3.650412000	-1.410739000	0.000016000
6	-3.790146000	1.359885000	-0.000233000
6	-4.900063000	-0.790101000	0.000044000
6	-4.973637000	0.603966000	-0.000079000
1	6.403541000	2.746047000	0.000205000
8	-6.133909000	1.320738000	0.000078000
6	-7.368113000	0.616182000	0.000359000
1	-7.471878000	-0.007892000	-0.893857000
1	-7.471639000	-0.007696000	0.894741000
1	-8.145772000	1.378171000	0.000418000
1	-1.651247000	1.320082000	-0.000388000
1	-3.869264000	2.440609000	-0.000360000
1	-5.794472000	-1.398450000	0.000156000
1	-3.603285000	-2.495039000	0.000098000

5f_2, optimization in gas phase B3LYP/6-311++G**, E= -874.463161356 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.221698 a.u. Sum of electronic and thermal Free Energies= -874.241464 a.u.			
0; 1			
6	5.687869000	1.963672000	0.000043000
6	4.287186000	1.971640000	-0.000568000
6	6.403769000	0.766100000	0.000655000
1	3.732904000	2.902609000	-0.001080000
6	3.638166000	0.747304000	-0.000478000
6	5.747748000	-0.471399000	0.000627000
1	6.305792000	-1.400214000	0.001034000
6	4.361949000	-0.462370000	0.000101000
6	2.140837000	-0.968148000	-0.000321000
7	2.289835000	0.402847000	-0.001005000
7	3.420320000	-1.487325000	-0.000335000
1	7.486940000	0.789913000	0.001123000
1	1.483140000	1.005571000	-0.001015000
1	3.594544000	-2.478359000	0.002138000
7	1.063480000	-1.690209000	0.000153000
7	-0.069501000	-0.895310000	0.000057000
6	-1.174404000	-1.551140000	-0.000023000
1	-1.149621000	-2.644474000	-0.000108000
6	-2.485662000	-0.908174000	0.000104000
6	-3.642940000	-1.707301000	-0.000273000
6	-2.654638000	0.483065000	0.000512000
6	-4.909750000	-1.146063000	-0.000253000
6	-3.919676000	1.060665000	0.000513000
6	-5.058696000	0.245277000	0.000090000
1	6.221823000	2.906402000	0.000017000
8	-6.341622000	0.709066000	-0.000082000
6	-6.560026000	2.113300000	0.000136000
1	-6.137989000	2.583723000	0.894839000
1	-6.137193000	2.584145000	-0.893958000
1	-7.640719000	2.245681000	-0.000310000
1	-3.541755000	-2.787844000	-0.000537000
1	-5.799243000	-1.764440000	-0.000506000
1	-1.776779000	1.117204000	0.000895000
1	-4.008198000	2.138966000	0.000848000

5f_3, optimization in gas phase B3LYP/6-311++G**, E= -874.459115635 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.222549 a.u. Sum of electronic and thermal Free Energies= -874.236567 a.u.			
0; 1			
6	6.324861000	-0.104463000	-0.000435000
6	5.246137000	-0.997160000	0.000864000
6	6.121457000	1.276332000	-0.001589000
1	5.405700000	-2.068735000	0.001779000
6	3.968433000	-0.459634000	0.000840000
6	4.830873000	1.819541000	-0.001404000
1	4.675332000	2.891897000	-0.002151000
6	3.764139000	0.934874000	-0.000272000
6	1.726196000	-0.079401000	0.000866000
7	2.706716000	-1.045004000	0.002008000

7	2.385516000	1.132084000	0.000831000
1	6.975412000	1.943104000	-0.002579000
1	2.452988000	-2.020781000	0.001515000
1	1.895728000	2.010839000	-0.004252000
7	0.432840000	-0.213262000	0.000068000
7	0.099548000	-1.557219000	-0.000065000
6	-1.150635000	-1.876000000	-0.000281000
1	-1.308082000	-2.954005000	-0.000626000
6	-2.387968000	-1.091006000	-0.000198000
6	-3.600088000	-1.814081000	-0.001500000
6	-2.473504000	0.311059000	0.001152000
6	-4.829084000	-1.181094000	-0.001523000
6	-3.707174000	0.959770000	0.001180000
6	-4.892222000	0.218407000	-0.000213000
1	7.335039000	-0.496084000	-0.000541000
8	-6.144929000	0.757073000	-0.000423000
6	-6.279020000	2.172014000	0.000576000
1	-5.829418000	2.615653000	0.895429000
1	-5.828128000	2.617045000	-0.892954000
1	-7.349897000	2.368838000	-0.000100000
1	-3.567404000	-2.898983000	-0.002461000
1	-5.754299000	-1.744705000	-0.002520000
1	-1.561031000	0.886608000	0.002158000
1	-3.729255000	2.041581000	0.002406000

5g_1, optimization in gas phase B3LYP/6-311++G**, E= -989.009625243 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.249346 a.u. Sum of electronic and thermal Free Energies= -988.760279 a.u.			
0; 1			
6	5.950319000	1.189139000	-0.001880000
6	4.575059000	1.456396000	-0.001579000
6	6.432254000	-0.120042000	-0.001033000
1	4.203297000	2.474102000	-0.002220000
6	3.708938000	0.374283000	-0.000467000
6	5.557745000	-1.214507000	0.000147000
1	5.933941000	-2.230740000	0.000830000
6	4.197650000	-0.949283000	0.000395000
6	1.922671000	-1.034648000	0.001074000
7	2.321930000	0.285031000	0.000253000
7	3.083237000	-1.783045000	0.001536000
1	7.501126000	-0.297328000	-0.001281000
1	1.626559000	1.015775000	-0.000963000
1	3.071749000	-2.789109000	0.001607000
7	0.724204000	-1.530858000	0.001377000
7	-0.209820000	-0.506555000	0.000527000
6	-1.428013000	-0.924061000	0.000876000
1	-1.613996000	-1.996125000	0.001708000
6	-2.612125000	-0.069417000	0.000159000
6	-2.607258000	1.349079000	0.000236000
6	-3.880521000	-0.709404000	-0.000524000
6	-3.804294000	2.074629000	-0.000337000
6	-5.072810000	0.015956000	-0.001091000

5g_2, optimization in gas phase B3LYP/6-311++G**, E= -989.007306476 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.250412 a.u. Sum of electronic and thermal Free Energies= -988.756894 a.u.			
0; 1			
6	5.892260000	1.137953000	-0.607571000
6	4.517790000	1.406507000	-0.609360000
6	6.382630000	-0.122226000	-0.262804000
1	4.138653000	2.385216000	-0.878031000
6	3.661378000	0.375157000	-0.257171000
6	5.517583000	-1.164792000	0.092595000
1	5.900363000	-2.142915000	0.358939000
6	4.157680000	-0.898312000	0.089412000
6	1.886926000	-0.961196000	0.230869000
7	2.276252000	0.303508000	-0.154165000
7	3.049290000	-1.688316000	0.383292000
1	7.451161000	-0.301248000	-0.269685000
1	1.582000000	1.006048000	-0.360490000
1	3.043438000	-2.655799000	0.659825000
7	0.691930000	-1.436201000	0.417290000
7	-0.246977000	-0.442030000	0.210612000
6	-1.466419000	-0.851890000	0.236954000
1	-1.671301000	-1.908773000	0.395895000
6	-2.622776000	0.018675000	0.022105000
6	-3.889959000	-0.603219000	-0.161845000
6	-2.589151000	1.429594000	-0.052096000
6	-5.036926000	0.140984000	-0.434358000
6	-3.736450000	2.170223000	-0.336634000

6	-5.021225000	1.404922000	-0.000995000	6	-4.951158000	1.528562000	-0.530184000
1	6.649628000	2.016789000	-0.002778000	1	6.584918000	1.925458000	-0.879519000
8	-3.854575000	-2.074635000	-0.000575000	8	-1.424421000	2.143303000	0.112204000
6	-5.079830000	-2.792842000	-0.001019000	6	-1.006217000	2.320022000	1.468553000
1	-5.672944000	-2.574163000	0.893280000	1	-1.782358000	2.836390000	2.044584000
1	-5.672188000	-2.574354000	-0.895859000	1	-0.763827000	1.364235000	1.938433000
1	-4.802658000	-3.845892000	-0.000787000	1	-0.111597000	2.942331000	1.434906000
8	-1.392981000	1.960429000	0.000957000	8	-3.898484000	-1.966112000	-0.069912000
6	-1.340370000	3.379893000	0.001825000	6	-5.121758000	-2.665489000	-0.250192000
1	-1.810371000	3.802498000	-0.892655000	1	-5.863483000	-2.375875000	0.501735000
1	-1.811719000	3.801435000	0.896092000	1	-5.532466000	-2.501144000	-1.252013000
1	-0.281414000	3.635604000	0.002770000	1	-4.878306000	-3.719851000	-0.129043000
1	-3.793634000	3.154637000	-0.000282000	1	-5.990009000	-0.346818000	-0.581049000
1	-5.943765000	1.974353000	-0.001444000	1	-5.842008000	2.105509000	-0.750770000
1	-6.029153000	-0.486401000	-0.001641000	1	-3.647999000	3.247679000	-0.400903000

5g_3, optimization in gas phase
B3LYP/6-311++G**, E= -989.004961555 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.250730 a.u.
Sum of electronic and thermal Free Energies= -988.754232 a.u.

0; 1

6	-6.125658000	-0.586377000	-0.243705000
6	-4.965651000	-0.950168000	-0.939776000
6	-6.058317000	0.158410000	0.934092000
1	-5.020028000	-1.529510000	-1.853747000
6	-3.748035000	-0.544894000	-0.416430000
6	-4.827771000	0.569465000	1.462634000
1	-4.777432000	1.147869000	2.377627000
6	-3.680901000	0.207905000	0.774109000
6	-1.553441000	-0.141348000	0.036397000
7	-2.437780000	-0.730449000	-0.843397000
7	-2.331076000	0.446736000	1.015401000
1	-6.971824000	0.425254000	1.452003000
1	-2.093163000	-1.248572000	-1.636218000
1	-1.924886000	0.914316000	1.808279000
7	-0.258497000	-0.104314000	0.015347000
7	0.222031000	-0.821752000	-1.068249000
6	1.494299000	-0.824376000	-1.234765000
1	1.846866000	-1.461640000	-2.042072000
6	2.523179000	-0.116207000	-0.437247000
6	3.548632000	-0.862272000	0.168542000
6	2.550695000	1.284205000	-0.311742000
6	4.549959000	-0.242818000	0.923022000
6	3.544886000	1.913705000	0.447631000
6	4.526676000	1.141634000	1.059013000
1	-7.091092000	-0.891052000	-0.629845000
8	3.471743000	-2.212812000	-0.023387000
6	4.457873000	-3.046815000	0.567585000
1	5.460296000	-2.812204000	0.193316000
1	4.447415000	-2.964481000	1.659669000
1	4.195064000	-4.063983000	0.280947000
8	1.596004000	1.961046000	-1.002630000
6	1.504755000	3.368286000	-0.850179000
1	1.330906000	3.646405000	0.194957000
1	2.404971000	3.874102000	-1.217170000
1	0.650811000	3.675761000	-1.451974000
1	3.565774000	2.989037000	0.553954000

1	5.296205000	1.630051000	1.646525000
1	5.328322000	-0.818789000	1.403075000

5h_1, optimization in gas phase B3LYP/6-311++G**, E= -989.019319977 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.250472 a.u. Sum of electronic and thermal Free Energies= -988.768848 a.u.			
0; 1			
6	6.258099000	1.603305000	0.000060000
6	4.862791000	1.721152000	-0.000238000
6	6.878358000	0.353110000	0.000336000
1	4.382780000	2.692430000	-0.000461000
6	4.120295000	0.550912000	-0.000210000
6	6.128050000	-0.829222000	0.000314000
1	6.611786000	-1.798784000	0.000486000
6	4.747192000	-0.711360000	0.000062000
6	2.494536000	-1.040745000	-0.000203000
7	2.749108000	0.312983000	-0.000495000
7	3.727393000	-1.659195000	-0.000172000
1	7.960079000	0.292410000	0.000556000
1	1.991810000	0.977326000	-0.000334000
1	3.822538000	-2.660992000	0.000866000
7	1.362040000	-1.677571000	0.000009000
7	0.300770000	-0.794411000	-0.000022000
6	-0.856728000	-1.350001000	0.000054000
1	-0.930892000	-2.440768000	0.000169000
6	-2.105657000	-0.584686000	0.000030000
6	-2.122510000	0.808957000	0.000021000
6	-3.318100000	-1.303547000	0.000086000
6	-3.342789000	1.489544000	-0.000007000
6	-4.525384000	-0.611694000	0.000085000
6	-4.548021000	0.789341000	0.000018000
1	6.864303000	2.501267000	0.000071000
8	-3.258421000	2.853227000	-0.000045000
6	-4.460769000	3.609989000	0.000207000
1	-5.061044000	3.408424000	-0.893664000
1	-5.060606000	3.408445000	0.894390000
1	-4.154258000	4.654919000	0.000108000
8	-5.756220000	-1.206282000	-0.000036000
6	-5.824664000	-2.625563000	-0.000058000
1	-5.354244000	-3.049094000	-0.894036000
1	-5.354531000	-3.049076000	0.894077000
1	-6.885419000	-2.871685000	-0.000232000
1	-1.199836000	1.372062000	-0.000068000
1	-3.289284000	-2.384610000	0.000172000
1	-5.509427000	1.282578000	-0.000033000

5h_2, optimization in gas phase B3LYP/6-311++G**, E= -989.019081926 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.250407 a.u. Sum of electronic and thermal Free Energies= -988.768675 a.u.			
0; 1			
6	6.202960000	1.392918000	-0.000797000
6	4.813332000	1.566215000	-0.000349000
6	6.772771000	0.119051000	-0.000770000
1	4.372937000	2.556125000	-0.000374000
6	4.024812000	0.426596000	0.000080000
6	5.975948000	-1.032417000	-0.000249000
1	6.420461000	-2.020542000	-0.000149000
6	4.600872000	-0.859650000	0.000130000
6	2.336447000	-1.100132000	0.000628000
7	2.644900000	0.242990000	0.000516000
7	3.544553000	-1.766305000	0.001015000
1	7.851195000	0.015295000	-0.001117000
1	1.915275000	0.936900000	0.000411000
1	3.600164000	-2.771103000	-0.001164000
7	1.181368000	-1.692958000	0.000481000
7	0.148710000	-0.774846000	0.000284000
6	-1.024036000	-1.299327000	0.000207000
1	-1.124919000	-2.387744000	0.000275000
6	-2.254581000	-0.507258000	-0.000012000
6	-3.476223000	-1.195622000	-0.000203000
6	-2.233531000	0.895421000	0.000162000
6	-4.675676000	-0.475771000	-0.000317000
6	-3.439233000	1.595187000	0.000017000
6	-4.660126000	0.916202000	-0.000242000
1	6.844525000	2.265947000	-0.001165000
8	-5.914830000	-1.050979000	-0.000512000
6	-6.008805000	-2.468557000	-0.000385000
1	-5.547306000	-2.901586000	-0.894550000
1	-5.547460000	-2.901524000	0.893883000
1	-7.073971000	-2.694748000	-0.000445000
8	-3.534218000	2.958541000	0.000169000
6	-2.337156000	3.722573000	0.000409000
1	-1.736063000	3.524608000	0.894629000
1	-1.735901000	3.524910000	-0.893777000
1	-2.650761000	4.765451000	0.000562000
1	-3.470685000	-2.277095000	-0.000242000
1	-1.279027000	1.399313000	0.000386000
1	-5.589432000	1.470542000	-0.000339000

5h_3, optimization in gas phase B3LYP/6-311++G**, E= -989.012918053 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.251048 a.u. Sum of electronic and thermal Free Energies= -988.761871 a.u.			
0; 1			
6	6.811540000	-0.419735000	-0.000277000
6	5.687194000	-1.253910000	0.000272000

6	6.681697000	0.970063000	-0.000686000
1	5.789738000	-2.332443000	0.000598000
6	4.439889000	-0.649135000	0.000337000
6	5.422003000	1.581085000	-0.000525000
1	5.323407000	2.660135000	-0.000763000
6	4.309686000	0.754224000	-0.000055000
6	2.222137000	-0.150112000	0.000453000
7	3.148734000	-1.166806000	0.000872000
7	2.943595000	1.023907000	0.000522000
1	7.569911000	1.590460000	-0.001100000
1	2.844382000	-2.127989000	0.000463000
1	2.498738000	1.926651000	-0.001582000
7	0.922359000	-0.210802000	0.000096000
7	0.512641000	-1.528972000	-0.000066000
6	-0.751643000	-1.782761000	-0.000209000
1	-0.967500000	-2.849880000	-0.000504000
6	-1.949345000	-0.928877000	-0.000153000
6	-3.180946000	-1.605394000	-0.000233000
6	-1.937492000	0.473529000	-0.000024000
6	-4.376959000	-0.895707000	-0.000143000
6	-3.143140000	1.172035000	0.000091000
6	-4.374124000	0.504255000	0.000034000
1	7.799527000	-0.864371000	-0.000386000
8	-3.031706000	2.536933000	0.000275000
6	-4.212544000	3.322751000	0.000163000
1	-4.818692000	3.139766000	-0.894464000
1	-4.818801000	3.139874000	0.894731000
1	-3.880065000	4.359886000	0.000121000
8	-5.518557000	-1.650905000	-0.000224000
6	-6.775548000	-0.992929000	-0.000174000
1	-6.905883000	-0.373714000	0.894586000
1	-6.905752000	-0.373359000	-0.894707000
1	-7.525029000	-1.783016000	-0.000374000
1	-1.005564000	1.013778000	-0.000029000
1	-5.300963000	1.056341000	0.000163000
1	-3.221070000	-2.687918000	-0.000355000

5i_1, optimization in gas phase B3LYP/6-311++G**, E= -1103.56018108 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.277884 a.u. Sum of electronic and thermal Free Energies= -1103.282298 a.u.			
0; 1			
6	-6.766072000	1.740077000	-0.152886000
6	-5.367128000	1.799788000	-0.177820000
6	-7.435575000	0.524178000	-0.008989000
1	-4.848830000	2.744521000	-0.290294000
6	-4.671819000	0.607343000	-0.054504000
6	-6.732865000	-0.680766000	0.115480000
1	-7.254850000	-1.623718000	0.227224000
6	-5.348542000	-0.620508000	0.090290000
6	-3.110747000	-1.040680000	0.105604000
7	-3.311352000	0.314806000	-0.039294000
7	-4.367738000	-1.603826000	0.186490000

5i_2, optimization in gas phase B3LYP/6-311++G**, E= -1103.56078026 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.278565 a.u. Sum of electronic and thermal Free Energies= -1103.282216 a.u.			
0; 1			
6	6.689291000	1.706465000	0.144404000
6	5.289903000	1.754999000	0.111107000
6	7.370595000	0.488871000	0.130602000
1	4.762650000	2.701499000	0.121933000
6	4.606707000	0.550327000	0.063946000
6	6.680028000	-0.728622000	0.083214000
1	7.211406000	-1.672858000	0.072529000
6	5.295432000	-0.679409000	0.050186000
6	3.061827000	-1.120518000	-0.016876000
7	3.249378000	0.245005000	0.022606000
7	4.325269000	-1.676214000	0.001705000

1	-8.518768000	0.508202000	0.006812000	1	8.453665000	0.481225000	0.156806000
1	-2.528248000	0.942667000	-0.125055000	1	2.460733000	0.870782000	0.017700000
1	-4.503406000	-2.595157000	0.293244000	1	4.471075000	-2.671579000	-0.024067000
7	-2.004924000	-1.719280000	0.161037000	7	1.965311000	-1.812180000	-0.062492000
7	-0.908476000	-0.884850000	0.056986000	7	0.853884000	-0.988744000	-0.071801000
6	0.224626000	-1.488549000	0.082709000	6	-0.266469000	-1.616468000	-0.114181000
1	0.252344000	-2.577553000	0.178525000	1	-0.271939000	-2.709058000	-0.136185000
6	1.503141000	-0.784999000	-0.014657000	6	-1.560110000	-0.936672000	-0.135398000
6	1.591035000	0.603668000	-0.114964000	6	-2.720899000	-1.707231000	-0.157503000
6	2.684152000	-1.545936000	-0.004277000	6	-1.667829000	0.465387000	-0.133702000
6	2.829746000	1.236505000	-0.198874000	6	-3.985214000	-1.109834000	-0.170205000
6	3.924985000	-0.924391000	-0.106259000	6	-2.917240000	1.066626000	-0.163107000
6	4.016973000	0.481477000	-0.195181000	6	-4.101118000	0.286950000	-0.171780000
1	-7.335875000	2.656657000	-0.247832000	1	7.249671000	2.632964000	0.181536000
8	2.797165000	2.594693000	-0.360875000	8	-5.046852000	-1.967046000	-0.257703000
6	3.709104000	3.421151000	0.367123000	6	-6.220354000	-1.731855000	0.524849000
1	3.813424000	3.070795000	1.399507000	1	-5.954210000	-1.424915000	1.541890000
1	4.687566000	3.455501000	-0.111762000	1	-6.861774000	-0.978641000	0.067667000
1	3.263437000	4.416295000	0.372141000	1	-6.741416000	-2.688655000	0.565834000
8	5.114123000	-1.597187000	-0.160794000	8	-3.111987000	2.418860000	-0.219677000
6	5.090778000	-3.018742000	-0.177890000	6	-1.972507000	3.262819000	-0.316911000
1	4.665618000	-3.424829000	0.746214000	1	-1.335393000	3.179343000	0.570167000
1	4.526671000	-3.396641000	-1.036767000	1	-1.384461000	3.033760000	-1.211628000
1	6.130701000	-3.330336000	-0.263343000	1	-2.361150000	4.277620000	-0.388572000
1	0.697828000	1.212743000	-0.125436000	1	-2.672546000	-2.789622000	-0.161844000
1	2.614345000	-2.623190000	0.065097000	1	-0.762042000	1.052898000	-0.127705000
8	5.217438000	1.110194000	-0.405102000	8	-5.336948000	0.863645000	-0.313146000
6	6.203535000	1.013174000	0.631794000	6	-5.793610000	1.717746000	0.744788000
1	5.813590000	1.417953000	1.572517000	1	-5.817838000	1.173351000	1.695481000
1	6.523505000	-0.018423000	0.778050000	1	-5.161765000	2.600562000	0.840562000
1	7.046605000	1.618223000	0.298598000	1	-6.805867000	2.015095000	0.471386000

5i_3, optimization in gas phase
B3LYP/6-311++G**, E= -1103.55920291 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.279113 a.u.
Sum of electronic and thermal Free Energies= -1103.280090 a.u.

0; 1

6	7.183183000	-0.515325000	0.088652000
6	6.047965000	-1.334438000	0.105293000
6	7.072134000	0.874769000	0.028848000
1	6.136158000	-2.413239000	0.151342000
6	4.809014000	-0.714389000	0.060271000
6	5.820792000	1.501162000	-0.016432000
1	5.736885000	2.580505000	-0.062445000
6	4.697916000	0.689041000	0.000185000
6	2.597734000	-0.188354000	0.004186000
7	3.511182000	-1.215107000	0.061136000
7	3.335088000	0.975957000	-0.032281000
1	7.968452000	1.483227000	0.017144000
1	3.192848000	-2.171238000	0.095002000
1	2.905171000	1.884264000	-0.078249000
7	1.297465000	-0.237619000	-0.014817000
7	0.880094000	-1.555858000	0.032126000
6	-0.385083000	-1.807231000	0.016960000
1	-0.598981000	-2.874515000	0.056641000
6	-1.581849000	-0.959962000	-0.042537000
6	-2.815226000	-1.636025000	-0.043614000

6	-1.566006000	0.442532000	-0.094362000
6	-4.015339000	-0.928978000	-0.094767000
6	-2.767903000	1.147416000	-0.151055000
6	-4.001854000	0.474769000	-0.154270000
1	8.164971000	-0.972171000	0.122777000
8	-2.850033000	2.509043000	-0.207742000
6	-1.641913000	3.255141000	-0.260446000
1	-1.037918000	3.103332000	0.640676000
1	-1.049334000	2.991713000	-1.142839000
1	-1.943111000	4.299860000	-0.324419000
8	-5.251221000	-1.504439000	-0.090280000
6	-5.336608000	-2.921629000	-0.078463000
1	-4.854251000	-3.359923000	-0.958987000
1	-4.891308000	-3.345199000	0.828860000
1	-6.400486000	-3.153235000	-0.098664000
1	-0.614404000	0.945299000	-0.093829000
1	-2.819180000	-2.716885000	-0.000807000
8	-5.176848000	1.158852000	-0.289894000
6	-5.678694000	1.765924000	0.905010000
1	-5.884412000	1.006537000	1.666725000
1	-4.973582000	2.505570000	1.294211000
1	-6.609094000	2.260293000	0.626292000

5j_1, optimization in gas phase B3LYP/6-311++G**, E= -949.714148124 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.225044 a.u. Sum of electronic and thermal Free Energies= -949.489104 a.u.			
0; 1			
6	-5.668724000	1.481903000	0.488971000
6	-4.459650000	1.447510000	1.193964000
6	-5.942792000	0.559246000	-0.521994000
1	-4.247114000	2.164603000	1.977762000
6	-3.547973000	0.462144000	0.851263000
6	-5.020670000	-0.435716000	-0.867050000
1	-5.236387000	-1.151243000	-1.651471000
6	-3.824936000	-0.469667000	-0.166538000
6	-1.761920000	-0.942385000	0.678066000
7	-2.278011000	0.153315000	1.339115000
7	-2.716942000	-1.308061000	-0.247624000
1	-6.886456000	0.611133000	-1.051620000
1	-1.808346000	0.583506000	2.117716000
1	-2.581535000	-2.085103000	-0.872754000
7	-0.636822000	-1.573636000	0.823565000
7	0.176195000	-0.998510000	1.776718000
6	1.246721000	-1.665314000	2.062221000
1	1.424928000	-2.622385000	1.568170000
6	2.233926000	-1.193902000	3.018445000
6	3.333287000	-2.013979000	3.332343000
6	2.113136000	0.067426000	3.651010000
6	4.287558000	-1.605912000	4.250066000
6	3.096783000	0.484031000	4.566712000
6	4.165387000	-0.355900000	4.862037000
1	-6.402434000	2.240063000	0.734715000

5j_2, optimization in gas phase B3LYP/6-311++G**, E= -949.714168537 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.225166 a.u. Sum of electronic and thermal Free Energies= -949.489003 a.u.			
0; 1			
6	-6.123213000	-1.093168000	1.539571000
6	-4.839794000	-0.788430000	2.008670000
6	-6.473195000	-0.885210000	0.204395000
1	-4.569396000	-0.948573000	3.045498000
6	-3.931424000	-0.274782000	1.097401000
6	-5.554113000	-0.366690000	-0.715238000
1	-5.828006000	-0.207572000	-1.751347000
6	-4.283414000	-0.066725000	-0.249395000
6	-2.111730000	0.570641000	0.017215000
7	-2.603374000	0.131154000	1.229213000
7	-3.153648000	0.447994000	-0.878475000
1	-7.474253000	-1.129374000	-0.130220000
1	-2.027211000	0.057394000	2.050449000
1	-3.060029000	0.718659000	-1.843306000
7	-0.939226000	1.017226000	-0.316224000
7	-0.074031000	1.093111000	0.754192000
6	1.142741000	1.413647000	0.455720000
1	1.408434000	1.575443000	-0.590727000
6	2.182295000	1.571558000	1.458429000
6	3.498280000	1.849517000	1.045710000
6	1.907070000	1.442988000	2.841692000
6	4.519806000	1.992504000	1.970559000
6	2.945206000	1.610558000	3.776455000
6	4.237126000	1.874520000	3.333636000
1	-6.855557000	-1.497041000	2.228115000

8	2.986673000	1.673363000	5.243568000
6	3.070962000	2.865941000	4.453409000
1	4.031004000	2.907992000	3.926652000
1	2.250404000	2.926162000	3.736444000
1	3.008350000	3.695608000	5.157063000
1	3.418835000	-2.979598000	2.845558000
1	4.894644000	-0.011315000	5.585913000
8	1.066353000	0.884043000	3.399109000
1	0.502203000	0.416897000	2.732772000
1	5.126309000	-2.247705000	4.491049000

8	2.731742000	1.439104000	5.121759000
6	1.868827000	2.391555000	5.755762000
1	2.269933000	3.405075000	5.642496000
1	0.857503000	2.344106000	5.348388000
1	1.854273000	2.124859000	6.812194000
1	3.702515000	1.944317000	-0.015406000
1	5.016101000	1.978991000	4.079865000
8	0.664332000	1.156172000	3.288097000
1	0.089421000	1.085359000	2.484953000
1	5.531551000	2.198374000	1.642771000

5j_3, optimization in gas phase
B3LYP/6-311++G**, E= -949.710360570 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.226069 a.u.
Sum of electronic and thermal Free Energies= -949.484291 a.u.

0; 1

6	-4.982683000	2.186047000	-0.909791000
6	-3.794049000	2.127361000	-0.173759000
6	-5.737627000	1.038387000	-1.160244000
1	-3.209226000	3.018570000	0.019099000
6	-3.395395000	0.886542000	0.297821000
6	-5.334617000	-0.213942000	-0.683556000
1	-5.922230000	-1.103195000	-0.877654000
6	-4.157397000	-0.269658000	0.045509000
6	-2.340745000	-0.872461000	1.266173000
7	-2.291251000	0.478879000	1.044187000
7	-3.484940000	-1.328744000	0.656400000
1	-6.653172000	1.115489000	-1.734116000
1	-1.534696000	1.029544000	1.420272000
1	-3.745881000	-2.301165000	0.645218000
7	-1.493260000	-1.620494000	1.913467000
7	-0.447458000	-0.874903000	2.433358000
6	0.514973000	-1.502194000	3.017674000
1	1.295294000	-0.822973000	3.355977000
6	0.830555000	-2.916557000	3.295396000
6	2.189356000	-3.154580000	3.600168000
6	-0.065496000	-4.017732000	3.322312000
6	2.670076000	-4.416952000	3.895985000
6	0.434021000	-5.299179000	3.654103000
6	1.780181000	-5.492257000	3.926447000
1	-5.320766000	3.141773000	-1.291711000
8	-0.393741000	-6.396476000	3.639558000
6	-1.383913000	-6.455050000	4.672313000
1	-0.907075000	-6.459882000	5.659438000
1	-2.081911000	-5.619144000	4.599944000
1	-1.916545000	-7.394512000	4.524907000
1	2.870750000	-2.310508000	3.591684000
1	2.114165000	-6.496756000	4.159270000
8	-1.383912000	-3.930162000	3.083577000
1	-1.575725000	-3.067851000	2.602803000
1	3.720690000	-4.568652000	4.112015000

5k_1, optimization in gas phase
B3LYP/6-311++G**, E= -949.722771010 a.u.

5k_2, optimization in gas phase
B3LYP/6-311++G**, E= -949.722798328 a.u.

Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.224517 a.u. Sum of electronic and thermal Free Energies= -949.498254 a.u.			
0; 1			
6	-5.362590000	1.785470000	0.097598000
6	-4.103392000	1.781665000	0.710715000
6	-5.875777000	0.636763000	-0.506095000
1	-3.706353000	2.673831000	1.180037000
6	-3.387001000	0.596032000	0.694337000
6	-5.150516000	-0.560882000	-0.522166000
1	-5.550850000	-1.451307000	-0.992084000
6	-3.904050000	-0.562748000	0.084139000
6	-1.846406000	-1.069131000	0.926788000
7	-2.134158000	0.253498000	1.201964000
7	-2.943272000	-1.556141000	0.242730000
1	-6.853260000	0.668528000	-0.972222000
1	-1.484638000	0.860362000	1.671998000
1	-2.991869000	-2.510522000	-0.072521000
7	-0.806154000	-1.791061000	1.202433000
7	0.157183000	-1.100123000	1.911613000
6	1.238507000	-1.770207000	2.151818000
1	1.319997000	-2.793956000	1.780607000
6	2.351093000	-1.222921000	2.899058000
6	3.511638000	-1.994688000	3.106822000
6	2.323021000	0.080420000	3.450785000
6	4.593298000	-1.514931000	3.816321000
6	3.411293000	0.577342000	4.173208000
6	4.541878000	-0.217056000	4.354056000
1	-5.946080000	2.698249000	0.094455000
1	3.548487000	-2.996837000	2.692148000
8	1.246025000	0.878881000	3.298581000
1	0.583560000	0.360425000	2.776092000
1	5.482682000	-2.111621000	3.972018000
8	5.648445000	0.179427000	5.039960000
6	5.667777000	1.479173000	5.617430000
1	5.571860000	2.256499000	4.852202000
1	4.871531000	1.596809000	6.359855000
1	6.635652000	1.571226000	6.107317000
1	3.335239000	1.578435000	4.573404000

Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.225079 a.u. Sum of electronic and thermal Free Energies= -949.497720 a.u.			
0; 1			
6	-6.578700000	0.007795000	1.287647000
6	-5.345223000	0.481579000	1.751725000
6	-6.678756000	-0.684747000	0.080260000
1	-5.268337000	1.018900000	2.689389000
6	-4.229806000	0.237865000	0.967114000
6	-5.550522000	-0.930512000	-0.711725000
1	-5.631080000	-1.468390000	-1.648808000
6	-4.330612000	-0.459870000	-0.251681000
6	-2.142758000	0.103540000	0.058248000
7	-2.883239000	0.560942000	1.130791000
7	-3.044302000	-0.526201000	-0.777615000
1	-7.646050000	-1.040520000	-0.253725000
1	-2.475842000	1.098412000	1.876701000
1	-2.757590000	-0.956414000	-1.640927000
7	-0.876993000	0.196523000	-0.204293000
7	-0.169825000	0.845762000	0.789032000
6	1.081811000	1.045157000	0.526046000
1	1.480859000	0.714455000	-0.435190000
6	1.984355000	1.689087000	1.457200000
6	3.329544000	1.910878000	1.100979000
6	1.568835000	2.110598000	2.743248000
6	4.223716000	2.519667000	1.957485000
6	2.465307000	2.726862000	3.620529000
6	3.786734000	2.931656000	3.228494000
1	-7.468978000	0.183592000	1.879357000
1	3.665277000	1.590984000	0.119853000
8	0.298902000	1.928017000	3.160783000
1	-0.177323000	1.473962000	2.420494000
1	5.255456000	2.688827000	1.677827000
8	4.729341000	3.523597000	4.011572000
6	4.360281000	3.966797000	5.311912000
1	3.576786000	4.730321000	5.264975000
1	4.021231000	3.133052000	5.935533000
1	5.261180000	4.398954000	5.744164000
1	2.094314000	3.027804000	4.590067000

5k_3, optimization in gas phase B3LYP/6-311++G**, E= -949.719728437 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.225675 a.u. Sum of electronic and thermal Free Energies= -949.494053 a.u.			
0; 1			
6	-4.972411000	2.028352000	-0.933937000
6	-3.715301000	1.948449000	-0.323562000
6	-5.831390000	0.928542000	-0.969247000
1	-3.049606000	2.802680000	-0.296917000
6	-3.355883000	0.736578000	0.244698000
6	-5.467659000	-0.295335000	-0.395498000
1	-6.135848000	-1.147738000	-0.424303000
6	-4.222999000	-0.372141000	0.208746000
6	-2.327350000	-0.991149000	1.296682000
7	-2.207511000	0.321020000	0.914931000
7	-3.562727000	-1.413657000	0.860953000
1	-6.798457000	1.020266000	-1.448813000
1	-1.372950000	0.840674000	1.139480000

1	-3.905381000	-2.347844000	1.013123000
7	-1.470510000	-1.726640000	1.941278000
7	-0.317762000	-1.018187000	2.250085000
6	0.629803000	-1.631989000	2.875560000
1	1.480505000	-0.974950000	3.048939000
6	0.856737000	-2.984892000	3.400369000
6	2.150846000	-3.187781000	3.940147000
6	-0.032839000	-4.093965000	3.456327000
6	2.572557000	-4.377069000	4.490783000
6	0.392295000	-5.308958000	4.018939000
6	1.675033000	-5.456415000	4.530592000
1	-5.281520000	2.962840000	-1.386489000
1	2.845034000	-2.354100000	3.914103000
8	-1.297368000	-4.082173000	3.014020000
1	-1.494608000	-3.202361000	2.564739000
1	3.569789000	-4.498982000	4.893025000
8	2.149043000	-6.602377000	5.089886000
6	1.288171000	-7.732112000	5.169705000
1	0.402082000	-7.515207000	5.775182000
1	0.977179000	-8.066944000	4.174720000
1	1.871996000	-8.515902000	5.649540000
1	-0.329259000	-6.113533000	4.033394000

5l_1, optimization in gas phase
B3LYP/6-311++G**, E= -949.703313584 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.223601 a.u.
Sum of electronic and thermal Free Energies= -949.479712 a.u.

0; 1			
6	-6.173396000	1.779040000	-0.035018000
6	-4.776706000	1.873145000	-0.072559000
6	-6.812600000	0.541775000	0.054883000
1	-4.282100000	2.834550000	-0.142654000
6	-4.052562000	0.692842000	-0.017156000
6	-6.080766000	-0.650775000	0.110722000
1	-6.579323000	-1.610247000	0.180831000
6	-4.698613000	-0.556375000	0.073337000
6	-2.451724000	-0.923502000	0.045116000
7	-2.685307000	0.432156000	-0.031856000
7	-3.694079000	-1.519613000	0.109418000
1	-7.894837000	0.499270000	0.081978000
1	-1.918510000	1.082565000	-0.089648000
1	-3.805195000	-2.517870000	0.170951000
7	-1.330380000	-1.578653000	0.059458000
7	-0.252115000	-0.718489000	-0.015639000
6	0.892784000	-1.301044000	-0.008466000
1	0.940009000	-2.391929000	0.052830000
6	2.156411000	-0.570242000	-0.078791000
6	2.228531000	0.828572000	-0.162301000
6	3.355543000	-1.298348000	-0.065206000
6	3.462159000	1.460907000	-0.217340000
6	4.593148000	-0.665388000	-0.135514000
6	4.655736000	0.736342000	-0.198242000
1	-6.765480000	2.685377000	-0.077023000
8	5.839600000	1.414646000	-0.324741000
6	6.762658000	1.309634000	0.767509000
1	6.302364000	1.676799000	1.691424000
1	7.102688000	0.281765000	0.904058000

5l_2, optimization in gas phase
B3LYP/6-311++G**, E= -949.703880596 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.223891 a.u.
Sum of electronic and thermal Free Energies= -949.479989 a.u.

0; 1			
6	5.882028000	1.973471000	-0.003443000
6	4.481930000	1.957027000	-0.032301000
6	6.617809000	0.789274000	0.055232000
1	3.912458000	2.877635000	-0.078188000
6	3.854050000	0.722115000	-0.000253000
6	5.983171000	-0.458595000	0.087624000
1	6.556527000	-1.376853000	0.133239000
6	4.597654000	-0.473593000	0.059257000
6	2.386427000	-1.018398000	0.033368000
7	2.511593000	0.353613000	-0.014854000
7	3.673403000	-1.514252000	0.078340000
1	7.700156000	0.832241000	0.076079000
1	1.695835000	0.942263000	-0.053128000
1	3.864093000	-2.501527000	0.118987000
7	1.322656000	-1.761654000	0.038613000
7	0.173571000	-0.994915000	-0.015897000
6	-0.915326000	-1.677611000	-0.010626000
1	-0.866681000	-2.768449000	0.036507000
6	-2.240986000	-1.067100000	-0.065414000
6	-3.374390000	-1.890028000	-0.040112000
6	-2.427096000	0.322398000	-0.149471000
6	-4.650609000	-1.336565000	-0.084064000
6	-3.698242000	0.874312000	-0.208654000
6	-4.834677000	0.040523000	-0.161398000
1	6.400098000	2.924668000	-0.027603000
8	-6.107581000	0.533094000	-0.275940000
6	-6.564107000	1.393233000	0.776821000
1	-6.538152000	0.866140000	1.736913000
1	-5.965230000	2.303545000	0.835043000

1	7.607345000	1.945954000	0.505726000	1	-7.594762000	1.645062000	0.529484000
1	1.313935000	1.406263000	-0.178590000	1	-3.255297000	-2.966192000	0.018054000
1	3.532999000	2.540485000	-0.283911000	1	-5.533513000	-1.964630000	-0.067463000
1	3.320179000	-2.383960000	-0.013540000	1	-1.555608000	0.968415000	-0.184669000
8	5.773910000	-1.363218000	-0.158981000	8	-3.907092000	2.224772000	-0.327370000
1	5.587392000	-2.307752000	-0.148174000	1	-3.056915000	2.672438000	-0.389594000

5l_3, optimization in gas phase
B3LYP/6-311++G**, E= -949.699995581 a.u.
Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.224760 a.u.
Sum of electronic and thermal Free Energies= -949.475235 a.u.

0; 1

6	-6.538451000	0.088792000	0.074562000
6	-5.473525000	0.997072000	0.099791000
6	-6.314893000	-1.287487000	0.007364000
1	-5.648775000	2.064888000	0.151793000
6	-4.188332000	0.479427000	0.055301000
6	-5.016995000	-1.810309000	-0.037349000
1	-4.845833000	-2.879004000	-0.089262000
6	-3.963897000	-0.909784000	-0.012534000
6	-1.941677000	0.134643000	0.002203000
7	-2.935085000	1.083374000	0.062909000
7	-2.581952000	-1.085226000	-0.042483000
1	-7.158975000	-1.966399000	-0.010749000
1	-2.695418000	2.061981000	0.103391000
1	-2.081049000	-1.955995000	-0.094121000
7	-0.649142000	0.290706000	-0.014197000
7	-0.342466000	1.638980000	0.044942000
6	0.898335000	1.991281000	0.029506000
1	1.029779000	3.071104000	0.080072000
6	2.155384000	1.240651000	-0.042519000
6	3.344950000	1.990473000	-0.040247000
6	2.259026000	-0.159610000	-0.118307000
6	4.582744000	1.364792000	-0.098863000
6	3.499054000	-0.783193000	-0.191965000
6	4.682585000	-0.023695000	-0.168048000
1	-7.554163000	0.464250000	0.107758000
8	5.924356000	-0.586886000	-0.294873000
6	6.335711000	-1.491961000	0.738583000
1	6.333483000	-0.985856000	1.710237000
1	5.692901000	-2.372579000	0.776239000
1	7.353583000	-1.787458000	0.486592000
1	3.294501000	3.072469000	0.011660000
1	5.501779000	1.938961000	-0.099545000
1	1.351485000	-0.748253000	-0.134117000
8	3.617035000	-2.146494000	-0.304467000
1	2.735967000	-2.532461000	-0.348293000

Radicals, anions and radical cations of the hydrazones **5a-l**

5a_A1, optimization in gas phase B3LYP/6-311++G**, E= -834.598949198 a.u. Sum of electronic and thermal Enthalpies= -834.357468 a.u.			
-1; 1			
6	-4.991220000	1.708229000	0.000242000
6	-3.587415000	1.753459000	0.000066000
6	-5.674924000	0.494644000	0.000286000
1	-3.056288000	2.697782000	0.000043000
6	-2.895658000	0.551035000	-0.000060000
6	-4.978665000	-0.726586000	0.000145000
1	-5.510892000	-1.671522000	0.000170000
6	-3.594103000	-0.683611000	-0.000024000
6	-1.354265000	-1.121310000	-0.000207000
7	-1.549010000	0.252480000	-0.000237000
7	-2.630548000	-1.682199000	-0.000247000
1	-6.759199000	0.486461000	0.000426000
1	-0.723162000	0.846957000	-0.000131000
1	-2.781266000	-2.675634000	0.000234000
7	-0.234793000	-1.757934000	-0.000142000
7	0.786887000	-0.796817000	-0.000125000
6	1.989929000	-1.259659000	-0.000007000
1	2.134621000	-2.349598000	0.000081000
6	3.183532000	-0.449891000	0.000024000
6	4.415666000	-1.136465000	0.000164000
6	3.161166000	1.020796000	-0.000079000
6	5.643209000	-0.493823000	0.000214000
6	4.476469000	1.636966000	-0.000020000
6	5.650657000	0.917883000	0.000120000
1	-5.549103000	2.638112000	0.000350000
1	4.386278000	-2.225539000	0.000236000
1	6.569869000	-1.057896000	0.000324000
1	4.489099000	2.723259000	-0.000094000
8	2.115495000	1.720180000	-0.000215000
1	6.602050000	1.447476000	0.000156000

5a_A2, optimization in gas phase B3LYP/6-311++G**, E= -834.625344290 a.u. Sum of electronic and thermal Enthalpies= -834.383842 a.u.			
-1; 1			
6	-5.217925000	1.543260000	0.000212000
6	-3.830236000	1.718628000	0.000114000
6	-5.794484000	0.266784000	0.000215000
1	-3.388121000	2.708891000	0.000113000
6	-3.005259000	0.588555000	0.000021000
6	-4.989601000	-0.882698000	0.000110000
1	-5.433703000	-1.873539000	0.000103000
6	-3.613614000	-0.702569000	0.000020000
6	-1.366242000	-0.819800000	-0.000123000
7	-1.634462000	0.490569000	-0.000074000
7	-2.545915000	-1.574139000	-0.000123000
1	-6.874575000	0.162550000	0.000293000
1	-2.557210000	-2.579949000	0.000035000
7	-0.214180000	-1.509862000	-0.000186000
7	0.874178000	-0.728805000	-0.000185000
6	2.038675000	-1.308316000	-0.000002000
1	2.107169000	-2.400365000	0.000129000
6	3.261489000	-0.529136000	0.000031000
6	4.515131000	-1.166904000	0.000212000
6	3.242939000	0.896914000	-0.000134000
6	5.709869000	-0.453044000	0.000230000
6	4.447178000	1.607343000	-0.000115000
6	5.672730000	0.943271000	0.000066000
1	-5.863933000	2.416031000	0.000289000
1	4.535845000	-2.253309000	0.000336000
1	6.658942000	-0.978851000	0.000369000
1	4.395287000	2.690718000	-0.000243000
8	2.088920000	1.588145000	-0.000299000
1	1.333116000	0.928282000	-0.000262000
1	6.594573000	1.516305000	0.000077000

5a_A3, optimization in gas phase B3LYP/6-311++G**, E= -834.625540739 a.u. Sum of electronic and thermal Enthalpies= -834.383958 a.u.			
-1; 1			
6	-5.113184000	1.597612000	-0.115370000
6	-3.717194000	1.727844000	-0.151799000
6	-5.711961000	0.335973000	0.003140000
1	-3.250301000	2.703738000	-0.241076000
6	-2.962757000	0.566084000	-0.068632000
6	-4.946502000	-0.830376000	0.086891000
1	-5.413714000	-1.804974000	0.178273000
6	-3.550661000	-0.726756000	0.050359000
6	-1.414472000	-1.063618000	0.033132000
7	-1.604350000	0.322445000	-0.067978000
7	-2.587710000	-1.701774000	0.109775000
1	-6.795133000	0.264574000	0.029982000
1	-0.865431000	0.991157000	-0.198076000
7	-0.217627000	-1.679894000	0.042859000

5a_Aw1, optimization in solv.water B3LYP/6-311++G**, E= -834.690503213 a.u. Sum of electronic and thermal Enthalpies= -834.448079 a.u.			
-1; 1			
6	-5.288719000	1.533091000	-0.037961000
6	-3.899037000	1.718983000	-0.037601000
6	-5.847842000	0.253059000	-0.015186000
1	-3.464335000	2.710982000	-0.055433000
6	-3.101244000	0.585042000	-0.014029000
6	-5.040506000	-0.892795000	0.008328000
1	-5.473524000	-1.885551000	0.025816000
6	-3.666022000	-0.706860000	0.008120000
6	-1.400234000	-0.926986000	0.016336000
7	-1.720532000	0.414718000	-0.007256000
7	-2.604266000	-1.605225000	0.026479000
1	-6.925563000	0.139400000	-0.015750000
1	-1.003504000	1.122908000	-0.019918000
1	-2.668127000	-2.610387000	0.045089000

7	0.817276000	-0.830483000	0.024358000	7	-0.232618000	-1.496394000	0.026653000
6	2.017869000	-1.348194000	-0.038903000	7	0.790583000	-0.541002000	0.018231000
1	2.123673000	-2.433505000	-0.094410000	6	1.972436000	-1.066029000	0.010619000
6	3.212433000	-0.529961000	-0.030676000	1	2.034512000	-2.161686000	0.007000000
6	4.485545000	-1.121074000	-0.143931000	6	3.255410000	-0.387971000	0.002029000
6	3.160714000	0.887659000	0.098204000	6	4.387142000	-1.234268000	-0.037402000
6	5.654208000	-0.365987000	-0.137619000	6	3.443612000	1.057982000	0.033307000
6	4.333216000	1.641789000	0.104583000	6	5.690306000	-0.761035000	-0.055935000
6	5.578158000	1.023117000	-0.014382000	6	4.816102000	1.498623000	0.008541000
1	-5.734037000	2.485178000	-0.179078000	6	5.891109000	0.631465000	-0.034138000
1	4.541737000	-2.201583000	-0.239183000	1	-5.937636000	2.400804000	-0.056483000
1	6.617440000	-0.856821000	-0.229091000	1	4.215579000	-2.308151000	-0.055117000
1	4.247370000	2.718350000	0.204835000	1	6.529731000	-1.445998000	-0.087296000
8	1.970444000	1.521645000	0.220120000	1	4.980284000	2.572661000	0.026916000
1	1.277947000	0.799498000	0.202763000	8	2.487972000	1.901891000	0.082044000
1	6.481301000	1.624505000	-0.008981000	1	6.901555000	1.031390000	-0.050091000
5a_Aw2, optimization in solv.water B3LYP/6-311++G**, E= -834.703249096 a.u. Sum of electronic and thermal Enthalpies= -834.461306 a.u.				**5a_Aw3,** optimization in solv.water B3LYP/6-311++G**, E= -834.702725220 a.u. Sum of electronic and thermal Enthalpies= -834.460444 a.u.			
-1; 1				-1; 1			
6	5.165569000	1.583183000	0.000102000	6	-5.169857000	1.567872000	0.000036000
6	3.774290000	1.731727000	0.000130000	6	-3.776699000	1.723923000	0.000027000
6	5.764119000	0.315465000	0.000025000	6	-5.751600000	0.292051000	0.000036000
1	3.319022000	2.716489000	0.000191000	1	-3.323730000	2.709211000	0.000026000
6	2.977257000	0.582439000	0.000076000	6	-3.006213000	0.568830000	0.000020000
6	4.984998000	-0.849662000	-0.000021000	6	-4.968230000	-0.866498000	0.000028000
1	5.445287000	-1.831486000	-0.000078000	1	-5.426979000	-1.849616000	0.000029000
6	3.604646000	-0.693504000	0.000003000	6	-3.574842000	-0.733406000	0.000021000
6	1.365484000	-0.870639000	0.000012000	6	-1.420908000	-1.025555000	0.000008000
7	1.600057000	0.450662000	0.000088000	7	-1.639087000	0.350642000	0.000004000
7	2.555913000	-1.592481000	-0.000008000	7	-2.586009000	-1.695358000	0.000015000
1	6.845215000	0.232350000	0.000003000	1	-6.832726000	0.202372000	0.000042000
1	2.611190000	-2.598811000	-0.000196000	1	-0.919322000	1.052946000	0.000047000
7	0.213946000	-1.568275000	-0.000019000	7	-0.223056000	-1.636544000	0.000008000
7	-0.877251000	-0.777339000	-0.000030000	7	0.826756000	-0.782897000	0.000004000
6	-2.050156000	-1.337805000	-0.000088000	6	2.017032000	-1.314498000	-0.000042000
1	-2.145428000	-2.426912000	-0.000062000	1	2.117984000	-2.402136000	-0.000052000
6	-3.258837000	-0.530916000	-0.000055000	6	3.232009000	-0.518778000	-0.000039000
6	-4.525351000	-1.144231000	0.000129000	6	4.488884000	-1.154113000	-0.000014000
6	-3.208444000	0.890776000	-0.000152000	6	3.211624000	0.900622000	-0.000038000
6	-5.699965000	-0.399137000	0.000242000	6	5.675266000	-0.428838000	0.000020000
6	-4.389979000	1.635017000	-0.000029000	6	4.401880000	1.627813000	0.000000000
6	-5.629403000	0.996845000	0.000165000	6	5.629974000	0.968290000	0.000029000
1	5.794656000	2.466959000	0.000140000	1	-5.803868000	2.447401000	0.000043000
1	-4.573823000	-2.228871000	0.000206000	1	4.519044000	-2.239190000	-0.000012000
1	-6.661423000	-0.899556000	0.000394000	1	6.627745000	-0.946013000	0.000043000
1	-4.320363000	2.717273000	-0.000114000	1	4.349277000	2.710891000	-0.000003000
8	-2.021306000	1.546693000	-0.000441000	8	2.030947000	1.573861000	-0.000101000
1	-1.300912000	0.843540000	-0.000670000	1	1.316975000	0.880770000	-0.000182000
1	-6.536994000	1.590173000	0.000250000	1	6.547879000	1.545287000	0.000054000
5a_R1, optimization in gas phase B3LYP/6-311++G**, E= -834.513880821 a.u. Sum of electronic and thermal Enthalpies= -834.270641 a.u.				**5a_R2,** optimization in gas phase B3LYP/6-311++G**, E= -834.531357576 a.u. Sum of electronic and thermal Enthalpies= -834.288141 a.u.			
0; 2				0; 2			
6	-5.017165000	1.679873000	0.000030000	6	5.203417000	1.534838000	0.000018000
6	-3.622460000	1.759913000	-0.000007000	6	3.832820000	1.722224000	0.000037000

6	-5.676415000	0.446198000	0.000059000	6	5.772298000	0.240283000	-0.000022000
1	-3.112615000	2.715392000	-0.000032000	1	3.389492000	2.710361000	0.000070000
6	-2.914406000	0.566012000	-0.000008000	6	3.009125000	0.581953000	0.000014000
6	-4.965278000	-0.756660000	0.000052000	6	4.985948000	-0.904906000	-0.000041000
1	-5.477253000	-1.711439000	0.000070000	1	5.430499000	-1.893122000	-0.000067000
6	-3.580294000	-0.676710000	0.000022000	6	3.603781000	-0.717366000	-0.000024000
6	-1.351128000	-1.064027000	-0.000021000	6	1.380628000	-0.814248000	-0.000012000
7	-1.553659000	0.287649000	-0.000044000	7	1.648200000	0.494707000	0.000025000
7	-2.586921000	-1.653717000	-0.000014000	7	2.541055000	-1.581581000	-0.000018000
1	-6.759388000	0.419980000	0.000086000	1	6.851576000	0.140384000	-0.000035000
1	-0.756428000	0.914721000	-0.000037000	1	2.553260000	-2.589343000	-0.000134000
1	-2.708564000	-2.653514000	0.000116000	7	0.203701000	-1.466535000	-0.000031000
7	-0.207618000	-1.718921000	-0.000006000	7	-0.855417000	-0.656200000	-0.000018000
7	0.798771000	-0.813594000	-0.000014000	6	-2.018703000	-1.262559000	-0.000029000
6	2.005332000	-1.303433000	-0.000005000	1	-2.056772000	-2.353937000	-0.000032000
1	2.139231000	-2.389769000	0.000003000	6	-3.240431000	-0.515065000	-0.000005000
6	3.178538000	-0.490316000	-0.000006000	6	-4.476486000	-1.202640000	0.000031000
6	4.428092000	-1.148125000	-0.000013000	6	-3.253198000	0.913682000	-0.000007000
6	3.158357000	0.996564000	-0.000001000	6	-5.678590000	-0.524861000	0.000068000
6	5.624219000	-0.460733000	-0.000022000	6	-4.481968000	1.588085000	0.000032000
6	4.460212000	1.657788000	-0.000016000	6	-5.672517000	0.879989000	0.000069000
6	5.632710000	0.961651000	-0.000025000	1	5.862332000	2.395286000	0.000034000
1	-5.598483000	2.594047000	0.000034000	1	-4.461181000	-2.287667000	0.000034000
1	4.436604000	-2.233836000	-0.000013000	1	-6.615642000	-1.067803000	0.000097000
1	6.561937000	-1.004209000	-0.000028000	1	-4.468378000	2.671130000	0.000028000
1	4.437281000	2.741403000	-0.000017000	8	-2.135385000	1.645582000	-0.000059000
8	2.117535000	1.675170000	0.000020000	1	-1.349612000	1.039285000	-0.000111000
1	6.581506000	1.487978000	-0.000034000	1	-6.611997000	1.421563000	0.000098000
5a_R3, optimization in gas phase B3LYP/6-311++G**, E= -834.529637936 a.u. Sum of electronic and thermal Enthalpies= -834.286450 a.u.				**5a_Rw1,** optimization in solv. water B3LYP/6-311++G**, E= -834.532666120 a.u. Sum of electronic and thermal Enthalpies= -834.289087 a.u.			
0; 2				0; 2			
6	-5.230181000	1.485878000	0.000069000	6	-5.258110000	1.531106000	0.000025000
6	-3.858343000	1.714057000	0.000062000	6	-3.877213000	1.728914000	0.000007000
6	-5.770416000	0.179232000	0.000038000	6	-5.814691000	0.242745000	0.000050000
1	-3.455509000	2.719973000	0.000083000	1	-3.446294000	2.721994000	-0.000013000
6	-3.036395000	0.589136000	0.000029000	6	-3.076734000	0.592800000	0.000014000
6	-4.955021000	-0.937689000	0.000003000	6	-5.011884000	-0.897772000	0.000057000
1	-5.357709000	-1.943075000	-0.000022000	1	-5.439154000	-1.892459000	0.000076000
6	-3.561311000	-0.739051000	-0.000001000	6	-3.635850000	-0.700117000	0.000040000
6	-1.420282000	-0.945114000	-0.000011000	6	-1.391005000	-0.902626000	0.000017000
7	-1.673681000	0.425849000	0.000002000	7	-1.697161000	0.424285000	0.000000000
7	-2.558094000	-1.656964000	-0.000029000	7	-2.567914000	-1.588867000	0.000037000
1	-6.847366000	0.058645000	0.000043000	1	-6.892073000	0.129997000	0.000064000
1	-0.971241000	1.146224000	0.000088000	1	-0.982111000	1.137568000	-0.000015000
7	-0.215311000	-1.529659000	-0.000016000	1	-2.618642000	-2.597052000	0.000071000
7	0.812964000	-0.663744000	-0.000010000	7	-0.202032000	-1.493428000	0.000016000
6	1.990942000	-1.246091000	-0.000007000	7	0.794850000	-0.587190000	-0.000007000
1	2.028590000	-2.336231000	0.000010000	6	1.991889000	-1.132875000	-0.000005000
6	3.222140000	-0.508203000	-0.000007000	1	2.048253000	-2.224983000	0.000014000
6	4.448474000	-1.210637000	0.000039000	6	3.230429000	-0.438092000	-0.000027000
6	3.258111000	0.915366000	-0.000052000	6	4.404934000	-1.239347000	-0.000021000
6	5.658955000	-0.544603000	0.000046000	6	3.381021000	1.035630000	-0.000058000
6	4.486600000	1.581285000	-0.000043000	6	5.667212000	-0.696288000	-0.000032000
6	5.670789000	0.858205000	0.000006000	6	4.745280000	1.543823000	-0.000050000
1	-5.905945000	2.333359000	0.000095000	6	5.831809000	0.719124000	-0.000043000

1	4.421846000	-2.295209000	0.000070000	1	-5.914621000	2.392797000	0.000020000
1	6.589276000	-1.098849000	0.000083000	1	4.286945000	-2.318219000	-0.000004000
1	4.485391000	2.664397000	-0.000078000	1	6.538709000	-1.339816000	-0.000025000
8	2.129639000	1.646539000	-0.000112000	1	4.854986000	2.622578000	-0.000055000
1	1.373668000	1.010736000	-0.000130000	8	2.414314000	1.828063000	-0.000032000
1	6.616369000	1.388706000	0.000012000	1	6.832780000	1.137348000	-0.000045000
5a_Rw2, optimization in solv. water B3LYP/6-311++G**, E= -834.545226034 a.u. Sum of electronic and thermal Enthalpies= -834.302209 a.u.				**5a_Rw3,** optimization in solv. water B3LYP/6-311++G**, E= -834.545123970 a.u. Sum of electronic and thermal Enthalpies= -834.301753 a.u.			
0; 2				0; 2			
6	-5.206081000	1.534405000	0.000052000	6	5.836290000	1.849111000	-0.000051000
6	-3.836309000	1.726749000	0.000049000	6	4.449892000	1.947875000	-0.000039000
6	-5.772581000	0.235670000	0.000025000	6	6.497718000	0.597138000	-0.000048000
1	-3.401735000	2.719173000	0.000068000	1	3.950288000	2.908754000	-0.000041000
6	-3.010064000	0.586417000	0.000019000	6	3.737737000	0.748829000	-0.000026000
6	-4.984964000	-0.907267000	-0.000005000	6	5.791771000	-0.592367000	-0.000034000
1	-5.422109000	-1.898013000	-0.000026000	1	6.294085000	-1.552286000	-0.000032000
6	-3.601689000	-0.714678000	-0.000007000	6	4.384678000	-0.523842000	-0.000023000
6	-1.383035000	-0.818470000	-0.000022000	6	2.264849000	-0.916382000	-0.000003000
7	-1.648101000	0.496781000	0.000011000	7	2.396207000	0.463041000	-0.000012000
7	-2.542228000	-1.578533000	-0.000035000	7	3.464547000	-1.528230000	-0.000008000
1	-6.851559000	0.134575000	0.000029000	1	7.581130000	0.578117000	-0.000057000
1	-2.569526000	-2.587846000	-0.000031000	1	1.637329000	1.125828000	-0.000013000
7	-0.204364000	-1.466971000	-0.000041000	7	1.123128000	-1.619529000	0.000011000
7	0.858859000	-0.656645000	-0.000031000	7	0.005888000	-0.870345000	0.000020000
6	2.022061000	-1.264321000	-0.000030000	6	-1.101088000	-1.578745000	0.000031000
1	2.064535000	-2.354485000	-0.000021000	1	-1.026282000	-2.666668000	0.000015000
6	3.244818000	-0.514539000	-0.000010000	6	-2.406321000	-0.983487000	0.000022000
6	4.480726000	-1.201908000	0.000051000	6	-3.542818000	-1.825908000	-0.000014000
6	3.258016000	0.912126000	-0.000039000	6	-2.608720000	0.425850000	0.000038000
6	5.682337000	-0.519234000	0.000091000	6	-4.822867000	-1.305156000	-0.000039000
6	4.480033000	1.592117000	0.000005000	6	-3.906243000	0.944143000	0.000010000
6	5.674663000	0.884564000	0.000070000	6	-4.998837000	0.087276000	-0.000028000
1	-5.867657000	2.392692000	0.000075000	1	6.430032000	2.755713000	-0.000061000
1	4.467464000	-2.286313000	0.000075000	1	-3.389618000	-2.899457000	-0.000027000
1	6.619965000	-1.060856000	0.000141000	1	-5.682088000	-1.964063000	-0.000069000
1	4.471248000	2.675445000	-0.000020000	1	-4.036489000	2.019622000	0.000025000
8	2.123262000	1.635234000	-0.000127000	8	-1.573675000	1.288489000	0.000098000
1	1.354085000	1.003170000	-0.000181000	1	-0.741722000	0.757983000	0.000147000
1	6.612453000	1.428377000	0.000101000	1	-5.999457000	0.504081000	-0.000048000
5a_RC, optimization in gas phase B3LYP/6-311++G**, E= -834.920546103 a.u. Sum of electronic and thermal Enthalpies= -834.662903 a.u.				**5a_RCw,** optimization in solv. water B3LYP/6-311++G**, E= -834.989126690 a.u. Sum of electronic and thermal Enthalpies= -834.731789 a.u.			
1; 2				1; 2			
6	-5.305117000	1.463708000	0.000064000	6	-5.300253000	1.461980000	-0.046850000
6	-3.939617000	1.715759000	0.000033000	6	-3.936876000	1.715715000	-0.069511000
6	-5.818892000	0.150315000	0.000078000	6	-5.814398000	0.146330000	0.009506000
1	-3.549868000	2.725741000	0.000023000	1	-3.541731000	2.721886000	-0.111828000
6	-3.100811000	0.604750000	0.000017000	6	-3.096374000	0.604340000	-0.033601000
6	-4.986350000	-0.959510000	0.000062000	6	-4.983570000	-0.962299000	0.045013000
1	-5.382870000	-1.966822000	0.000073000	1	-5.373845000	-1.970394000	0.088124000
6	-3.614946000	-0.710832000	0.000031000	6	-3.610602000	-0.712508000	0.022289000
6	-1.366837000	-0.831245000	-0.000017000	6	-1.372372000	-0.825737000	0.007584000
7	-1.717642000	0.483945000	-0.000011000	7	-1.720623000	0.486882000	-0.040392000
7	-2.518866000	-1.554957000	0.000012000	7	-2.520577000	-1.552013000	0.044116000
1	-6.892051000	0.006076000	0.000103000	1	-6.887614000	0.003411000	0.025174000

1	-1.046634000	1.237569000	-0.000032000	1	-1.057026000	1.246871000	-0.089028000
1	-2.520875000	-2.566154000	0.000003000	1	-2.531492000	-2.563223000	0.084095000
7	-0.175764000	-1.423371000	-0.000043000	7	-0.178815000	-1.418171000	0.018353000
7	0.858356000	-0.580364000	-0.000068000	7	0.857153000	-0.575661000	0.009540000
6	2.034004000	-1.195401000	0.000004000	6	2.025810000	-1.193305000	-0.014545000
1	2.042215000	-2.285253000	0.000065000	1	2.038136000	-2.282452000	-0.038262000
6	3.266658000	-0.499944000	0.000001000	6	3.264221000	-0.495347000	-0.012053000
6	4.477805000	-1.248685000	0.000066000	6	4.468703000	-1.246807000	-0.061001000
6	3.350839000	0.935613000	-0.000068000	6	3.352179000	0.931925000	0.041407000
6	5.696920000	-0.619729000	0.000061000	6	5.696017000	-0.624546000	-0.059745000
6	4.602099000	1.560369000	-0.000075000	6	4.606206000	1.550532000	0.042714000
6	5.751892000	0.793184000	-0.000011000	6	5.757695000	0.782089000	-0.007343000
1	-5.995722000	2.297766000	0.000079000	1	-5.992461000	2.294341000	-0.072435000
1	4.416855000	-2.331056000	0.000119000	1	4.399840000	-2.327864000	-0.101053000
1	6.613104000	-1.195935000	0.000111000	1	6.607371000	-1.207190000	-0.098620000
1	4.640379000	2.642238000	-0.000128000	1	4.652229000	2.631641000	0.083657000
8	2.259570000	1.701348000	-0.000125000	8	2.262390000	1.708406000	0.093477000
1	1.473614000	1.111217000	-0.000101000	1	1.466376000	1.129016000	0.083642000
1	6.716839000	1.286943000	-0.000015000	1	6.722812000	1.275276000	-0.005775000
5a_M, optimization in gas phase B3LYP/6-311++G**, E= -835.164800326 a.u. Sum of electronic and thermal Enthalpies= -834.908173 a.u.				**5a_Mw,** optimization in solv. water B3LYP/6-311++G**, E= -835.179289044 a.u. Sum of electronic and thermal Enthalpies= -834.922971 a.u.			
0; 1				0; 1			
6	-5.223588000	1.547972000	0.026893000	6	-5.235768000	1.542543000	-0.039469000
6	-3.837861000	1.718059000	0.131475000	6	-3.848100000	1.727038000	-0.045093000
6	-5.788048000	0.278628000	-0.108916000	6	-5.798056000	0.262247000	-0.008290000
1	-3.400530000	2.703643000	0.236976000	1	-3.411124000	2.717640000	-0.069253000
6	-3.049570000	0.579289000	0.094971000	6	-3.055713000	0.589137000	-0.018630000
6	-4.990310000	-0.871016000	-0.145466000	6	-4.996167000	-0.884510000	0.018293000
1	-5.430954000	-1.855160000	-0.251113000	1	-5.430495000	-1.876250000	0.042228000
6	-3.618473000	-0.700920000	-0.041662000	6	-3.620987000	-0.698715000	0.012568000
6	-1.356115000	-0.945886000	0.088004000	6	-1.360154000	-0.923002000	0.014701000
7	-1.669155000	0.395224000	0.171604000	7	-1.671769000	0.415018000	-0.015286000
7	-2.561013000	-1.605435000	-0.042078000	7	-2.558289000	-1.596117000	0.032461000
1	-6.863840000	0.177512000	-0.187385000	1	-6.875995000	0.152404000	-0.004638000
1	-0.968271000	1.109300000	0.272161000	1	-0.980109000	1.145487000	-0.045030000
1	-2.612067000	-2.607341000	-0.122441000	1	-2.618663000	-2.602025000	0.057407000
7	-0.213184000	-1.560662000	0.115065000	7	-0.205359000	-1.536469000	0.024671000
7	0.855246000	-0.700341000	0.250363000	7	0.868515000	-0.675976000	0.015526000
6	2.014981000	-1.272252000	0.281855000	6	2.029619000	-1.247890000	-0.007301000
1	2.072537000	-2.359759000	0.202944000	1	2.090802000	-2.337883000	-0.024106000
6	3.254379000	-0.528400000	0.418115000	6	3.275200000	-0.498927000	-0.009732000
6	4.478551000	-1.221104000	0.443218000	6	4.499077000	-1.192759000	-0.050563000
6	3.279156000	0.885280000	0.527766000	6	3.309076000	0.917494000	0.031033000
6	5.686730000	-0.552635000	0.571083000	6	5.714038000	-0.520785000	-0.052837000
6	4.497440000	1.555981000	0.656547000	6	4.531842000	1.592004000	0.029441000
6	5.689222000	0.842116000	0.677830000	6	5.725015000	0.877508000	-0.012666000
1	-5.866461000	2.419536000	0.052393000	1	-5.883819000	2.410614000	-0.059749000
1	4.462817000	-2.303153000	0.359914000	1	4.478719000	-2.277206000	-0.080944000
1	6.618081000	-1.105583000	0.588270000	1	6.643950000	-1.075523000	-0.085423000
1	4.484721000	2.636300000	0.737938000	1	4.528641000	2.675430000	0.060979000
8	2.138898000	1.609111000	0.510209000	8	2.166416000	1.644824000	0.073149000
1	1.397630000	0.963303000	0.412560000	1	1.414270000	1.001467000	0.067060000
1	6.627765000	1.375840000	0.778457000	1	6.667271000	1.413761000	-0.014047000

5b_A1, optimization in gas phase B3LYP/6-311++G**, E= -909.879034547 a.u. Sum of electronic and thermal Enthalpies= -909.632062 a.u.			
-1; 1			
6	-5.390873000	1.739033000	0.319179000
6	-4.154801000	1.689948000	0.971785000
6	-5.838508000	0.680164000	-0.480920000
1	-3.812196000	2.512003000	1.590616000
6	-3.352941000	0.553940000	0.817683000
6	-5.053442000	-0.470064000	-0.651887000
1	-5.398282000	-1.292394000	-1.271390000
6	-3.828282000	-0.513234000	-0.001522000
6	-1.807010000	-0.954615000	0.881639000
7	-2.117568000	0.261149000	1.344843000
7	-2.822652000	-1.454410000	0.059179000
1	-6.802130000	0.747157000	-0.975154000
1	-2.780920000	-2.356906000	-0.383079000
7	-0.735141000	-1.743725000	1.063414000
7	0.192684000	-1.194230000	1.856947000
6	1.273591000	-1.874629000	2.105817000
1	1.410652000	-2.869931000	1.674390000
6	2.308459000	-1.320426000	2.957840000
6	3.488897000	-2.037217000	3.245774000
6	2.164239000	-0.036455000	3.528982000
6	4.477773000	-1.502602000	4.062445000
6	3.167845000	0.493050000	4.351243000
6	4.323919000	-0.229464000	4.622909000
1	-6.018362000	2.617509000	0.434925000
1	5.376890000	-2.073551000	4.269193000
8	1.079033000	0.750252000	3.329211000
1	0.445950000	0.244214000	2.725999000
1	3.613722000	-3.025574000	2.814459000
1	5.082146000	0.207155000	5.262653000
8	2.984897000	1.744137000	4.884591000
1	2.121700000	2.046196000	4.563198000

5b_A2, optimization in gas phase B3LYP/6-311++G**, E= -909.877524807 a.u. Sum of electronic and thermal Enthalpies= -909.630515 a.u.			
-1; 1			
6	-5.219352000	1.863877000	0.217386000
6	-3.948316000	1.802156000	0.806764000
6	-5.773606000	0.739325000	-0.409215000
1	-3.518004000	2.670402000	1.295979000
6	-3.269257000	0.593882000	0.740189000
6	-5.084420000	-0.474682000	-0.472784000
1	-5.516161000	-1.342406000	-0.959644000
6	-3.811778000	-0.560206000	0.104819000
6	-1.865345000	-1.162767000	0.829248000
7	-2.037251000	0.178493000	1.204925000
7	-2.937763000	-1.615653000	0.171741000
1	-6.760619000	0.814739000	-0.855372000
1	-1.323128000	0.749614000	1.622197000
7	-0.765905000	-1.898460000	1.080124000
7	0.132692000	-1.267696000	1.845354000
6	1.278633000	-1.866845000	2.053476000
1	1.469097000	-2.831152000	1.579751000
6	2.293293000	-1.286711000	2.908374000
6	3.545891000	-1.911081000	3.092959000
6	2.064445000	-0.077438000	3.600664000
6	4.513747000	-1.355289000	3.920502000
6	3.041151000	0.473756000	4.434255000
6	4.270736000	-0.156090000	4.598756000
1	-5.778200000	2.793288000	0.249671000
1	5.469180000	-1.854191000	4.043868000
8	0.886557000	0.601800000	3.498809000
1	0.316528000	0.044220000	2.881450000
1	3.743513000	-2.842269000	2.571990000
1	5.012631000	0.292825000	5.248631000
8	2.768073000	1.648356000	5.091494000
1	1.866516000	1.896278000	4.841310000

5b_A3, optimization in gas phase B3LYP/6-311++G**, E= -909.862443693 a.u. Sum of electronic and thermal Enthalpies= -909.615050 a.u.			
-1; 1			
6	-5.270966000	1.772285000	0.368379000
6	-4.017209000	1.644630000	0.988109000
6	-5.786659000	0.757069000	-0.434036000
1	-3.616634000	2.434547000	1.612119000
6	-3.302602000	0.474499000	0.778805000
6	-5.066333000	-0.430426000	-0.649054000
1	-5.468052000	-1.220847000	-1.273446000
6	-3.829420000	-0.557730000	-0.038281000
6	-1.788736000	-1.222661000	0.737382000
7	-2.072472000	0.042242000	1.230857000
7	-2.886955000	-1.576606000	-0.043981000
1	-6.757197000	0.880001000	-0.901558000
1	-1.381512000	0.483746000	1.831952000
1	-2.941117000	-2.455510000	-0.528070000
7	-0.736345000	-1.934901000	0.947958000
7	0.108018000	-1.194826000	1.786772000
6	1.216560000	-1.766184000	2.110164000

5b_A4, optimization in gas phase B3LYP/6-311++G**, E= -909.845544686 a.u. Sum of electronic and thermal Enthalpies= -909.598004 a.u.			
-1; 1			
6	-5.407872000	1.747465000	0.149663000
6	-4.172991000	1.718806000	0.816821000
6	-5.859280000	0.648246000	-0.577555000
1	-3.822525000	2.573502000	1.383167000
6	-3.416021000	0.561845000	0.728594000
6	-5.093332000	-0.525001000	-0.667854000
1	-5.445921000	-1.379299000	-1.234496000
6	-3.874027000	-0.553510000	-0.009996000
6	-1.832537000	-1.077707000	0.879401000
7	-2.182959000	0.212652000	1.258498000
7	-2.896372000	-1.530397000	0.100271000
1	-6.816709000	0.694958000	-1.083788000
1	-1.560050000	0.780065000	1.810220000
1	-2.902185000	-2.450339000	-0.304770000
7	-0.782675000	-1.767712000	1.144630000
7	0.110334000	-1.068536000	1.959768000
6	1.226488000	-1.693156000	2.188472000

1	1.428653000	-2.771315000	1.720669000
6	2.219459000	-1.174547000	2.962760000
6	3.388191000	-1.939600000	3.228400000
6	2.085739000	0.135089000	3.545574000
6	4.412035000	-1.477080000	4.029174000
6	3.194579000	0.571550000	4.378830000
6	4.310196000	-0.191114000	4.616420000
1	-5.844744000	2.679771000	0.520014000
1	5.290161000	-2.087842000	4.211391000
8	1.118112000	0.957822000	3.421791000
1	3.462813000	-2.926193000	2.776410000
1	5.101186000	0.198683000	5.250716000
8	3.017120000	1.819918000	4.904855000
1	2.132494000	2.049315000	4.528730000

1	1.368036000	-2.675513000	1.728213000
6	2.301154000	-1.189010000	3.006085000
6	3.471036000	-1.998180000	3.124890000
6	2.227064000	0.050863000	3.673001000
6	4.521428000	-1.538396000	3.899552000
6	3.315779000	0.569320000	4.495770000
6	4.449604000	-0.306280000	4.558751000
1	-6.017092000	2.642285000	0.204599000
1	5.420248000	-2.143135000	4.000310000
8	1.114213000	0.830863000	3.576809000
1	0.480602000	0.342174000	3.015039000
1	3.516024000	-2.950694000	2.607332000
1	5.284274000	0.038881000	5.162803000
8	3.241527000	1.683478000	5.085289000

5b_A5, optimization in gas phase
B3LYP/6-311++G**, E= -909.857906359 a.u.
Sum of electronic and thermal Enthalpies= -909.610488 a.u.

5b_Aw1, optimization in solv.water
B3LYP/6-311++G**, E= -909.954625694 a.u.
Sum of electronic and thermal Enthalpies= -909.707513 a.u.

-1; 1			
6	-5.326619000	1.752238000	0.327658000
6	-4.076165000	1.649744000	0.957403000
6	-5.820503000	0.721083000	-0.468583000
1	-3.692897000	2.452060000	1.576485000
6	-3.343793000	0.488488000	0.763830000
6	-5.081448000	-0.456816000	-0.666970000
1	-5.466455000	-1.259126000	-1.286439000
6	-3.847369000	-0.558920000	-0.045868000
6	-1.802756000	-1.186512000	0.750682000
7	-2.108899000	0.077839000	1.229227000
7	-2.888859000	-1.563229000	-0.034287000
1	-6.789192000	0.824762000	-0.944220000
1	-1.437665000	0.541925000	1.830433000
1	-2.925266000	-2.448210000	-0.509266000
7	-0.746347000	-1.890314000	0.968555000
7	0.104166000	-1.156352000	1.805789000
6	1.205096000	-1.743837000	2.115822000
1	1.400208000	-2.747436000	1.718842000
6	2.233664000	-1.175824000	2.968165000
6	3.393054000	-1.971254000	3.215137000
6	2.169053000	0.087542000	3.561491000
6	4.412869000	-1.493144000	4.019418000
6	3.222348000	0.615514000	4.408021000
6	4.340444000	-0.221573000	4.611731000
1	-5.915250000	2.652054000	0.466193000
1	5.288469000	-2.112695000	4.197429000
8	1.139145000	0.960798000	3.425997000
1	1.488860000	1.705948000	3.990969000
1	3.457521000	-2.955498000	2.762049000
1	5.146391000	0.144103000	5.241114000
8	3.027176000	1.794442000	4.886634000

-1; 1			
6	-5.358110000	1.756065000	0.344999000
6	-4.117899000	1.689017000	0.988937000
6	-5.821382000	0.704255000	-0.457942000
1	-3.766911000	2.507107000	1.609058000
6	-3.335313000	0.542304000	0.818929000
6	-5.053764000	-0.453697000	-0.642648000
1	-5.409762000	-1.268775000	-1.262949000
6	-3.823775000	-0.512590000	0.000514000
6	-1.805862000	-0.995843000	0.859405000
7	-2.092731000	0.224607000	1.336812000
7	-2.830029000	-1.471508000	0.045898000
1	-6.787058000	0.785198000	-0.944305000
1	-2.823168000	-2.369041000	-0.412561000
7	-0.731924000	-1.788635000	1.041162000
7	0.196432000	-1.230614000	1.840973000
6	1.282832000	-1.897223000	2.099609000
1	1.440702000	-2.892867000	1.678273000
6	2.307367000	-1.323941000	2.956196000
6	3.491863000	-2.029914000	3.250770000
6	2.143090000	-0.038366000	3.517992000
6	4.469494000	-1.477977000	4.069765000
6	3.134663000	0.508174000	4.342370000
6	4.296441000	-0.203720000	4.621316000
1	-5.974665000	2.639861000	0.469637000
1	5.373908000	-2.035046000	4.285390000
8	1.038459000	0.724480000	3.296040000
1	0.436310000	0.181657000	2.689840000
1	3.630648000	-3.018445000	2.826053000
1	5.049405000	0.240491000	5.261873000
8	2.949709000	1.758742000	4.875427000
1	2.090316000	2.082719000	4.568128000

5b_Aw2, optimization in solv.water
B3LYP/6-311++G**, E= -909.953486005 a.u.
Sum of electronic and thermal Enthalpies= -909.706017 a.u.

5b_Aw3, optimization in solv.water
B3LYP/6-311++G**, E= -909.949919136 a.u.
Sum of electronic and thermal Enthalpies= -909.702005 a.u.

-1; 1			
6	-5.278919000	1.833155000	0.195965000
6	-4.012535000	1.793574000	0.795533000
6	-5.808522000	0.703313000	-0.443823000

-1; 1			
6	-5.518901000	1.664234000	0.174009000
6	-4.292285000	1.664316000	0.852894000
6	-5.911087000	0.578254000	-0.612591000

1	-3.600776000	2.664985000	1.292603000	1	-3.987209000	2.505871000	1.462896000
6	-3.311622000	0.597086000	0.725065000	6	-3.483790000	0.546123000	0.714480000
6	-5.095564000	-0.497804000	-0.510748000	6	-5.092958000	-0.551389000	-0.752109000
1	-5.512557000	-1.366473000	-1.009211000	1	-5.396186000	-1.393709000	-1.362019000
6	-3.827267000	-0.557984000	0.078446000	6	-3.880043000	-0.549425000	-0.079500000
6	-1.865723000	-1.120899000	0.824547000	6	-1.836751000	-1.021705000	0.804197000
7	-2.070850000	0.205638000	1.199228000	7	-2.235003000	0.225502000	1.237888000
7	-2.924596000	-1.599129000	0.151110000	7	-2.855678000	-1.487324000	-0.003709000
1	-6.792203000	0.763184000	-0.897269000	1	-6.864826000	0.605871000	-1.126380000
1	-1.384306000	0.796236000	1.637154000	1	-1.656199000	0.775444000	1.852999000
7	-0.764264000	-1.850787000	1.078563000	1	-2.828801000	-2.385369000	-0.459483000
7	0.141045000	-1.216543000	1.856255000	7	-0.744665000	-1.677166000	1.063753000
6	1.273873000	-1.826809000	2.068493000	7	0.092326000	-0.941906000	1.908258000
1	1.461817000	-2.794498000	1.599107000	6	1.191383000	-1.556553000	2.198359000
6	2.303629000	-1.268342000	2.926832000	1	1.345725000	-2.553392000	1.767467000
6	3.536635000	-1.932107000	3.098124000	6	2.271291000	-1.080671000	3.043048000
6	2.104034000	-0.058957000	3.624285000	6	3.374765000	-1.964425000	3.202979000
6	4.522545000	-1.408021000	3.925018000	6	2.297065000	0.189186000	3.708593000
6	3.100724000	0.461792000	4.456812000	6	4.476119000	-1.650357000	3.976256000
6	4.311240000	-0.206286000	4.609346000	6	3.470614000	0.467807000	4.503898000
1	-5.855171000	2.750932000	0.229757000	6	4.524641000	-0.405120000	4.641836000
1	5.464375000	-1.931097000	4.043301000	1	-6.171937000	2.524387000	0.263455000
8	0.943989000	0.651429000	3.530816000	1	5.298300000	-2.349898000	4.074920000
1	0.358354000	0.135606000	2.907014000	8	1.397363000	1.111136000	3.680633000
1	3.706061000	-2.864480000	2.570527000	1	3.337791000	-2.922235000	2.691458000
1	5.070934000	0.215209000	5.257094000	1	5.377256000	-0.132190000	5.255851000
8	2.877694000	1.638222000	5.125534000	8	3.444827000	1.693730000	5.118718000
1	1.991505000	1.949931000	4.892198000	1	2.575218000	2.044754000	4.816752000
5b_Aw4, optimization in solv.water B3LYP/6-311++G**, E= -909.947740901 a.u. Sum of electronic and thermal Enthalpies= -909.699663 a.u.				**5b_Aw5,** optimization in solv.water B3LYP/6-311++G**, E= -909.948118767 a.u. Sum of electronic and thermal Enthalpies= -909.700160 a.u.			
-1; 1				-1; 1			
6	-5.467672000	1.711335000	0.194517000	6	-5.489448000	1.683201000	0.196616000
6	-4.238274000	1.707340000	0.866195000	6	-4.258707000	1.669807000	0.866490000
6	-5.880228000	0.615646000	-0.569307000	6	-5.900717000	0.600680000	-0.585879000
1	-3.917499000	2.555609000	1.458352000	1	-3.939085000	2.508345000	1.473071000
6	-3.448617000	0.574118000	0.743210000	6	-3.465338000	0.541249000	0.723272000
6	-5.080900000	-0.527761000	-0.692137000	6	-5.098083000	-0.538612000	-0.730096000
1	-5.399317000	-1.377191000	-1.283898000	1	-5.415710000	-1.377968000	-1.336626000
6	-3.864221000	-0.529321000	-0.025609000	6	-3.880473000	-0.549785000	-0.065920000
6	-1.823912000	-1.014603000	0.855323000	6	-1.839107000	-1.045273000	0.803175000
7	-2.199339000	0.244684000	1.267438000	7	-2.216583000	0.205105000	1.238628000
7	-2.852362000	-1.478830000	0.064267000	7	-2.866156000	-1.499741000	0.004289000
1	-6.836496000	0.647989000	-1.077917000	1	-6.857818000	0.639537000	-1.092539000
1	-1.627801000	0.821942000	1.861393000	1	-1.625708000	0.751549000	1.845501000
1	-2.838564000	-2.386940000	-0.372468000	1	-2.852889000	-2.399682000	-0.448812000
7	-0.748873000	-1.707990000	1.102764000	7	-0.752223000	-1.718997000	1.053763000
7	0.151688000	-1.043541000	1.919249000	7	0.098094000	-1.000647000	1.889129000
6	1.235208000	-1.704368000	2.176672000	6	1.193243000	-1.618306000	2.170634000
1	1.356800000	-2.702457000	1.748100000	1	1.353299000	-2.615269000	1.745606000
6	2.317827000	-1.203000000	3.006916000	6	2.273684000	-1.123613000	3.017397000
6	3.447454000	-2.040336000	3.198557000	6	3.389987000	-1.990538000	3.192785000
6	2.279528000	0.065997000	3.613548000	6	2.310514000	0.113843000	3.666563000
6	4.499230000	-1.593254000	3.982416000	6	4.466914000	-1.613947000	3.979343000
6	3.356740000	0.564531000	4.435307000	6	3.414808000	0.534087000	4.490827000
6	4.454977000	-0.329540000	4.582163000	6	4.488860000	-0.368467000	4.625205000

1	-6.108153000	2.581966000	0.270914000	1	-6.131655000	2.551049000	0.289479000
1	5.367992000	-2.226787000	4.135207000	1	5.306777000	-2.291522000	4.099124000
8	1.199495000	0.890765000	3.445070000	8	1.317726000	1.047449000	3.592398000
1	0.563337000	0.411266000	2.866524000	1	1.697789000	1.759707000	4.165045000
1	3.470457000	-3.017279000	2.728407000	1	3.382240000	-2.955745000	2.698011000
1	5.287062000	0.008392000	5.193864000	1	5.337107000	-0.081895000	5.239883000
8	3.309695000	1.730158000	4.984454000	8	3.317640000	1.712195000	5.037081000
5b_Ab1, optimization in solv. benzene B3LYP/6-311++G**, E= -909.917745480 a.u. Sum of electronic and thermal Enthalpies= -909.670568 a.u.				**5b_Ab2,** optimization in solv. benzene B3LYP/6-311++G**, E= -909.916351372 a.u. Sum of electronic and thermal Enthalpies= -909.669007 a.u.			
-1; 1				-1; 1			
6	-5.374581000	1.745449000	0.337725000	6	-5.211586000	1.868010000	0.205399000
6	-4.135247000	1.687635000	0.983227000	6	-3.934367000	1.808393000	0.780347000
6	-5.830776000	0.691416000	-0.464848000	6	-5.780546000	0.737514000	-0.397281000
1	-3.787933000	2.505775000	1.604862000	1	-3.492374000	2.680587000	1.250754000
6	-3.341759000	0.547607000	0.817857000	6	-3.264035000	0.594504000	0.723140000
6	-5.053221000	-0.461367000	-0.646455000	6	-5.099143000	-0.481645000	-0.451015000
1	-5.404425000	-1.279125000	-1.267403000	1	-5.544701000	-1.352442000	-0.919547000
6	-3.824227000	-0.512267000	-0.002617000	6	-3.820280000	-0.563984000	0.112243000
6	-1.803735000	-0.974047000	0.867399000	6	-1.865046000	-1.163636000	0.826415000
7	-2.103100000	0.242622000	1.339044000	7	-2.027864000	0.180398000	1.182271000
7	-2.823589000	-1.461256000	0.047537000	7	-2.947396000	-1.624544000	0.187027000
1	-6.796796000	0.765206000	-0.952635000	1	-6.772288000	0.811653000	-0.831893000
1	-2.798603000	-2.361159000	-0.402897000	1	-1.304615000	0.760194000	1.571938000
7	-0.731218000	-1.765870000	1.048774000	7	-0.767489000	-1.902590000	1.076188000
7	0.195272000	-1.212205000	1.846127000	7	0.135152000	-1.269068000	1.843274000
6	1.278656000	-1.885556000	2.100809000	6	1.281621000	-1.862614000	2.048238000
1	1.425507000	-2.880848000	1.674008000	1	1.481544000	-2.824066000	1.572437000
6	2.307448000	-1.322566000	2.956203000	6	2.295077000	-1.281647000	2.907657000
6	3.488295000	-2.034817000	3.251817000	6	3.550367000	-1.902391000	3.081119000
6	2.153901000	-0.036740000	3.520089000	6	2.058372000	-0.081508000	3.611734000
6	4.470326000	-1.492021000	4.071510000	6	4.517149000	-1.349461000	3.911996000
6	3.150876000	0.501219000	4.344309000	6	3.034137000	0.466416000	4.449560000
6	4.307640000	-0.216970000	4.624939000	6	4.267080000	-0.159093000	4.603012000
1	-5.997539000	2.625563000	0.461220000	1	-5.764736000	2.800657000	0.230320000
1	5.370487000	-2.057432000	4.286319000	1	5.475685000	-1.842931000	4.028598000
8	1.062492000	0.740462000	3.306961000	8	0.876164000	0.591608000	3.519255000
1	0.441645000	0.218946000	2.703158000	1	0.307481000	0.042468000	2.897546000
1	3.619429000	-3.024133000	2.825367000	1	3.751846000	-2.826915000	2.550359000
1	5.061564000	0.223736000	5.266917000	1	5.008732000	0.286004000	5.255831000
8	2.966345000	1.754012000	4.872715000	8	2.761492000	1.631518000	5.122354000
1	2.106150000	2.065212000	4.552921000	1	1.858147000	1.888684000	4.888399000
5b_Ab3, optimization in solv. benzene B3LYP/6-311++G**, E= -909.906626421 a.u. Sum of electronic and thermal Enthalpies= -909.658794 a.u.				**5b_Ab4,** optimization in solv. benzene B3LYP/6-311++G**, E= -909.897007716 a.u. Sum of electronic and thermal Enthalpies= -909.649007 a.u.			
-1; 1				-1; 1			
6	-5.436467000	1.701852000	0.239460000	6	-5.378670000	1.770248000	0.107645000
6	-4.197281000	1.657256000	0.896655000	6	-4.147501000	1.742141000	0.778277000
6	-5.874421000	0.638802000	-0.549849000	6	-5.845089000	0.657400000	-0.593002000
1	-3.857367000	2.483354000	1.509634000	1	-3.785358000	2.605365000	1.323550000
6	-3.420545000	0.520058000	0.736160000	6	-3.410166000	0.570376000	0.718692000
6	-5.089316000	-0.513138000	-0.713911000	6	-5.098321000	-0.527933000	-0.653213000
1	-5.429670000	-1.339256000	-1.327547000	1	-5.460960000	-1.391207000	-1.198630000
6	-3.865497000	-0.556801000	-0.064985000	6	-3.880464000	-0.554065000	0.008656000
6	-1.817669000	-1.095523000	0.780561000	6	-1.851474000	-1.082873000	0.908626000
7	-2.178004000	0.161304000	1.233813000	7	-2.180178000	0.214163000	1.260963000

7	-2.869952000	-1.524036000	-0.018214000	7	-2.913345000	-1.541832000	0.144284000
1	-6.835858000	0.698649000	-1.046904000	1	-6.800807000	0.706088000	-1.101780000
1	-1.553061000	0.669596000	1.844802000	1	-1.552414000	0.798474000	1.788182000
1	-2.869596000	-2.417193000	-0.481071000	1	-2.936385000	-2.471825000	-0.239501000
7	-0.741197000	-1.766341000	1.023114000	7	-0.803739000	-1.787887000	1.183326000
7	0.095784000	-1.020110000	1.863955000	7	0.098892000	-1.098431000	1.989512000
6	1.195548000	-1.621998000	2.170007000	6	1.222304000	-1.712474000	2.189979000
1	1.364450000	-2.625086000	1.756936000	1	1.376436000	-2.684362000	1.712556000
6	2.251590000	-1.108557000	3.015236000	6	2.301590000	-1.198894000	3.007747000
6	3.378012000	-1.955209000	3.209975000	6	3.495557000	-1.969816000	3.083466000
6	2.225692000	0.177655000	3.654500000	6	2.203081000	0.016242000	3.711776000
6	4.457193000	-1.592993000	3.990822000	6	4.549980000	-1.500114000	3.848391000
6	3.384578000	0.507602000	4.462698000	6	3.286241000	0.538435000	4.526916000
6	4.458733000	-0.330899000	4.631548000	6	4.451196000	-0.289529000	4.543059000
1	-6.061282000	2.580688000	0.349909000	1	-5.975561000	2.674265000	0.137310000
1	5.298455000	-2.265787000	4.116663000	1	5.468965000	-2.077399000	3.912046000
8	1.306363000	1.066429000	3.598538000	8	1.063248000	0.765827000	3.658654000
1	3.375244000	-2.924567000	2.717657000	1	0.434255000	0.279100000	3.085241000
1	5.293557000	-0.019553000	5.252430000	1	3.560744000	-2.905995000	2.539369000
8	3.305291000	1.742279000	5.048323000	1	5.288245000	0.066263000	5.137534000
1	2.425059000	2.045307000	4.718890000	8	3.184962000	1.638787000	5.159858000

5b_Ab5, optimization in solv. benzene
B3LYP/6-311++G**, E= -909.903926123 a.u.
Sum of electronic and thermal Enthalpies= -909.656026 a.u.

-1; 1

6	-5.438297000	1.707707000	0.223778000
6	-4.203131000	1.664232000	0.887119000
6	-5.874921000	0.640688000	-0.561696000
1	-3.864389000	2.493151000	1.496884000
6	-3.429588000	0.523699000	0.736305000
6	-5.092954000	-0.513887000	-0.715122000
1	-5.432210000	-1.342658000	-1.325561000
6	-3.872730000	-0.556219000	-0.059251000
6	-1.831169000	-1.095384000	0.798735000
7	-2.188907000	0.163963000	1.242428000
7	-2.879233000	-1.525665000	-0.000450000
1	-6.833588000	0.700461000	-1.063869000
1	-1.570468000	0.682854000	1.849124000
1	-2.876801000	-2.421491000	-0.458581000
7	-0.759432000	-1.776690000	1.043063000
7	0.089526000	-1.047672000	1.880773000
6	1.187766000	-1.654833000	2.166404000
1	1.356081000	-2.653181000	1.745789000
6	2.257084000	-1.139224000	3.008614000
6	3.393094000	-1.981930000	3.191335000
6	2.263600000	0.103923000	3.645353000
6	4.459148000	-1.571484000	3.973657000
6	3.362171000	0.561390000	4.467972000
6	4.454981000	-0.318846000	4.607624000
1	-6.061655000	2.588445000	0.325868000
1	5.314770000	-2.229089000	4.100466000
8	1.257551000	1.014962000	3.571556000
1	1.639492000	1.732419000	4.144213000
1	3.405947000	-2.951858000	2.704961000
1	5.295450000	-0.005488000	5.220018000
8	3.231797000	1.735504000	4.995933000

5b_R1, optimization in gas phase B3LYP/6-311++G**, E= -909.781486437 a.u. Sum of electronic and thermal Enthalpies= -909.532916 a.u.			
0; 2			
6	-5.403346000	1.707813000	0.296372000
6	-4.185900000	1.685601000	0.952576000
6	-5.830165000	0.624472000	-0.506127000
1	-3.852199000	2.511266000	1.568922000
6	-3.373542000	0.547035000	0.801635000
6	-5.051131000	-0.513104000	-0.675033000
1	-5.386568000	-1.338524000	-1.291732000
6	-3.823406000	-0.537096000	-0.013399000
6	-1.824394000	-0.935155000	0.878255000
7	-2.147702000	0.278526000	1.335382000
7	-2.815300000	-1.461712000	0.056826000
1	-6.791851000	0.684829000	-1.002370000
1	-2.763267000	-2.366285000	-0.384656000
7	-0.727757000	-1.684470000	1.092083000
7	0.167618000	-1.098963000	1.888339000
6	1.249411000	-1.801857000	2.126012000
1	1.359689000	-2.792266000	1.680521000
6	2.288171000	-1.281746000	2.965506000
6	3.451135000	-2.049898000	3.217482000
6	2.176998000	0.001029000	3.557855000
6	4.456929000	-1.558328000	4.024869000
6	3.211434000	0.486533000	4.377633000
6	4.338663000	-0.286617000	4.607520000
1	-6.049933000	2.571890000	0.395061000
1	5.343806000	-2.150567000	4.214020000
8	1.123104000	0.822526000	3.393652000
1	0.457832000	0.377673000	2.801799000
1	3.535912000	-3.031198000	2.764654000
1	5.119780000	0.112596000	5.243436000
8	3.096741000	1.718655000	4.942274000
1	2.248524000	2.093819000	4.665596000

5b_R2, optimization in gas phase B3LYP/6-311++G**, E= -909.778308168 a.u. Sum of electronic and thermal Enthalpies= -909.529772 a.u.			
0; 2			
6	-5.470179000	1.651369000	0.339726000
6	-4.273049000	1.652945000	1.047787000
6	-5.806347000	0.612059000	-0.557851000
1	-4.025990000	2.455837000	1.732175000
6	-3.415810000	0.576523000	0.830872000
6	-4.956040000	-0.456989000	-0.773096000
1	-5.203498000	-1.258874000	-1.457672000
6	-3.737018000	-0.484509000	-0.069334000
6	-1.810319000	-0.967642000	0.755664000
7	-2.182298000	0.245050000	1.334855000
7	-2.745965000	-1.414366000	-0.096654000
1	-6.752120000	0.661019000	-1.084493000
1	-1.656681000	0.738798000	2.036340000
7	-0.679080000	-1.644895000	0.987667000
7	0.168353000	-1.028183000	1.830418000
6	1.235505000	-1.739103000	2.117957000
1	1.325101000	-2.737392000	1.688722000
6	2.280811000	-1.250051000	2.972672000
6	3.385432000	-2.079043000	3.279453000
6	2.241796000	0.053348000	3.517778000
6	4.399809000	-1.621910000	4.099316000
6	3.277333000	0.507316000	4.346783000
6	4.347915000	-0.327930000	4.635231000
1	-6.165868000	2.470824000	0.478940000
1	5.242026000	-2.261713000	4.332152000
8	1.232229000	0.923653000	3.276606000
1	0.593775000	0.460529000	2.677596000
1	3.420669000	-3.078685000	2.862103000
1	5.136150000	0.044564000	5.278439000
8	3.232309000	1.764634000	4.866042000
1	2.424628000	2.192891000	4.551479000

5b_R3, optimization in gas phase B3LYP/6-311++G**, E= -909.774701276 a.u. Sum of electronic and thermal Enthalpies= -909.525625 a.u.			
0; 2			
6	-5.302306000	1.762982000	0.345814000
6	-4.059177000	1.665755000	0.977391000
6	-5.793117000	0.729276000	-0.457420000
1	-3.679772000	2.467008000	1.599557000
6	-3.329643000	0.502651000	0.776914000
6	-5.059162000	-0.443065000	-0.660371000
1	-5.441050000	-1.243291000	-1.282920000
6	-3.825695000	-0.538964000	-0.033215000
6	-1.797268000	-1.160958000	0.760891000
7	-2.089103000	0.086224000	1.244037000
7	-2.858492000	-1.541792000	-0.019372000
1	-6.760579000	0.836091000	-0.932997000
1	-1.428597000	0.558697000	1.849293000
1	-2.888229000	-2.429754000	-0.493387000
7	-0.726802000	-1.892282000	0.973019000
7	0.114745000	-1.203871000	1.789434000
6	1.222150000	-1.804752000	2.092961000

5b_R4, optimization in gas phase B3LYP/6-311++G**, E= -909.769404503 a.u. Sum of electronic and thermal Enthalpies= -909.520474 a.u.			
0; 2			
6	-5.467783000	1.698372000	0.318768000
6	-4.236239000	1.669505000	0.982645000
6	-5.870866000	0.645754000	-0.505555000
1	-3.923683000	2.487124000	1.620928000
6	-3.434623000	0.555713000	0.790781000
6	-5.059816000	-0.477965000	-0.698057000
1	-5.375042000	-1.293603000	-1.337657000
6	-3.840642000	-0.505255000	-0.038559000
6	-1.790655000	-1.020131000	0.809240000
7	-2.176494000	0.212496000	1.288850000
7	-2.815816000	-1.447186000	-0.004975000
1	-6.829620000	0.697027000	-1.007269000
1	-1.626967000	0.738877000	1.946636000
1	-2.777164000	-2.328042000	-0.490679000
7	-0.716569000	-1.725045000	1.017032000
7	0.189089000	-1.093490000	1.834101000
6	1.237276000	-1.785369000	2.143235000

1	1.420815000	-2.803716000	1.693251000
6	2.222546000	-1.221439000	2.942604000
6	3.382519000	-1.959074000	3.215910000
6	2.096193000	0.111571000	3.543616000
6	4.401788000	-1.469584000	4.029840000
6	3.209817000	0.570030000	4.393409000
6	4.325042000	-0.199041000	4.626770000
1	-5.895814000	2.658827000	0.483070000
1	5.277372000	-2.083149000	4.208490000
8	1.139440000	0.903412000	3.409983000
1	3.483930000	-2.945511000	2.776420000
1	5.120567000	0.176805000	5.258480000
8	3.053524000	1.791388000	4.920521000
1	2.182721000	2.093313000	4.587813000

1	1.336636000	-2.805189000	1.767569000
6	2.298392000	-1.244304000	2.977669000
6	3.397299000	-2.046868000	3.316839000
6	2.256744000	0.085939000	3.457892000
6	4.448830000	-1.565221000	4.122270000
6	3.334565000	0.624548000	4.301367000
6	4.426024000	-0.279777000	4.601457000
1	-6.117776000	2.555128000	0.448572000
1	5.276861000	-2.223366000	4.359657000
8	1.250711000	0.897781000	3.168009000
1	0.625090000	0.377319000	2.592026000
1	3.430878000	-3.066093000	2.946876000
1	5.220537000	0.115208000	5.223409000
8	3.296085000	1.794650000	4.726414000

5b_R5, optimization in gas phase
B3LYP/6-311++G**, E= -909.769110037 a.u.
Sum of electronic and thermal Enthalpies= -909.519938 a.u.

0; 2			
6	-5.378670000	1.735545000	0.295770000
6	-4.137179000	1.667041000	0.938410000
6	-5.842294000	0.684975000	-0.498450000
1	-3.778974000	2.482954000	1.554472000
6	-3.384453000	0.517032000	0.757490000
6	-5.082501000	-0.476244000	-0.681293000
1	-5.444176000	-1.290593000	-1.297764000
6	-3.853360000	-0.542823000	-0.044149000
6	-1.814305000	-1.122712000	0.774328000
7	-2.138577000	0.128839000	1.240189000
7	-2.868374000	-1.527877000	-0.011639000
1	-6.807505000	0.766700000	-0.983622000
1	-1.500540000	0.626947000	1.843495000
1	-2.879512000	-2.420677000	-0.476172000
7	-0.744570000	-1.835538000	0.994955000
7	0.110963000	-1.142215000	1.817886000
6	1.202504000	-1.753741000	2.108200000
1	1.391402000	-2.753195000	1.705873000
6	2.236956000	-1.185991000	2.965586000
6	3.382616000	-1.950752000	3.226474000
6	2.189415000	0.087540000	3.567691000
6	4.449060000	-1.502978000	4.042407000
6	3.281279000	0.585520000	4.421096000
6	4.417420000	-0.267780000	4.633666000
1	-5.989138000	2.622032000	0.419028000
1	5.299279000	-2.158186000	4.193815000
8	1.180100000	0.938707000	3.425694000
1	1.454652000	1.717738000	3.962717000
1	3.449343000	-2.935972000	2.777914000
1	5.218711000	0.100455000	5.262015000
8	3.139411000	1.733050000	4.907357000

5b_R6, optimization in gas phase
B3LYP/6-311++G**, E= -909.737939855 a.u.
Sum of electronic and thermal Enthalpies= -909.488402 a.u.

0; 2			
6	-5.184205000	1.883449000	-0.083338000
6	-3.920306000	1.832391000	0.516793000
6	-5.803294000	0.728531000	-0.564095000
1	-3.441835000	2.729105000	0.891984000
6	-3.307853000	0.593562000	0.611774000
6	-5.183204000	-0.522506000	-0.466562000
1	-5.665495000	-1.417329000	-0.841293000
6	-3.930567000	-0.570478000	0.125032000
6	-1.906563000	-1.164791000	0.984593000
7	-2.080946000	0.194757000	1.147178000
7	-3.053953000	-1.623194000	0.373218000
1	-6.782590000	0.798069000	-1.022097000
1	-1.340079000	0.794691000	1.469637000
1	-3.185337000	-2.595642000	0.148898000
7	-0.913166000	-1.941371000	1.293573000
7	0.088730000	-1.265727000	1.967268000
6	1.247515000	-1.725565000	2.126924000
6	2.325892000	-1.197139000	2.926243000
6	3.619463000	-1.748058000	2.855636000
6	2.088937000	-0.130705000	3.818393000
6	4.639980000	-1.242006000	3.646317000
6	3.124200000	0.367059000	4.620190000
6	4.395138000	-0.186266000	4.529342000
1	-5.688348000	2.838025000	-0.173319000
1	5.634550000	-1.666945000	3.585787000
8	0.874111000	0.468134000	3.955568000
1	0.245408000	0.004815000	3.363280000
1	3.795370000	-2.571566000	2.174954000
1	5.181360000	0.217363000	5.156080000
8	2.886840000	1.395305000	5.484856000
1	1.951684000	1.630753000	5.423014000

5b_Rw1, optimization in solv. water
B3LYP/6-311++G**, E= -909.795418724 a.u.
Sum of electronic and thermal Enthalpies= -909.547255 a.u.

0; 2			
6	-5.406639000	1.708991000	0.293808000
6	-4.190291000	1.691775000	0.951643000
6	-5.831064000	0.621171000	-0.509126000

5b_Rw2, optimization in solv. water
B3LYP/6-311++G**, E= -909.794825209 a.u.
Sum of electronic and thermal Enthalpies= -909.546489 a.u.

0; 2			
6	-5.437236000	1.702575000	0.189840000
6	-4.222027000	1.745064000	0.863005000
6	-5.834997000	0.574449000	-0.568393000

1	-3.864238000	2.522417000	1.566013000	1	-3.924753000	2.610802000	1.441595000
6	-3.375450000	0.552557000	0.802029000	6	-3.408598000	0.617444000	0.756189000
6	-5.051035000	-0.514582000	-0.676325000	6	-5.028634000	-0.543895000	-0.675199000
1	-5.379622000	-1.343364000	-1.290962000	1	-5.328489000	-1.409333000	-1.253842000
6	-3.822709000	-0.534113000	-0.012285000	6	-3.790335000	-0.529991000	-0.003118000
6	-1.827279000	-0.936832000	0.875142000	6	-1.850615000	-0.966769000	0.830481000
7	-2.149287000	0.282466000	1.335165000	7	-2.176180000	0.306168000	1.271530000
7	-2.817907000	-1.457942000	0.057320000	7	-2.822587000	-1.485510000	0.054984000
1	-6.792459000	0.679912000	-1.005778000	1	-6.793626000	0.595322000	-1.073046000
1	-2.779056000	-2.361544000	-0.391778000	1	-1.597547000	0.896371000	1.847391000
7	-0.729458000	-1.682013000	1.091643000	7	-0.733935000	-1.657198000	1.098402000
7	0.168999000	-1.097135000	1.891025000	7	0.138851000	-1.026248000	1.905019000
6	1.250710000	-1.801091000	2.126261000	6	1.236747000	-1.713570000	2.126265000
1	1.365048000	-2.789939000	1.680739000	1	1.350515000	-2.688135000	1.651224000
6	2.290850000	-1.281070000	2.968105000	6	2.295470000	-1.233639000	2.969038000
6	3.452454000	-2.050266000	3.217770000	6	3.455055000	-2.025324000	3.149498000
6	2.179571000	0.000963000	3.561692000	6	2.214690000	0.013332000	3.631393000
6	4.459820000	-1.558654000	4.026125000	6	4.487670000	-1.584780000	3.955856000
6	3.212511000	0.485533000	4.380048000	6	3.269876000	0.448974000	4.446350000
6	4.341315000	-0.287811000	4.609453000	6	4.396949000	-0.345413000	4.605930000
1	-6.055726000	2.571351000	0.390126000	1	-6.101649000	2.556862000	0.246087000
1	5.346829000	-2.150531000	4.214654000	1	5.372986000	-2.193523000	4.090580000
8	1.116009000	0.814741000	3.389862000	8	1.149798000	0.840255000	3.527098000
1	0.466167000	0.346194000	2.793752000	1	0.494869000	0.407175000	2.927169000
1	3.536884000	-3.030845000	2.764187000	1	3.518654000	-2.981624000	2.643949000
1	5.125216000	0.107446000	5.244820000	1	5.200413000	0.010206000	5.240216000
8	3.102403000	1.721132000	4.949914000	8	3.188936000	1.653159000	5.083426000
1	2.256719000	2.107561000	4.679918000	1	2.343310000	2.066871000	4.858755000
5b_Rw3, optimization in solv. water B3LYP/6-311++G**, E= -909.791450658 a.u. Sum of electronic and thermal Enthalpies= -909.542779 a.u.				**5b_Rw4,** optimization in solv. water B3LYP/6-311++G**, E= -909.791243721 a.u. Sum of electronic and thermal Enthalpies= -909.542487 a.u.			
0; 2				0; 2			
6	-5.475261000	1.683472000	0.211939000	6	-5.384713000	1.778793000	0.125137000
6	-4.251953000	1.677508000	0.884723000	6	-4.142300000	1.772329000	0.768938000
6	-5.879782000	0.600119000	-0.581301000	6	-5.861042000	0.648088000	-0.547448000
1	-3.938632000	2.513371000	1.497394000	1	-3.772544000	2.646454000	1.290503000
6	-3.452813000	0.550937000	0.734684000	6	-3.404090000	0.599362000	0.710909000
6	-5.076768000	-0.531544000	-0.732320000	6	-5.113928000	-0.533233000	-0.604981000
1	-5.386789000	-1.368961000	-1.344565000	1	-5.480685000	-1.408642000	-1.126358000
6	-3.859858000	-0.536853000	-0.061863000	6	-3.881605000	-0.536371000	0.033284000
6	-1.833912000	-1.019636000	0.807156000	6	-1.843275000	-1.038701000	0.895870000
7	-2.205634000	0.215658000	1.250271000	7	-2.156709000	0.254148000	1.232594000
7	-2.840107000	-1.478903000	0.008306000	7	-2.903190000	-1.516208000	0.167287000
1	-6.835980000	0.640480000	-1.088879000	1	-6.827787000	0.685157000	-1.035255000
1	-1.615812000	0.761858000	1.861225000	1	-1.532489000	0.868263000	1.728751000
1	-2.815885000	-2.378859000	-0.447824000	1	-2.936499000	-2.455845000	-0.196846000
7	-0.729735000	-1.705574000	1.058483000	7	-0.783288000	-1.765656000	1.152654000
7	0.098080000	-1.014766000	1.875766000	7	0.143061000	-1.128421000	1.935622000
6	1.205679000	-1.647596000	2.161510000	6	1.250539000	-1.771940000	2.124495000
1	1.358410000	-2.641989000	1.733140000	1	1.402107000	-2.743650000	1.652896000
6	2.253589000	-1.152084000	2.997579000	6	2.313201000	-1.240139000	2.964037000
6	3.374976000	-1.985052000	3.200106000	6	3.511900000	-1.947609000	3.109756000
6	2.241976000	0.157841000	3.654991000	6	2.166595000	-0.015618000	3.657503000
6	4.445572000	-1.602555000	3.991448000	6	4.566200000	-1.469733000	3.920731000
6	3.409467000	0.501559000	4.479212000	6	3.239574000	0.509620000	4.511347000
6	4.471994000	-0.348055000	4.641398000	6	4.444052000	-0.285823000	4.599597000

1	-6.125033000	2.545186000	0.306077000	1	-5.987507000	2.678709000	0.150287000
1	5.283995000	-2.277282000	4.117717000	1	5.475502000	-2.053716000	3.999125000
8	1.332730000	1.017100000	3.583059000	8	1.056532000	0.705004000	3.569702000
1	3.390735000	-2.955709000	2.717148000	1	0.436759000	0.210303000	2.956704000
1	5.314336000	-0.057704000	5.257975000	1	3.630962000	-2.887541000	2.582795000
8	3.358111000	1.715392000	5.064503000	1	5.241111000	0.097072000	5.225964000
1	2.502670000	2.096425000	4.780747000	8	3.098820000	1.594084000	5.123889000
5b_Rw5, optimization in solv. water B3LYP/6-311++G**, E= -909.785800626 a.u. Sum of electronic and thermal Enthalpies= -909.536909 a.u.				**5b_Rw6,** optimization in solv. water B3LYP/6-311++G**, E= -909.754659096 a.u. Sum of electronic and thermal Enthalpies= -909.505553 a.u.			
0; 2				0; 2			
6	-5.433425000	1.713920000	0.248551000	6	-5.201145000	1.875716000	-0.098331000
6	-4.197211000	1.675221000	0.903994000	6	-3.925945000	1.840019000	0.477501000
6	-5.872084000	0.644617000	-0.539370000	6	-5.827937000	0.708897000	-0.548133000
1	-3.856714000	2.502687000	1.514140000	1	-3.439228000	2.741913000	0.827501000
6	-3.425541000	0.533786000	0.740958000	6	-3.310672000	0.601495000	0.581117000
6	-5.092166000	-0.505858000	-0.703498000	6	-5.204541000	-0.539395000	-0.442463000
1	-5.430525000	-1.334248000	-1.313580000	1	-5.688478000	-1.443322000	-0.790915000
6	-3.867399000	-0.542018000	-0.052527000	6	-3.939544000	-0.571246000	0.126906000
6	-1.831140000	-1.077683000	0.788608000	6	-1.908606000	-1.142691000	0.962586000
7	-2.176869000	0.170507000	1.239638000	7	-2.072446000	0.213625000	1.095983000
7	-2.866741000	-1.509117000	-0.000772000	7	-3.055512000	-1.617051000	0.377366000
1	-6.834167000	0.704897000	-1.034130000	1	-6.816377000	0.769288000	-0.987789000
1	-1.568637000	0.701767000	1.844121000	1	-1.344276000	0.828382000	1.422870000
1	-2.871514000	-2.406363000	-0.460468000	1	-3.206249000	-2.594415000	0.180551000
7	-0.747745000	-1.778774000	1.023033000	7	-0.904082000	-1.921154000	1.280167000
7	0.108404000	-1.086114000	1.847515000	7	0.103997000	-1.244766000	1.935264000
6	1.201226000	-1.704144000	2.131044000	6	1.257850000	-1.707137000	2.115500000
1	1.383406000	-2.701440000	1.720878000	6	2.333209000	-1.185907000	2.925845000
6	2.253753000	-1.164241000	2.986021000	6	3.626635000	-1.739124000	2.849381000
6	3.386269000	-1.958203000	3.217677000	6	2.096695000	-0.134398000	3.836844000
6	2.239788000	0.099043000	3.610290000	6	4.648439000	-1.252525000	3.651925000
6	4.472555000	-1.545747000	4.027394000	6	3.134634000	0.344768000	4.647871000
6	3.352022000	0.559109000	4.456647000	6	4.404764000	-0.210908000	4.552801000
6	4.472501000	-0.320582000	4.639269000	1	-5.710220000	2.827213000	-0.195075000
1	-6.060543000	2.590965000	0.355901000	1	5.641521000	-1.679845000	3.585733000
1	5.310545000	-2.220385000	4.156064000	8	0.886497000	0.466182000	3.985781000
8	1.238133000	0.963148000	3.487501000	1	0.258289000	0.056325000	3.356815000
1	1.507282000	1.740158000	4.025207000	1	3.804629000	-2.550676000	2.154631000
1	3.428933000	-2.936668000	2.752885000	1	5.193818000	0.177576000	5.185923000
1	5.291866000	0.016038000	5.262374000	8	2.901559000	1.361919000	5.531583000
8	3.244721000	1.703520000	4.968079000	1	1.974159000	1.627964000	5.460090000
5b_Rb1, optimization in solv. benzene B3LYP/6-311++G**, E= -909.787317884 a.u. Sum of electronic and thermal Enthalpies= -909.538929 a.u.				**5b_Rb2,** optimization in solv. benzene B3LYP/6-311++G**, E= -909.785102496 a.u. Sum of electronic and thermal Enthalpies= -909.536612 a.u.			
0; 2				0; 2			
6	-5.404880000	1.708574000	0.293563000	6	-5.473884000	1.672516000	0.332578000
6	-4.188978000	1.687679000	0.952359000	6	-4.274804000	1.676977000	1.036534000
6	-5.829621000	0.624062000	-0.510492000	6	-5.818571000	0.622828000	-0.551196000
1	-3.858979000	2.514907000	1.568788000	1	-4.019054000	2.485553000	1.710664000
6	-3.375740000	0.548538000	0.802692000	6	-3.424075000	0.592700000	0.829839000
6	-5.050374000	-0.513121000	-0.677972000	6	-4.974898000	-0.453455000	-0.756299000
1	-5.382849000	-1.338814000	-1.295352000	1	-5.231378000	-1.261382000	-1.430535000
6	-3.823730000	-0.536404000	-0.012914000	6	-3.753123000	-0.477727000	-0.056127000
6	-1.827561000	-0.936824000	0.879974000	6	-1.823633000	-0.954253000	0.771751000
7	-2.150524000	0.279306000	1.337593000	7	-2.191550000	0.262862000	1.335670000

7	-2.817353000	-1.461204000	0.058728000	7	-2.763527000	-1.410620000	-0.074071000
1	-6.790189000	0.684344000	-1.008821000	1	-6.765953000	0.670007000	-1.075048000
1	-2.770219000	-2.365488000	-0.385773000	1	-1.660667000	0.773054000	2.021807000
7	-0.730406000	-1.684379000	1.095689000	7	-0.694031000	-1.635045000	1.003614000
7	0.166328000	-1.098964000	1.893126000	7	0.160723000	-1.023150000	1.843424000
6	1.248656000	-1.801730000	2.128474000	6	1.233701000	-1.733410000	2.110009000
1	1.360752000	-2.791254000	1.682478000	1	1.326797000	-2.724779000	1.666212000
6	2.288932000	-1.281651000	2.967797000	6	2.286072000	-1.253808000	2.961366000
6	3.452173000	-2.049693000	3.216675000	6	3.400351000	-2.082473000	3.233007000
6	2.178116000	0.000622000	3.561004000	6	2.245496000	0.036677000	3.537021000
6	4.459905000	-1.557740000	4.022622000	6	4.424204000	-1.637322000	4.047938000
6	3.213409000	0.486123000	4.378264000	6	3.290864000	0.477941000	4.360538000
6	4.342072000	-0.286451000	4.605889000	6	4.371530000	-0.355849000	4.613748000
1	-6.052276000	2.572179000	0.390794000	1	-6.165200000	2.496955000	0.463432000
1	5.347505000	-2.149435000	4.209669000	1	5.274044000	-2.276182000	4.253744000
8	1.119912000	0.818529000	3.395977000	8	1.226162000	0.904348000	3.332643000
1	0.459428000	0.364938000	2.803345000	1	0.577955000	0.452857000	2.736294000
1	3.536673000	-3.030612000	2.763205000	1	3.435581000	-3.071827000	2.792073000
1	5.125355000	0.111408000	5.240163000	1	5.167769000	0.005838000	5.253413000
8	3.100811000	1.719829000	4.945064000	8	3.246217000	1.723903000	4.910884000
1	2.252938000	2.099204000	4.672351000	1	2.430460000	2.156346000	4.622750000
5b_Rb3, optimization in solv. benzene B3LYP/6-311++G**, E= -909.781724622 a.u. Sum of electronic and thermal Enthalpies= -909.532813 a.u.				**5b_Rb4,** optimization in solv. benzene B3LYP/6-311++G**, E= -909.778814986 a.u. Sum of electronic and thermal Enthalpies= -909.529935 a.u.			
0; 2				0; 2			
6	-5.361100000	1.738343000	0.299471000	6	-5.380028000	1.778091000	0.146795000
6	-4.123657000	1.671292000	0.944855000	6	-4.138834000	1.761591000	0.792564000
6	-5.824287000	0.687017000	-0.500030000	6	-5.854022000	0.658462000	-0.542493000
1	-3.765096000	2.484727000	1.563348000	1	-3.771699000	2.628648000	1.328135000
6	-3.371730000	0.518962000	0.761637000	6	-3.399712000	0.591125000	0.719484000
6	-5.067791000	-0.473083000	-0.685006000	6	-5.105987000	-0.521501000	-0.614868000
1	-5.426434000	-1.286465000	-1.303814000	1	-5.473990000	-1.388138000	-1.150345000
6	-3.839136000	-0.539210000	-0.042826000	6	-3.875721000	-0.535390000	0.025454000
6	-1.811232000	-1.115487000	0.776716000	6	-1.835943000	-1.051535000	0.887694000
7	-2.128291000	0.128785000	1.245229000	7	-2.152984000	0.239488000	1.239610000
7	-2.854571000	-1.523193000	-0.009184000	7	-2.897107000	-1.517714000	0.148712000
1	-6.788494000	0.771926000	-0.986537000	1	-6.819555000	0.702048000	-1.031922000
1	-1.490279000	0.627778000	1.851230000	1	-1.526829000	0.842646000	1.745932000
1	-2.869071000	-2.416757000	-0.475431000	1	-2.924601000	-2.454102000	-0.221862000
7	-0.728500000	-1.831990000	1.002995000	7	-0.780832000	-1.778252000	1.140155000
7	0.108030000	-1.142275000	1.819619000	7	0.141633000	-1.136818000	1.927213000
6	1.216911000	-1.752480000	2.115243000	6	1.246535000	-1.779365000	2.128889000
1	1.402014000	-2.749259000	1.704247000	1	1.395110000	-2.755969000	1.665801000
6	2.234033000	-1.198546000	2.960583000	6	2.306697000	-1.240839000	2.967021000
6	3.382777000	-1.967993000	3.209034000	6	3.502819000	-1.953039000	3.125533000
6	2.145380000	0.127257000	3.582347000	6	2.161268000	-0.006090000	3.642423000
6	4.419993000	-1.514083000	4.016288000	6	4.555639000	-1.469728000	3.931258000
6	3.277983000	0.547556000	4.424505000	6	3.235774000	0.529419000	4.490394000
6	4.376911000	-0.248513000	4.633042000	6	4.435843000	-0.274178000	4.591955000
1	-5.973166000	2.623773000	0.422004000	1	-5.982868000	2.677384000	0.184404000
1	5.284359000	-2.148011000	4.176628000	1	5.462655000	-2.056104000	4.021739000
8	1.202979000	0.941087000	3.469310000	8	1.053267000	0.714515000	3.540920000
1	3.456074000	-2.949420000	2.753386000	1	0.436875000	0.206985000	2.939523000
1	5.188929000	0.098484000	5.260495000	1	3.617143000	-2.900632000	2.610517000
8	3.155769000	1.767223000	4.973023000	1	5.231007000	0.117238000	5.215378000
1	2.289060000	2.096341000	4.657396000	8	3.103712000	1.620294000	5.083476000

5b_Rb5, optimization in solv. benzene
B3LYP/6-311++G**, E= -909.776242240 a.u.
Sum of electronic and thermal Enthalpies= -909.527166 a.u.

0; 2

6	-5.400329000	1.728125000	0.272328000
6	-4.161700000	1.671596000	0.921641000
6	-5.853735000	0.669186000	-0.518551000
1	-3.810465000	2.492762000	1.534539000
6	-3.402113000	0.524159000	0.750348000
6	-5.086540000	-0.488618000	-0.691222000
1	-5.438685000	-1.309127000	-1.304626000
6	-3.860095000	-0.543197000	-0.046539000
6	-1.823303000	-1.105139000	0.783746000
7	-2.155657000	0.145992000	1.241102000
7	-2.869670000	-1.521839000	-0.003357000
1	-6.816996000	0.742388000	-1.009068000
1	-1.529831000	0.659072000	1.843960000
1	-2.879236000	-2.417714000	-0.463710000
7	-0.748106000	-1.813439000	1.011310000
7	0.107901000	-1.120173000	1.834053000
6	1.201158000	-1.733454000	2.119204000
1	1.388012000	-2.731409000	1.712416000
6	2.244010000	-1.177101000	2.974411000
6	3.386020000	-1.952501000	3.219486000
6	2.209660000	0.091255000	3.588214000
6	4.461701000	-1.519019000	4.031719000
6	3.310829000	0.573752000	4.437708000
6	4.442441000	-0.289149000	4.634133000
1	-6.017040000	2.611467000	0.387270000
1	5.308338000	-2.181251000	4.170838000
8	1.201706000	0.946182000	3.457468000
1	1.473243000	1.723790000	3.995733000
1	3.443427000	-2.933990000	2.762022000
1	5.251784000	0.066174000	5.259740000
8	3.182254000	1.719016000	4.937128000

5b_RC, optimization in gas phase
B3LYP/6-311++G**, E= -910.166588693 a.u.
Sum of electronic and thermal Enthalpies= -909.903926 a.u.

1; 2

6	-5.539693000	1.647133000	0.186612000
6	-4.341068000	1.700817000	0.885186000
6	-5.886263000	0.537203000	-0.612008000
1	-4.079517000	2.554879000	1.496881000
6	-3.495828000	0.601755000	0.758212000
6	-5.047272000	-0.559873000	-0.741042000
1	-5.315319000	-1.410849000	-1.354188000
6	-3.842878000	-0.510229000	-0.041054000
6	-1.824361000	-0.902431000	0.875576000
7	-2.249587000	0.319040000	1.301031000
7	-2.792500000	-1.403714000	0.061326000
1	-6.833028000	0.543536000	-1.137411000
1	-1.716673000	0.906689000	1.924279000
1	-2.708076000	-2.308060000	-0.383382000
7	-0.712935000	-1.586412000	1.129376000
7	0.151466000	-0.967363000	1.935971000
6	1.239888000	-1.688369000	2.176625000

5b_RCw, optimization in solv. water
B3LYP/6-311++G**, E= -910.238314307 a.u.
Sum of electronic and thermal Enthalpies= -909.975753 a.u.

1; 2

6	-5.537476000	1.643010000	0.190830000
6	-4.342216000	1.700401000	0.891290000
6	-5.881057000	0.530908000	-0.612442000
1	-4.079187000	2.550564000	1.506339000
6	-3.492438000	0.602364000	0.763363000
6	-5.041534000	-0.563321000	-0.742802000
1	-5.300843000	-1.416127000	-1.355934000
6	-3.836835000	-0.511315000	-0.039505000
6	-1.827447000	-0.892830000	0.877386000
7	-2.253289000	0.325503000	1.304809000
7	-2.791200000	-1.397987000	0.061673000
1	-6.827255000	0.537283000	-1.138873000
1	-1.731757000	0.922975000	1.930308000
1	-2.712772000	-2.300627000	-0.389597000
7	-0.714038000	-1.578681000	1.129291000
7	0.155190000	-0.964928000	1.937039000
6	1.234519000	-1.690518000	2.173058000

1	1.312807000	-2.673745000	1.717332000
6	2.299519000	-1.235078000	2.998382000
6	3.424099000	-2.085048000	3.205951000
6	2.280868000	0.046615000	3.626497000
6	4.465385000	-1.670294000	3.999372000
6	3.353828000	0.454394000	4.433231000
6	4.431473000	-0.401987000	4.612890000
1	-6.228645000	2.479688000	0.255724000
1	5.321335000	-2.312780000	4.160788000
8	1.265324000	0.916816000	3.488474000
1	0.591200000	0.504415000	2.904154000
1	3.439946000	-3.057597000	2.729471000
1	5.249963000	-0.068438000	5.239842000
8	3.352624000	1.664169000	5.035201000
1	2.540670000	2.140369000	4.816259000

1	1.309511000	-2.676307000	1.715610000
6	2.299947000	-1.235524000	3.000087000
6	3.419924000	-2.083992000	3.210713000
6	2.281757000	0.042230000	3.621769000
6	4.466810000	-1.671282000	4.004382000
6	3.358764000	0.447247000	4.426409000
6	4.437365000	-0.403730000	4.613193000
1	-6.229548000	2.473021000	0.259426000
1	5.319746000	-2.317909000	4.165803000
8	1.271517000	0.919469000	3.487294000
1	0.585886000	0.515557000	2.906650000
1	3.432485000	-3.057873000	2.737064000
1	5.257984000	-0.072109000	5.238354000
8	3.347207000	1.670837000	5.022663000
1	2.527034000	2.128943000	4.789907000

5b_RCb, optimization in solv. benzene
B3LYP/6-311++G**, E= -910.205028066 a.u.
Sum of electronic and thermal Enthalpies= -909.942316 a.u.

5b_M, optimization in gas phase
B3LYP/6-311++G**, E= -910.413957329 a.u.
Sum of electronic and thermal Enthalpies= -910.151871 a.u.

1; 2			
6	-5.536177000	1.647609000	0.183874000
6	-4.338413000	1.704063000	0.882148000
6	-5.883182000	0.534250000	-0.612404000
1	-4.074754000	2.558021000	1.492671000
6	-3.493236000	0.604004000	0.758450000
6	-5.045904000	-0.563559000	-0.738013000
1	-5.311591000	-1.416104000	-1.349478000
6	-3.841515000	-0.512023000	-0.036558000
6	-1.826159000	-0.897256000	0.879287000
7	-2.249514000	0.325619000	1.300275000
7	-2.794335000	-1.403086000	0.068815000
1	-6.829533000	0.540129000	-1.138402000
1	-1.719869000	0.925804000	1.915108000
1	-2.716251000	-2.310890000	-0.370636000
7	-0.714485000	-1.583370000	1.132342000
7	0.154323000	-0.966192000	1.935914000
6	1.239454000	-1.689235000	2.172943000
1	1.313091000	-2.674520000	1.713787000
6	2.301658000	-1.234950000	2.996070000
6	3.426364000	-2.082178000	3.202279000
6	2.280366000	0.042881000	3.625416000
6	4.469020000	-1.667974000	3.996751000
6	3.352929000	0.448933000	4.433820000
6	4.433385000	-0.402691000	4.613152000
1	-6.225276000	2.480256000	0.249948000
1	5.325367000	-2.310450000	4.155852000
8	1.264208000	0.913638000	3.490586000
1	0.587016000	0.501950000	2.907209000
1	3.443312000	-3.053920000	2.724450000
1	5.251547000	-0.070360000	5.240985000
8	3.342434000	1.661845000	5.039095000
1	2.522470000	2.125010000	4.819820000

0; 1			
6	-5.346038000	1.797055000	0.100833000
6	-4.104231000	1.775604000	0.746972000
6	-5.839585000	0.667868000	-0.554762000
1	-3.723075000	2.652036000	1.257241000
6	-3.384164000	0.592600000	0.708644000
6	-5.110674000	-0.526475000	-0.592896000
1	-5.495443000	-1.401162000	-1.103466000
6	-3.880288000	-0.545182000	0.045398000
6	-1.842940000	-1.073246000	0.919455000
7	-2.144726000	0.234575000	1.240461000
7	-2.918681000	-1.540272000	0.193369000
1	-6.804622000	0.713387000	-1.044944000
1	-1.492534000	0.838774000	1.710597000
1	-2.956826000	-2.484823000	-0.152117000
7	-0.800361000	-1.799112000	1.185795000
7	0.125003000	-1.143417000	1.969177000
6	1.244980000	-1.769824000	2.133504000
1	1.395317000	-2.731471000	1.639728000
6	2.315990000	-1.244267000	2.961400000
6	3.537305000	-1.939090000	3.064560000
6	2.161893000	-0.046207000	3.684180000
6	4.564191000	-1.449170000	3.856959000
6	3.202149000	0.440947000	4.486729000
6	4.399603000	-0.257536000	4.570087000
1	-5.932234000	2.707964000	0.112686000
1	5.500465000	-1.989431000	3.928436000
8	1.018864000	0.690524000	3.653914000
1	0.388389000	0.201469000	3.065752000
1	3.662773000	-2.863780000	2.512398000
1	5.190535000	0.139100000	5.195301000
8	3.034229000	1.601100000	5.184099000
1	2.141489000	1.926714000	5.006067000

5b_Mw, optimization in solv. water
B3LYP/6-311++G**, E= -910.429583289 a.u.
Sum of electronic and thermal Enthalpies= -910.168057 a.u.

5b_Mb, optimization in solv. benzene
B3LYP/6-311++G**, E= -910.420675694 a.u.
Sum of electronic and thermal Enthalpies= -910.158797 a.u.

0; 1			
6	-5.401320000	1.762395000	0.157402000

0; 1			
6	-5.366042000	1.785105000	0.127356000

6	-4.162385000	1.752362000	0.808982000	6	-4.125067000	1.766917000	0.774935000
6	-5.860411000	0.644798000	-0.547350000	6	-5.846783000	0.661006000	-0.548755000
1	-3.805868000	2.616700000	1.355575000	1	-3.752678000	2.637988000	1.300475000
6	-3.410456000	0.589861000	0.725982000	6	-3.393201000	0.591283000	0.716976000
6	-5.099309000	-0.526718000	-0.629924000	6	-5.105852000	-0.524960000	-0.606246000
1	-5.453274000	-1.392299000	-1.176079000	1	-5.479122000	-1.395262000	-1.132161000
6	-3.871392000	-0.533692000	0.016376000	6	-3.876199000	-0.540376000	0.034838000
6	-1.832914000	-1.037694000	0.882562000	6	-1.837958000	-1.060339000	0.903231000
7	-2.163344000	0.245045000	1.247518000	7	-2.150297000	0.237468000	1.243211000
7	-2.884456000	-1.506978000	0.132951000	7	-2.904654000	-1.527511000	0.168611000
1	-6.824280000	0.683541000	-1.040769000	1	-6.811493000	0.704888000	-1.039870000
1	-1.550486000	0.848981000	1.769318000	1	-1.513353000	0.843097000	1.732494000
1	-2.906115000	-2.436927000	-0.255636000	1	-2.938695000	-2.467321000	-0.192188000
7	-0.769685000	-1.756941000	1.134293000	7	-0.786694000	-1.784442000	1.162112000
7	0.148442000	-1.115775000	1.932583000	7	0.136448000	-1.135671000	1.951107000
6	1.250345000	-1.765584000	2.133220000	6	1.249046000	-1.771785000	2.131466000
1	1.394004000	-2.740202000	1.663482000	1	1.397362000	-2.739255000	1.648823000
6	2.318852000	-1.249796000	2.973148000	6	2.317913000	-1.248561000	2.964994000
6	3.510553000	-1.985776000	3.130410000	6	3.528319000	-1.958427000	3.092662000
6	2.194274000	-0.021519000	3.650681000	6	2.172854000	-0.037336000	3.667853000
6	4.537787000	-1.508691000	3.932421000	6	4.553441000	-1.471246000	3.890070000
6	3.235498000	0.452940000	4.459799000	6	3.211404000	0.447162000	4.474038000
6	4.403505000	-0.286379000	4.599946000	6	4.398153000	-0.266283000	4.583153000
1	-6.014117000	2.654796000	0.202306000	1	-5.962343000	2.689212000	0.153577000
1	5.450165000	-2.081693000	4.045556000	1	5.481024000	-2.023537000	3.980493000
8	1.082799000	0.756725000	3.565749000	8	1.040527000	0.713983000	3.611825000
1	0.450046000	0.285173000	2.964716000	1	0.412407000	0.228457000	3.016272000
1	3.613847000	-2.932836000	2.612896000	1	3.647361000	-2.892744000	2.555574000
1	5.197148000	0.098747000	5.229446000	1	5.188839000	0.127346000	5.210800000
8	3.098831000	1.647524000	5.113016000	8	3.052821000	1.622607000	5.151942000
1	2.230466000	2.015162000	4.894981000	1	2.169263000	1.963790000	4.955890000

5c_A1, optimization in gas phase B3LYP/6-311++G**, E= -909.872968103 a.u. Sum of electronic and thermal Enthalpies= -909.626280 a.u.			
-1; 1			
6	-5.399096000	1.743810000	0.239687000
6	-4.157537000	1.713037000	0.884025000
6	-5.860396000	0.656494000	-0.512489000
1	-3.804591000	2.557597000	1.465728000
6	-3.363559000	0.566505000	0.770618000
6	-5.083417000	-0.505492000	-0.641974000
1	-5.438744000	-1.350406000	-1.224224000
6	-3.853314000	-0.530371000	-0.000635000
6	-1.825546000	-0.948808000	0.883574000
7	-2.126172000	0.287960000	1.298993000
7	-2.853795000	-1.475135000	0.091141000
1	-6.827710000	0.709466000	-1.001335000
1	-2.819635000	-2.393347000	-0.318000000
7	-0.760315000	-1.737756000	1.086260000
7	0.185697000	-1.167098000	1.849819000
6	1.256015000	-1.855061000	2.111930000
1	1.368541000	-2.869233000	1.716822000
6	2.317523000	-1.296230000	2.929334000
6	3.475933000	-2.033455000	3.220224000
6	2.226671000	0.020271000	3.468389000
6	4.514411000	-1.531215000	4.000280000
6	3.268470000	0.527444000	4.252224000
6	4.399280000	-0.241498000	4.514249000
1	-6.019750000	2.630799000	0.324414000
1	5.399856000	-2.117993000	4.212541000
1	3.167891000	1.534452000	4.647437000
8	1.159452000	0.801632000	3.246431000
1	0.513156000	0.282488000	2.671833000
8	5.440139000	0.243534000	5.287851000
1	5.218047000	1.137406000	5.565977000
1	3.558210000	-3.038524000	2.816615000

5c_A2, optimization in gas phase B3LYP/6-311++G**, E= -909.872506677 a.u. Sum of electronic and thermal Enthalpies= -909.625657 a.u.			
-1; 1			
6	-5.356999000	1.749671000	0.423432000
6	-4.121829000	1.658973000	1.083047000
6	-5.782057000	0.732430000	-0.441432000
1	-3.787928000	2.446428000	1.751617000
6	-3.350058000	0.530633000	0.847058000
6	-4.999182000	-0.401786000	-0.675761000
1	-5.332760000	-1.187192000	-1.345410000
6	-3.763519000	-0.516939000	-0.026882000
6	-1.832737000	-1.129471000	0.733822000
7	-2.115111000	0.120328000	1.307799000
7	-2.824494000	-1.514677000	-0.079001000
1	-6.741716000	0.828398000	-0.940500000
1	-1.547471000	0.568224000	2.005736000
7	-0.725484000	-1.853638000	0.970627000
7	0.161823000	-1.227135000	1.760391000
6	1.228698000	-1.894241000	2.113904000
1	1.344388000	-2.927436000	1.780186000
6	2.270404000	-1.300453000	2.929526000
6	3.386344000	-2.048283000	3.342389000
6	2.218562000	0.060625000	3.341346000
6	4.405893000	-1.510073000	4.122431000
6	3.237101000	0.607626000	4.122738000
6	4.322734000	-0.175084000	4.511527000
1	-5.986796000	2.618152000	0.585867000
1	5.256221000	-2.105999000	4.430974000
1	3.160005000	1.650980000	4.415338000
8	1.183255000	0.847268000	2.979237000
1	0.583468000	0.261285000	2.423045000
8	5.345778000	0.339183000	5.288444000
1	5.153280000	1.263741000	5.472145000
1	3.448021000	-3.088565000	3.037602000

5c_A3, optimization in gas phase B3LYP/6-311++G**, E= -909.850765436 a.u. Sum of electronic and thermal Enthalpies= -909.603832 a.u.			
-1; 1			
6	-5.299910000	1.757083000	0.320819000
6	-4.038535000	1.650187000	0.929773000
6	-5.825843000	0.714487000	-0.438287000
1	-3.630154000	2.461374000	1.520602000
6	-3.326830000	0.472649000	0.754384000
6	-5.108371000	-0.480866000	-0.619337000
1	-5.518025000	-1.292654000	-1.210356000
6	-3.864272000	-0.587943000	-0.019321000
6	-1.815735000	-1.228365000	0.758714000
7	-2.092418000	0.055668000	1.207220000
7	-2.922542000	-1.606727000	-0.001074000
1	-6.801982000	0.821339000	-0.898153000
1	-1.395007000	0.514424000	1.787617000
1	-2.989160000	-2.507197000	-0.441907000
7	-0.764465000	-1.934133000	0.988412000
7	0.089580000	-1.165861000	1.794890000
6	1.196407000	-1.737810000	2.128134000

5c_A4, optimization in gas phase B3LYP/6-311++G**, E= -909.867831555 a.u. Sum of electronic and thermal Enthalpies= -909.620120 a.u.			
-1; 1			
6	-5.503887000	1.680917000	0.244271000
6	-4.255427000	1.675856000	0.890249000
6	-5.919671000	0.597121000	-0.523843000
1	-3.932048000	2.520375000	1.487495000
6	-3.450692000	0.558191000	0.740813000
6	-5.105320000	-0.538163000	-0.676940000
1	-5.432065000	-1.381914000	-1.274218000
6	-3.874565000	-0.544824000	-0.039419000
6	-1.801135000	-1.026939000	0.807984000
7	-2.193359000	0.243163000	1.230123000
7	-2.859477000	-1.484454000	0.015326000
1	-6.886629000	0.623856000	-1.013399000
1	-1.616470000	0.779752000	1.856345000
1	-2.839051000	-2.387165000	-0.425804000
7	-0.732139000	-1.687622000	1.051849000
7	0.165471000	-0.992259000	1.861731000
6	1.238637000	-1.684045000	2.173537000

1	1.388005000	-2.758143000	1.766347000
6	2.222182000	-1.147002000	2.949608000
6	3.361000000	-1.932902000	3.209003000
6	2.130348000	0.208592000	3.517577000
6	4.432074000	-1.511902000	3.981451000
6	3.276075000	0.600906000	4.315884000
6	4.360308000	-0.218700000	4.530776000
1	-5.871244000	2.670072000	0.446925000
1	5.296541000	-2.137215000	4.166228000
1	3.240034000	1.598618000	4.749736000
8	1.161081000	0.989110000	3.349135000
8	5.440499000	0.192858000	5.303552000
1	5.250876000	1.086616000	5.606423000
1	3.394832000	-2.930469000	2.774486000

1	1.312107000	-2.706951000	1.792384000
6	2.308447000	-1.205320000	2.968035000
6	3.416389000	-2.052998000	3.264872000
6	2.355162000	0.123137000	3.514543000
6	4.473579000	-1.647424000	4.029697000
6	3.409789000	0.546717000	4.285697000
6	4.537898000	-0.305015000	4.597324000
1	-6.149306000	2.545573000	0.348805000
1	5.304356000	-2.312554000	4.242309000
1	3.410347000	1.556899000	4.680173000
8	1.324951000	0.986175000	3.257865000
1	0.683535000	0.498446000	2.692688000
8	5.504872000	0.076151000	5.302600000
1	3.399849000	-3.062574000	2.857782000

5c_Aw1, optimization in solv.water
B3LYP/6-311++G**, E= -909.954329994 a.u.
Sum of electronic and thermal Enthalpies= -909.707281 a.u.

5c_Aw2, optimization in solv.water
B3LYP/6-311++G**, E= -909.953852394 a.u.
Sum of electronic and thermal Enthalpies=-909.706366 a.u.

-1; 1			
6	-5.367678000	1.761083000	0.269552000
6	-4.122858000	1.709720000	0.907666000
6	-5.842367000	0.684274000	-0.491384000
1	-3.763361000	2.548110000	1.495090000
6	-3.347310000	0.553321000	0.774912000
6	-5.081798000	-0.484799000	-0.638108000
1	-5.446778000	-1.319959000	-1.225777000
6	-3.848323000	-0.527990000	-0.001362000
6	-1.825033000	-0.993331000	0.861988000
7	-2.103383000	0.247745000	1.295769000
7	-2.860653000	-1.491159000	0.073017000
1	-6.810734000	0.752915000	-0.974354000
1	-2.861972000	-2.403712000	-0.354519000
7	-0.759179000	-1.785710000	1.064161000
7	0.188429000	-1.205095000	1.836297000
6	1.263297000	-1.880407000	2.109601000
1	1.394563000	-2.895799000	1.725991000
6	2.315590000	-1.302904000	2.929219000
6	3.479864000	-2.030544000	3.229964000
6	2.211260000	0.013657000	3.455424000
6	4.503291000	-1.506247000	4.009135000
6	3.235917000	0.548120000	4.239231000
6	4.373981000	-0.208917000	4.513374000
1	-5.977900000	2.652835000	0.366224000
1	5.393154000	-2.082697000	4.230289000
1	3.129951000	1.556016000	4.626987000
8	1.121057000	0.775547000	3.209465000
1	0.503350000	0.219495000	2.635069000
8	5.403172000	0.278752000	5.279429000
1	5.200918000	1.176698000	5.568000000
1	3.577250000	-3.037744000	2.837386000

-1; 1			
6	-5.399699000	1.731946000	0.375760000
6	-4.165167000	1.666210000	1.038291000
6	-5.817852000	0.695173000	-0.469887000
1	-3.837727000	2.466987000	1.692307000
6	-3.385053000	0.538459000	0.822979000
6	-5.025020000	-0.437946000	-0.681994000
1	-5.357866000	-1.235627000	-1.337776000
6	-3.790038000	-0.524939000	-0.028721000
6	-1.843238000	-1.098576000	0.753224000
7	-2.143653000	0.149931000	1.297543000
7	-2.831896000	-1.516797000	-0.058166000
1	-6.777225000	0.773210000	-0.970406000
1	-1.583004000	0.632469000	1.979048000
7	-0.733145000	-1.813734000	0.991458000
7	0.164210000	-1.177484000	1.788798000
6	1.227846000	-1.846550000	2.128886000
1	1.345299000	-2.878279000	1.789049000
6	2.284164000	-1.273246000	2.944491000
6	3.392129000	-2.050394000	3.328288000
6	2.256495000	0.076902000	3.379458000
6	4.424051000	-1.539770000	4.104104000
6	3.288348000	0.601545000	4.157391000
6	4.365989000	-0.205913000	4.519161000
1	-6.036468000	2.597404000	0.520965000
1	5.267845000	-2.154926000	4.391440000
1	3.236000000	1.638407000	4.472213000
8	1.223527000	0.888057000	3.043106000
1	0.600257000	0.331462000	2.497688000
8	5.401245000	0.264175000	5.286074000
1	5.251577000	1.190164000	5.511588000
1	3.435901000	-3.085348000	3.004884000

5c_Aw3, optimization in solv.water
B3LYP/6-311++G**, E= -909.944333682 a.u.
Sum of electronic and thermal Enthalpies= -909.696689 a.u.

5c_Aw4, optimization in solv.water
B3LYP/6-311++G**, E= -909.958554428 a.u.
Sum of electronic and thermal Enthalpies= -909.710711 a.u.

-1; 1			
6	-5.527635000	1.657821000	0.110803000
6	-4.292436000	1.681290000	0.774397000
6	-5.944468000	0.531728000	-0.602778000

-1; 1			
6	-5.499393000	1.685580000	0.256884000
6	-4.260746000	1.679365000	0.913691000
6	-5.907018000	0.604896000	-0.529031000

1	-3.968095000	2.554096000	1.328022000	1	-3.943446000	2.516817000	1.523068000
6	-3.500863000	0.545452000	0.695412000	6	-3.458218000	0.560231000	0.754159000
6	-5.143307000	-0.616255000	-0.682319000	6	-5.094075000	-0.525528000	-0.689309000
1	-5.466008000	-1.489844000	-1.235712000	1	-5.409866000	-1.363893000	-1.298186000
6	-3.921934000	-0.591040000	-0.025774000	6	-3.869595000	-0.530010000	-0.037415000
6	-1.872383000	-1.037605000	0.860329000	6	-1.812777000	-1.015256000	0.814237000
7	-2.250444000	0.239757000	1.222725000	7	-2.198569000	0.235890000	1.254304000
7	-2.909299000	-1.536787000	0.093529000	7	-2.847274000	-1.469914000	0.017392000
1	-6.904230000	0.541452000	-1.105960000	1	-6.869575000	0.637178000	-1.025804000
1	-1.653199000	0.818076000	1.792321000	1	-1.642239000	0.789546000	1.883807000
1	-2.902780000	-2.462235000	-0.304175000	1	-2.831101000	-2.367571000	-0.439667000
7	-0.785854000	-1.687296000	1.146736000	7	-0.733529000	-1.697754000	1.046087000
7	0.068377000	-0.911036000	1.942642000	7	0.176575000	-1.027879000	1.859250000
6	1.168133000	-1.521644000	2.245434000	6	1.234544000	-1.722581000	2.165627000
1	1.300848000	-2.538202000	1.853446000	1	1.316251000	-2.746660000	1.790781000
6	2.273904000	-1.036257000	3.045437000	6	2.314180000	-1.225641000	2.969941000
6	3.362748000	-1.923562000	3.184700000	6	3.418937000	-2.057278000	3.280224000
6	2.337446000	0.267426000	3.700473000	6	2.347930000	0.101815000	3.489999000
6	4.508154000	-1.632542000	3.907612000	6	4.478275000	-1.627133000	4.045977000
6	3.544777000	0.532385000	4.438969000	6	3.405945000	0.549354000	4.259920000
6	4.580280000	-0.377445000	4.536519000	6	4.526739000	-0.287362000	4.583141000
1	-6.167411000	2.531409000	0.154790000	1	-6.149238000	2.546139000	0.363331000
1	5.326222000	-2.336842000	3.993744000	1	5.307068000	-2.292821000	4.265418000
1	3.619252000	1.497516000	4.933799000	1	3.390419000	1.567987000	4.634768000
8	1.407857000	1.136590000	3.646181000	8	1.318450000	0.959592000	3.225644000
8	5.728892000	-0.105639000	5.249354000	1	0.665698000	0.464039000	2.670734000
1	5.664229000	0.776064000	5.635494000	8	5.503667000	0.124081000	5.298972000
1	3.294576000	-2.890737000	2.693108000	1	3.416131000	-3.073121000	2.892933000
5c_R1, optimization in gas phase B3LYP/6-311++G**, E= -909.782418535 a.u. Sum of electronic and thermal Enthalpies= -909.533874 a.u.				**5c_R2,** optimization in gas phase B3LYP/6-311++G**, E= -909.780246727 a.u. Sum of electronic and thermal Enthalpies= -909.531729 a.u.			
0; 2				0; 2			
6	-5.405176000	1.715524000	0.221384000	6	-5.444872000	1.682561000	0.273937000
6	-4.180648000	1.712051000	0.866893000	6	-4.229666000	1.703125000	0.950733000
6	-5.848009000	0.602313000	-0.527930000	6	-5.836026000	0.583319000	-0.523029000
1	-3.834966000	2.561628000	1.442930000	1	-3.939218000	2.551802000	1.558727000
6	-3.378592000	0.562383000	0.759042000	6	-3.412457000	0.584159000	0.806180000
6	-5.078162000	-0.547794000	-0.653006000	6	-5.024560000	-0.528316000	-0.666071000
1	-5.425558000	-1.397192000	-1.229377000	1	-5.315274000	-1.376286000	-1.273944000
6	-3.844498000	-0.552034000	-0.002583000	6	-3.789456000	-0.537034000	0.007745000
6	-1.839078000	-0.925989000	0.887015000	6	-1.856933000	-1.012108000	0.823172000
7	-2.147850000	0.307387000	1.292869000	7	-2.176958000	0.255163000	1.308066000
7	-2.841884000	-1.480932000	0.099336000	7	-2.826130000	-1.498281000	0.035119000
1	-6.813943000	0.647681000	-1.017593000	1	-6.793277000	0.618291000	-1.029857000
1	-2.799730000	-2.403560000	-0.303815000	1	-1.609615000	0.795174000	1.939464000
7	-0.745909000	-1.678295000	1.121739000	7	-0.736841000	-1.701488000	1.084767000
7	0.165745000	-1.072921000	1.880533000	7	0.139910000	-1.047290000	1.864048000
6	1.241452000	-1.783305000	2.135518000	6	1.211252000	-1.751883000	2.161175000
1	1.327155000	-2.793446000	1.729715000	1	1.279180000	-2.772502000	1.782488000
6	2.297560000	-1.253826000	2.935985000	6	2.280943000	-1.233054000	2.955652000
6	3.445959000	-2.037003000	3.201427000	6	3.390555000	-2.053952000	3.264678000
6	2.238914000	0.063451000	3.492642000	6	2.282153000	0.102074000	3.456117000
6	4.489274000	-1.571881000	3.968074000	6	4.445353000	-1.602063000	4.025499000
6	3.300269000	0.532892000	4.270423000	6	3.348110000	0.563037000	4.226305000
6	4.408413000	-0.273047000	4.504422000	6	4.418212000	-0.281855000	4.508202000
1	-6.043610000	2.588780000	0.288245000	1	-6.110698000	2.533635000	0.359376000

1	5.365706000	-2.173573000	4.169312000
1	3.233053000	1.534567000	4.681275000
8	1.199821000	0.877082000	3.299896000
1	0.525570000	0.411201000	2.734298000
8	5.462151000	0.144118000	5.255292000
1	5.308032000	1.041288000	5.571837000
1	3.494256000	-3.036275000	2.781943000

1	5.291887000	-2.233311000	4.261211000
1	3.321320000	1.583557000	4.592848000
8	1.268861000	0.944293000	3.200595000
1	0.615230000	0.448245000	2.645291000
8	5.480450000	0.119294000	5.254476000
1	5.366109000	1.035270000	5.531364000
1	3.400289000	-3.070605000	2.886906000

5c_R3, optimization in gas phase
B3LYP/6-311++G**, E= -909.764597346 a.u.
Sum of electronic and thermal Enthalpies= -909.515924 a.u.

5c_R4, optimization in gas phase
B3LYP/6-311++G**, E= -909.774995850 a.u.
Sum of electronic and thermal Enthalpies= -909.526195 a.u.

0; 2			
6	-5.288759000	1.763323000	0.325163000
6	-4.039045000	1.671357000	0.942204000
6	-5.804946000	0.709759000	-0.437013000
1	-3.639869000	2.487008000	1.532263000
6	-3.327454000	0.491965000	0.769829000
6	-5.090315000	-0.477908000	-0.611772000
1	-5.491429000	-1.292948000	-1.202098000
6	-3.848855000	-0.568984000	0.001354000
6	-1.820719000	-1.188574000	0.786923000
7	-2.086710000	0.074738000	1.233070000
7	-2.894190000	-1.583295000	0.035170000
1	-6.777787000	0.814464000	-0.901912000
1	-1.406397000	0.554736000	1.813142000
1	-2.941423000	-2.486592000	-0.407987000
7	-0.748955000	-1.924177000	1.012798000
7	0.094570000	-1.210985000	1.791002000
6	1.214167000	-1.805669000	2.109927000
1	1.398076000	-2.819553000	1.740795000
6	2.213180000	-1.203127000	2.918670000
6	3.376343000	-1.964819000	3.196564000
6	2.109830000	0.172646000	3.489565000
6	4.405110000	-1.490339000	3.968612000
6	3.233902000	0.614751000	4.299801000
6	4.321430000	-0.176040000	4.524916000
1	-5.869118000	2.670772000	0.440538000
1	5.286701000	-2.084766000	4.172730000
1	3.158856000	1.614586000	4.715239000
8	1.138464000	0.920503000	3.303167000
8	5.395719000	0.201682000	5.277340000
1	5.258002000	1.095735000	5.610191000
1	3.446968000	-2.964153000	2.779069000

0; 2			
6	-5.464233000	1.699967000	0.219687000
6	-4.231532000	1.705044000	0.878023000
6	-5.880606000	0.599375000	-0.535680000
1	-3.910034000	2.558255000	1.462754000
6	-3.438917000	0.573993000	0.751801000
6	-5.081499000	-0.539760000	-0.662115000
1	-5.406315000	-1.391441000	-1.247352000
6	-3.858072000	-0.533850000	-0.007658000
6	-1.812196000	-1.006323000	0.857003000
7	-2.182960000	0.250801000	1.264642000
7	-2.839830000	-1.478270000	0.079356000
1	-6.842031000	0.627862000	-1.033840000
1	-1.604476000	0.821601000	1.858791000
1	-2.810403000	-2.390885000	-0.346110000
7	-0.732156000	-1.705878000	1.101106000
7	0.161403000	-1.050345000	1.881337000
6	1.247476000	-1.737354000	2.163943000
1	1.337397000	-2.749525000	1.767758000
6	2.303551000	-1.221837000	2.959869000
6	3.437281000	-2.056031000	3.219859000
6	2.293242000	0.110407000	3.524649000
6	4.484611000	-1.632153000	3.975668000
6	3.340432000	0.550268000	4.287080000
6	4.492108000	-0.287980000	4.558586000
1	-6.108095000	2.567468000	0.297769000
1	5.343358000	-2.261370000	4.175396000
1	3.326366000	1.548253000	4.706943000
8	1.241526000	0.931951000	3.300116000
1	0.603798000	0.438541000	2.738006000
8	5.446609000	0.104897000	5.251664000
1	3.438348000	-3.053573000	2.791826000

5c_Rw1, optimization in solv. water
B3LYP/6-311++G**, E= -909.800028339 a.u.
Sum of electronic and thermal Enthalpies= -909.551626 a.u.

5c_Rw2, optimization in solv. water
B3LYP/6-311++G**, E= -909.799911965 a.u.
Sum of electronic and thermal Enthalpies=-909.551348 a.u.

0; 2			
6	-5.418125000	1.713528000	0.209612000
6	-4.195826000	1.719095000	0.860546000
6	-5.853530000	0.593762000	-0.538317000
1	-3.861984000	2.576250000	1.433154000
6	-3.388626000	0.571144000	0.759123000
6	-5.078749000	-0.552920000	-0.656324000
1	-5.415023000	-1.408084000	-1.229562000
6	-3.846625000	-0.547787000	0.000185000
6	-1.845820000	-0.920449000	0.891499000
7	-2.156378000	0.317849000	1.296604000

0; 2			
6	-5.450262000	1.693036000	0.181901000
6	-4.227987000	1.742979000	0.843260000
6	-5.863203000	0.547643000	-0.538321000
1	-3.917483000	2.622618000	1.393493000
6	-3.425402000	0.605596000	0.762502000
6	-5.065973000	-0.581504000	-0.618127000
1	-5.379086000	-1.460679000	-1.168603000
6	-3.823129000	-0.559110000	0.042081000
6	-1.879595000	-0.989629000	0.870528000
7	-2.189281000	0.298716000	1.275361000

7	-2.844567000	-1.473615000	0.105967000	7	-2.860658000	-1.523214000	0.121957000
1	-6.817681000	0.633787000	-1.031600000	1	-6.825712000	0.560789000	-1.036040000
1	-2.812759000	-2.396966000	-0.301124000	1	-1.604046000	0.895305000	1.837654000
7	-0.749307000	-1.667816000	1.130983000	7	-0.761839000	-1.679739000	1.152572000
7	0.164885000	-1.062641000	1.891151000	7	0.127484000	-1.021829000	1.913719000
6	1.242631000	-1.775445000	2.142046000	6	1.215994000	-1.719011000	2.171123000
1	1.329507000	-2.783423000	1.734069000	1	1.298855000	-2.725642000	1.760189000
6	2.301619000	-1.250599000	2.940855000	6	2.291304000	-1.216359000	2.962961000
6	3.449378000	-2.039113000	3.198604000	6	3.427865000	-2.030844000	3.190523000
6	2.250790000	0.063475000	3.503166000	6	2.278515000	0.085552000	3.546601000
6	4.494613000	-1.574785000	3.963076000	6	4.494103000	-1.598292000	3.944532000
6	3.309344000	0.534403000	4.277907000	6	3.355212000	0.527444000	4.310736000
6	4.419295000	-0.276456000	4.504706000	6	4.453854000	-0.307573000	4.506705000
1	-6.060851000	2.583990000	0.270511000	1	-6.106031000	2.555104000	0.218616000
1	5.369531000	-2.181526000	4.157108000	1	5.359976000	-2.224861000	4.114445000
1	3.252446000	1.533039000	4.696165000	1	3.322386000	1.520487000	4.744391000
8	1.198639000	0.873692000	3.306788000	8	1.235227000	0.917275000	3.377973000
1	0.537731000	0.386929000	2.738768000	1	0.568440000	0.449913000	2.817405000
8	5.474062000	0.135192000	5.250210000	8	5.528464000	0.072265000	5.239441000
1	5.331969000	1.033674000	5.575016000	1	5.411764000	0.969165000	5.578532000
1	3.495126000	-3.036911000	2.776848000	1	3.448077000	-3.022627000	2.753137000
5c_Rw3, optimization in solv. water B3LYP/6-311++G**, E= -909.787845130 a.u. Sum of electronic and thermal Enthalpies= -909.538915 a.u.				**5c_Rw4,** optimization in solv. water B3LYP/6-311++G**, E= -909.800806054 a.u. Sum of electronic and thermal Enthalpies= -909.551627 a.u.			
0; 2				0; 2			
6	-5.504134000	1.661915000	0.133489000	6	-5.494109000	1.685036000	0.172202000
6	-4.278981000	1.696248000	0.799118000	6	-4.270078000	1.723336000	0.839357000
6	-5.915171000	0.531413000	-0.590087000	6	-5.893223000	0.559503000	-0.566013000
1	-3.960815000	2.567235000	1.357795000	1	-3.961348000	2.590254000	1.409420000
6	-3.482559000	0.560051000	0.714020000	6	-3.463536000	0.595814000	0.740079000
6	-5.116939000	-0.608662000	-0.675680000	6	-5.084287000	-0.571399000	-0.664992000
1	-5.431548000	-1.481787000	-1.233092000	1	-5.389530000	-1.440765000	-1.233257000
6	-3.895851000	-0.574268000	-0.011923000	6	-3.864167000	-0.532808000	0.000900000
6	-1.869115000	-1.003803000	0.872499000	6	-1.832367000	-0.955520000	0.884667000
7	-2.233694000	0.254737000	1.241283000	7	-2.210292000	0.297182000	1.266346000
7	-2.877587000	-1.510930000	0.110832000	7	-2.837973000	-1.459492000	0.115324000
1	-6.874080000	0.543622000	-1.093844000	1	-6.851729000	0.568713000	-1.070535000
1	-1.638815000	0.836046000	1.814355000	1	-1.648761000	0.899479000	1.847758000
1	-2.855874000	-2.437708000	-0.289138000	1	-2.804382000	-2.380839000	-0.296550000
7	-0.760009000	-1.677447000	1.159253000	7	-0.734206000	-1.652952000	1.145086000
7	0.070756000	-0.948799000	1.926729000	7	0.155800000	-1.009316000	1.913204000
6	1.187884000	-1.586835000	2.225965000	6	1.249011000	-1.712940000	2.176339000
1	1.308739000	-2.596482000	1.823827000	1	1.327742000	-2.718857000	1.763743000
6	2.252160000	-1.093425000	3.013625000	6	2.309377000	-1.222001000	2.963062000
6	3.369844000	-1.964424000	3.179089000	6	3.446895000	-2.062069000	3.194473000
6	2.293522000	0.239722000	3.669584000	6	2.319204000	0.098204000	3.560088000
6	4.476041000	-1.619836000	3.903836000	6	4.505830000	-1.653933000	3.943257000
6	3.493353000	0.550913000	4.416461000	6	3.381666000	0.517762000	4.315045000
6	4.529535000	-0.334278000	4.528707000	6	4.530015000	-0.325752000	4.550446000
1	-6.152581000	2.528600000	0.176718000	1	-6.151214000	2.544508000	0.225804000
1	5.315607000	-2.294012000	4.016947000	1	5.360818000	-2.298006000	4.112228000
1	3.534826000	1.524026000	4.894397000	1	3.371435000	1.508771000	4.753595000
8	1.357338000	1.064670000	3.598867000	8	1.271250000	0.932199000	3.374746000
8	5.669608000	-0.077236000	5.225820000	1	0.608538000	0.464952000	2.814056000
1	5.631384000	0.805676000	5.616129000	8	5.505755000	0.054535000	5.241594000
1	3.332501000	-2.938846000	2.703677000	1	3.442017000	-3.051489000	2.749405000

5c_RC, optimization in gas phase B3LYP/6-311++G**, E= -910.176589432 a.u. Sum of electronic and thermal Enthalpies= -909.913501 a.u.			
1; 2			
6	-5.515378000	1.665864000	0.157367000
6	-4.300200000	1.726562000	0.828459000
6	-5.900207000	0.527894000	-0.578332000
1	-4.008363000	2.603216000	1.392739000
6	-3.480456000	0.605698000	0.738143000
6	-5.084670000	-0.591986000	-0.670217000
1	-5.382703000	-1.465576000	-1.235948000
6	-3.865850000	-0.534325000	0.001709000
6	-1.835460000	-0.925852000	0.895512000
7	-2.227162000	0.322951000	1.269760000
7	-2.829711000	-1.445166000	0.126081000
1	-6.857275000	0.527628000	-1.084778000
1	-1.668531000	0.928967000	1.851190000
1	-2.772798000	-2.371019000	-0.275566000
7	-0.731141000	-1.617961000	1.161113000
7	0.153902000	-0.975577000	1.923306000
6	1.242730000	-1.693448000	2.181076000
1	1.302626000	-2.698876000	1.765109000
6	2.310732000	-1.210867000	2.963835000
6	3.439375000	-2.052152000	3.196247000
6	2.320347000	0.106328000	3.549574000
6	4.500375000	-1.637783000	3.948094000
6	3.400675000	0.526212000	4.313700000
6	4.480209000	-0.333805000	4.513084000
1	-6.185097000	2.515680000	0.200493000
1	5.359660000	-2.269405000	4.129926000
1	3.382481000	1.521432000	4.742723000
8	1.302221000	0.948909000	3.375485000
1	0.628141000	0.497924000	2.816831000
8	5.552230000	0.003875000	5.237163000
1	5.478851000	0.899433000	5.592304000
1	3.441867000	-3.044216000	2.759652000

5c_RCw, optimization in solv. water B3LYP/6-311++G**, E= -910.246616815 a.u. Sum of electronic and thermal Enthalpies= -909.983658 a.u.			
1; 2			
6	-5.512679000	1.664694000	0.141499000
6	-4.300799000	1.731133000	0.816057000
6	-5.896127000	0.519820000	-0.589234000
1	-4.006690000	2.608078000	1.377396000
6	-3.479629000	0.608476000	0.735569000
6	-5.081898000	-0.600642000	-0.671096000
1	-5.372564000	-1.480393000	-1.229985000
6	-3.864099000	-0.537844000	0.005384000
6	-1.844664000	-0.917436000	0.905445000
7	-2.233607000	0.331950000	1.270788000
7	-2.834116000	-1.444807000	0.138224000
1	-6.851664000	0.517096000	-1.098767000
1	-1.682062000	0.951807000	1.846301000
1	-2.785884000	-2.373313000	-0.260597000
7	-0.737562000	-1.610818000	1.175202000
7	0.148874000	-0.971096000	1.937556000
6	1.236215000	-1.689178000	2.184710000
1	1.302125000	-2.690935000	1.761630000
6	2.308292000	-1.208293000	2.969966000
6	3.438669000	-2.046775000	3.183971000
6	2.317564000	0.097345000	3.568675000
6	4.508988000	-1.636036000	3.931116000
6	3.404758000	0.513956000	4.327698000
6	4.490737000	-0.341684000	4.505867000
1	-6.183009000	2.514513000	0.176447000
1	5.368899000	-2.272210000	4.093463000
1	3.391590000	1.502815000	4.770643000
8	1.293016000	0.943005000	3.416380000
1	0.609725000	0.503136000	2.857206000
8	5.572636000	0.005660000	5.224915000
1	5.487264000	0.902629000	5.575882000
1	3.439124000	-3.034092000	2.737521000

5c_M, optimization in gas phase B3LYP/6-311++G**, E= -910.413748482 a.u. Sum of electronic and thermal Enthalpies= -910.151814 a.u.			
0; 1			
6	-5.480322000	1.684057000	0.312699000
6	-4.243032000	1.662382000	0.968305000
6	-5.885790000	0.624946000	-0.500588000
1	-3.928453000	2.485751000	1.598349000
6	-3.438713000	0.550187000	0.780413000
6	-5.071800000	-0.498456000	-0.689635000
1	-5.389386000	-1.319827000	-1.320838000
6	-3.848138000	-0.518988000	-0.038823000
6	-1.789242000	-1.023698000	0.800595000
7	-2.176885000	0.215402000	1.271204000
7	-2.822450000	-1.458476000	-0.005794000
1	-6.848009000	0.669244000	-0.996477000
1	-1.624298000	0.739286000	1.928093000
1	-2.786413000	-2.342412000	-0.485411000
7	-0.714802000	-1.717697000	1.011869000
7	0.194037000	-1.066620000	1.822546000

5c_Mw, optimization in solv. water B3LYP/6-311++G**, E= -910.431654022 a.u. Sum of electronic and thermal Enthalpies= -910.170113 a.u.			
0; 1			
6	-5.478782000	1.697578000	0.254616000
6	-4.245885000	1.687076000	0.918659000
6	-5.887974000	0.617125000	-0.533049000
1	-3.927650000	2.523538000	1.528622000
6	-3.449467000	0.562351000	0.764085000
6	-5.081993000	-0.517075000	-0.687582000
1	-5.397886000	-1.354556000	-1.297314000
6	-3.861553000	-0.525300000	-0.027628000
6	-1.815651000	-1.017434000	0.832271000
7	-2.193601000	0.230088000	1.272099000
7	-2.842606000	-1.469702000	0.035870000
1	-6.847351000	0.654927000	-1.035292000
1	-1.639097000	0.787633000	1.900058000
1	-2.823073000	-2.366641000	-0.423570000
7	-0.737801000	-1.717462000	1.061182000
7	0.177048000	-1.067850000	1.864467000

6	1.234026000	-1.765508000	2.146382000	6	1.232866000	-1.758161000	2.157651000
1	1.314163000	-2.794386000	1.789473000	1	1.328185000	-2.778414000	1.780331000
6	2.307378000	-1.238088000	2.963494000	6	2.313961000	-1.234597000	2.969882000
6	3.392566000	-2.059819000	3.319274000	6	3.423135000	-2.046836000	3.271034000
6	2.315439000	0.103481000	3.424246000	6	2.308634000	0.088230000	3.479898000
6	4.441228000	-1.600998000	4.095670000	6	4.482203000	-1.591548000	4.037899000
6	3.369611000	0.575055000	4.206486000	6	3.370386000	0.557398000	4.253137000
6	4.422426000	-0.272995000	4.539392000	6	4.449840000	-0.279877000	4.529041000
1	-6.131456000	2.540290000	0.441035000	1	-6.125200000	2.561272000	0.355282000
1	5.271536000	-2.239947000	4.366554000	1	5.329580000	-2.226744000	4.262788000
1	3.346408000	1.606515000	4.542433000	1	3.339440000	1.573705000	4.630692000
8	1.314099000	0.952911000	3.118702000	8	1.278023000	0.927504000	3.229362000
1	0.676072000	0.444465000	2.556573000	1	0.627522000	0.426656000	2.673130000
8	5.474850000	0.143422000	5.304039000	8	5.512980000	0.131738000	5.280671000
1	5.357269000	1.068451000	5.544957000	1	5.390777000	1.047290000	5.560186000
1	3.399500000	-3.087370000	2.970615000	1	3.442409000	-3.061354000	2.887355000

5d_A1, optimization in gas phase B3LYP/6-311++G**, E= -909.848955653 a.u. Sum of electronic and thermal Enthalpies= -909.601568 a.u.			
-1; 1			
6	6.606941000	0.095199000	0.009377000
6	5.693678000	-0.959494000	0.008392000
6	6.172573000	1.436025000	0.006100000
1	6.029929000	-1.992415000	0.010885000
6	4.325890000	-0.657263000	0.004069000
6	4.814073000	1.755316000	0.001761000
1	4.479972000	2.788636000	-0.000801000
6	3.882476000	0.710287000	0.000647000
6	2.220610000	-0.569096000	-0.002063000
7	3.221469000	-1.472150000	0.002229000
7	2.506050000	0.734577000	-0.003294000
7	0.921385000	-1.095555000	-0.004879000
7	-0.190957000	-0.390616000	-0.007120000
6	-1.326678000	-1.011671000	-0.006483000
1	-1.369505000	-2.108946000	-0.003763000
1	0.888959000	-2.113108000	-0.002046000
1	6.910819000	2.233189000	0.006969000
6	-2.596244000	-0.300320000	-0.008290000
6	-3.800683000	-1.025594000	-0.003557000
6	-2.663278000	1.107583000	-0.012464000
1	-3.773623000	-2.109997000	0.000456000
1	-1.748799000	1.687795000	-0.011797000
6	-5.031731000	-0.370801000	-0.008017000
6	-3.886348000	1.756043000	-0.012213000
6	-5.077792000	1.015094000	-0.010819000
1	7.672427000	-0.117779000	0.012675000
8	-3.936062000	3.125942000	-0.012750000
1	-4.864777000	3.386169000	0.023583000
8	-6.252648000	1.760502000	-0.022357000
1	-6.998230000	1.186764000	0.174842000
1	-5.956554000	-0.942267000	-0.012852000

5d_A2, optimization in gas phase B3LYP/6-311++G**, E= -909.855972006 a.u. Sum of electronic and thermal Enthalpies= -909.609034 a.u.			
-1; 1			
6	6.403491000	0.406507000	0.011140000
6	5.647183000	-0.769616000	0.019461000
6	5.793691000	1.668052000	-0.003643000
1	6.123241000	-1.744303000	0.030890000
6	4.250422000	-0.676459000	0.012699000
6	4.395830000	1.788844000	-0.010586000
1	3.921191000	2.765172000	-0.022150000
6	3.649273000	0.618586000	-0.002245000
6	2.118701000	-1.025471000	0.007004000
7	3.295769000	-1.662300000	0.018031000
7	2.296452000	0.361462000	-0.005328000
1	1.518481000	0.999921000	-0.015638000
7	0.912293000	-1.627780000	0.007367000
7	-0.088700000	-0.739148000	-0.002211000
6	-1.297931000	-1.224126000	-0.006005000
1	-1.439860000	-2.308598000	-0.003157000
1	6.407044000	2.563274000	-0.009989000
6	-2.479750000	-0.385637000	-0.012791000
6	-3.757789000	-0.984998000	-0.021343000
6	-2.422948000	1.026363000	-0.008752000
1	-3.834887000	-2.066893000	-0.024039000
1	-1.461798000	1.523447000	0.004207000
6	-4.918577000	-0.215343000	-0.034069000
6	-3.577669000	1.789174000	-0.012482000
6	-4.834790000	1.170143000	-0.026359000
1	7.487551000	0.342191000	0.016202000
8	-3.495243000	3.161854000	-0.000485000
1	-4.397994000	3.501944000	0.035156000
8	-5.939281000	2.025647000	-0.048702000
1	-6.711355000	1.551985000	0.272751000
1	-5.893916000	-0.695759000	-0.054919000

5d_A3, optimization in gas phase B3LYP/6-311++G**, E= -909.850703679 a.u. Sum of electronic and thermal Enthalpies= -909.603515 a.u.			
-1; 1			
6	6.490153000	0.202987000	0.684920000
6	5.667822000	-0.913645000	0.524726000
6	5.966376000	1.503469000	0.685634000
1	6.074028000	-1.918739000	0.524811000
6	4.295685000	-0.711817000	0.362799000
6	4.595407000	1.728335000	0.524341000
1	4.187760000	2.733136000	0.525041000
6	3.784776000	0.613244000	0.365314000
6	2.183791000	-0.889927000	0.092590000
7	3.271359000	-1.629976000	0.191437000
7	2.417107000	0.459585000	0.184952000
1	1.681316000	1.149878000	0.165579000
7	0.926035000	-1.359045000	-0.112483000
7	-0.131291000	-0.474443000	-0.045530000
6	-1.310454000	-0.992281000	-0.070351000
1	-1.416345000	-2.085338000	-0.126450000
1	0.782274000	-2.359364000	-0.017703000

5d_A4, optimization in gas phase B3LYP/6-311++G**, E= -909.874617338 a.u. Sum of electronic and thermal Enthalpies= -909.626868 a.u.			
-1; 1			
6	6.522088000	0.240170000	0.112844000
6	5.693078000	-0.883022000	0.106110000
6	5.997109000	1.537793000	0.036020000
1	6.100479000	-1.885826000	0.166242000
6	4.312677000	-0.690960000	0.020163000
6	4.617765000	1.752913000	-0.051427000
1	4.209216000	2.755647000	-0.110846000
6	3.800499000	0.631445000	-0.057905000
6	2.187474000	-0.884065000	-0.091073000
7	3.281299000	-1.616590000	-0.001436000
7	2.424009000	0.467757000	-0.132326000
1	1.687250000	1.156315000	-0.162757000
7	0.920493000	-1.363843000	-0.169897000
7	-0.134231000	-0.474082000	-0.112475000
6	-1.311913000	-0.994334000	-0.033354000
1	-1.415226000	-2.088366000	-0.002391000
1	0.785731000	-2.352950000	0.013254000

1	6.632222000	2.349813000	0.812979000	1	6.668386000	2.389384000	0.043948000
6	-2.552226000	-0.242576000	-0.029142000	6	-2.550306000	-0.246821000	0.019278000
6	-3.743650000	-0.990760000	-0.048417000	6	-3.738212000	-0.992942000	0.114368000
6	-2.595673000	1.158104000	0.031004000	6	-2.589578000	1.164815000	-0.020668000
1	-3.720402000	-2.074338000	-0.095359000	1	-3.695344000	-2.077418000	0.142633000
1	-1.670778000	1.723505000	0.044276000	1	-1.667351000	1.728935000	-0.095378000
6	-4.963071000	-0.303849000	-0.006452000	6	-4.976485000	-0.337168000	0.170100000
6	-3.810087000	1.916106000	0.076656000	6	-3.810443000	1.865049000	0.033569000
6	-5.009583000	1.079278000	0.054822000	6	-5.006751000	1.043055000	0.131025000
1	7.558514000	0.062809000	0.812092000	1	7.596892000	0.107394000	0.179123000
8	-3.868430000	3.172982000	0.130786000	8	-3.999122000	3.133438000	0.007360000
8	-6.212801000	1.749628000	0.097392000	8	-6.148223000	1.770015000	0.178790000
1	-6.915379000	1.091618000	0.083331000	1	-5.770447000	2.689049000	0.128320000
1	-5.898269000	-0.865111000	-0.021328000	1	-5.904651000	-0.895540000	0.243113000
5d_A5, optimization in gas phase B3LYP/6-311++G**, E= -909.881755922 a.u. Sum of electronic and thermal Enthalpies= -909.633750 a.u.				**5d_Aw1,** optimization in solv.water B3LYP/6-311++G**, E= -909.941751931 a.u. Sum of electronic and thermal Enthalpies= -909.693770 a.u.			
-1; 1				-1; 1			
6	6.313529000	0.420526000	0.949492000	6	6.602584000	0.133541000	0.006299000
6	5.584389000	-0.753345000	0.748283000	6	5.711683000	-0.943508000	0.005324000
6	5.691437000	1.676389000	0.957904000	6	6.138873000	1.462262000	0.004020000
1	6.067857000	-1.723677000	0.743287000	1	6.076603000	-1.966434000	0.007093000
6	4.204854000	-0.656646000	0.552573000	6	4.338334000	-0.670108000	0.001962000
6	4.310722000	1.796595000	0.762893000	6	4.770690000	1.750273000	0.000674000
1	3.826508000	2.767045000	0.769046000	1	4.419287000	2.777923000	-0.001096000
6	3.593216000	0.626085000	0.563618000	6	3.866266000	0.682363000	-0.000447000
6	2.118902000	-0.992743000	0.223956000	6	2.215248000	-0.644398000	-0.003128000
7	3.261348000	-1.647473000	0.339986000	7	3.247479000	-1.513449000	0.000241000
7	2.246602000	0.370212000	0.344259000	7	2.484197000	0.670152000	-0.003772000
1	1.458641000	0.999174000	0.319134000	7	0.927465000	-1.170181000	-0.006902000
7	0.909566000	-1.548562000	-0.022230000	7	-0.181181000	-0.414816000	-0.004997000
7	-0.222601000	-0.749033000	0.036544000	6	-1.321974000	-1.013952000	-0.002438000
6	-1.353407000	-1.381591000	-0.041683000	1	-1.382910000	-2.107572000	-0.000903000
1	-1.346122000	-2.477629000	-0.129350000	1	0.855084000	-2.183520000	-0.002036000
1	0.841306000	-2.557900000	0.057636000	1	6.856887000	2.276089000	0.004865000
1	6.285850000	2.569259000	1.117231000	6	-2.590297000	-0.288160000	-0.001628000
6	-2.650297000	-0.776939000	-0.023136000	6	-3.790623000	-1.013797000	0.002813000
6	-3.788675000	-1.607045000	-0.101740000	6	-2.651952000	1.117911000	-0.005282000
6	-2.848562000	0.631562000	0.075415000	1	-3.765314000	-2.097662000	0.005632000
1	-3.643026000	-2.682760000	-0.177001000	1	-1.741987000	1.704903000	-0.008923000
1	-1.994220000	1.296027000	0.136863000	6	-5.022771000	-0.359495000	0.003646000
6	-5.077019000	-1.096676000	-0.086142000	6	-3.873578000	1.768857000	-0.004395000
6	-4.117391000	1.140345000	0.092134000	6	-5.069523000	1.028247000	0.000067000
6	-5.310700000	0.305775000	0.011905000	1	7.671137000	-0.056395000	0.008859000
1	7.385957000	0.360180000	1.103378000	8	-3.912905000	3.136821000	-0.007964000
8	-4.388071000	2.474072000	0.183552000	1	-4.838102000	3.419043000	-0.006781000
1	-5.372179000	2.475615000	0.166740000	8	-6.220838000	1.775581000	0.000451000
8	-6.438136000	0.891532000	0.035334000	1	-7.001342000	1.209141000	0.003502000
1	-5.939199000	-1.752743000	-0.148320000	1	-5.946023000	-0.929331000	0.007104000
5d_Aw2, optimization in solv.water B3LYP/6-311++G**, E= -909.943189803 a.u. Sum of electronic and thermal Enthalpies= -909.695875 a.u.				**5d_Aw3,** optimization in solv.water B3LYP/6-311++G**, E= -909.945050503 a.u. Sum of electronic and thermal Enthalpies= -909.697140 a.u.			
-1; 1				-1; 1			
6	6.425863000	0.389984000	0.001682000	6	6.529809000	0.242098000	0.006648000
6	5.662661000	-0.783176000	0.002015000	6	5.698894000	-0.879733000	0.006025000
6	5.821453000	1.654486000	0.000934000	6	6.003177000	1.543296000	0.003463000

1	6.140064000	-1.757550000	0.002637000	1	6.110161000	-1.882905000	0.008504000
6	4.267254000	-0.676842000	0.001567000	6	4.316628000	-0.677523000	0.002089000
6	4.424651000	1.784640000	0.000481000	6	4.622913000	1.765516000	-0.000490000
1	3.953917000	2.761729000	-0.000114000	1	4.213737000	2.768963000	-0.002970000
6	3.673763000	0.616764000	0.000794000	6	3.804287000	0.643286000	-0.001113000
6	2.119590000	-1.005958000	0.000997000	6	2.181733000	-0.861647000	-0.003289000
7	3.296417000	-1.657867000	0.001872000	7	3.275945000	-1.600381000	0.000705000
7	2.312897000	0.372753000	0.000370000	7	2.422904000	0.486183000	-0.004679000
1	1.554603000	1.036028000	0.000447000	1	1.708679000	1.198512000	-0.006665000
7	0.920100000	-1.612493000	0.001157000	7	0.915649000	-1.358611000	-0.007109000
7	-0.101505000	-0.717390000	0.000680000	7	-0.154032000	-0.507780000	-0.005907000
6	-1.300661000	-1.204509000	0.000019000	6	-1.323682000	-1.044809000	-0.003282000
1	-1.447839000	-2.289231000	-0.000066000	1	-1.427055000	-2.135505000	-0.001258000
1	6.439158000	2.545657000	0.000708000	1	0.795489000	-2.366570000	-0.000575000
6	-2.498509000	-0.371073000	-0.000792000	1	6.677026000	2.392322000	0.004055000
6	-3.762750000	-0.985304000	-0.001295000	6	-2.565733000	-0.280237000	-0.002146000
6	-2.445418000	1.037575000	-0.001019000	6	-3.769731000	-0.999385000	0.001986000
1	-3.832787000	-2.067474000	-0.001156000	6	-2.595502000	1.125852000	-0.005078000
1	-1.488894000	1.545362000	-0.000678000	1	-3.766151000	-2.083532000	0.004276000
6	-4.933542000	-0.226724000	-0.001923000	1	-1.661176000	1.677454000	-0.008313000
6	-3.606787000	1.791676000	-0.001652000	6	-4.981405000	-0.299078000	0.002964000
6	-4.862418000	1.160271000	-0.002093000	6	-3.796352000	1.884609000	-0.004038000
1	7.508494000	0.319260000	0.002035000	6	-5.005518000	1.087006000	0.000005000
8	-3.526449000	3.160185000	-0.001823000	1	7.605629000	0.106591000	0.009654000
1	-4.424175000	3.520004000	-0.002391000	8	-3.830944000	3.171025000	-0.006668000
8	-5.948338000	2.005673000	-0.002646000	8	-6.193126000	1.787382000	0.000842000
1	-6.773092000	1.506192000	-0.003221000	1	-6.927277000	1.161810000	0.003403000
1	-5.902444000	-0.715801000	-0.002272000	1	-5.921119000	-0.846422000	0.006096000
5d_Aw4, optimization in solv.water B3LYP/6-311++G**, E= -909.956177849 a.u. Sum of electronic and thermal Enthalpies= -909.708177 a.u.				**5d_Aw5,** optimization in solv.water B3LYP/6-311++G**, E= -909.959616926 a.u. Sum of electronic and thermal Enthalpies= -909.711572 a.u.			
-1; 1				-1; 1			
6	6.527334000	0.249990000	0.006510000	6	6.347399000	0.535501000	0.069222000
6	5.699758000	-0.874385000	0.005567000	6	5.623857000	-0.652553000	0.191866000
6	5.996891000	1.549599000	0.003790000	6	5.704966000	1.766177000	-0.136241000
1	6.114169000	-1.876266000	0.007680000	1	6.125790000	-1.600422000	0.350788000
6	4.316850000	-0.676484000	0.001786000	6	4.230813000	-0.590695000	0.104741000
6	4.615908000	1.767586000	-0.000004000	6	4.311776000	1.848408000	-0.226324000
1	4.203661000	2.769788000	-0.002111000	1	3.812781000	2.797344000	-0.384978000
6	3.800700000	0.642920000	-0.000947000	6	3.600798000	0.661588000	-0.103027000
6	2.182378000	-0.866803000	-0.003492000	6	2.123727000	-0.982225000	0.042247000
7	3.278909000	-1.602408000	0.000145000	7	3.281264000	-1.602678000	0.192083000
7	2.419852000	0.481795000	-0.004433000	7	2.241963000	0.370524000	-0.139902000
1	1.703384000	1.191850000	-0.006134000	1	1.463759000	1.002708000	-0.250571000
7	0.917483000	-1.366064000	-0.007323000	7	0.910484000	-1.593625000	0.037608000
7	-0.153021000	-0.515315000	-0.005762000	7	-0.232067000	-0.830350000	-0.020073000
6	-1.323082000	-1.052581000	-0.003024000	6	-1.351176000	-1.461579000	0.112800000
1	-1.427417000	-2.143115000	-0.001340000	1	-1.352333000	-2.545390000	0.274377000
1	0.798327000	-2.374083000	-0.001005000	1	0.874839000	-2.576584000	0.289097000
1	6.668153000	2.400676000	0.004632000	1	6.296739000	2.669754000	-0.227366000
6	-2.562305000	-0.285949000	-0.002052000	6	-2.648230000	-0.826004000	0.062276000
6	-3.767874000	-1.002791000	0.002146000	6	-3.800064000	-1.614517000	0.229295000
6	-2.578398000	1.126858000	-0.005200000	6	-2.811959000	0.569598000	-0.150315000
1	-3.754148000	-2.087252000	0.004483000	1	-3.686097000	-2.682731000	0.391910000
1	-1.641961000	1.674168000	-0.008559000	1	-1.943959000	1.206005000	-0.282460000
6	-4.993211000	-0.318887000	0.003277000	6	-5.078955000	-1.064459000	0.191185000

6	-3.785353000	1.848798000	-0.004099000	6	-4.072151000	1.110056000	-0.188152000
6	-4.995517000	1.062039000	0.000235000	6	-5.274763000	0.323415000	-0.019798000
1	7.603556000	0.117663000	0.009402000	1	7.429488000	0.507482000	0.133819000
8	-3.926137000	3.139447000	-0.006722000	8	-4.294328000	2.446959000	-0.390094000
8	-6.144525000	1.799027000	0.001099000	1	-5.274214000	2.502761000	-0.362937000
1	-5.790390000	2.718835000	-0.001576000	8	-6.403457000	0.941897000	-0.075244000
1	-5.932809000	-0.861909000	0.006515000	1	-5.952058000	-1.695927000	0.323308000
5d_Ab1, optimization in solv. benzene B3LYP/6-311++G**, E= -909.894952267 a.u. Sum of electronic and thermal Enthalpies= -909.647225 a.u.				**5d_Ab2,** optimization in solv. benzene B3LYP/6-311++G**, E= -909.899244929 a.u. Sum of electronic and thermal Enthalpies= -909.652220 a.u.			
-1; 1				-1; 1			
6	6.605535000	0.110524000	0.005960000	6	6.423121000	0.385182000	-0.001966000
6	5.700676000	-0.952929000	0.005456000	6	5.656774000	-0.784979000	0.010047000
6	6.159535000	1.446183000	0.003366000	6	5.823694000	1.651620000	-0.014910000
1	6.047164000	-1.982391000	0.007419000	1	6.128155000	-1.761965000	0.019834000
6	4.331160000	-0.661540000	0.002257000	6	4.261094000	-0.678403000	0.008861000
6	4.796845000	1.753117000	0.000183000	6	4.426848000	1.784462000	-0.015781000
1	4.456569000	2.784328000	-0.001884000	1	3.959846000	2.764048000	-0.025883000
6	3.875673000	0.699742000	-0.000448000	6	3.671461000	0.620064000	-0.003658000
6	2.218142000	-0.598581000	-0.002539000	6	2.120785000	-1.005811000	0.011002000
7	3.232117000	-1.487813000	0.000949000	7	3.294057000	-1.656118000	0.017549000
7	2.496602000	0.709549000	-0.003625000	7	2.313814000	0.377192000	-0.001419000
7	0.923991000	-1.126283000	-0.005887000	1	1.549679000	1.032522000	-0.007792000
7	-0.187671000	-0.401362000	-0.004267000	7	0.915730000	-1.603872000	0.014859000
6	-1.324595000	-1.012428000	-0.002019000	7	-0.093498000	-0.712051000	0.010005000
1	-1.376597000	-2.108419000	-0.000540000	6	-1.297032000	-1.200471000	0.007093000
1	0.876407000	-2.142019000	-0.001704000	1	-1.438063000	-2.285392000	0.005349000
1	6.889495000	2.250265000	0.003841000	1	6.444216000	2.541365000	-0.024340000
6	-2.595030000	-0.294691000	-0.001507000	6	-2.490473000	-0.369443000	0.004615000
6	-3.796617000	-1.020400000	0.002193000	6	-3.758135000	-0.982796000	-0.018112000
6	-2.658691000	1.111752000	-0.004664000	6	-2.444870000	1.040844000	0.026286000
1	-3.769963000	-2.104609000	0.004517000	1	-3.825362000	-2.065125000	-0.032768000
1	-1.744852000	1.692697000	-0.007605000	1	-1.489796000	1.549473000	0.050263000
6	-5.028290000	-0.365607000	0.002901000	6	-4.928233000	-0.225154000	-0.025796000
6	-3.880999000	1.761793000	-0.004009000	6	-3.607009000	1.792860000	0.021085000
6	-5.074142000	1.020856000	-0.000135000	6	-4.859008000	1.161031000	-0.007066000
1	7.672171000	-0.093669000	0.008425000	1	7.506118000	0.311366000	-0.001407000
8	-3.925300000	3.130588000	-0.007211000	8	-3.533199000	3.164133000	0.044325000
1	-4.851984000	3.403194000	-0.006445000	1	-4.434939000	3.509707000	0.064194000
8	-6.238049000	1.767294000	0.000300000	8	-5.959129000	2.005919000	-0.019226000
1	-7.006229000	1.187281000	0.002736000	1	-6.768750000	1.493706000	0.071891000
1	-5.952578000	-0.936095000	0.005845000	1	-5.897472000	-0.715829000	-0.048632000
5d_Ab3, optimization in solv. benzene B3LYP/6-311++G**, E= -909.897798544 a.u. Sum of electronic and thermal Enthalpies= -909.650174 a.u.				**5d_Ab4,** optimization in solv. benzene B3LYP/6-311++G**, E= -909.916699919 a.u. Sum of electronic and thermal Enthalpies= -909.668589 a.u.			
-1; 1				-1; 1			
6	6.524983000	0.233660000	0.115056000	6	6.497399000	0.213091000	0.648553000
6	5.691977000	-0.886101000	0.093859000	6	5.673779000	-0.905146000	0.508066000
6	6.003776000	1.534711000	0.057060000	6	5.971899000	1.513661000	0.652411000
1	6.096690000	-1.890861000	0.139174000	1	6.082414000	-1.909327000	0.505436000
6	4.312580000	-0.684512000	0.012535000	6	4.299067000	-0.702585000	0.369199000
6	4.625942000	1.757759000	-0.024593000	6	4.598626000	1.737772000	0.515024000
1	4.221044000	2.762347000	-0.068991000	1	4.189983000	2.741849000	0.518083000
6	3.804808000	0.638451000	-0.045473000	6	3.787045000	0.620073000	0.375597000
6	2.184180000	-0.867017000	-0.098187000	6	2.180259000	-0.882380000	0.134228000
7	3.274305000	-1.605822000	-0.021325000	7	3.269644000	-1.621972000	0.217326000

7	2.426117000	0.482317000	-0.118462000	7	2.415222000	0.465776000	0.219898000
1	1.703285000	1.185428000	-0.151577000	1	1.690180000	1.166824000	0.199178000
7	0.917632000	-1.354619000	-0.178306000	7	0.921712000	-1.363380000	-0.045609000
7	-0.144669000	-0.484357000	-0.133006000	7	-0.143731000	-0.495914000	0.000176000
6	-1.317204000	-1.012028000	-0.077627000	6	-1.317864000	-1.023990000	-0.042466000
1	-1.419214000	-2.105001000	-0.056623000	1	-1.420895000	-2.115343000	-0.099145000
1	0.789848000	-2.352254000	-0.041387000	1	0.789195000	-2.367899000	0.013347000
1	6.678456000	2.383129000	0.075688000	1	6.639525000	2.360586000	0.763558000
6	-2.560405000	-0.257866000	-0.037455000	6	-2.558175000	-0.268922000	-0.020580000
6	-3.753246000	-0.995663000	0.034302000	6	-3.756266000	-0.999777000	-0.059518000
6	-2.601236000	1.145548000	-0.064280000	6	-2.584042000	1.141864000	0.039678000
1	-3.735543000	-2.079973000	0.052768000	1	-3.729187000	-2.083729000	-0.105764000
1	-1.673470000	1.704577000	-0.118613000	1	-1.653312000	1.696456000	0.066716000
6	-4.969856000	-0.304518000	0.080802000	6	-4.988415000	-0.329287000	-0.036895000
6	-3.810539000	1.902319000	-0.020868000	6	-3.797518000	1.854036000	0.063597000
6	-5.009938000	1.080112000	0.056304000	6	-5.002733000	1.050120000	0.023578000
1	7.599051000	0.096183000	0.177803000	1	7.567664000	0.074632000	0.757280000
8	-3.865068000	3.171544000	-0.044173000	8	-3.959910000	3.132010000	0.116149000
8	-6.205848000	1.762763000	0.105650000	8	-6.147829000	1.782338000	0.049816000
1	-6.920035000	1.118534000	0.159675000	1	-5.778906000	2.700309000	0.090336000
1	-5.904542000	-0.861001000	0.137408000	1	-5.924461000	-0.878124000	-0.065576000

5d_Ab5, optimization in solv. benzene
B3LYP/6-311++G**, E= -909.921968945 a.u.
Sum of electronic and thermal Enthalpies= -909.673870 a.u.

-1; 1

6	6.354041000	0.501860000	0.142670000
6	5.619909000	-0.685364000	0.112928000
6	5.725459000	1.753395000	0.070994000
1	6.109595000	-1.650827000	0.170111000
6	4.229429000	-0.604234000	0.009237000
6	4.334371000	1.856554000	-0.033277000
1	3.845720000	2.822868000	-0.088336000
6	3.612330000	0.671437000	-0.062291000
6	2.124482000	-0.968027000	-0.130841000
7	3.275038000	-1.610393000	-0.034677000
7	2.253438000	0.397926000	-0.155318000
1	1.472430000	1.034961000	-0.190362000
7	0.906059000	-1.556696000	-0.232516000
7	-0.229988000	-0.770536000	-0.169433000
6	-1.352668000	-1.410602000	-0.090042000
1	-1.347057000	-2.508239000	-0.060924000
1	0.860021000	-2.554210000	-0.050349000
1	6.324793000	2.656488000	0.096536000
6	-2.649961000	-0.794355000	-0.033248000
6	-3.790352000	-1.614297000	0.070038000
6	-2.835727000	0.616147000	-0.072466000
1	-3.656979000	-2.693121000	0.099086000
1	-1.977734000	1.273529000	-0.154055000
6	-5.073584000	-1.086846000	0.135060000
6	-4.099327000	1.138719000	-0.008451000
6	-5.293273000	0.317453000	0.100591000
1	7.434845000	0.456306000	0.222882000
8	-4.350531000	2.481832000	-0.042435000
1	-5.331579000	2.504274000	0.019089000
8	-6.419941000	0.918598000	0.154184000
1	-5.938083000	-1.738438000	0.213725000

5d_R1, optimization in gas phase B3LYP/6-311++G**, E= -909.750426255 a.u. Sum of electronic and thermal Enthalpies= -909.502105 a.u.			
0; 2			
6	6.560397000	0.058529000	0.002124000
6	5.679747000	-0.993077000	0.002839000
6	6.115611000	1.425890000	0.000754000
1	6.014709000	-2.023369000	0.003856000
6	4.294819000	-0.685967000	0.002170000
6	4.783102000	1.764380000	0.000076000
1	4.453074000	2.796124000	-0.000954000
6	3.842231000	0.709912000	0.000764000
6	2.195263000	-0.574845000	0.001575000
7	3.225441000	-1.486383000	0.002567000
7	2.497188000	0.741304000	0.000365000
7	0.938873000	-1.080363000	0.001690000
7	-0.174237000	-0.328931000	0.000547000
6	-1.297162000	-0.961897000	0.000766000
1	-1.327688000	-2.058707000	0.001863000
1	0.883632000	-2.099034000	0.002579000
1	6.866693000	2.208054000	0.000243000
6	-2.574775000	-0.269298000	-0.000288000
6	-3.757349000	-1.022924000	0.000087000
6	-2.648849000	1.135760000	-0.001690000
1	-3.710935000	-2.105972000	0.001159000
1	-1.743643000	1.729548000	-0.001994000
6	-4.996262000	-0.388338000	-0.000926000
6	-3.878470000	1.767990000	-0.002700000
6	-5.058801000	0.998933000	-0.002320000
1	7.627564000	-0.133236000	0.002581000
8	-3.943170000	3.126190000	-0.004054000
1	-4.871134000	3.394475000	-0.004596000
8	-6.222937000	1.723913000	-0.003394000
1	-6.990254000	1.142665000	-0.003196000
1	-5.912183000	-0.970996000	-0.000635000

5d_R2, optimization in gas phase B3LYP/6-311++G**, E= -909.769512741 a.u. Sum of electronic and thermal Enthalpies= -909.521241 a.u.			
0; 2			
6	6.444420000	0.276912000	0.002131000
6	5.641233000	-0.849673000	0.002641000
6	5.889623000	1.576935000	0.000866000
1	6.056543000	-1.850037000	0.003537000
6	4.245979000	-0.668359000	0.001855000
6	4.515343000	1.788472000	0.000065000
1	4.100660000	2.789612000	-0.000854000
6	3.704805000	0.654338000	0.000583000
6	2.111514000	-0.897509000	0.001140000
7	3.252146000	-1.599548000	0.001931000
7	2.346291000	0.473369000	0.000206000
1	1.609434000	1.160646000	-0.000245000
7	0.895717000	-1.470843000	0.001113000
7	-0.095088000	-0.564188000	0.000094000
6	-1.284986000	-1.105116000	0.000022000
1	-1.366352000	-2.194008000	0.000859000
1	6.555401000	2.432424000	0.000522000
6	-2.501265000	-0.325560000	-0.000729000
6	-3.735887000	-0.998510000	-0.000544000
6	-2.491330000	1.084003000	-0.001623000
1	-3.757048000	-2.081971000	0.000140000
1	-1.552919000	1.621817000	-0.001780000
6	-4.929465000	-0.285827000	-0.001250000
6	-3.675703000	1.794922000	-0.002317000
6	-4.903368000	1.103858000	-0.002130000
1	7.522710000	0.167931000	0.002681000
8	-3.651853000	3.155993000	-0.003183000
1	-4.560712000	3.483216000	-0.003642000
8	-6.018103000	1.901228000	-0.002848000
1	-6.821147000	1.370159000	-0.002884000
1	-5.881319000	-0.807839000	-0.001109000

5d_R3, optimization in gas phase B3LYP/6-311++G**, E= -909.756263865 a.u. Sum of electronic and thermal Enthalpies= -909.507607 a.u.			
0; 2			
6	6.519011000	0.253634000	0.006091000
6	5.690967000	-0.865822000	0.005808000
6	5.992523000	1.555322000	0.002769000
1	6.095282000	-1.870886000	0.008349000
6	4.310057000	-0.661307000	0.002103000
6	4.616053000	1.780691000	-0.000960000
1	4.211504000	2.786251000	-0.003525000
6	3.797636000	0.657971000	-0.001214000
6	2.188059000	-0.851105000	-0.002654000
7	3.270190000	-1.585124000	0.001107000
7	2.413970000	0.498917000	-0.004426000
1	1.696025000	1.205576000	-0.006200000
7	0.915795000	-1.371682000	-0.005589000
7	-0.156894000	-0.564426000	-0.004340000
6	-1.327184000	-1.095648000	-0.002436000
1	-1.448067000	-2.184433000	-0.001267000
1	0.834796000	-2.384341000	-0.000724000

5d_R4, optimization in gas phase B3LYP/6-311++G**, E= -909.771680851 a.u. Sum of electronic and thermal Enthalpies= -909.522434 a.u.			
0; 2			
6	6.525166000	0.238244000	0.005359000
6	5.690773000	-0.875936000	0.005226000
6	6.006278000	1.543385000	0.002408000
1	6.088702000	-1.883494000	0.007481000
6	4.310866000	-0.662634000	0.002054000
6	4.631534000	1.777660000	-0.000786000
1	4.233451000	2.785751000	-0.003071000
6	3.806154000	0.659926000	-0.000893000
6	2.188150000	-0.839267000	-0.001971000
7	3.266087000	-1.579817000	0.001293000
7	2.421782000	0.509272000	-0.003643000
1	1.708065000	1.220240000	-0.005095000
7	0.913599000	-1.353791000	-0.004429000
7	-0.154800000	-0.544191000	-0.003511000
6	-1.327713000	-1.074629000	-0.002009000
1	-1.448170000	-2.163111000	-0.000987000
1	0.829291000	-2.366587000	-0.000247000

1	6.667871000	2.402961000	0.003090000	1	6.686972000	2.386706000	0.002596000
6	-2.549638000	-0.293162000	-0.001816000	6	-2.547017000	-0.273219000	-0.001671000
6	-3.797442000	-0.978204000	0.001098000	6	-3.794438000	-0.978197000	0.000732000
6	-2.550256000	1.087607000	-0.003953000	6	-2.543610000	1.108131000	-0.003575000
1	-3.805955000	-2.062898000	0.002719000	1	-3.777887000	-2.062796000	0.002153000
1	-1.623846000	1.647215000	-0.006296000	1	-1.617842000	1.668281000	-0.005487000
6	-5.007713000	-0.294173000	0.001903000	6	-5.014563000	-0.323812000	0.001274000
6	-3.767801000	1.861921000	-0.003274000	6	-3.770955000	1.842959000	-0.003115000
6	-5.025601000	1.095296000	-0.000172000	6	-5.020660000	1.066817000	-0.000600000
1	7.594776000	0.120132000	0.008909000	1	7.600093000	0.098554000	0.007766000
8	-3.772848000	3.107108000	-0.005176000	8	-3.877398000	3.092458000	-0.004651000
8	-6.151408000	1.823513000	0.000462000	8	-6.142689000	1.776180000	-0.000268000
1	-6.924183000	1.245523000	0.002588000	1	-5.848036000	2.713226000	-0.001948000
1	-5.941823000	-0.848639000	0.004165000	1	-5.950022000	-0.869559000	0.003096000
5d_R5, optimization in gas phase B3LYP/6-311++G**, E= -909.779381655 a.u. Sum of electronic and thermal Enthalpies= -909.530120 a.u.				**5d_R6,** optimization in gas phase B3LYP/6-311++G**, E= -909.731551960 a.u. Sum of electronic and thermal Enthalpies= -909.482318 a.u.			
0; 2				0; 2			
6	6.331090000	0.505998000	0.001997000	6	6.404262000	0.358338000	0.254776000
6	5.592925000	-0.672789000	0.002121000	6	5.638634000	-0.699604000	-0.230506000
6	5.705088000	1.764458000	0.000726000	6	5.809651000	1.546582000	0.706882000
1	6.072609000	-1.643982000	0.003099000	1	6.096624000	-1.617255000	-0.579753000
6	4.199233000	-0.573893000	0.000936000	6	4.251439000	-0.549737000	-0.258017000
6	4.316570000	1.885388000	-0.000479000	6	4.424720000	1.715711000	0.687238000
1	3.836916000	2.857205000	-0.001476000	1	3.966432000	2.634041000	1.036320000
6	3.586096000	0.702942000	-0.000338000	6	3.670009000	0.656004000	0.200257000
6	2.099193000	-0.923854000	-0.000457000	6	2.145360000	-0.788054000	-0.486758000
7	3.235598000	-1.573315000	0.000818000	7	3.264360000	-1.435056000	-0.680187000
7	2.219908000	0.438990000	-0.001358000	7	2.299540000	0.470372000	0.034704000
1	1.449611000	1.088556000	-0.001679000	1	1.545429000	1.094004000	0.273801000
7	0.873530000	-1.544197000	-0.001238000	7	0.903454000	-1.286230000	-0.812258000
7	-0.257152000	-0.833654000	-0.000871000	7	-0.206139000	-0.637413000	-0.343347000
6	-1.382814000	-1.489268000	-0.000128000	6	-1.336977000	-1.162503000	-0.338973000
1	-1.381746000	-2.583824000	0.000419000	1	0.849617000	-2.278692000	-1.014488000
1	0.879621000	-2.561644000	0.000618000	1	6.436465000	2.349212000	1.077830000
1	6.314126000	2.660840000	0.000666000	6	-2.665567000	-0.662362000	-0.136685000
6	-2.654719000	-0.833175000	0.000028000	6	-3.571770000	-1.369582000	0.673248000
6	-3.831422000	-1.650058000	0.001139000	6	-3.096509000	0.506979000	-0.797746000
6	-2.779267000	0.576553000	-0.000875000	1	-3.252741000	-2.278811000	1.166601000
1	-3.710919000	-2.728567000	0.001790000	1	-2.420404000	1.058422000	-1.438522000
1	-1.896791000	1.202533000	-0.001755000	6	-4.868266000	-0.899619000	0.844351000
6	-5.082851000	-1.105268000	0.001376000	6	-4.391344000	0.968666000	-0.630594000
6	-4.026757000	1.143514000	-0.000652000	6	-5.280136000	0.260478000	0.196713000
6	-5.254817000	0.328612000	0.000499000	1	7.483859000	0.264005000	0.284675000
1	7.413817000	0.456599000	0.002891000	8	-4.792074000	2.102731000	-1.267186000
8	-4.216425000	2.468300000	-0.001469000	1	-5.715858000	2.274731000	-1.042644000
1	-5.187552000	2.588351000	-0.001085000	8	-6.538566000	0.798791000	0.293436000
8	-6.350563000	0.921662000	0.000637000	1	-7.099825000	0.260456000	0.860697000
1	-5.976956000	-1.716848000	0.002214000	1	-5.565166000	-1.438081000	1.479219000
5d_Rw1, optimization in solv. water B3LYP/6-311++G**, E= -909.774919774 a.u. Sum of electronic and thermal Enthalpies= -909.526282 a.u.				**5d_Rw2,** optimization in solv. water B3LYP/6-311++G**, E= -909.790869268 a.u. Sum of electronic and thermal Enthalpies= -909.542443 a.u.			
0; 2				0; 2			
6	6.565767000	0.068161000	0.002018000	6	6.449600000	0.276843000	0.002079000
6	5.686302000	-0.988359000	0.002930000	6	5.646955000	-0.851548000	0.002728000
6	6.114955000	1.429649000	0.000541000	6	5.893888000	1.577849000	0.000695000

1	6.030359000	-2.016008000	0.004052000	1	6.069460000	-1.849365000	0.003708000
6	4.301617000	-0.687336000	0.002352000	6	4.251708000	-0.668753000	0.001952000
6	4.776929000	1.758511000	-0.000054000	6	4.519688000	1.788460000	-0.000087000
1	4.446088000	2.790494000	-0.001173000	1	4.099785000	2.786760000	-0.001096000
6	3.844234000	0.698520000	0.000840000	6	3.710698000	0.652128000	0.000565000
6	2.192485000	-0.601032000	0.001699000	6	2.110389000	-0.886860000	0.001309000
7	3.231629000	-1.497807000	0.002952000	7	3.249115000	-1.597177000	0.002102000
7	2.492997000	0.719017000	0.000522000	7	2.350858000	0.475570000	0.000243000
7	0.935358000	-1.098787000	0.001853000	1	1.625860000	1.177692000	-0.000331000
7	-0.166843000	-0.326825000	0.000737000	7	0.894278000	-1.467518000	0.001339000
6	-1.298798000	-0.955904000	0.000871000	7	-0.102526000	-0.569369000	0.000286000
1	-1.333646000	-2.048912000	0.001815000	6	-1.295320000	-1.110107000	0.000033000
1	0.855952000	-2.116319000	0.002786000	1	-1.385620000	-2.198156000	0.000764000
1	6.859802000	2.217323000	-0.000113000	1	6.559421000	2.433232000	0.000240000
6	-2.568212000	-0.260289000	-0.000297000	6	-2.504776000	-0.328675000	-0.000780000
6	-3.751252000	-1.018077000	-0.000127000	6	-3.742070000	-1.001204000	-0.000782000
6	-2.648911000	1.146965000	-0.001594000	6	-2.491143000	1.083630000	-0.001516000
1	-3.699538000	-2.100477000	0.000821000	1	-3.764409000	-2.084449000	-0.000233000
1	-1.748688000	1.747967000	-0.001769000	1	-1.551319000	1.620344000	-0.001528000
6	-4.992101000	-0.390518000	-0.001185000	6	-4.934830000	-0.290074000	-0.001497000
6	-3.879750000	1.772015000	-0.002644000	6	-3.675197000	1.791892000	-0.002204000
6	-5.061567000	0.999161000	-0.002421000	6	-4.908365000	1.102246000	-0.002176000
1	7.633199000	-0.120179000	0.002423000	1	7.527813000	0.167907000	0.002604000
8	-3.951300000	3.133141000	-0.003871000	8	-3.653086000	3.155091000	-0.002889000
1	-4.881407000	3.399716000	-0.004425000	1	-4.562392000	3.485571000	-0.003277000
8	-6.217161000	1.718142000	-0.003489000	8	-6.011685000	1.897436000	-0.002828000
1	-6.992591000	1.143352000	-0.003136000	1	-6.825172000	1.377429000	-0.002664000
1	-5.905415000	-0.974976000	-0.001058000	1	-5.886333000	-0.809979000	-0.001512000
5d_Rw3, optimization in solv. water B3LYP/6-311++G**, E= -909.783399606 a.u. Sum of electronic and thermal Enthalpies= -909.534426 a.u.				**5d_Rw4,** optimization in solv. water B3LYP/6-311++G**, E= -909.790875298 a.u. Sum of electronic and thermal Enthalpies= -909.541811 a.u.			
0; 2				0; 2			
6	6.508891000	0.273521000	0.005058000	6	6.512972000	0.262011000	0.003866000
6	5.691759000	-0.856364000	0.004434000	6	5.691051000	-0.863799000	0.003680000
6	5.967147000	1.570000000	0.002993000	6	5.977005000	1.561318000	0.002156000
1	6.112622000	-1.855295000	0.006034000	1	6.106920000	-1.864763000	0.004995000
6	4.307404000	-0.666601000	0.001654000	6	4.307377000	-0.667189000	0.001720000
6	4.586686000	1.779576000	0.000204000	6	4.597976000	1.777872000	0.000188000
1	4.167249000	2.778552000	-0.001395000	1	4.183363000	2.778808000	-0.001141000
6	3.780061000	0.647548000	-0.000425000	6	3.785959000	0.649521000	0.000009000
6	2.179092000	-0.872349000	-0.002111000	6	2.178929000	-0.862592000	-0.000874000
7	3.275637000	-1.599977000	0.000524000	7	3.271738000	-1.595400000	0.001110000
7	2.400941000	0.476099000	-0.003007000	7	2.406268000	0.484599000	-0.001777000
1	1.681980000	1.183971000	-0.003968000	1	1.690728000	1.195999000	-0.002455000
7	0.914460000	-1.395553000	-0.004719000	7	0.912173000	-1.382158000	-0.002614000
7	-0.154973000	-0.577809000	-0.003741000	7	-0.153701000	-0.564625000	-0.002314000
6	-1.326328000	-1.108864000	-0.002078000	6	-1.327203000	-1.095716000	-0.001406000
1	-1.454828000	-2.194131000	-0.000895000	1	-1.454914000	-2.180892000	-0.000515000
1	0.819165000	-2.407344000	-0.000530000	1	0.815847000	-2.394231000	0.000400000
1	6.632680000	2.425463000	0.003564000	1	6.646793000	2.413429000	0.002355000
6	-2.539295000	-0.292819000	-0.001780000	6	-2.536652000	-0.280100000	-0.001520000
6	-3.794322000	-0.975132000	0.001404000	6	-3.791376000	-0.975871000	0.000461000
6	-2.528408000	1.086384000	-0.004443000	6	-2.519312000	1.101732000	-0.003462000
1	-3.805954000	-2.059032000	0.003471000	1	-3.784846000	-2.059726000	0.001936000
1	-1.595404000	1.636161000	-0.007008000	1	-1.585308000	1.649341000	-0.005060000
6	-4.998392000	-0.288919000	0.001983000	6	-5.002246000	-0.307759000	0.000553000

6	-3.740891000	1.860834000	-0.004071000	6	-3.737004000	1.847220000	-0.003450000
6	-5.002997000	1.103231000	-0.000665000	6	-4.993147000	1.083517000	-0.001361000
1	7.586070000	0.150923000	0.007176000	1	7.589572000	0.134745000	0.005349000
8	-3.745519000	3.114697000	-0.006564000	8	-3.828243000	3.103962000	-0.005087000
8	-6.119910000	1.840513000	-0.000314000	8	-6.115325000	1.797026000	-0.001399000
1	-6.905539000	1.275790000	0.001831000	1	-5.831902000	2.735710000	-0.002933000
1	-5.935227000	-0.835285000	0.004521000	1	-5.942326000	-0.845238000	0.002072000
5d_Rw5, optimization in solv. water B3LYP/6-311++G**, E= -909.798714196 a.u. Sum of electronic and thermal Enthalpies= -909.549523 a.u.				**5d_Rw6,** optimization in solv. water B3LYP/6-311++G**, E= -909.750433510 a.u. Sum of electronic and thermal Enthalpies= -909.501557 a.u.			
0; 2				0; 2			
6	6.309015000	0.536566000	0.001185000	6	6.415666000	0.368519000	0.256399000
6	5.588012000	-0.654273000	0.001375000	6	5.654306000	-0.697233000	-0.224234000
6	5.662825000	1.786512000	0.000449000	6	5.813401000	1.553220000	0.710482000
1	6.087273000	-1.616165000	0.001942000	1	6.123192000	-1.610084000	-0.573589000
6	4.191506000	-0.575552000	0.000809000	6	4.264659000	-0.557136000	-0.244589000
6	4.271934000	1.886533000	-0.000132000	6	4.425583000	1.711271000	0.698020000
1	3.774046000	2.848673000	-0.000709000	1	3.958320000	2.624105000	1.048099000
6	3.558585000	0.692289000	0.000066000	6	3.676296000	0.644688000	0.216229000
6	2.090001000	-0.949940000	0.000200000	6	2.149943000	-0.803005000	-0.461780000
7	3.240878000	-1.587580000	0.000855000	7	3.279108000	-1.447468000	-0.662837000
7	2.199327000	0.410874000	-0.000419000	7	2.308016000	0.451117000	0.060456000
1	1.425296000	1.058834000	-0.000429000	1	1.558595000	1.085274000	0.292980000
7	0.872994000	-1.580610000	-0.000130000	7	0.913994000	-1.302262000	-0.780540000
7	-0.255041000	-0.869854000	-0.000104000	7	-0.198799000	-0.627044000	-0.340842000
6	-1.382148000	-1.526959000	0.000311000	6	-1.333707000	-1.143486000	-0.371960000
1	-1.388997000	-2.618789000	0.000763000	1	0.843702000	-2.293132000	-0.987363000
1	0.873018000	-2.598850000	0.001011000	1	6.435520000	2.361330000	1.077527000
1	6.258338000	2.692014000	0.000321000	6	-2.665799000	-0.649357000	-0.197603000
6	-2.642589000	-0.852059000	0.000196000	6	-3.572371000	-1.331235000	0.635864000
6	-3.831881000	-1.649372000	0.000791000	6	-3.104172000	0.486227000	-0.914203000
6	-2.746722000	0.561653000	-0.000517000	1	-3.249999000	-2.214940000	1.171811000
1	-3.730767000	-2.729112000	0.001333000	1	-2.427769000	1.016555000	-1.572803000
1	-1.853623000	1.173336000	-0.000979000	6	-4.874943000	-0.869238000	0.778443000
6	-5.073637000	-1.080151000	0.000674000	6	-4.405360000	0.936875000	-0.775711000
6	-3.984262000	1.146669000	-0.000636000	6	-5.296381000	0.257509000	0.076642000
6	-5.221441000	0.353259000	-0.000061000	1	7.496110000	0.281553000	0.280621000
1	7.392451000	0.503050000	0.001608000	8	-4.816388000	2.039563000	-1.465932000
8	-4.146320000	2.482011000	-0.001303000	1	-5.742570000	2.216853000	-1.249345000
1	-5.111865000	2.631073000	-0.001249000	8	-6.554169000	0.783273000	0.138616000
8	-6.316336000	0.963987000	-0.000230000	1	-7.116442000	0.278012000	0.738412000
1	-5.974692000	-1.681906000	0.001119000	1	-5.571706000	-1.385144000	1.430012000
5d_Rb1, optimization in solv. benzene B3LYP/6-311++G**, E= -909.760443922 a.u. Sum of electronic and thermal Enthalpies= -909.512000 a.u.				**5d_Rb2,** optimization in solv. benzene B3LYP/6-311++G**, E= -909.778426951 a.u. Sum of electronic and thermal Enthalpies= -909.530100 a.u.			
0; 2				0; 2			
6	6.563214000	0.060159000	0.001883000	6	6.447706000	0.275044000	0.002010000
6	5.682449000	-0.992959000	0.003178000	6	5.644234000	-0.851884000	0.002621000
6	6.116871000	1.425560000	0.000017000	6	5.893412000	1.575886000	0.000711000
1	6.020552000	-2.022368000	0.004603000	1	6.061904000	-1.851445000	0.003548000
6	4.297839000	-0.687531000	0.002609000	6	4.249015000	-0.669306000	0.001900000
6	4.782522000	1.760858000	-0.000588000	6	4.519274000	1.787814000	-0.000022000
1	4.452544000	2.792753000	-0.002005000	1	4.102769000	2.788009000	-0.000969000
6	3.844157000	0.704655000	0.000699000	6	3.708881000	0.653090000	0.000593000
6	2.194271000	-0.584843000	0.001993000	6	2.111638000	-0.892407000	0.001283000
7	3.227499000	-1.491305000	0.003554000	7	3.250999000	-1.598719000	0.002076000

7	2.496915000	0.732844000	0.000453000
7	0.937037000	-1.084324000	0.002360000
7	-0.170393000	-0.321652000	0.001055000
6	-1.295864000	-0.954357000	0.000961000
1	-1.323923000	-2.049700000	0.001728000
1	0.867343000	-2.102232000	0.003544000
1	6.865994000	2.209420000	-0.000925000
6	-2.572119000	-0.263794000	-0.000296000
6	-3.753642000	-1.020910000	-0.000632000
6	-2.650347000	1.141920000	-0.001155000
1	-3.704284000	-2.103773000	-0.000032000
1	-1.747398000	1.738908000	-0.000915000
6	-4.994184000	-0.390422000	-0.001754000
6	-3.881275000	1.769762000	-0.002274000
6	-5.060998000	0.997711000	-0.002540000
1	7.630425000	-0.130734000	0.002280000
8	-3.950594000	3.129079000	-0.003071000
1	-4.879751000	3.395575000	-0.003730000
8	-6.223008000	1.718224000	-0.003594000
1	-6.992400000	1.137936000	-0.003535000
1	-5.908959000	-0.974133000	-0.002013000

5d_Rb3, optimization in solv. benzene
B3LYP/6-311++G**, E= -909.767633612 a.u.
Sum of electronic and thermal Enthalpies= -909.518737 a.u.

0; 2			
6	6.513948000	0.264244000	0.005709000
6	5.691954000	-0.860668000	0.005583000
6	5.979605000	1.563165000	0.002435000
1	6.104422000	-1.862698000	0.008098000
6	4.309363000	-0.664147000	0.002087000
6	4.601192000	1.780167000	-0.001068000
1	4.188860000	2.782443000	-0.003602000
6	3.789263000	0.652381000	-0.001178000
6	2.184797000	-0.862879000	-0.002363000
7	3.273745000	-1.593136000	0.001263000
7	2.407749000	0.486586000	-0.004203000
1	1.688631000	1.192959000	-0.005937000
7	0.915756000	-1.384878000	-0.005171000
7	-0.155350000	-0.572497000	-0.003948000
6	-1.326514000	-1.102495000	-0.002108000
1	-1.451690000	-2.189731000	-0.001019000
1	0.827990000	-2.397107000	-0.000220000
1	6.649867000	2.414894000	0.002622000
6	-2.544415000	-0.293079000	-0.001556000
6	-3.795882000	-0.975648000	0.000842000
6	-2.539609000	1.086840000	-0.003281000
1	-3.807135000	-2.059959000	0.002273000
1	-1.610211000	1.641838000	-0.005132000
6	-5.003263000	-0.290066000	0.001392000
6	-3.754904000	1.862453000	-0.002735000
6	-5.015031000	1.100635000	-0.000400000
1	7.590495000	0.136630000	0.008362000
8	-3.758648000	3.110974000	-0.004175000
8	-6.137045000	1.831773000	-0.000089000
1	-6.915081000	1.259067000	0.001445000
1	-5.939002000	-0.840271000	0.003213000

7	2.349805000	0.474890000	0.000284000
1	1.618212000	1.168632000	-0.000208000
7	0.895350000	-1.467421000	0.001309000
7	-0.097613000	-0.563358000	0.000286000
6	-1.288570000	-1.104215000	0.000138000
1	-1.373318000	-2.192796000	0.000904000
1	6.559698000	2.430889000	0.000285000
6	-2.502874000	-0.324687000	-0.000673000
6	-3.737604000	-0.998924000	-0.000675000
6	-2.493268000	1.085903000	-0.001447000
1	-3.758009000	-2.082284000	-0.000092000
1	-1.555035000	1.624487000	-0.001460000
6	-4.931643000	-0.288127000	-0.001448000
6	-3.678403000	1.794419000	-0.002198000
6	-4.907312000	1.102513000	-0.002200000
1	7.525916000	0.165434000	0.002506000
8	-3.656685000	3.156619000	-0.002936000
1	-4.565997000	3.484529000	-0.003411000
8	-6.019107000	1.896530000	-0.002959000
1	-6.825130000	1.367763000	-0.003034000
1	-5.882967000	-0.810032000	-0.001474000

5d_Rb4, optimization in solv. benzene
B3LYP/6-311++G**, E= -909.779867292 a.u.
Sum of electronic and thermal Enthalpies= -909.530703 a.u.

0; 2			
6	6.518128000	0.252195000	0.005225000
6	5.691212000	-0.868500000	0.004557000
6	5.989754000	1.553999000	0.003094000
1	6.098541000	-1.872570000	0.006186000
6	4.309330000	-0.664911000	0.001693000
6	4.612817000	1.778208000	0.000223000
1	4.205562000	2.782517000	-0.001427000
6	3.795320000	0.654274000	-0.000426000
6	2.184456000	-0.853096000	-0.002151000
7	3.269833000	-1.588583000	0.000540000
7	2.413276000	0.495173000	-0.003061000
1	1.697487000	1.204936000	-0.004086000
7	0.913336000	-1.370747000	-0.004621000
7	-0.153844000	-0.557570000	-0.003726000
6	-1.327499000	-1.087070000	-0.002319000
1	-1.452410000	-2.174082000	-0.001339000
1	0.823702000	-2.383236000	-0.001128000
1	6.664384000	2.402240000	0.003687000
6	-2.541605000	-0.277689000	-0.001919000
6	-3.793386000	-0.976383000	0.001547000
6	-2.530199000	1.103712000	-0.004692000
1	-3.783155000	-2.060581000	0.003708000
1	-1.600299000	1.657273000	-0.007470000
6	-5.008518000	-0.314156000	0.002288000
6	-3.752227000	1.845431000	-0.004067000
6	-5.005983000	1.076787000	-0.000458000
1	7.594042000	0.119775000	0.007414000
8	-3.849416000	3.098102000	-0.006356000
8	-6.127330000	1.789238000	0.000000000
1	-5.837257000	2.726798000	-0.002378000
1	-5.946889000	-0.854735000	0.004941000

5d_Rb5, optimization in solv. benzene B3LYP/6-311++G**, E= -909.787589566 a.u. Sum of electronic and thermal Enthalpies= -909.538501 a.u.			
0; 2			
6	6.328975000	0.508394000	0.001611000
6	5.592213000	-0.671765000	0.001956000
6	5.700680000	1.766388000	0.000371000
1	6.075221000	-1.641514000	0.002909000
6	4.197816000	-0.574372000	0.001029000
6	4.311707000	1.885360000	-0.000572000
1	3.829618000	2.855722000	-0.001542000
6	3.582522000	0.701596000	-0.000213000
6	2.095257000	-0.924498000	0.000018000
7	3.234802000	-1.574332000	0.001130000
7	2.217708000	0.437011000	-0.000957000
1	1.449898000	1.090701000	-0.001261000
7	0.871277000	-1.545097000	-0.000521000
7	-0.258311000	-0.834267000	-0.000399000
6	-1.382390000	-1.494574000	0.000040000
1	-1.377999000	-2.588078000	0.000402000
1	0.871391000	-2.562742000	0.001082000
1	6.308426000	2.663685000	0.000129000
6	-2.652887000	-0.837375000	0.000070000
6	-3.830879000	-1.652061000	0.000780000
6	-2.776274000	0.573393000	-0.000568000
1	-3.713406000	-2.730674000	0.001270000
1	-1.892728000	1.198111000	-0.001115000
6	-5.081040000	-1.103348000	0.000849000
6	-4.022364000	1.141833000	-0.000502000
6	-5.250312000	0.329737000	0.000200000
1	7.411804000	0.460314000	0.002302000
8	-4.206274000	2.470352000	-0.001080000
1	-5.175530000	2.599190000	-0.000887000
8	-6.348700000	0.924305000	0.000201000
1	-5.975045000	-1.715235000	0.001382000

5d_Rb6, optimization in solv. benzene B3LYP/6-311++G**, E= -909.739695530 a.u. Sum of electronic and thermal Enthalpies= -909.490632 a.u.			
0; 2			
6	6.398949000	0.388139000	0.307448000
6	5.644255000	-0.705344000	-0.114417000
6	5.791548000	1.595878000	0.685856000
1	6.114423000	-1.637033000	-0.406350000
6	4.255235000	-0.570845000	-0.153440000
6	4.404410000	1.749535000	0.653662000
1	3.934964000	2.682025000	0.945177000
6	3.661111000	0.654685000	0.230562000
6	2.148159000	-0.838837000	-0.372768000
7	3.276557000	-1.488012000	-0.525258000
7	2.293639000	0.447604000	0.074439000
1	1.536506000	1.084027000	0.268948000
7	0.913618000	-1.362883000	-0.670335000
7	-0.203709000	-0.678303000	-0.271770000
6	-1.337319000	-1.198868000	-0.268226000
1	0.856976000	-2.363908000	-0.823904000
1	6.409541000	2.425817000	1.008489000
6	-2.666513000	-0.679030000	-0.130433000
6	-3.604906000	-1.339078000	0.682985000
6	-3.063545000	0.463414000	-0.857639000
1	-3.312290000	-2.228388000	1.226631000
1	-2.361876000	0.977088000	-1.502483000
6	-4.900426000	-0.848468000	0.794751000
6	-4.356647000	0.945418000	-0.748778000
6	-5.279148000	0.286590000	0.083970000
1	7.479384000	0.306094000	0.344573000
8	-4.725981000	2.054892000	-1.447780000
1	-5.653411000	2.249152000	-1.256126000
8	-6.529159000	0.843629000	0.118435000
1	-7.113345000	0.351576000	0.705749000
1	-5.622487000	-1.350044000	1.431119000

5d_RC, optimization in gas phase B3LYP/6-311++G**, E= -910.157599623 a.u. Sum of electronic and thermal Enthalpies= -909.895365 a.u.			
1; 2			
6	6.348010000	0.424989000	0.000521000
6	5.588323000	-0.723301000	0.000948000
6	5.747792000	1.712155000	-0.000073000
1	6.031057000	-1.711005000	0.001393000
6	4.183746000	-0.574659000	0.000782000
6	4.365961000	1.892135000	-0.000266000
1	3.927300000	2.881910000	-0.000735000
6	3.599689000	0.737446000	0.000180000
6	2.074026000	-0.843187000	0.000750000
7	3.218754000	-1.527410000	0.001120000
7	2.233667000	0.513566000	0.000107000
1	1.484398000	1.190143000	0.000097000
7	0.874117000	-1.455218000	0.000963000
7	-0.267978000	-0.751134000	0.000640000
6	-1.372252000	-1.442008000	0.000911000
1	-1.336784000	-2.535786000	0.001389000
1	0.891557000	-2.477025000	0.001409000

5d_RCw, optimization in solv. water B3LYP/6-311++G**, E= -910.228407305 a.u. Sum of electronic and thermal Enthalpies= -909.966466 a.u.			
1; 2			
6	6.307961000	0.485516000	0.000388000
6	5.578426000	-0.684893000	0.000688000
6	5.674395000	1.756294000	0.000050000
1	6.053645000	-1.657714000	0.000942000
6	4.172224000	-0.576609000	0.000651000
6	4.291295000	1.895118000	-0.000010000
1	3.817433000	2.868151000	-0.000275000
6	3.554265000	0.716198000	0.000300000
6	2.067932000	-0.896604000	0.000721000
7	3.227636000	-1.556446000	0.000907000
7	2.200293000	0.461428000	0.000297000
1	1.438064000	1.125786000	0.000386000
7	0.873172000	-1.522680000	0.000902000
7	-0.261714000	-0.821007000	0.000715000
6	-1.371669000	-1.507451000	0.000969000
1	-1.350996000	-2.598932000	0.001340000
1	0.885335000	-2.544762000	0.001190000

1	6.389442000	2.585190000	-0.000398000
6	-2.668361000	-0.830060000	0.000626000
6	-3.802925000	-1.672436000	0.000986000
6	-2.839748000	0.570637000	-0.000011000
1	-3.678316000	-2.748826000	0.001471000
1	-1.984844000	1.233029000	-0.000296000
6	-5.076363000	-1.131268000	0.000711000
6	-4.105049000	1.116233000	-0.000289000
6	-5.235348000	0.255300000	0.000074000
1	7.428686000	0.356274000	0.000631000
8	-4.261026000	2.455096000	-0.000903000
1	-5.201508000	2.681300000	-0.001005000
8	-6.424521000	0.892200000	-0.000247000
1	-7.171228000	0.280641000	0.000033000
1	-5.949426000	-1.774717000	0.000983000

1	6.292082000	2.646286000	-0.000176000
6	-2.650540000	-0.863286000	0.000702000
6	-3.809316000	-1.672623000	0.000970000
6	-2.781265000	0.543974000	0.000132000
1	-3.712023000	-2.751397000	0.001410000
1	-1.903667000	1.176862000	-0.000073000
6	-5.067040000	-1.096527000	0.000650000
6	-4.030551000	1.120572000	-0.000199000
6	-5.186152000	0.295020000	0.000036000
1	7.390248000	0.444200000	0.000407000
8	-4.158681000	2.470861000	-0.000770000
1	-5.097469000	2.706506000	-0.000938000
8	-6.356353000	0.963282000	-0.000380000
1	-7.116554000	0.366599000	-0.000282000
1	-5.959573000	-1.711515000	0.000855000

5d_RCb, optimization in gas phase
B3LYP/6-311++G**, E= -910.195571425 a.u.
Sum of electronic and thermal Enthalpies= -909.933204 a.u.

1; 2

6	6.337116000	0.444893000	-0.023526000
6	5.584871000	-0.708320000	0.013300000
6	5.728805000	1.727833000	-0.064905000
1	6.035921000	-1.691699000	0.045428000
6	4.179934000	-0.569614000	0.008693000
6	4.347222000	1.897583000	-0.071520000
1	3.898494000	2.882122000	-0.102795000
6	3.587729000	0.736965000	-0.034794000
6	2.070789000	-0.848944000	0.020983000
7	3.219713000	-1.528066000	0.042053000
7	2.225618000	0.506886000	-0.026079000
1	1.475469000	1.183272000	-0.049182000
7	0.871875000	-1.461519000	0.048630000
7	-0.267155000	-0.756969000	0.024045000
6	-1.370364000	-1.447884000	0.086103000
1	-1.332673000	-2.537614000	0.167557000
1	0.880522000	-2.482756000	0.082635000
1	6.364871000	2.604399000	-0.091985000
6	-2.663369000	-0.830931000	0.051781000
6	-3.802982000	-1.661551000	0.136649000
6	-2.825622000	0.566617000	-0.069067000
1	-3.684519000	-2.734407000	0.229897000
1	-1.964362000	1.217464000	-0.136945000
6	-5.072689000	-1.112905000	0.101013000
6	-4.087428000	1.117460000	-0.106493000
6	-5.222997000	0.269076000	-0.022220000
1	7.418206000	0.382859000	-0.020934000
8	-4.239811000	2.455578000	-0.224028000
1	-5.181152000	2.678697000	-0.238926000
8	-6.409750000	0.908033000	-0.071603000
1	-7.156326000	0.297757000	-0.015043000
1	-5.951424000	-1.744212000	0.167847000

5d_M, optimization in gas phase
B3LYP/6-311++G**, E= -910.403405101 a.u.
Sum of electronic and thermal Enthalpies= -910.141696 a.u.

0; 1

6	6.312687000	0.556319000	0.003950000
6	5.597824000	-0.639485000	0.003620000
6	5.661582000	1.799660000	0.001771000
1	6.099692000	-1.599674000	0.005308000
6	4.203689000	-0.573191000	0.001031000
6	4.268864000	1.887166000	-0.000842000
1	3.766876000	2.847995000	-0.002551000
6	3.564700000	0.689844000	-0.001154000
6	2.109324000	-0.971348000	-0.002346000
7	3.259986000	-1.594942000	0.000242000
7	2.203609000	0.395362000	-0.003476000
1	1.418348000	1.026041000	-0.004516000
7	0.894013000	-1.607351000	-0.004566000
7	-0.254019000	-0.897350000	-0.003076000
6	-1.365820000	-1.540536000	-0.001300000
1	-1.377667000	-2.636315000	-0.000582000
1	0.903827000	-2.622507000	-0.000815000
1	6.249877000	2.709953000	0.002095000
6	-2.664517000	-0.873581000	-0.000269000
6	-3.827526000	-1.654206000	0.002026000
6	-2.783005000	0.526629000	-0.001537000
1	-3.754186000	-2.735823000	0.002984000
1	-1.900337000	1.152424000	-0.003363000
6	-5.085204000	-1.052852000	0.003074000
6	-4.029418000	1.127074000	-0.000519000
6	-5.188740000	0.330365000	0.001818000
1	7.396452000	0.528350000	0.005923000
8	-4.126572000	2.485550000	-0.001820000
1	-5.061589000	2.728461000	-0.000557000
8	-6.374082000	1.026761000	0.002696000
1	-7.124332000	0.424044000	0.004389000
1	-5.983490000	-1.662631000	0.004864000

5d_Mw, optimization in solv. water
B3LYP/6-311++G**, E= -910.423657288 a.u.
Sum of electronic and thermal Enthalpies= -910.162145 a.u.

0; 1

6	6.300335000	0.580230000	0.003177000

5d_Mb, optimization in solv. water
B3LYP/6-311++G**, E= -910.411968821 a.u.
Sum of electronic and thermal Enthalpies= -910.150574 a.u.

0; 1

6	6.308578000	0.564774000	0.003840000

6	5.600029000	-0.626831000	0.002721000	6	5.598795000	-0.635107000	0.003126000
6	5.631699000	1.815089000	0.001714000	6	5.651270000	1.805127000	0.002208000
1	6.120561000	-1.577792000	0.003877000	1	6.107656000	-1.591840000	0.004419000
6	4.203891000	-0.578838000	0.000750000	6	4.203899000	-0.575378000	0.000721000
6	4.236147000	1.883099000	-0.000272000	6	4.257390000	1.885482000	-0.000198000
1	3.717708000	2.834695000	-0.001412000	1	3.749525000	2.843006000	-0.001463000
6	3.547751000	0.675971000	-0.000708000	6	3.558798000	0.684740000	-0.000883000
6	2.104396000	-0.998611000	-0.001857000	6	2.107011000	-0.980777000	-0.002497000
7	3.270988000	-1.611758000	0.000004000	7	3.263903000	-1.600917000	-0.000336000
7	2.192612000	0.366589000	-0.002500000	7	2.199992000	0.385284000	-0.003081000
1	1.404980000	0.996981000	-0.003165000	1	1.414583000	1.016894000	-0.003887000
7	0.898346000	-1.637418000	-0.003713000	7	0.895171000	-1.617060000	-0.004676000
7	-0.249688000	-0.914279000	-0.002539000	7	-0.253002000	-0.901582000	-0.003204000
6	-1.362272000	-1.556901000	-0.000961000	6	-1.364280000	-1.545967000	-0.001348000
1	-1.380180000	-2.650397000	-0.000204000	1	-1.376117000	-2.640852000	-0.000478000
1	0.893126000	-2.652885000	-0.000485000	1	0.897476000	-2.632289000	-0.001451000
1	6.207164000	2.733623000	0.002119000	1	6.234906000	2.718469000	0.002819000
6	-2.655706000	-0.878331000	-0.000114000	6	-2.661732000	-0.876064000	-0.000276000
6	-3.824954000	-1.650748000	0.002039000	6	-3.827051000	-1.653740000	0.002536000
6	-2.763722000	0.524263000	-0.001448000	6	-2.776288000	0.524987000	-0.002026000
1	-3.758330000	-2.732672000	0.003089000	1	-3.756436000	-2.735573000	0.003912000
1	-1.875724000	1.143831000	-0.003140000	1	-1.891616000	1.148318000	-0.004260000
6	-5.079710000	-1.042201000	0.002835000	6	-5.083790000	-1.049675000	0.003592000
6	-4.007211000	1.130243000	-0.000644000	6	-4.021414000	1.127408000	-0.000970000
6	-5.175014000	0.343424000	0.001490000	6	-5.184060000	0.334609000	0.001842000
1	7.384468000	0.565799000	0.004692000	1	7.392519000	0.541513000	0.005693000
8	-4.097354000	2.493580000	-0.001956000	8	-4.115893000	2.487940000	-0.002702000
1	-5.031967000	2.743529000	-0.001066000	1	-5.050814000	2.733616000	-0.001539000
8	-6.348751000	1.047311000	0.002063000	8	-6.364304000	1.034276000	0.002619000
1	-7.110501000	0.455494000	0.003613000	1	-7.119883000	0.436779000	0.004668000
1	-5.982270000	-1.643882000	0.004507000	1	-5.983943000	-1.656196000	0.005782000

5e_A1, optimization in gas phase B3LYP/6-311++G**, E= -985.127417097 a.u. Sum of electronic and thermal Enthalpies= -984.874954 a.u.			
-1; 1			
6	-6.116973000	1.604239000	0.000403000
6	-4.731033000	1.794882000	0.000229000
6	-6.679358000	0.321822000	0.000414000
1	-4.300482000	2.790280000	0.000218000
6	-3.893495000	0.674226000	0.000069000
6	-5.861392000	-0.818714000	0.000246000
1	-6.294328000	-1.814467000	0.000249000
6	-4.487764000	-0.623410000	0.000081000
6	-2.239207000	-0.718056000	-0.000189000
7	-2.521596000	0.590627000	-0.000121000
7	-3.410640000	-1.484255000	-0.000116000
1	-7.758170000	0.205505000	0.000549000
1	-3.412396000	-2.490097000	-0.000104000
7	-1.077515000	-1.388962000	-0.000372000
7	-0.006329000	-0.580172000	-0.000464000
6	1.177114000	-1.117599000	-0.000306000
1	1.292147000	-2.205056000	-0.000122000
6	2.358725000	-0.274175000	-0.000345000
6	3.661006000	-0.806503000	-0.000179000
6	2.232567000	1.135714000	-0.000581000
6	4.794564000	0.003137000	-0.000244000
6	3.370071000	1.941412000	-0.000644000
6	4.648011000	1.389074000	-0.000475000
1	-6.772412000	2.469944000	0.000530000
1	5.791590000	-0.421034000	-0.000119000
8	1.045011000	1.781215000	-0.000740000
1	0.320505000	1.069283000	-0.000640000
1	3.778658000	-1.885446000	0.000000000
8	3.248111000	3.316266000	-0.000884000
1	2.297300000	3.502952000	-0.000985000
8	5.753689000	2.211176000	-0.000543000
1	5.430856000	3.121131000	-0.000710000

5e_A2, optimization in gas phase B3LYP/6-311++G**, E= -985.125266511 a.u. Sum of electronic and thermal Enthalpies= -984.872826 a.u.			
-1; 1			
6	-6.029312000	1.689706000	0.021844000
6	-4.641946000	1.816959000	0.187545000
6	-6.608757000	0.436928000	-0.219379000
1	-4.190220000	2.785352000	0.379205000
6	-3.877139000	0.662874000	0.099008000
6	-5.832557000	-0.722237000	-0.306979000
1	-6.285311000	-1.689725000	-0.495163000
6	-4.444935000	-0.620349000	-0.149316000
6	-2.314041000	-0.956568000	0.015969000
7	-2.522862000	0.418064000	0.217028000
7	-3.474520000	-1.588316000	-0.195602000
1	-7.685462000	0.366403000	-0.341092000
1	-1.789344000	1.101804000	0.283848000
7	-1.114128000	-1.562588000	0.021835000
7	-0.104174000	-0.745062000	0.358073000
6	1.111746000	-1.222137000	0.286688000
1	1.265565000	-2.243356000	-0.065729000
6	2.257706000	-0.426998000	0.681664000
6	3.577283000	-0.905249000	0.569245000
6	2.089991000	0.872192000	1.214335000
6	4.676984000	-0.143873000	0.957483000
6	3.188635000	1.631204000	1.603237000
6	4.484386000	1.134186000	1.477874000
1	-6.657793000	2.571966000	0.083856000
1	5.686669000	-0.525569000	0.863554000
8	0.863922000	1.435853000	1.381199000
1	0.210541000	0.729090000	1.060737000
1	3.735088000	-1.900220000	0.166440000
8	3.020538000	2.897291000	2.128326000
1	2.067338000	3.060637000	2.157401000
8	5.559159000	1.902208000	1.866894000
1	5.208453000	2.735389000	2.205690000

5e_A3, optimization in gas phase B3LYP/6-311++G**, E= -985.114074842 a.u. Sum of electronic and thermal Enthalpies= -984.860996 a.u.			
-1; 1			
6	-6.048732000	1.617593000	0.000187000
6	-4.650204000	1.746265000	-0.000017000
6	-6.658551000	0.365267000	0.000373000
1	-4.176734000	2.720804000	-0.000156000
6	-3.888607000	0.587070000	-0.000026000
6	-5.891083000	-0.812237000	0.000357000
1	-6.366019000	-1.787131000	0.000497000
6	-4.511549000	-0.686832000	0.000157000
6	-2.249226000	-0.990960000	-0.000073000
7	-2.525765000	0.368791000	-0.000197000
7	-3.490128000	-1.626109000	0.000062000
1	-7.740366000	0.292531000	0.000529000
1	-1.741058000	1.014200000	-0.000262000
1	-3.581085000	-2.626837000	0.000374000
7	-1.096653000	-1.563994000	-0.000074000
7	-0.121559000	-0.556065000	-0.000217000

5e_A4, optimization in gas phase B3LYP/6-311++G**, E= -985.111790321 a.u. Sum of electronic and thermal Enthalpies= -984.858317 a.u.			
-1; 1			
6	-6.231839000	1.529535000	0.061910000
6	-4.863085000	1.702674000	0.323206000
6	-6.740571000	0.290888000	-0.321759000
1	-4.467766000	2.666297000	0.621987000
6	-4.033130000	0.601862000	0.186573000
6	-5.900841000	-0.826081000	-0.460391000
1	-6.298358000	-1.789352000	-0.759279000
6	-4.549740000	-0.655664000	-0.203370000
6	-2.291492000	-0.874429000	0.094147000
7	-2.668609000	0.435790000	0.367769000
7	-3.475177000	-1.530533000	-0.244268000
1	-7.801232000	0.182638000	-0.517830000
1	-1.982747000	1.134283000	0.604401000
1	-3.487172000	-2.501666000	-0.503214000
7	-1.134643000	-1.429336000	0.122399000
7	-0.133830000	-0.536885000	0.512981000

6	1.099593000	-0.968358000	-0.000232000
1	1.291846000	-2.049955000	-0.000143000
6	2.254651000	-0.105943000	-0.000356000
6	3.532851000	-0.720836000	-0.000361000
6	2.174361000	1.336976000	-0.000471000
6	4.720480000	-0.011996000	-0.000473000
6	3.438134000	2.024889000	-0.000585000
6	4.657772000	1.396461000	-0.000589000
1	-6.661128000	2.512435000	0.000202000
1	5.685135000	-0.505008000	-0.000476000
8	1.133972000	2.076106000	-0.000495000
1	3.571161000	-1.807365000	-0.000274000
8	3.351752000	3.399499000	-0.000694000
1	2.370456000	3.513611000	-0.000650000
8	5.827792000	2.135812000	-0.000703000
1	5.559946000	3.063678000	-0.000772000

5e_A5, optimization in gas phase
B3LYP/6-311++G**, E= -985.117585857 a.u.
Sum of electronic and thermal Enthalpies= -984.863949 a.u.

-1; 1

6	-6.105545000	1.584150000	0.000170000
6	-4.710286000	1.740452000	-0.000049000
6	-6.690007000	0.319599000	0.000383000
1	-4.256956000	2.724548000	-0.000212000
6	-3.927451000	0.596080000	-0.000042000
6	-5.900260000	-0.842202000	0.000383000
1	-6.355716000	-1.826168000	0.000545000
6	-4.523508000	-0.689116000	0.000171000
6	-2.255456000	-0.949891000	-0.000069000
7	-2.558717000	0.403399000	-0.000226000
7	-3.483045000	-1.607720000	0.000085000
1	-7.770057000	0.225641000	0.000550000
1	-1.795211000	1.069269000	-0.000288000
1	-3.553193000	-2.610298000	0.000407000
7	-1.097238000	-1.510915000	-0.000059000
7	-0.117149000	-0.508605000	-0.000211000
6	1.095525000	-0.940649000	-0.000242000
1	1.269985000	-2.023203000	-0.000168000
6	2.276458000	-0.102377000	-0.000363000
6	3.535282000	-0.758167000	-0.000384000
6	2.271115000	1.306926000	-0.000456000
6	4.730281000	-0.045481000	-0.000494000
6	3.470002000	2.062299000	-0.000567000
6	4.689635000	1.347099000	-0.000584000
1	-6.735589000	2.466447000	0.000172000
1	5.688226000	-0.555231000	-0.000510000
8	1.139714000	2.075657000	-0.000446000
1	1.527072000	2.979576000	-0.000524000
1	3.553248000	-1.843051000	-0.000314000
8	3.445174000	3.361779000	-0.000657000
8	5.820170000	2.121039000	-0.000695000
1	5.446586000	3.026930000	-0.000734000

5e_A7, optimization in gas phase
B3LYP/6-311++G**, E= -985.115010121 a.u.
Sum of electronic and thermal Enthalpies= -984.861553 a.u.

-1; 1

6	1.070181000	-1.027568000	0.453063000
1	1.189065000	-2.056482000	0.101200000
6	2.264815000	-0.315804000	0.812635000
6	3.501051000	-0.990523000	0.641837000
6	2.244004000	1.016233000	1.315339000
6	4.694712000	-0.355264000	0.956488000
6	3.442664000	1.699630000	1.644614000
6	4.650511000	0.949624000	1.440720000
1	-6.899946000	2.377197000	0.161976000
1	5.651813000	-0.851895000	0.833688000
8	1.059518000	1.677559000	1.496973000
1	0.354228000	1.052938000	1.236219000
1	3.497432000	-2.006408000	0.260804000
8	3.562797000	2.895595000	2.100892000
8	5.766644000	1.648705000	1.775065000
1	5.349577000	2.502757000	2.070149000

5e_A6, optimization in gas phase
B3LYP/6-311++G**, E= -985.111353986 a.u.
Sum of electronic and thermal Enthalpies= -984.858117 a.u.

-1; 1

6	-6.260592000	1.514022000	0.000374000
6	-4.875327000	1.753125000	0.000256000
6	-6.765728000	0.217041000	0.000287000
1	-4.483106000	2.763403000	0.000330000
6	-4.027010000	0.658058000	0.000049000
6	-5.907225000	-0.895740000	0.000077000
1	-6.302751000	-1.905132000	0.000011000
6	-4.541016000	-0.661261000	-0.000039000
6	-2.252783000	-0.789287000	-0.000219000
7	-2.645628000	0.549328000	-0.000113000
7	-3.450155000	-1.513421000	-0.000263000
1	-7.838047000	0.057387000	0.000383000
1	-1.964825000	1.289888000	0.000095000
1	-3.460900000	-2.518319000	-0.000145000
7	-1.084307000	-1.312068000	-0.000246000
7	-0.057972000	-0.369755000	-0.000236000
6	1.146131000	-0.901560000	0.000149000
1	1.223013000	-1.992256000	0.000342000
6	2.349231000	-0.157804000	-0.000088000
6	3.613676000	-0.809378000	-0.000081000
6	2.373094000	1.273353000	-0.000459000
6	4.791608000	-0.109903000	-0.000416000
6	3.544746000	1.990352000	-0.000824000
6	4.847675000	1.344121000	-0.000829000
1	-6.942259000	2.356903000	0.000539000
1	5.748168000	-0.622357000	-0.000407000
8	1.195309000	1.992011000	-0.000332000
1	0.467174000	1.324511000	0.000223000
1	3.626502000	-1.897109000	0.000178000
8	3.501806000	3.369122000	-0.001194000
1	2.565311000	3.604852000	-0.001157000
8	5.923036000	1.985155000	-0.001156000

5e_Aw1, optimization in solv.water
B3LYP/6-311++G**, E= -985.203873001 a.u.
Sum of electronic and thermal Enthalpies= -984.951442 a.u.

-1; 1

6	-6.203323000	1.521035000	0.000204000	6	-6.098156000	1.617803000	0.000011000
6	-4.812254000	1.718957000	-0.000021000	6	-4.709981000	1.796298000	-0.000074000
6	-6.748695000	0.239939000	0.000402000	6	-6.669394000	0.337975000	0.000181000
1	-4.389532000	2.716731000	-0.000170000	1	-4.276618000	2.790941000	-0.000204000
6	-3.994644000	0.599341000	-0.000036000	6	-3.887735000	0.664827000	0.000012000
6	-5.923499000	-0.897935000	0.000379000	6	-5.864616000	-0.810252000	0.000271000
1	-6.349135000	-1.895179000	0.000529000	1	-6.303472000	-1.801891000	0.000402000
6	-4.551594000	-0.704419000	0.000160000	6	-4.488286000	-0.624458000	0.000184000
6	-2.274189000	-0.897815000	-0.000090000	6	-2.244661000	-0.754458000	0.000084000
7	-2.621227000	0.447827000	-0.000234000	7	-2.508442000	0.562553000	-0.000040000
7	-3.485736000	-1.591200000	0.000055000	7	-3.420516000	-1.501246000	0.000224000
1	-7.825425000	0.112997000	0.000574000	1	-7.748421000	0.231324000	0.000244000
1	-1.879662000	1.135860000	-0.000269000	1	-3.454988000	-2.508430000	0.000364000
1	-3.527268000	-2.595270000	0.000374000	7	-1.078887000	-1.423688000	0.000105000
7	-1.102350000	-1.421958000	-0.000081000	7	-0.006422000	-0.601352000	-0.000032000
7	-0.136741000	-0.403917000	-0.000228000	6	1.182681000	-1.124662000	-0.000198000
6	1.081458000	-0.842974000	-0.000239000	1	1.316732000	-2.209313000	-0.000225000
1	1.238154000	-1.928223000	-0.000146000	6	2.357702000	-0.269504000	-0.000368000
6	2.276715000	-0.047702000	-0.000360000	6	3.659873000	-0.802216000	-0.000554000
6	3.521320000	-0.728604000	-0.000352000	6	2.222148000	1.139290000	-0.000339000
6	2.337806000	1.377341000	-0.000489000	6	4.785458000	0.014770000	-0.000702000
6	4.749125000	-0.093124000	-0.000460000	6	3.351749000	1.956747000	-0.000486000
6	3.558418000	2.007601000	-0.000595000	6	4.631960000	1.401770000	-0.000668000
6	4.826518000	1.333348000	-0.000590000	1	-6.745820000	2.488119000	-0.000055000
1	-6.859603000	2.384069000	0.000224000	1	5.783912000	-0.405481000	-0.000843000
1	5.673777000	-0.660681000	-0.000449000	8	1.015033000	1.760308000	-0.000171000
8	1.194522000	2.148634000	-0.000510000	1	0.319129000	1.020151000	-0.000098000
1	1.502821000	3.065054000	-0.000613000	1	3.783523000	-1.879733000	-0.000578000
1	3.490705000	-1.815324000	-0.000256000	8	3.243610000	3.327107000	-0.000456000
8	3.626113000	3.385682000	-0.000720000	1	2.303430000	3.556490000	-0.000314000
1	4.600364000	3.525286000	-0.000774000	8	5.738425000	2.211463000	-0.000812000
8	5.879109000	2.053702000	-0.000699000	1	5.447884000	3.133688000	-0.000765000
5e_Aw2, optimization in solv.water B3LYP/6-311++G**, E= -985.202752026 a.u. Sum of electronic and thermal Enthalpies= -984.949972 a.u.				**5e_Aw3,** optimization in solv.water B3LYP/6-311++G**, E= -985.200891614 a.u. Sum of electronic and thermal Enthalpies= -984.947547 a.u.			
-1; 1				-1; 1			
6	-6.126331000	1.612761000	0.000163000	6	-6.329026000	1.437120000	0.000644000
6	-4.737906000	1.810465000	0.000053000	6	-4.952164000	1.702510000	0.000512000
6	-6.668892000	0.320107000	0.000277000	6	-6.813707000	0.126975000	0.000462000
1	-4.314554000	2.808877000	-0.000036000	1	-4.575170000	2.717989000	0.000652000
6	-3.933195000	0.679419000	0.000064000	6	-4.090651000	0.616043000	0.000202000
6	-5.850626000	-0.814511000	0.000288000	6	-5.941860000	-0.970923000	0.000146000
1	-6.279541000	-1.811050000	0.000378000	1	-6.317431000	-1.986988000	0.000003000
6	-4.461738000	-0.639742000	0.000182000	6	-4.580333000	-0.706392000	0.000030000
6	-2.298380000	-0.866901000	0.000044000	6	-2.305736000	-0.796468000	-0.000249000
7	-2.559774000	0.503061000	-0.000034000	7	-2.702485000	0.524965000	-0.000014000
7	-3.444740000	-1.570990000	0.000170000	7	-3.468895000	-1.542777000	-0.000274000
1	-7.746831000	0.197548000	0.000359000	1	-7.883135000	-0.048300000	0.000564000
1	-1.864684000	1.229404000	-0.000051000	1	-2.026120000	1.272206000	0.000146000
7	-1.085294000	-1.441950000	0.000009000	1	-3.475583000	-2.550173000	-0.000329000
7	-0.055322000	-0.558072000	-0.000130000	7	-1.107065000	-1.296537000	-0.000422000
6	1.147740000	-1.058642000	-0.000190000	7	-0.141874000	-0.282474000	-0.000470000
1	1.279898000	-2.142652000	-0.000109000	6	1.069589000	-0.733317000	-0.000387000
6	2.336027000	-0.224202000	-0.000347000	1	1.205148000	-1.821915000	-0.000200000
6	3.624536000	-0.791562000	-0.000355000	6	2.299433000	0.033812000	-0.000470000
6	2.243784000	1.185440000	-0.000489000	6	3.504260000	-0.716518000	0.000014000

6	4.770722000	-0.004691000	-0.000486000
6	3.390624000	1.975904000	-0.000616000
6	4.655809000	1.385986000	-0.000613000
1	-6.786542000	2.472811000	0.000159000
1	5.757374000	-0.451844000	-0.000487000
8	1.047628000	1.833311000	-0.000519000
1	0.353168000	1.112170000	-0.000445000
1	3.719893000	-1.871756000	-0.000250000
8	3.322119000	3.348147000	-0.000752000
1	2.391331000	3.611326000	-0.000699000
8	5.783013000	2.164393000	-0.000738000
1	5.518871000	3.094606000	-0.000807000

6	2.386353000	1.470837000	-0.001007000
6	4.762828000	-0.140972000	0.000072000
6	3.709940000	2.021863000	-0.000906000
6	4.858879000	1.262909000	-0.000382000
1	-7.026727000	2.266335000	0.000893000
1	5.664162000	-0.741864000	0.000464000
8	1.420857000	2.322571000	-0.001591000
1	3.427804000	-1.799828000	0.000373000
8	3.783239000	3.397528000	-0.001385000
1	2.831921000	3.646452000	-0.001694000
8	6.103618000	1.854474000	-0.000308000
1	5.981387000	2.813217000	-0.000647000

5e_Aw4, optimization in solv.water
B3LYP/6-311++G**, E= -985.207553854 a.u.
Sum of electronic and thermal Enthalpies= -984.953916 a.u.

5e_Aw5, optimization in solv.water
B3LYP/6-311++G**, E= -985.204111545 a.u.
Sum of electronic and thermal Enthalpies= -984.950479 a.u.

-1; 1			
6	-6.242169000	1.517191000	0.044901000
6	-4.862189000	1.760165000	0.047371000
6	-6.748570000	0.214877000	0.012849000
1	-4.467749000	2.768578000	0.071981000
6	-4.021040000	0.658534000	0.017109000
6	-5.896656000	-0.896783000	-0.017778000
1	-6.288724000	-1.906116000	-0.042503000
6	-4.530783000	-0.653554000	-0.014944000
6	-2.258369000	-0.780861000	-0.022614000
7	-2.631990000	0.545355000	0.009365000
7	-3.431867000	-1.505439000	-0.038964000
1	-7.820777000	0.058069000	0.011545000
1	-1.968670000	1.301211000	0.043019000
1	-3.451831000	-2.512591000	-0.064229000
7	-1.078575000	-1.330460000	-0.035722000
7	-0.048394000	-0.400701000	-0.027821000
6	1.142148000	-0.912388000	0.001158000
1	1.248267000	-2.000071000	0.025076000
6	2.360437000	-0.127797000	0.002263000
6	3.594646000	-0.812007000	0.054811000
6	2.349666000	1.290194000	-0.049413000
6	4.794837000	-0.107813000	0.058929000
6	3.549426000	2.041713000	-0.046884000
6	4.755306000	1.281794000	0.009429000
1	-6.926317000	2.357148000	0.068316000
1	5.748796000	-0.622407000	0.099866000
8	1.166770000	1.981260000	-0.105443000
1	0.447112000	1.308113000	-0.098746000
1	3.595670000	-1.895669000	0.092241000
8	3.646454000	3.340926000	-0.090557000
8	5.894112000	2.041437000	0.010745000
1	5.523939000	2.953559000	-0.030334000

-1; 1			
6	-6.274979000	1.478860000	0.000185000
6	-4.894594000	1.721644000	0.000021000
6	-6.781642000	0.176569000	0.000340000
1	-4.500489000	2.730545000	-0.000100000
6	-4.051910000	0.620379000	0.000024000
6	-5.929015000	-0.935611000	0.000336000
1	-6.321331000	-1.945244000	0.000454000
6	-4.563305000	-0.693050000	0.000179000
6	-2.292319000	-0.820489000	-0.000024000
7	-2.664975000	0.505803000	-0.000131000
7	-3.464808000	-1.547148000	0.000109000
1	-7.853861000	0.019597000	0.000464000
1	-1.978403000	1.243660000	-0.000147000
1	-3.486935000	-2.554453000	0.000326000
7	-1.101338000	-1.346067000	-0.000047000
7	-0.119782000	-0.355744000	-0.000191000
6	1.083157000	-0.818814000	-0.000218000
1	1.223539000	-1.905435000	-0.000132000
6	2.310434000	-0.035745000	-0.000355000
6	3.527244000	-0.762922000	-0.000360000
6	2.397356000	1.369834000	-0.000483000
6	4.765413000	-0.126581000	-0.000490000
6	3.638739000	2.050687000	-0.000619000
6	4.811861000	1.265153000	-0.000619000
1	-6.958993000	2.319348000	0.000191000
1	5.686479000	-0.699408000	-0.000492000
8	1.305516000	2.198392000	-0.000489000
1	1.718747000	3.087775000	-0.000591000
1	3.483120000	-1.846353000	-0.000263000
8	3.688425000	3.358604000	-0.000737000
8	6.000012000	1.953951000	-0.000752000
1	5.721729000	2.890080000	-0.000819000

5e_Aw6, optimization in solv.water
B3LYP/6-311++G**, E= -985.205477114 a.u.
Sum of electronic and thermal Enthalpies= -984.952101 a.u.

5e_Aw7, optimization in solv.water
B3LYP/6-311++G**, E= -985.201482675 a.u.
Sum of electronic and thermal Enthalpies= -984.947996 a.u.

-1; 1			
6	-6.250300000	1.495432000	0.408862000
6	-4.872111000	1.742563000	0.339006000
6	-6.764973000	0.209683000	0.225135000
1	-4.471081000	2.738780000	0.480504000

-1; 1			
6	-6.308132000	1.455357000	0.000203000
6	-4.929437000	1.710724000	0.000038000
6	-6.802249000	0.148715000	0.000348000
1	-4.544926000	2.723385000	-0.000076000

6	-4.041979000	0.662669000	0.081509000	6	-4.076033000	0.617910000	0.000030000
6	-5.923748000	-0.880853000	-0.034478000	6	-5.938516000	-0.955543000	0.000333000
1	-6.322952000	-1.877718000	-0.176364000	1	-6.321542000	-1.968797000	0.000443000
6	-4.560251000	-0.634141000	-0.102542000	6	-4.575049000	-0.700877000	0.000176000
6	-2.293789000	-0.745947000	-0.308283000	6	-2.301029000	-0.807120000	-0.000031000
7	-2.658703000	0.560909000	-0.051791000	7	-2.688447000	0.517046000	-0.000130000
7	-3.472739000	-1.467469000	-0.336904000	7	-3.469423000	-1.544957000	0.000096000
1	-7.834911000	0.048104000	0.283930000	1	-7.872928000	-0.018708000	0.000472000
1	-1.992203000	1.309337000	0.034713000	1	-2.008964000	1.261150000	-0.000133000
1	-3.501699000	-2.459431000	-0.510673000	1	-3.483226000	-2.552272000	0.000311000
7	-1.124199000	-1.277264000	-0.495735000	7	-1.106333000	-1.317492000	-0.000058000
7	-0.083708000	-0.355776000	-0.433139000	7	-0.131518000	-0.315066000	-0.000205000
6	1.102451000	-0.873435000	-0.581427000	6	1.075901000	-0.776307000	-0.000223000
1	1.191881000	-1.952854000	-0.728950000	1	1.212434000	-1.863806000	-0.000127000
6	2.312518000	-0.102735000	-0.564515000	6	2.305595000	-0.012921000	-0.000359000
6	3.574249000	-0.720355000	-0.717520000	6	3.519098000	-0.741473000	-0.000344000
6	2.308782000	1.309576000	-0.397668000	6	2.421598000	1.404663000	-0.000509000
6	4.747241000	0.007216000	-0.704490000	6	4.772348000	-0.147636000	-0.000467000
6	3.478312000	2.046643000	-0.385611000	6	3.669395000	1.993430000	-0.000632000
6	4.771839000	1.436320000	-0.537901000	6	4.901320000	1.268924000	-0.000621000
1	-6.925212000	2.319267000	0.608776000	1	-6.999819000	2.289589000	0.000217000
1	5.703714000	-0.492218000	-0.822965000	1	5.671171000	-0.755807000	-0.000448000
8	1.135147000	2.003061000	-0.242883000	8	1.305905000	2.208324000	-0.000534000
1	0.404847000	1.332214000	-0.272730000	1	1.614279000	3.125519000	-0.000652000
1	3.609519000	-1.798386000	-0.847140000	1	3.452570000	-1.825489000	-0.000231000
8	3.418379000	3.419755000	-0.223192000	8	3.769948000	3.369404000	-0.000777000
1	2.484290000	3.655143000	-0.138463000	1	4.739221000	3.512416000	-0.000842000
8	5.852214000	2.120120000	-0.524678000	8	5.998836000	1.946792000	-0.000747000
5e_R1, optimization in gas phase B3LYP/6-311++G**, E= -985.033663819 a.u. Sum of electronic and thermal Enthalpies= -984.779451 a.u.				**5e_R2,** optimization in gas phase B3LYP/6-311++G**, E= -985.030006472 a.u. Sum of electronic and thermal Enthalpies= -984.775967 a.u.			
0; 2				0; 2			
6	-6.150556000	1.553039000	0.000175000	6	-6.201434000	1.521060000	0.000223000
6	-4.784854000	1.778038000	0.000043000	6	-4.838569000	1.799970000	0.000138000
6	-6.683452000	0.244134000	0.000308000	6	-6.691414000	0.195625000	0.000245000
1	-4.369995000	2.778527000	-0.000060000	1	-4.473980000	2.820482000	0.000120000
6	-3.930147000	0.661826000	0.000046000	6	-3.975106000	0.706830000	0.000078000
6	-5.864748000	-0.878486000	0.000313000	6	-5.833688000	-0.889994000	0.000185000
1	-6.281242000	-1.878893000	0.000413000	1	-6.198492000	-1.909772000	0.000202000
6	-4.488499000	-0.652397000	0.000181000	6	-4.449038000	-0.639271000	0.000101000
6	-2.263689000	-0.689384000	-0.000003000	6	-2.301436000	-0.766579000	-0.000023000
7	-2.565449000	0.610850000	-0.000065000	7	-2.606159000	0.594414000	-0.000020000
7	-3.401679000	-1.487723000	0.000137000	7	-3.410769000	-1.519426000	0.000042000
1	-7.759491000	0.114030000	0.000408000	1	-7.762982000	0.033904000	0.000311000
1	-3.386482000	-2.495414000	0.000240000	1	-1.933123000	1.341727000	0.000026000
7	-1.066499000	-1.308763000	-0.000056000	7	-1.074780000	-1.307094000	-0.000084000
7	-0.036039000	-0.466462000	-0.000194000	7	-0.074898000	-0.411091000	-0.000188000
6	1.152935000	-1.027123000	-0.000243000	6	1.122944000	-0.959015000	-0.000085000
1	1.238439000	-2.115340000	-0.000150000	1	1.194327000	-2.047022000	0.000047000
6	2.331192000	-0.221686000	-0.000370000	6	2.322141000	-0.180760000	-0.000252000
6	3.615447000	-0.819040000	-0.000353000	6	3.587474000	-0.814210000	-0.000260000
6	2.250213000	1.199489000	-0.000506000	6	2.287234000	1.237867000	-0.000458000
6	4.766465000	-0.060672000	-0.000457000	6	4.759675000	-0.086514000	-0.000469000
6	3.418085000	1.957161000	-0.000607000	6	3.468831000	1.968113000	-0.000678000
6	4.669197000	1.340014000	-0.000584000	6	4.703739000	1.314678000	-0.000685000
1	-6.832521000	2.395388000	0.000176000	1	-6.908271000	2.342808000	0.000272000

1	5.749130000	-0.514092000	-0.000443000
8	1.097197000	1.892101000	-0.000560000
1	0.338745000	1.243137000	-0.000517000
1	3.682956000	-1.900926000	-0.000251000
8	3.385699000	3.325989000	-0.000737000
1	2.460007000	3.607310000	-0.000734000
8	5.797404000	2.087560000	-0.000684000
1	5.549065000	3.022746000	-0.000765000

1	5.728835000	-0.568105000	-0.000479000
8	1.133614000	1.944571000	-0.000406000
1	0.397594000	1.277382000	-0.000131000
1	3.625629000	-1.897343000	-0.000110000
8	3.478803000	3.337928000	-0.000884000
1	2.565809000	3.654557000	-0.000856000
8	5.852245000	2.029535000	-0.000896000
1	5.633436000	2.971916000	-0.001027000

5e_R3, optimization in gas phase
B3LYP/6-311++G**, E= -985.022836715 a.u.
Sum of electronic and thermal Enthalpies= -984.768410 a.u.

5e_R4, optimization in gas phase
B3LYP/6-311++G**, E= -985.030905764 a.u.
Sum of electronic and thermal Enthalpies= -984.776141 a.u.

0; 2			
6	-6.070095000	1.605857000	0.000539000
6	-4.681836000	1.763387000	0.000365000
6	-6.659346000	0.337441000	0.000475000
1	-4.226617000	2.746096000	0.000416000
6	-3.908323000	0.610955000	0.000125000
6	-5.882170000	-0.823929000	0.000234000
1	-6.339944000	-1.805810000	0.000187000
6	-4.503806000	-0.667069000	0.000063000
6	-2.255551000	-0.930625000	-0.000277000
7	-2.533906000	0.408539000	-0.000087000
7	-3.458081000	-1.587264000	-0.000189000
1	-7.739162000	0.250847000	0.000617000
1	-1.775012000	1.079984000	-0.000078000
1	-3.524286000	-2.592250000	-0.000245000
7	-1.080915000	-1.523153000	-0.000488000
7	-0.114658000	-0.571640000	-0.000549000
6	1.108888000	-1.015780000	-0.000283000
1	1.284711000	-2.095623000	0.000022000
6	2.250886000	-0.160192000	-0.000356000
6	3.530623000	-0.748678000	-0.000003000
6	2.169729000	1.312988000	-0.000799000
6	4.696385000	-0.002016000	-0.000050000
6	3.431423000	2.038059000	-0.000833000
6	4.650503000	1.410783000	-0.000469000
1	-6.701483000	2.486183000	0.000728000
1	5.667290000	-0.482383000	0.000231000
8	1.127244000	2.002452000	-0.001182000
1	3.601075000	-1.830663000	0.000323000
8	3.359827000	3.392113000	-0.001248000
1	2.402731000	3.589527000	-0.001437000
8	5.824218000	2.104829000	-0.000502000
1	5.621116000	3.049397000	-0.000807000

0; 2			
6	-6.217678000	1.541423000	0.000216000
6	-4.837666000	1.774886000	0.000088000
6	-6.732296000	0.243542000	0.000311000
1	-4.439379000	2.782361000	0.000013000
6	-4.003704000	0.668497000	0.000062000
6	-5.888325000	-0.872658000	0.000281000
1	-6.289857000	-1.878882000	0.000353000
6	-4.521692000	-0.639537000	0.000157000
6	-2.247678000	-0.783453000	-0.000020000
7	-2.613440000	0.545909000	-0.000059000
7	-3.426118000	-1.498327000	0.000091000
1	-7.805296000	0.094298000	0.000408000
1	-1.944452000	1.296675000	-0.000094000
1	-3.436920000	-2.504808000	0.000180000
7	-1.079003000	-1.352539000	-0.000069000
7	-0.040129000	-0.450954000	-0.000189000
6	1.144583000	-0.972895000	-0.000186000
1	1.249790000	-2.059241000	-0.000093000
6	2.345218000	-0.157924000	-0.000328000
6	3.614711000	-0.779258000	-0.000320000
6	2.277136000	1.248211000	-0.000484000
6	4.813397000	-0.065964000	-0.000454000
6	3.492565000	2.043854000	-0.000629000
6	4.761312000	1.315487000	-0.000605000
1	-6.896292000	2.385785000	0.000241000
1	5.769392000	-0.573720000	-0.000442000
8	1.119428000	1.900054000	-0.000494000
1	0.408868000	1.199664000	-0.000374000
1	3.650707000	-1.863517000	-0.000203000
8	3.522591000	3.294214000	-0.000764000
8	5.859420000	2.075489000	-0.000740000
1	5.533721000	2.998795000	-0.000833000

5e_R5, optimization in gas phase
B3LYP/6-311++G**, E= -985.026789415 a.u.
Sum of electronic and thermal Enthalpies= -984.771809 a.u.

5e_R6, optimization in gas phase
B3LYP/6-311++G**, E= -985.023265483 a.u.
Sum of electronic and thermal Enthalpies= -984.768772 a.u.

0; 2			
6	-6.152189000	1.559165000	0.000152000
6	-4.765343000	1.747677000	-0.000018000
6	-6.709528000	0.279008000	0.000332000
1	-4.334664000	2.741687000	-0.000160000
6	-3.964557000	0.615925000	0.000006000
6	-5.901591000	-0.863950000	0.000347000
1	-6.335738000	-1.856669000	0.000481000
6	-4.528325000	-0.676038000	0.000185000

0; 2			
6	-6.236103000	1.522705000	0.000195000
6	-4.860425000	1.773069000	0.000075000
6	-6.736384000	0.217814000	0.000294000
1	-4.474191000	2.785120000	-0.000003000
6	-4.013822000	0.675294000	0.000059000
6	-5.881617000	-0.888320000	0.000276000
1	-6.271551000	-1.898955000	0.000351000
6	-4.517110000	-0.638580000	0.000159000

6	-2.265946000	-0.890600000	-0.000015000	6	-2.246137000	-0.755317000	-0.000009000
7	-2.583804000	0.446754000	-0.000140000	7	-2.622935000	0.567260000	-0.000052000
7	-3.461787000	-1.572160000	0.000132000	7	-3.411773000	-1.484036000	0.000108000
1	-7.786870000	0.164731000	0.000459000	1	-7.807668000	0.057406000	0.000385000
1	-1.850974000	1.141388000	-0.000197000	1	-1.958421000	1.322431000	-0.000094000
1	-3.506573000	-2.577616000	0.000358000	1	-3.409602000	-2.491136000	0.000176000
7	-1.093370000	-1.460093000	-0.000026000	7	-1.065728000	-1.313522000	-0.000058000
7	-0.112675000	-0.495800000	-0.000169000	7	-0.042822000	-0.414575000	-0.000188000
6	1.091501000	-0.945597000	-0.000216000	6	1.153236000	-0.949021000	-0.000170000
1	1.266754000	-2.025354000	-0.000150000	1	1.241153000	-2.035920000	-0.000064000
6	2.269395000	-0.088150000	-0.000355000	6	2.345404000	-0.162764000	-0.000315000
6	3.542733000	-0.723116000	-0.000393000	6	3.623822000	-0.817244000	-0.000322000
6	2.261011000	1.306155000	-0.000452000	6	2.317038000	1.252499000	-0.000469000
6	4.765391000	-0.051369000	-0.000520000	6	4.787194000	-0.116570000	-0.000470000
6	3.500888000	2.056058000	-0.000584000	6	3.487596000	1.993910000	-0.000625000
6	4.758650000	1.330215000	-0.000616000	6	4.801600000	1.344086000	-0.000634000
1	-6.803160000	2.425214000	0.000142000	1	-6.925105000	2.358509000	0.000212000
1	5.702356000	-0.593180000	-0.000544000	1	5.753158000	-0.606228000	-0.000476000
8	1.147381000	2.054349000	-0.000431000	8	1.148989000	1.956485000	-0.000455000
1	1.461174000	2.979454000	-0.000518000	1	0.421541000	1.287549000	-0.000304000
1	3.553720000	-1.807705000	-0.000320000	1	3.636423000	-1.902126000	-0.000207000
8	3.493333000	3.314963000	-0.000671000	8	3.449603000	3.337592000	-0.000770000
8	5.876144000	2.064918000	-0.000740000	1	2.519932000	3.609035000	-0.000744000
1	5.589752000	2.997554000	-0.000787000	8	5.851552000	2.000832000	-0.000772000

5e_R7, optimization in gas phase
B3LYP/6-311++G**, E= -985.025054850 a.u.
Sum of electronic and thermal Enthalpies= -984.770081 a.u.

0; 2

6	-6.141960000	1.555291000	0.000120000
6	-4.758657000	1.753136000	-0.000034000
6	-6.693507000	0.270318000	0.000306000
1	-4.333249000	2.749175000	-0.000181000
6	-3.952250000	0.623890000	0.000012000
6	-5.882629000	-0.867807000	0.000344000
1	-6.311436000	-1.862637000	0.000483000
6	-4.509438000	-0.670850000	0.000198000
6	-2.253508000	-0.870165000	0.000015000
7	-2.571486000	0.460713000	-0.000115000
7	-3.437482000	-1.560247000	0.000169000
1	-7.770285000	0.152062000	0.000420000
1	-1.836151000	1.155110000	-0.000193000
1	-3.474462000	-2.566785000	0.000376000
7	-1.066433000	-1.433790000	0.000003000
7	-0.110242000	-0.472308000	-0.000146000
6	1.114971000	-0.923642000	-0.000211000
1	1.277174000	-2.004242000	-0.000150000
6	2.270567000	-0.090178000	-0.000356000
6	3.547300000	-0.756432000	-0.000406000
6	2.265407000	1.335472000	-0.000452000
6	4.739223000	-0.098889000	-0.000537000
6	3.465366000	2.007614000	-0.000584000
6	4.760401000	1.346609000	-0.000635000
1	-6.798734000	2.416792000	0.000092000
1	5.687331000	-0.621965000	-0.000572000
8	1.099519000	2.045509000	-0.000414000
1	1.340273000	2.982967000	-0.000504000

1	3.532978000	-1.840932000	-0.000333000
8	3.471597000	3.362454000	-0.000675000
1	4.417077000	3.610883000	-0.000761000
8	5.784771000	2.061954000	-0.000758000

5e_Rw1, optimization in solv. water B3LYP/6-311++G**, E= -985.048471090 a.u. Sum of electronic and thermal Enthalpies= -984.794787 a.u.			
0; 2			
6	-6.169870000	1.543276000	0.000063000
6	-4.805664000	1.779397000	-0.000066000
6	-6.693864000	0.228277000	0.000268000
1	-4.403817000	2.785628000	-0.000222000
6	-3.943439000	0.667339000	0.000011000
6	-5.868209000	-0.888410000	0.000348000
1	-6.273071000	-1.892861000	0.000504000
6	-4.492314000	-0.650906000	0.000217000
6	-2.271064000	-0.683444000	0.000062000
7	-2.576935000	0.620769000	-0.000084000
7	-3.404242000	-1.480689000	0.000239000
1	-7.768896000	0.091288000	0.000362000
1	-3.398738000	-2.490344000	0.000361000
7	-1.069412000	-1.294674000	0.000054000
7	-0.036883000	-0.450291000	-0.000115000
6	1.152214000	-1.013647000	-0.000208000
1	1.238864000	-2.100856000	-0.000136000
6	2.334010000	-0.212538000	-0.000363000
6	3.612909000	-0.820734000	-0.000439000
6	2.261768000	1.209147000	-0.000436000
6	4.767606000	-0.067306000	-0.000584000
6	3.431531000	1.963793000	-0.000577000
6	4.678754000	1.333926000	-0.000653000
1	-6.858030000	2.380499000	0.000007000
1	5.746249000	-0.529865000	-0.000644000
8	1.100565000	1.894741000	-0.000373000
1	0.356231000	1.226230000	-0.000273000
1	3.673821000	-1.902523000	-0.000382000
8	3.414718000	3.331702000	-0.000651000
1	2.496857000	3.637775000	-0.000577000
8	5.816027000	2.069340000	-0.000793000
1	5.589158000	3.010900000	-0.000820000

5e_Rw2, optimization in solv. water B3LYP/6-311++G**, E= -985.047937276 a.u. Sum of electronic and thermal Enthalpies= -984.794033 a.u.			
0; 2			
6	-6.232161000	1.497862000	0.048999000
6	-4.872430000	1.788220000	0.066724000
6	-6.711222000	0.167769000	-0.007480000
1	-4.511777000	2.808446000	0.109647000
6	-3.999882000	0.701507000	0.026013000
6	-5.844550000	-0.910877000	-0.047807000
1	-6.207643000	-1.930810000	-0.091038000
6	-4.461895000	-0.646653000	-0.030796000
6	-2.307896000	-0.740639000	-0.023636000
7	-2.630496000	0.605958000	0.027152000
7	-3.408136000	-1.512805000	-0.059198000
1	-7.781232000	-0.003150000	-0.019132000
1	-1.972896000	1.367399000	0.077134000
7	-1.076589000	-1.277140000	-0.036652000
7	-0.074969000	-0.383415000	-0.021597000
6	1.122176000	-0.933970000	0.000112000
1	1.198564000	-2.021386000	0.016721000
6	2.324209000	-0.163449000	0.003796000
6	3.580344000	-0.816509000	0.047011000
6	2.307261000	1.256205000	-0.038366000
6	4.761373000	-0.104906000	0.051897000
6	3.499959000	1.971569000	-0.033175000
6	4.723916000	1.297473000	0.012207000
1	-6.946418000	2.312409000	0.078916000
1	5.722058000	-0.602440000	0.086149000
8	1.166928000	1.978534000	-0.086367000
1	0.412933000	1.337395000	-0.080857000
1	3.602452000	-1.899243000	0.077676000
8	3.535194000	3.338092000	-0.072486000
1	2.631913000	3.683286000	-0.094739000
8	5.885834000	1.991823000	0.018041000
1	5.693265000	2.940616000	-0.010875000

5e_Rw3, optimization in solv. water B3LYP/6-311++G**, E= -985.041855997 a.u. Sum of electronic and thermal Enthalpies= -984.787521 a.u.			
0; 2			
6	-6.281941000	1.463406000	0.000086000
6	-4.912978000	1.730660000	0.000027000
6	-6.773115000	0.148447000	0.000207000
1	-4.532553000	2.744108000	-0.000067000
6	-4.056480000	0.636048000	0.000092000
6	-5.914376000	-0.950250000	0.000272000
1	-6.291322000	-1.965074000	0.000364000
6	-4.549883000	-0.683559000	0.000213000
6	-2.298642000	-0.772681000	0.000145000
7	-2.670686000	0.536918000	0.000056000
7	-3.438898000	-1.517470000	0.000244000
1	-7.843487000	-0.018047000	0.000248000

5e_Rw4, optimization in solv. water B3LYP/6-311++G**, E= -985.050913298 a.u. Sum of electronic and thermal Enthalpies= -984.796600 a.u.			
0; 2			
6	-6.229974000	1.533718000	0.047680000
6	-4.851479000	1.775357000	0.057773000
6	-6.739187000	0.231400000	0.003442000
1	-4.455031000	2.782534000	0.091644000
6	-4.013618000	0.670794000	0.022600000
6	-5.891447000	-0.881185000	-0.032065000
1	-6.284751000	-1.889577000	-0.066169000
6	-4.524985000	-0.638602000	-0.021507000
6	-2.257799000	-0.769026000	-0.020612000
7	-2.623569000	0.553986000	0.019687000
7	-3.425771000	-1.490661000	-0.047166000
1	-7.811718000	0.077823000	-0.003555000

1	-1.990624000	1.283819000	-0.000007000
1	-3.439462000	-2.527149000	0.000336000
7	-1.079680000	-1.300334000	0.000148000
7	-0.133964000	-0.341793000	0.000008000
6	1.092558000	-0.820790000	-0.000149000
1	1.214236000	-1.907222000	-0.000127000
6	2.280670000	-0.049787000	-0.000340000
6	3.515500000	-0.756814000	-0.000437000
6	2.325412000	1.421212000	-0.000443000
6	4.731293000	-0.118189000	-0.000608000
6	3.638682000	2.032914000	-0.000617000
6	4.795491000	1.302123000	-0.000699000
1	-6.981142000	2.290841000	0.000037000
1	5.659219000	-0.676959000	-0.000676000
8	1.335425000	2.193873000	-0.000400000
1	3.486934000	-1.840372000	-0.000369000
8	3.686593000	3.396089000	-0.000705000
1	2.752525000	3.679521000	-0.000621000
8	6.027181000	1.888836000	-0.000868000
1	5.918971000	2.850037000	-0.000907000

5e_Rw5, optimization in solv. water
B3LYP/6-311++G**, E= -985.043565327 a.u.
Sum of electronic and thermal Enthalpies= -984.789179 a.u.

0; 2

6	-6.238759000	1.503841000	0.000133000
6	-4.858392000	1.735196000	-0.000012000
6	-6.758375000	0.204938000	0.000303000
1	-4.454610000	2.740072000	-0.000145000
6	-4.027073000	0.624498000	0.000026000
6	-5.918739000	-0.914626000	0.000334000
1	-6.319853000	-1.920605000	0.000463000
6	-4.550606000	-0.682775000	0.000196000
6	-2.287861000	-0.830247000	0.000020000
7	-2.640581000	0.495256000	-0.000098000
7	-3.458421000	-1.546084000	0.000164000
1	-7.832081000	0.059491000	0.000411000
1	-1.947028000	1.227626000	-0.000157000
1	-3.486942000	-2.553760000	0.000355000
7	-1.096090000	-1.376635000	0.000000000
7	-0.117007000	-0.410267000	-0.000148000
6	1.087362000	-0.869846000	-0.000191000
1	1.248968000	-1.951428000	-0.000116000
6	2.288135000	-0.044408000	-0.000343000
6	3.539312000	-0.727103000	-0.000404000
6	2.329294000	1.348192000	-0.000436000
6	4.781780000	-0.096743000	-0.000553000
6	3.592383000	2.057586000	-0.000594000
6	4.822944000	1.284898000	-0.000650000
1	-6.915883000	2.349728000	0.000111000
1	5.698114000	-0.672812000	-0.000593000
8	1.232858000	2.124198000	-0.000385000
1	1.553964000	3.045792000	-0.000470000
1	3.514629000	-1.810965000	-0.000331000
8	3.627968000	3.317233000	-0.000681000
8	5.972369000	1.970136000	-0.000799000
1	5.741312000	2.917441000	-0.000840000

1	-1.965976000	1.314214000	0.066922000
1	-3.444251000	-2.498100000	-0.081374000
7	-1.078818000	-1.338109000	-0.032781000
7	-0.038049000	-0.443353000	-0.021688000
6	1.145693000	-0.969660000	0.007764000
1	1.255690000	-2.054719000	0.031282000
6	2.348162000	-0.155472000	0.006985000
6	3.617050000	-0.779779000	0.056741000
6	2.288090000	1.245344000	-0.047499000
6	4.817463000	-0.068474000	0.057125000
6	3.503690000	2.038130000	-0.050769000
6	4.770615000	1.311340000	0.005080000
1	-6.913459000	2.373959000	0.074614000
1	5.769497000	-0.582006000	0.097163000
8	1.131508000	1.906360000	-0.099450000
1	0.409465000	1.214375000	-0.088629000
1	3.651824000	-1.862774000	0.096232000
8	3.526928000	3.292883000	-0.098262000
8	5.878517000	2.062790000	0.002635000
1	5.578606000	2.991953000	-0.038824000

5e_Rw6, optimization in solv. water
B3LYP/6-311++G**, E= -985.050090738 a.u.
Sum of electronic and thermal Enthalpies= -984.795589 a.u.

0; 2

6	-6.260430000	1.499524000	0.045557000
6	-4.891733000	1.771747000	0.063024000
6	-6.745175000	0.184029000	-0.004889000
1	-4.515698000	2.786144000	0.101461000
6	-4.031971000	0.681372000	0.028501000
6	-5.880774000	-0.910440000	-0.039565000
1	-6.252963000	-1.926295000	-0.078534000
6	-4.517817000	-0.638114000	-0.021778000
6	-2.260648000	-0.719312000	-0.011625000
7	-2.642623000	0.590077000	0.032301000
7	-3.402657000	-1.465199000	-0.044593000
1	-7.814694000	0.012437000	-0.017287000
1	-1.995359000	1.360764000	0.080317000
1	-3.397182000	-2.474019000	-0.081714000
7	-1.059324000	-1.274537000	-0.020952000
7	-0.047433000	-0.388284000	-0.012037000
6	1.154599000	-0.934156000	0.009156000
1	1.236692000	-2.020842000	0.028743000
6	2.342704000	-0.162079000	0.007305000
6	3.612744000	-0.828494000	0.047443000
6	2.337628000	1.263213000	-0.036502000
6	4.783811000	-0.137328000	0.048001000
6	3.515035000	1.979857000	-0.036148000
6	4.811336000	1.317497000	0.006613000
1	-6.962775000	2.323859000	0.071348000
1	5.740735000	-0.644476000	0.079414000
8	1.182072000	1.981159000	-0.081619000
1	0.435388000	1.334753000	-0.074896000
1	3.615922000	-1.912390000	0.078769000
8	3.504862000	3.337125000	-0.077532000
1	2.582337000	3.632009000	-0.100261000
8	5.880239000	1.967682000	0.007069000

5e_Rw7, optimization in solv. water B3LYP/6-311++G**, E= -985.045749695 a.u. Sum of electronic and thermal Enthalpies= -984.791003 a.u.			
0; 2			
6	-6.253371000	1.480562000	0.000155000
6	-4.882330000	1.739238000	0.000024000
6	-6.752328000	0.169038000	0.000301000
1	-4.495817000	2.750420000	-0.000091000
6	-4.032490000	0.639786000	0.000049000
6	-5.899648000	-0.934892000	0.000323000
1	-6.282674000	-1.947472000	0.000435000
6	-4.533873000	-0.676500000	0.000197000
6	-2.282713000	-0.780003000	0.000023000
7	-2.646628000	0.532225000	-0.000063000
7	-3.427615000	-1.517658000	0.000166000
1	-7.823645000	0.008623000	0.000398000
1	-1.961567000	1.274749000	-0.000146000
1	-3.434524000	-2.527184000	0.000288000
7	-1.066901000	-1.314176000	-0.000022000
7	-0.119086000	-0.358853000	-0.000166000
6	1.108773000	-0.833502000	-0.000205000
1	1.240787000	-1.917723000	-0.000119000
6	2.290565000	-0.049990000	-0.000351000
6	3.535338000	-0.771941000	-0.000370000
6	2.358031000	1.379210000	-0.000483000
6	4.754316000	-0.162233000	-0.000507000
6	3.585145000	1.997515000	-0.000624000
6	4.841880000	1.277584000	-0.000644000
1	-6.947324000	2.312419000	0.000141000
1	5.675216000	-0.732767000	-0.000518000
8	1.219878000	2.129056000	-0.000470000
1	1.476620000	3.062565000	-0.000572000
1	3.477860000	-1.854642000	-0.000270000
8	3.644299000	3.356653000	-0.000751000
1	4.594206000	3.578033000	-0.000833000
8	5.911668000	1.940939000	-0.000776000

5e_RC, optimization in gas phase B3LYP/6-311++G**, E= -985.424931493 a.u. Sum of electronic and thermal Enthalpies= -985.156369 a.u.			
1; 2			
6	-6.324532000	1.442504000	0.000067000
6	-4.971446000	1.759381000	-0.000021000
6	-6.773111000	0.107409000	0.000233000
1	-4.631356000	2.787228000	-0.000149000
6	-4.079900000	0.691194000	0.000061000
6	-5.885779000	-0.960613000	0.000319000
1	-6.232999000	-1.986037000	0.000447000
6	-4.528832000	-0.646104000	0.000229000
6	-2.275639000	-0.659478000	0.000141000
7	-2.690225000	0.637391000	0.000012000
7	-3.391652000	-1.437349000	0.000275000
1	-7.837745000	-0.090114000	0.000296000
1	-2.057530000	1.422486000	-0.000107000
1	-3.344783000	-2.447084000	0.000377000
7	-1.058758000	-1.195147000	0.000154000
7	-0.060686000	-0.311187000	0.000006000
6	1.140001000	-0.881780000	-0.000174000
1	1.190329000	-1.970047000	-0.000159000
6	2.339045000	-0.139417000	-0.000360000
6	3.588814000	-0.832472000	-0.000465000
6	2.355544000	1.291275000	-0.000433000
6	4.778069000	-0.157566000	-0.000622000
6	3.560445000	1.971466000	-0.000586000
6	4.771750000	1.257110000	-0.000681000
1	-7.053942000	2.242821000	0.000005000
1	5.731466000	-0.669051000	-0.000701000
8	1.234710000	2.037797000	-0.000377000
1	0.467795000	1.420694000	-0.000318000
1	3.579324000	-1.915648000	-0.000411000
8	3.656744000	3.326970000	-0.000663000
1	2.777221000	3.727783000	-0.000593000
8	5.933586000	1.904648000	-0.000832000
1	5.783466000	2.863630000	-0.000856000

5e_RCw, optimization in solv. water B3LYP/6-311++G**, E= -985.494167308 a.u. Sum of electronic and thermal Enthalpies= -985.226024 a.u.			
1; 2			
6	-6.299302000	1.455119000	0.053738000
6	-4.945636000	1.762577000	0.077462000
6	-6.758709000	0.121898000	-0.009497000
1	-4.591350000	2.783692000	0.125250000
6	-4.061428000	0.686642000	0.035527000
6	-5.881506000	-0.952079000	-0.051385000
1	-6.230881000	-1.975009000	-0.099887000
6	-4.520539000	-0.647720000	-0.027669000
6	-2.277733000	-0.671374000	-0.012010000
7	-2.679440000	0.624885000	0.042330000
7	-3.394582000	-1.443644000	-0.053698000
1	-7.825067000	-0.065924000	-0.025689000
1	-2.047765000	1.410325000	0.099743000
1	-3.363524000	-2.454087000	-0.098766000
7	-1.058876000	-1.213039000	-0.023730000

5e_M, optimization in gas phase B3LYP/6-311++G**, E= -985.663792068 a.u. Sum of electronic and thermal Enthalpies= -985.396306 a.u.			
0; 1			
6	-6.223717000	1.539138000	0.000304000
6	-4.843138000	1.773556000	0.000146000
6	-6.736340000	0.241110000	0.000341000
1	-4.446414000	2.781759000	0.000113000
6	-4.007115000	0.669015000	0.000042000
6	-5.890084000	-0.874124000	0.000222000
1	-6.290474000	-1.880853000	0.000244000
6	-4.523696000	-0.640389000	0.000079000
6	-2.247476000	-0.782324000	-0.000126000
7	-2.617249000	0.548359000	-0.000141000
7	-3.428395000	-1.498153000	-0.000089000
1	-7.809124000	0.090001000	0.000460000
1	-1.947439000	1.297755000	0.000014000
1	-3.438792000	-2.504477000	0.000121000
7	-1.080465000	-1.346547000	-0.000147000

7	-0.060653000	-0.329658000	-0.013130000	7	-0.037422000	-0.442841000	-0.000234000
6	1.137110000	-0.897581000	0.010980000	6	1.142578000	-0.977007000	-0.000146000
1	1.197356000	-1.984969000	0.033993000	1	1.233208000	-2.064716000	0.000016000
6	2.335306000	-0.145757000	0.009750000	6	2.354300000	-0.184680000	-0.000269000
6	3.584372000	-0.828218000	0.058165000	6	3.619443000	-0.802224000	-0.000212000
6	2.343648000	1.281076000	-0.042171000	6	2.307238000	1.226446000	-0.000497000
6	4.772466000	-0.143315000	0.059121000	6	4.790199000	-0.061129000	-0.000381000
6	3.548962000	1.969515000	-0.040805000	6	3.481744000	1.971413000	-0.000679000
6	4.759294000	1.265880000	0.009676000	6	4.723543000	1.334907000	-0.000623000
1	-7.023911000	2.259370000	0.084060000	1	-6.903160000	2.382897000	0.000396000
1	5.725410000	-0.654431000	0.097327000	1	5.762528000	-0.536808000	-0.000343000
8	1.224747000	2.025478000	-0.096144000	8	1.140980000	1.922482000	-0.000542000
1	0.450484000	1.415206000	-0.088453000	1	0.417941000	1.240333000	-0.000327000
1	3.581065000	-1.910402000	0.096605000	1	3.671131000	-1.885241000	-0.000044000
8	3.624122000	3.329775000	-0.088879000	8	3.467199000	3.344213000	-0.000913000
1	2.734316000	3.708489000	-0.115618000	1	2.546480000	3.637230000	-0.000904000
8	5.927622000	1.927310000	0.011436000	8	5.868836000	2.068182000	-0.000791000
1	5.764017000	2.882664000	-0.023515000	1	5.632548000	3.005411000	-0.000975000

5e_Mw, optimization in solv. water
B3LYP/6-311++G**, E= -985.680214250 a.u.
Sum of electronic and thermal Enthalpies= -985.413327 a.u.

0; 1

6	-6.229314000	1.534328000	0.065865000
6	-4.849484000	1.772152000	0.078909000
6	-6.741193000	0.234436000	0.003318000
1	-4.450830000	2.777971000	0.126849000
6	-4.013653000	0.666955000	0.027933000
6	-5.895028000	-0.879578000	-0.048254000
1	-6.290743000	-1.886527000	-0.096525000
6	-4.528124000	-0.640982000	-0.034665000
6	-2.258951000	-0.777105000	-0.035981000
7	-2.624092000	0.547540000	0.022777000
7	-3.431454000	-1.495637000	-0.072754000
1	-7.814039000	0.082842000	-0.005535000
1	-1.963337000	1.303825000	0.083341000
1	-3.453378000	-2.502217000	-0.120878000
7	-1.082490000	-1.343690000	-0.055874000
7	-0.038731000	-0.443072000	-0.032436000
6	1.141944000	-0.975299000	-0.002438000
1	1.242071000	-2.062194000	0.013094000
6	2.355079000	-0.180631000	0.008358000
6	3.616875000	-0.802399000	0.061308000
6	2.312461000	1.230110000	-0.039022000
6	4.790816000	-0.063349000	0.070433000
6	3.490335000	1.974097000	-0.030282000
6	4.728677000	1.331834000	0.024977000
1	-6.910583000	2.375941000	0.104971000
1	5.759119000	-0.546278000	0.112438000
8	1.149584000	1.927820000	-0.095915000
1	0.417834000	1.255580000	-0.093279000
1	3.665605000	-1.884788000	0.095882000
8	3.483956000	3.344749000	-0.075368000
1	2.568119000	3.654578000	-0.102471000
8	5.882040000	2.060284000	0.034750000
1	5.660305000	3.001398000	0.000588000

5f_A1, optimization in gas phase B3LYP/6-311++G**, E= -873.916059528 a.u. Sum of electronic and thermal Enthalpies= -873.645069 a.u.			
-1; 1			
6	6.407428000	0.692671000	0.000271000
6	5.743034000	-0.538009000	0.000418000
6	5.703414000	1.904013000	-0.000215000
1	6.292408000	-1.473418000	0.000801000
6	4.343064000	-0.552279000	0.000076000
6	4.299997000	1.917277000	-0.000616000
1	3.752042000	2.854631000	-0.001031000
6	3.645077000	0.693580000	-0.000441000
6	2.243474000	-1.063572000	-0.000277000
7	3.466921000	-1.608068000	0.000172000
7	2.315849000	0.333846000	-0.000890000
1	1.491391000	0.910770000	-0.000122000
7	1.087224000	-1.754437000	-0.000012000
7	0.020533000	-0.941971000	-0.000039000
6	-1.148347000	-1.515482000	0.000200000
1	-1.208896000	-2.607864000	0.000417000
1	6.246509000	2.843555000	-0.000306000
6	-2.389052000	-0.764605000	0.000151000
6	-2.441383000	0.650343000	-0.000193000
6	-3.624299000	-1.436698000	0.000456000
6	-3.644568000	1.332909000	-0.000228000
6	-4.845142000	-0.757126000	0.000432000
6	-4.860826000	0.636806000	0.000086000
1	7.493271000	0.711156000	0.000554000
8	-6.005223000	1.413964000	0.000027000
6	-7.251222000	0.750129000	0.000377000
1	-7.378781000	0.123633000	-0.891830000
1	-7.378518000	0.124086000	0.892938000
1	-8.012446000	1.531098000	0.000289000
1	-3.630498000	-2.522514000	0.000730000
1	-5.765149000	-1.328576000	0.000682000
1	-3.669434000	2.417429000	-0.000496000
1	-1.507701000	1.198970000	-0.000437000

5f_A2, optimization in gas phase B3LYP/6-311++G**, E= -873.910146563 a.u. Sum of electronic and thermal Enthalpies= -873.638730 a.u.			
-1; 1			
6	6.650374000	0.302873000	0.006598000
6	5.807402000	-0.809079000	0.006663000
6	6.129023000	1.612159000	0.002206000
1	6.209901000	-1.818048000	0.010017000
6	4.423356000	-0.596507000	0.002220000
6	4.752586000	1.842307000	-0.002205000
1	4.352304000	2.851941000	-0.005527000
6	3.890546000	0.739017000	-0.002233000
6	2.315930000	-0.646766000	-0.003604000
7	3.373381000	-1.481818000	0.001169000
7	2.515942000	0.672899000	-0.005973000
7	1.052143000	-1.254083000	-0.006690000
7	-0.100354000	-0.615031000	-0.004625000
6	-1.200393000	-1.296232000	-0.002561000
1	-1.185320000	-2.394583000	-0.001830000
1	1.081218000	-2.271490000	-0.002560000
1	6.813554000	2.455943000	0.002271000
6	-2.503476000	-0.647234000	-0.001339000
6	-2.644061000	0.758785000	-0.002555000
6	-3.678547000	-1.410180000	0.001142000
6	-3.892625000	1.352771000	-0.001321000
6	-4.945438000	-0.818845000	0.002388000
6	-5.056153000	0.570284000	0.001158000
1	7.727429000	0.159720000	0.009945000
8	-6.248824000	1.262121000	0.002195000
6	-7.448443000	0.514410000	0.004663000
1	-7.533502000	-0.118657000	-0.887433000
1	-7.530873000	-0.116988000	0.898186000
1	-8.259486000	1.242884000	0.005174000
1	-3.607959000	-2.493945000	0.002100000
1	-5.823113000	-1.452598000	0.004311000
1	-3.994846000	2.432255000	-0.002242000
1	-1.746995000	1.366238000	-0.004470000

5f_Aw1, optimization in solv.water B3LYP/6-311++G**, E= -873.999957193 a.u. Sum of electronic and thermal Enthalpies= -873.728302 a.u.			
-1; 1			
6	-6.440194000	0.658632000	-0.000080000
6	-5.762170000	-0.565929000	-0.000079000
6	-5.747616000	1.876962000	0.000006000
1	-6.307506000	-1.503970000	-0.000156000
6	-4.362690000	-0.559172000	0.000017000
6	-4.344880000	1.907385000	0.000126000
1	-3.805609000	2.848403000	0.000205000
6	-3.679044000	0.689245000	0.000120000
6	-2.243333000	-1.039905000	0.000152000
7	-3.464173000	-1.606400000	-0.000005000
7	-2.338868000	0.349441000	0.000338000
1	-1.535562000	0.957290000	-0.000468000
7	-1.090617000	-1.729579000	-0.000079000

5f_Aw2, optimization in solv.water B3LYP/6-311++G**, E= -873.998689685 a.u. Sum of electronic and thermal Enthalpies= -873.726526 a.u.			
-1; 1			
6	6.653924000	0.331591000	0.006653000
6	5.824858000	-0.793893000	0.006051000
6	6.115965000	1.631954000	0.003311000
1	6.246847000	-1.794613000	0.008641000
6	4.438408000	-0.598419000	0.001953000
6	4.733620000	1.842308000	-0.000736000
1	4.325330000	2.848723000	-0.003292000
6	3.890454000	0.725311000	-0.001492000
6	2.317035000	-0.692859000	-0.003917000
7	3.396972000	-1.502095000	0.000394000
7	2.511210000	0.635106000	-0.005357000
7	1.061610000	-1.290677000	-0.007988000
7	-0.088390000	-0.598090000	-0.005625000

7	-0.006966000	-0.908254000	-0.000278000	6	-1.193778000	-1.260343000	-0.002600000
6	1.153943000	-1.480100000	-0.000097000	1	-1.191700000	-2.356039000	-0.001009000
1	1.221238000	-2.573215000	0.000181000	1	1.046565000	-2.306465000	-0.002257000
1	-6.300357000	2.809832000	-0.000016000	1	6.786916000	2.484998000	0.003890000
6	2.408323000	-0.734501000	-0.000050000	6	-2.500649000	-0.607574000	-0.001375000
6	2.468746000	0.676375000	-0.000190000	6	-2.656521000	0.793880000	-0.004460000
6	3.628087000	-1.428080000	0.000119000	6	-3.661608000	-1.391254000	0.002881000
6	3.680948000	1.344220000	-0.000181000	6	-3.913090000	1.372022000	-0.003336000
6	4.857969000	-0.766352000	0.000121000	6	-4.935533000	-0.820280000	0.004070000
6	4.889767000	0.629704000	-0.000027000	6	-5.066736000	0.570172000	0.000924000
1	-7.525132000	0.664932000	-0.000165000	1	7.731459000	0.201992000	0.009750000
8	6.031620000	1.383874000	-0.000025000	8	-6.257142000	1.237553000	0.001607000
6	7.290263000	0.709589000	0.000118000	6	-7.466620000	0.475820000	0.005748000
1	7.407426000	0.089622000	0.894025000	1	-7.540875000	-0.152153000	-0.886809000
1	7.407525000	0.089426000	-0.893639000	1	-7.537492000	-0.147784000	0.901635000
1	8.047122000	1.491634000	0.000075000	1	-8.275321000	1.203828000	0.005497000
1	3.620821000	-2.513572000	0.000235000	1	-3.574795000	-2.473071000	0.005285000
1	5.770600000	-1.347313000	0.000243000	1	-5.803829000	-1.464966000	0.007398000
1	3.716630000	2.427996000	-0.000297000	1	-4.027994000	2.449952000	-0.005770000
1	1.545495000	1.243043000	-0.000313000	1	-1.776168000	1.424841000	-0.007843000
5f_R1, optimization in gas phase B3LYP/6-311++G**, E= -873.830953773 a.u. Sum of electronic and thermal Enthalpies= -873.558420 a.u.				**5f_R2,** optimization in gas phase B3LYP/6-311++G**, E= -873.812348959 a.u. Sum of electronic and thermal Enthalpies= -873.539748 a.u.			
0; 2				0; 2			
6	6.475526000	0.505078000	0.000291000	6	6.616965000	0.241546000	0.000031000
6	5.746747000	-0.671498000	0.000298000	6	5.795001000	-0.856875000	0.000002000
6	5.837935000	1.766054000	0.000083000	6	6.097724000	1.581819000	0.000039000
1	6.226552000	-1.642606000	0.000375000	1	6.185865000	-1.867300000	-0.000020000
6	4.343020000	-0.581592000	0.000087000	6	4.395508000	-0.626332000	-0.000023000
6	4.452553000	1.887188000	-0.000137000	6	4.748245000	1.846263000	0.000020000
1	3.973548000	2.859289000	-0.000259000	1	4.362332000	2.858462000	0.000026000
6	3.717501000	0.702822000	-0.000120000	6	3.866871000	0.741891000	-0.000018000
6	2.227986000	-0.949540000	-0.000028000	6	2.292806000	-0.631729000	0.000065000
7	3.411101000	-1.575854000	-0.000170000	7	3.371617000	-1.484775000	-0.000080000
7	2.373257000	0.433789000	-0.000215000	7	2.521561000	0.699034000	-0.000030000
1	1.592944000	1.071004000	0.000088000	7	1.066247000	-1.205791000	0.000067000
7	1.050737000	-1.599822000	-0.000034000	7	-0.086874000	-0.517231000	-0.000038000
7	0.003742000	-0.759242000	-0.000155000	6	-1.173493000	-1.212725000	-0.000047000
6	-1.149381000	-1.377155000	-0.000167000	1	-1.140288000	-2.309842000	0.000062000
1	-1.156993000	-2.469353000	0.000010000	1	1.067552000	-2.225989000	0.000053000
1	6.446463000	2.663177000	0.000095000	1	6.804459000	2.404309000	0.000054000
6	-2.412292000	-0.681085000	-0.000098000	6	-2.485274000	-0.593672000	-0.000026000
6	-2.510425000	0.729399000	-0.000167000	6	-2.651396000	0.808151000	-0.000047000
6	-3.604899000	-1.423018000	0.000050000	6	-3.630810000	-1.399132000	0.000019000
6	-3.738680000	1.353697000	-0.000110000	6	-3.912123000	1.365844000	-0.000039000
6	-4.850199000	-0.804237000	0.000102000	6	-4.908725000	-0.846249000	0.000023000
6	-4.922836000	0.593396000	0.000027000	6	-5.054227000	0.544596000	-0.000005000
1	7.558616000	0.465865000	0.000412000	1	7.693036000	0.108449000	0.000035000
8	-6.077000000	1.305404000	0.000079000	8	-6.245342000	1.194732000	0.000001000
6	-7.318702000	0.606753000	0.000225000	6	-7.447346000	0.431098000	0.000045000
1	-7.423804000	-0.014577000	-0.894767000	1	-7.519678000	-0.195214000	-0.894979000
1	-7.423656000	-0.014468000	0.895310000	1	-7.519645000	-0.195165000	0.895105000
1	-8.089337000	1.375092000	0.000243000	1	-8.258166000	1.156991000	0.000040000
1	-3.554295000	-2.506756000	0.000106000	1	-3.525785000	-2.479416000	0.000041000
1	-5.745662000	-1.410559000	0.000203000	1	-5.770504000	-1.499320000	0.000050000
1	-3.821775000	2.433826000	-0.000173000	1	-4.050584000	2.440188000	-0.000059000

1	-1.601580000	1.317158000	-0.000282000	1	-1.772064000	1.440369000	-0.000078000
5f_Rw1, optimization in solv. water B3LYP/6-311++G**, E= -873.848565758 a.u. Sum of electronic and thermal Enthalpies= -873.575923 a.u.				**5f_Rw2,** optimization in solv. water B3LYP/6-311++G**, E= -873.832585954 a.u. Sum of electronic and thermal Enthalpies= -873.559717 a.u.			
0; 2				0; 2			
6	-6.473309000	0.515270000	0.000042000	6	-6.626514000	0.240324000	0.000112000
6	-5.750239000	-0.666182000	0.000133000	6	-5.800072000	-0.858553000	0.000098000
6	-5.829344000	1.774426000	-0.000077000	6	-6.108687000	1.577204000	0.000057000
1	-6.241515000	-1.632025000	0.000154000	1	-6.194280000	-1.868061000	0.000131000
6	-4.346039000	-0.580777000	0.000075000	6	-4.402461000	-0.626425000	0.000020000
6	-4.443707000	1.889003000	-0.000103000	6	-4.755591000	1.839053000	-0.000014000
1	-3.955741000	2.856018000	-0.000134000	1	-4.374178000	2.853457000	-0.000060000
6	-3.715238000	0.699205000	-0.000042000	6	-3.876714000	0.734304000	-0.000034000
6	-2.225090000	-0.946914000	0.000128000	6	-2.291545000	-0.645715000	0.000037000
7	-3.409317000	-1.576906000	-0.000103000	7	-3.373883000	-1.489488000	-0.000027000
7	-2.370644000	0.428676000	0.000199000	7	-2.525438000	0.687271000	-0.000108000
1	-1.597769000	1.077896000	-0.000229000	7	-1.061359000	-1.207081000	0.000012000
7	-1.049593000	-1.608231000	0.000130000	7	0.080652000	-0.495891000	-0.000088000
7	0.003218000	-0.777746000	-0.000062000	6	1.176264000	-1.188849000	-0.000157000
6	1.160273000	-1.394315000	-0.000254000	1	1.145283000	-2.282650000	-0.000071000
1	1.178796000	-2.486147000	0.000010000	1	-1.036216000	-2.227339000	0.000018000
1	-6.433927000	2.673957000	-0.000129000	1	-6.813238000	2.401133000	0.000062000
6	2.414058000	-0.690959000	-0.000138000	6	2.482058000	-0.569921000	-0.000094000
6	2.499829000	0.722556000	-0.000081000	6	2.662046000	0.831845000	-0.000118000
6	3.613533000	-1.427894000	-0.000056000	6	3.623303000	-1.388304000	0.000002000
6	3.723603000	1.353791000	-0.000024000	6	3.927266000	1.377820000	-0.000064000
6	4.852705000	-0.801536000	-0.000009000	6	4.904013000	-0.848439000	0.000054000
6	4.914677000	0.599220000	0.000000000	6	5.063047000	0.543382000	0.000022000
1	-7.556484000	0.480710000	0.000035000	1	-7.701941000	0.104786000	0.000155000
8	6.060549000	1.314895000	0.000083000	8	6.256734000	1.177921000	0.000070000
6	7.317099000	0.623125000	0.000118000	6	7.461326000	0.399499000	0.000138000
1	7.421923000	0.005666000	0.895475000	1	7.522900000	-0.223965000	0.895535000
1	7.421986000	0.005700000	-0.895255000	1	7.522960000	-0.224028000	-0.895211000
1	8.077871000	1.400084000	0.000160000	1	8.274972000	1.120955000	0.000140000
1	3.570692000	-2.511650000	-0.000071000	1	3.507259000	-2.466675000	0.000025000
1	5.752543000	-1.400676000	0.000023000	1	5.759510000	-1.508945000	0.000121000
1	3.795567000	2.434798000	-0.000002000	1	4.072437000	2.451387000	-0.000092000
1	1.589147000	1.307833000	-0.000116000	1	1.794438000	1.479552000	-0.000189000
5f_RC, optimization in gas phase B3LYP/6-311++G**, E= -874.220854808 a.u. Sum of electronic and thermal Enthalpies= -873.934312 a.u.				**5f_RCw,** optimization in solv. water B3LYP/6-311++G**, E= -874.286705705 a.u. Sum of electronic and thermal Enthalpies= -874.000322 a.u.			
1; 2				1; 2			
6	6.579611000	0.322569000	0.000215000	6	6.537286000	0.405493000	0.000153000
6	5.774699000	-0.795353000	0.000187000	6	5.766534000	-0.738944000	0.000113000
6	6.031061000	1.631649000	0.000101000	6	5.948993000	1.697181000	0.000124000
1	6.178613000	-1.799572000	0.000255000	1	6.207538000	-1.727749000	0.000114000
6	4.377972000	-0.591790000	0.000057000	6	4.365617000	-0.581395000	0.000057000
6	4.657561000	1.865064000	-0.000060000	6	4.571608000	1.883948000	0.000032000
1	4.257816000	2.871217000	-0.000173000	1	4.132174000	2.872942000	-0.000006000
6	3.846277000	0.740922000	-0.000057000	6	3.793419000	0.731541000	0.000010000
6	2.259433000	-0.778718000	-0.000106000	6	2.251618000	-0.828047000	-0.000040000
7	3.374743000	-1.506838000	0.000019000	7	3.386298000	-1.528020000	0.000025000
7	2.472071000	0.570983000	-0.000315000	7	2.431430000	0.524691000	-0.000214000
1	1.750151000	1.276226000	0.000308000	1	1.693764000	1.215923000	0.000597000
7	1.035136000	-1.343635000	-0.000128000	7	1.034422000	-1.411351000	-0.000072000
7	-0.080081000	-0.600053000	-0.000109000	7	-0.075152000	-0.671661000	-0.000127000

6	-1.208470000	-1.256668000	-0.000092000	6	-1.207385000	-1.325227000	-0.000149000
1	-1.203422000	-2.351386000	-0.000068000	1	-1.215408000	-2.416911000	-0.000211000
1	1.014765000	-2.365423000	-0.000010000	1	1.010651000	-2.433414000	0.000098000
1	6.706303000	2.478953000	0.000119000	1	6.597073000	2.565322000	0.000154000
6	-2.481860000	-0.610774000	-0.000055000	6	-2.465230000	-0.649800000	-0.000151000
6	-2.626794000	0.801665000	-0.000102000	6	-2.572666000	0.766001000	-0.000306000
6	-3.648317000	-1.407451000	0.000031000	6	-3.650364000	-1.418367000	0.000044000
6	-3.871404000	1.374828000	-0.000061000	6	-3.804150000	1.369804000	-0.000255000
6	-4.907999000	-0.840840000	0.000073000	6	-4.895780000	-0.819135000	0.000130000
6	-5.032228000	0.562451000	0.000031000	6	-4.982506000	0.585695000	-0.000025000
1	7.656699000	0.210760000	0.000318000	1	7.617463000	0.325883000	0.000202000
8	-6.189927000	1.220687000	0.000068000	8	-6.130726000	1.272300000	0.000027000
6	-7.435523000	0.502230000	0.000164000	6	-7.386730000	0.569473000	0.000361000
1	-7.524489000	-0.113321000	-0.897846000	1	-7.482831000	-0.046001000	-0.896099000
1	-7.524376000	-0.113278000	0.898215000	1	-7.482511000	-0.045704000	0.897060000
1	-8.207081000	1.267380000	0.000195000	1	-8.149195000	1.343808000	0.000365000
1	-3.555918000	-2.488270000	0.000060000	1	-3.582417000	-2.500396000	0.000161000
1	-5.782414000	-1.476188000	0.000136000	1	-5.785470000	-1.432463000	0.000316000
1	-4.001737000	2.449702000	-0.000102000	1	-3.902780000	2.448094000	-0.000385000
1	-1.742697000	1.425823000	-0.000179000	1	-1.672831000	1.367332000	-0.000469000
5f_M, optimization in gas phase B3LYP/6-311++G**, E= -874.464309704 a.u. Sum of electronic and thermal Enthalpies= -874.178386 a.u.				**5f_Mw,** optimization in solv. water B3LYP/6-311++G**, E= -874.480851420 a.u. Sum of electronic and thermal Enthalpies= -874.195070 a.u.			
0; 1				0; 1			
6	6.539314000	0.504350000	0.008459000	6	6.527085000	0.535952000	0.006374000
6	5.789084000	-0.669725000	0.008605000	6	5.791373000	-0.649883000	0.005669000
6	5.925676000	1.766456000	0.002845000	6	5.895352000	1.789979000	0.003305000
1	6.262185000	-1.644403000	0.012950000	1	6.283616000	-1.615796000	0.008080000
6	4.397570000	-0.562260000	0.002942000	6	4.397246000	-0.560954000	0.001786000
6	4.536022000	1.895132000	-0.002854000	6	4.502344000	1.899041000	-0.000615000
1	4.063011000	2.870600000	-0.007212000	1	4.012431000	2.865673000	-0.002997000
6	3.796526000	0.719389000	-0.002693000	6	3.778453000	0.712850000	-0.001294000
6	2.291998000	-0.898304000	-0.004108000	6	2.286337000	-0.918839000	-0.003338000
7	3.424108000	-1.555527000	0.002025000	7	3.434630000	-1.565933000	0.000441000
7	2.427311000	0.465282000	-0.007514000	7	2.414609000	0.443349000	-0.004764000
1	1.660673000	1.118204000	-0.010449000	1	1.645448000	1.096188000	-0.006274000
7	1.058579000	-1.496371000	-0.008402000	7	1.062554000	-1.521656000	-0.006814000
7	-0.068961000	-0.750657000	-0.006375000	7	-0.065436000	-0.764665000	-0.005178000
6	-1.198295000	-1.363288000	-0.003000000	6	-1.194878000	-1.377832000	-0.002143000
1	-1.237331000	-2.458894000	-0.001160000	1	-1.238592000	-2.471042000	-0.000244000
1	1.036608000	-2.511204000	-0.000930000	1	1.027274000	-2.536462000	-0.000525000
1	6.540794000	2.658854000	0.002884000	1	6.497658000	2.691138000	0.003970000
6	-2.478668000	-0.665145000	-0.001674000	6	-2.470793000	-0.669515000	-0.001245000
6	-2.578737000	0.740381000	-0.004358000	6	-2.562476000	0.737015000	-0.005123000
6	-3.664331000	-1.406881000	0.002434000	6	-3.660722000	-1.407196000	0.003501000
6	-3.810242000	1.364130000	-0.002891000	6	-3.792376000	1.366751000	-0.004264000
6	-4.914940000	-0.789466000	0.003954000	6	-4.908380000	-0.783839000	0.004430000
6	-4.992287000	0.604757000	0.001351000	6	-4.978743000	0.611954000	0.000497000
1	7.621767000	0.444037000	0.012748000	1	7.610331000	0.489346000	0.009353000
8	-6.151695000	1.317259000	0.002347000	8	-6.135730000	1.327450000	0.000837000
6	-7.386909000	0.611723000	0.006439000	6	-7.380198000	0.621208000	0.005446000
1	-7.491471000	-0.013218000	-0.886759000	1	-7.481809000	-0.002265000	-0.887080000
1	-7.487532000	-0.009625000	0.902584000	1	-7.478177000	0.003000000	0.902031000
1	-8.163967000	1.373962000	0.006661000	1	-8.153601000	1.386272000	0.004765000
1	-3.616390000	-2.491246000	0.004465000	1	-3.617691000	-2.491370000	0.006565000
1	-5.807571000	-1.400108000	0.007192000	1	-5.803578000	-1.390308000	0.008157000

1	-3.892049000	2.444435000	-0.004959000	1	-3.863569000	2.448128000	-0.007289000
1	-1.673102000	1.333950000	-0.007639000	1	-1.656136000	1.330095000	-0.008928000

5g_A1, optimization in gas phase B3LYP/6-311++G**, E= -988.450822696 a.u. Sum of electronic and thermal Enthalpies= -988.143919 a.u.			
-1; 1			
6	6.087662000	0.684886000	-0.583495000
6	4.820537000	1.220330000	-0.821056000
6	6.243619000	-0.565722000	0.046795000
1	4.702517000	2.184579000	-1.307784000
6	3.698352000	0.484862000	-0.418876000
6	5.136219000	-1.312148000	0.454063000
1	5.257201000	-2.275953000	0.940119000
6	3.857154000	-0.791523000	0.224457000
6	1.813377000	-0.339898000	0.054320000
7	2.357066000	0.756523000	-0.517017000
7	2.613996000	-1.303133000	0.516938000
7	0.411068000	-0.373587000	0.095267000
7	-0.285769000	-1.230045000	0.814404000
6	-1.582026000	-1.174229000	0.911837000
1	-2.003932000	-2.020663000	1.441235000
1	-0.013922000	0.478807000	-0.249302000
1	7.244301000	-0.954023000	0.216208000
6	-2.580287000	-0.249758000	0.338713000
6	-3.809578000	-0.789302000	-0.117418000
6	-2.453486000	1.157096000	0.273688000
6	-4.822989000	0.011889000	-0.646993000
6	-3.456475000	1.969133000	-0.268620000
6	-4.632869000	1.389994000	-0.727399000
1	6.970676000	1.240194000	-0.888311000
8	-1.305613000	1.666141000	0.808316000
6	-1.025339000	3.055274000	0.700576000
1	-1.029319000	3.383448000	-0.344005000
1	-1.742197000	3.650272000	1.278145000
1	-0.023843000	3.180617000	1.107722000
8	-3.924220000	-2.150539000	-0.011008000
6	-5.109423000	-2.775967000	-0.462551000
1	-5.989577000	-2.428777000	0.092339000
1	-5.271136000	-2.609782000	-1.534280000
1	-4.969004000	-3.841685000	-0.283187000
1	-3.329939000	3.041894000	-0.314512000
1	-5.413393000	2.016102000	-1.145590000
1	-5.744841000	-0.422906000	-1.007622000

5g_A2, optimization in gas phase B3LYP/6-311++G**, E= -988.454352556 a.u. Sum of electronic and thermal Enthalpies= -988.148416 a.u.			
-1; 1			
6	5.998530000	0.437302000	-0.737109000
6	4.778103000	1.020294000	-1.096362000
6	6.056672000	-0.664832000	0.124879000
1	4.739164000	1.873451000	-1.765513000
6	3.592157000	0.485550000	-0.579435000
6	4.881635000	-1.220149000	0.657243000
1	4.923369000	-2.074774000	1.325833000
6	3.673734000	-0.639401000	0.298219000
6	1.550088000	0.011522000	-0.046759000
7	2.288116000	0.864962000	-0.773721000
7	2.362744000	-0.910966000	0.620227000
1	1.970430000	-1.629473000	1.206678000
7	0.210566000	0.035645000	0.046464000
7	-0.243090000	-0.946761000	0.847595000
6	-1.524757000	-1.049046000	1.049858000
1	-1.832344000	-1.925741000	1.610895000
1	7.017681000	-1.096510000	0.385577000
6	-2.598573000	-0.195464000	0.510341000
6	-3.733141000	-0.798546000	-0.082337000
6	-2.579242000	1.211524000	0.565308000
6	-4.756625000	-0.045131000	-0.657156000
6	-3.592211000	1.976581000	-0.028223000
6	-4.666812000	1.348950000	-0.640993000
1	6.921699000	0.847731000	-1.135884000
8	-1.607071000	1.808640000	1.317408000
6	-0.843107000	2.846128000	0.697323000
1	-0.354745000	2.460309000	-0.198804000
1	-1.463082000	3.723101000	0.470461000
1	-0.080548000	3.129284000	1.422750000
8	-3.736434000	-2.174873000	-0.073893000
6	-4.782398000	-2.853528000	-0.735758000
1	-5.759444000	-2.647390000	-0.279552000
1	-4.824618000	-2.592921000	-1.800593000
1	-4.559845000	-3.916442000	-0.636492000
1	-3.546448000	3.057608000	0.023071000
1	-5.455343000	1.941088000	-1.093935000
1	-5.605703000	-0.521283000	-1.128609000

5g_Aw1, optimization in solv.water B3LYP/6-311++G**, E= -988.547807006 a.u. Sum of electronic and thermal Enthalpies= -988.240057 a.u.			
-1; 1			
6	6.149301000	0.518085000	-0.591369000
6	4.919412000	1.157654000	-0.770233000
6	6.223523000	-0.782032000	-0.057019000
1	4.870438000	2.161406000	-1.182215000
6	3.754041000	0.472756000	-0.403991000
6	5.068892000	-1.477210000	0.314088000
1	5.132716000	-2.479756000	0.726996000
6	3.829796000	-0.849405000	0.141627000
6	1.801959000	-0.239988000	0.040402000
7	2.428065000	0.846225000	-0.458494000
7	2.549306000	-1.289801000	0.415734000

5g_Aw2, optimization in solv.water B3LYP/6-311++G**, E= -988.543531315 a.u. Sum of electronic and thermal Enthalpies= -988.236717 a.u.			
-1; 1			
6	6.035303000	-0.220001000	-1.141495000
6	4.815943000	0.259718000	-1.635120000
6	6.102112000	-0.956881000	0.048289000
1	4.775077000	0.829915000	-2.557484000
6	3.646056000	-0.010614000	-0.916315000
6	4.941498000	-1.239959000	0.785050000
1	4.989171000	-1.811603000	1.705596000
6	3.736246000	-0.762192000	0.289180000
6	1.611353000	-0.182029000	-0.167066000
7	2.336125000	0.336029000	-1.177311000
7	2.432101000	-0.850952000	0.738968000

7	0.404623000	-0.222730000	0.086601000	1	2.078418000	-1.314223000	1.560495000
7	-0.263150000	-1.076856000	0.893305000	7	0.278810000	-0.063648000	-0.052973000
6	-1.549861000	-1.027897000	0.994173000	7	-0.182973000	-0.719020000	1.050529000
1	-1.960011000	-1.823290000	1.608475000	6	-1.448477000	-0.681707000	1.305779000
1	-0.007236000	0.688869000	-0.090417000	1	-1.766343000	-1.271796000	2.163148000
1	7.194260000	-1.251037000	0.067837000	1	7.060863000	-1.315363000	0.406226000
6	-2.560698000	-0.166176000	0.341742000	6	-2.511005000	0.025462000	0.537754000
6	-3.733588000	-0.795680000	-0.144862000	6	-3.436824000	-0.714768000	-0.219168000
6	-2.489403000	1.238792000	0.243809000	6	-2.667464000	1.422595000	0.595634000
6	-4.767060000	-0.059410000	-0.728188000	6	-4.471722000	-0.086762000	-0.923162000
6	-3.516950000	1.983360000	-0.344686000	6	-3.695101000	2.063844000	-0.108040000
6	-4.642759000	1.324081000	-0.824303000	6	-4.582013000	1.299188000	-0.860737000
1	7.064334000	1.031659000	-0.868789000	1	6.947959000	-0.016368000	-1.691810000
8	-1.372718000	1.815693000	0.782141000	8	-1.779682000	2.088420000	1.390353000
6	-1.265308000	3.244999000	0.809371000	6	-1.879684000	3.508629000	1.493840000
1	-1.247119000	3.658840000	-0.201793000	1	-1.741788000	3.989236000	0.520849000
1	-2.087750000	3.684386000	1.378697000	1	-2.841136000	3.811504000	1.919474000
1	-0.321184000	3.456110000	1.306676000	1	-1.077027000	3.812507000	2.163346000
8	-3.764721000	-2.151461000	-0.013996000	8	-3.241777000	-2.069177000	-0.220879000
6	-4.936249000	-2.860629000	-0.426613000	6	-4.153878000	-2.893211000	-0.947924000
1	-5.817333000	-2.522625000	0.125498000	1	-5.173921000	-2.790150000	-0.566285000
1	-5.106778000	-2.748798000	-1.500776000	1	-4.136184000	-2.658918000	-2.016291000
1	-4.741229000	-3.906211000	-0.197182000	1	-3.812373000	-3.915612000	-0.796850000
1	-3.451329000	3.059188000	-0.417674000	1	-3.813747000	3.137294000	-0.068748000
1	-5.441177000	1.898803000	-1.279429000	1	-5.378507000	1.793566000	-1.405659000
1	-5.652489000	-0.547509000	-1.109032000	1	-5.176303000	-0.656518000	-1.512190000
5g_R1, optimization in gas phase B3LYP/6-311++G**, E= -988.359066740 a.u. Sum of electronic and thermal Enthalpies= -988.050911 a.u.				**5g_R2,** optimization in gas phase B3LYP/6-311++G**, E= -988.372285530 a.u. Sum of electronic and thermal Enthalpies= -988.064707 a.u.			
0; 2				0; 2			
6	6.047068000	0.469601000	-0.732555000	6	5.896298000	0.755880000	-0.585662000
6	4.855453000	1.141580000	-0.836062000	6	4.697027000	1.008158000	-1.230002000
6	6.131971000	-0.849659000	-0.167474000	6	5.969908000	-0.131023000	0.511195000
1	4.792596000	2.135689000	-1.262475000	1	4.632417000	1.683533000	-2.074512000
6	3.689708000	0.485446000	-0.362950000	6	3.542491000	0.355888000	-0.761825000
6	5.026838000	-1.518152000	0.303030000	6	4.845741000	-0.790553000	0.996754000
1	5.095557000	-2.511916000	0.728814000	1	4.912635000	-1.469703000	1.838608000
6	3.777882000	-0.860855000	0.214846000	6	3.637248000	-0.535241000	0.350411000
6	1.793016000	-0.200023000	0.246356000	6	1.557918000	-0.394656000	-0.428764000
7	2.416789000	0.885299000	-0.333445000	7	2.261058000	0.422112000	-1.223973000
7	2.553102000	-1.265422000	0.589618000	7	2.356621000	-0.983924000	0.545696000
7	0.454520000	-0.114634000	0.406425000	1	2.010022000	-1.666216000	1.202142000
7	-0.260931000	-1.044548000	1.070754000	7	0.235847000	-0.593242000	-0.557065000
6	-1.551733000	-1.010123000	1.038736000	7	-0.237980000	-1.476464000	0.333789000
1	-1.994551000	-1.842667000	1.575054000	6	-1.506209000	-1.435276000	0.611888000
1	0.031683000	0.779201000	0.157417000	1	-1.875155000	-2.297860000	1.157989000
1	7.106418000	-1.322860000	-0.116397000	1	6.929007000	-0.301763000	0.986738000
6	-2.534148000	-0.147209000	0.350044000	6	-2.485963000	-0.408431000	0.252028000
6	-3.688308000	-0.793742000	-0.163602000	6	-3.772718000	-0.833416000	-0.153111000
6	-2.476341000	1.257932000	0.236467000	6	-2.235561000	0.980325000	0.336693000
6	-4.713054000	-0.073892000	-0.780008000	6	-4.751363000	0.085015000	-0.534369000
6	-3.498412000	1.983635000	-0.380003000	6	-3.211462000	1.901670000	-0.058726000
6	-4.603597000	1.308576000	-0.882555000	6	-4.448657000	1.443461000	-0.494840000
1	6.960391000	0.936810000	-1.083881000	1	6.802011000	1.243835000	-0.926760000
8	-1.377191000	1.857526000	0.784477000	8	-1.051480000	1.345218000	0.881882000
6	-1.289339000	3.284427000	0.822164000	6	-0.638724000	2.706171000	0.801062000

1	-1.262862000	3.705700000	-0.186440000	1	-0.611555000	3.044831000	-0.238397000
1	-2.125041000	3.707436000	1.385766000	1	-1.290892000	3.357576000	1.392122000
1	-0.352759000	3.503219000	1.330577000	1	0.367507000	2.732440000	1.214580000
8	-3.707334000	-2.144673000	-0.022441000	8	-3.956411000	-2.183014000	-0.172585000
6	-4.838400000	-2.878491000	-0.482261000	6	-5.218584000	-2.702774000	-0.574981000
1	-5.752464000	-2.563227000	0.030476000	1	-6.021475000	-2.356547000	0.083833000
1	-4.964788000	-2.772418000	-1.564036000	1	-5.447327000	-2.429188000	-1.609798000
1	-4.627666000	-3.919103000	-0.243450000	1	-5.128583000	-3.784964000	-0.499155000
1	-3.441921000	3.059297000	-0.461130000	1	-3.018633000	2.963699000	-0.012356000
1	-5.396185000	1.870792000	-1.362732000	1	-5.201144000	2.161778000	-0.800404000
1	-5.581402000	-0.576148000	-1.181008000	1	-5.724777000	-0.240898000	-0.871123000
5g_Rw1, optimization in solv. water B3LYP/6-311++G**, E= -988.380108296 a.u. Sum of electronic and thermal Enthalpies= -988.071944 a.u.				**5g_Rw2,** optimization in solv. water B3LYP/6-311++G**, E= -988.390456126 a.u. Sum of electronic and thermal Enthalpies= -988.082873 a.u.			
0; 2				0; 2			
6	6.078790000	0.438158000	-0.718139000	6	5.900231000	0.707543000	-0.661723000
6	4.901036000	1.141010000	-0.795164000	6	4.722736000	0.838919000	-1.377977000
6	6.133365000	-0.896727000	-0.192753000	6	5.945875000	-0.006946000	0.558538000
1	4.863620000	2.148803000	-1.191774000	1	4.684666000	1.384567000	-2.313359000
6	3.723672000	0.498607000	-0.334360000	6	3.561660000	0.238127000	-0.855887000
6	5.011219000	-1.551160000	0.264655000	6	4.815478000	-0.609959000	1.098392000
1	5.063398000	-2.558738000	0.660110000	1	4.856904000	-1.156234000	2.032626000
6	3.781041000	-0.860117000	0.201233000	6	3.628305000	-0.476263000	0.378419000
6	1.801971000	-0.147897000	0.264401000	6	1.575535000	-0.500285000	-0.470875000
7	2.457039000	0.931321000	-0.285329000	7	2.293523000	0.207352000	-1.360340000
7	2.541078000	-1.242617000	0.570957000	7	2.350551000	-0.923633000	0.595837000
7	0.469313000	-0.046543000	0.440956000	1	2.008740000	-1.490640000	1.357733000
7	-0.246708000	-1.010047000	1.066373000	7	0.262532000	-0.732353000	-0.623516000
6	-1.541337000	-0.996583000	0.999662000	7	-0.245669000	-1.541838000	0.319891000
1	-1.976852000	-1.851028000	1.507202000	6	-1.513436000	-1.458709000	0.584907000
1	0.032763000	0.857137000	0.236971000	1	-1.904546000	-2.286764000	1.168966000
1	7.095004000	-1.396082000	-0.159872000	1	6.889257000	-0.085418000	1.086260000
6	-2.526135000	-0.143592000	0.321439000	6	-2.465292000	-0.419522000	0.190601000
6	-3.682520000	-0.805498000	-0.178908000	6	-3.757372000	-0.829757000	-0.219885000
6	-2.479636000	1.265629000	0.208341000	6	-2.197990000	0.967378000	0.292301000
6	-4.720844000	-0.092900000	-0.779169000	6	-4.730680000	0.104114000	-0.578260000
6	-3.516585000	1.979448000	-0.392884000	6	-3.172445000	1.902610000	-0.072250000
6	-4.622238000	1.290984000	-0.879957000	6	-4.417637000	1.459119000	-0.506906000
1	7.000854000	0.893879000	-1.060183000	1	6.810532000	1.158753000	-1.038775000
8	-1.386207000	1.876056000	0.750631000	8	-0.997134000	1.311700000	0.816264000
6	-1.326347000	3.312556000	0.805373000	6	-0.672032000	2.697730000	0.962757000
1	-1.307431000	3.739998000	-0.198950000	1	-0.663026000	3.203548000	-0.006124000
1	-2.172514000	3.706271000	1.371009000	1	-1.371969000	3.197835000	1.637357000
1	-0.397199000	3.542197000	1.321248000	1	0.326656000	2.718668000	1.393455000
8	-3.681777000	-2.154966000	-0.050153000	8	-3.947013000	-2.174547000	-0.266226000
6	-4.837794000	-2.898082000	-0.457879000	6	-5.239495000	-2.682077000	-0.616955000
1	-5.725067000	-2.574731000	0.091696000	1	-6.003471000	-2.326319000	0.078949000
1	-5.005786000	-2.798553000	-1.532923000	1	-5.506110000	-2.400097000	-1.638713000
1	-4.614947000	-3.935175000	-0.217889000	1	-5.156582000	-3.764463000	-0.547723000
1	-3.474930000	3.055633000	-0.472105000	1	-2.976209000	2.962591000	-0.003688000
1	-5.426453000	1.846549000	-1.347945000	1	-5.167505000	2.189155000	-0.789546000
1	-5.590290000	-0.600797000	-1.169805000	1	-5.708467000	-0.207449000	-0.915520000
5g_RC, optimization in gas phase B3LYP/6-311++G**, E= -988.774511829 a.u. Sum of electronic and thermal Enthalpies= -988.452575 a.u.				**5g_RCw,** optimization in solv. water B3LYP/6-311++G**, E= -988.834031596 a.u. Sum of electronic and thermal Enthalpies= -988.512611 a.u.			
1; 2				1; 2			

6	6.244723000	0.464222000	-0.432669000	6	6.230444000	0.439649000	-0.485452000
6	5.079635000	1.187312000	-0.543286000	6	5.069370000	1.171959000	-0.586397000
6	6.237427000	-0.899763000	-0.031890000	6	6.219650000	-0.919744000	-0.065296000
1	5.069370000	2.225957000	-0.847748000	1	5.066919000	2.206617000	-0.904735000
6	3.867748000	0.522859000	-0.243084000	6	3.857563000	0.522642000	-0.256372000
6	5.062374000	-1.584041000	0.270222000	6	5.046033000	-1.587492000	0.265914000
1	5.077768000	-2.623055000	0.573837000	1	5.049808000	-2.621477000	0.584672000
6	3.886084000	-0.858744000	0.159523000	6	3.872022000	-0.852009000	0.164938000
6	1.844359000	-0.044403000	0.104019000	6	1.836753000	-0.030056000	0.136253000
7	2.602334000	0.997799000	-0.268304000	7	2.593468000	1.005190000	-0.265767000
7	2.560102000	-1.179987000	0.368048000	7	2.553899000	-1.161792000	0.402283000
1	2.156368000	-2.052213000	0.679505000	1	2.162522000	-2.036816000	0.724005000
7	0.511878000	0.029776000	0.199610000	7	0.506118000	0.050019000	0.254122000
7	-0.175770000	-1.040834000	0.641754000	7	-0.178779000	-1.011480000	0.714598000
6	-1.481020000	-1.062057000	0.604665000	6	-1.484216000	-1.040875000	0.665386000
1	-1.851141000	-2.020697000	0.948708000	1	-1.853980000	-1.992230000	1.029587000
1	0.045811000	0.939673000	0.062325000	1	0.037197000	0.957537000	0.107520000
1	7.182432000	-1.424914000	0.040020000	1	7.161639000	-1.451069000	-0.002414000
6	-2.537849000	-0.171274000	0.158260000	6	-2.536111000	-0.164946000	0.183597000
6	-3.780124000	-0.820657000	-0.156482000	6	-3.763113000	-0.822728000	-0.164434000
6	-2.513029000	1.250459000	0.073819000	6	-2.514211000	1.256524000	0.098393000
6	-4.900567000	-0.086688000	-0.542485000	6	-4.876744000	-0.097126000	-0.582644000
6	-3.635102000	1.972317000	-0.311800000	6	-3.629435000	1.972426000	-0.322242000
6	-4.813451000	1.296162000	-0.618199000	6	-4.793712000	1.287803000	-0.659270000
1	7.194751000	0.934644000	-0.653510000	1	7.180212000	0.899484000	-0.728849000
8	-1.348273000	1.867793000	0.430981000	8	-1.367719000	1.872394000	0.494773000
6	-1.302202000	3.303743000	0.560664000	6	-1.318429000	3.311368000	0.599155000
1	-1.464992000	3.784473000	-0.405660000	1	-1.440186000	3.771649000	-0.382215000
1	-2.042272000	3.638299000	1.289043000	1	-2.086277000	3.662135000	1.289303000
1	-0.300559000	3.528655000	0.919762000	1	-0.331129000	3.534790000	0.994839000
8	-3.773240000	-2.163522000	-0.074337000	8	-3.747712000	-2.167938000	-0.084259000
6	-4.981596000	-2.902814000	-0.309632000	6	-4.952186000	-2.908887000	-0.336304000
1	-5.764143000	-2.601850000	0.390666000	1	-5.746685000	-2.602496000	0.347193000
1	-5.320053000	-2.771048000	-1.339901000	1	-5.273520000	-2.782419000	-1.372302000
1	-4.717547000	-3.943938000	-0.141797000	1	-4.691372000	-3.948977000	-0.157356000
1	-3.609266000	3.050218000	-0.365973000	1	-3.606552000	3.050224000	-0.377881000
1	-5.683686000	1.866172000	-0.921568000	1	-5.658252000	1.851691000	-0.988952000
1	-5.828265000	-0.581226000	-0.788762000	1	-5.794279000	-0.596734000	-0.855044000
5g_M, optimization in gas phase B3LYP/6-311++G**, E= -989.014836737 a.u. Sum of electronic and thermal Enthalpies= -988.693184 a.u.				**5g_Mw,** optimization in solv. water B3LYP/6-311++G**, E= -989.031386620 a.u. Sum of electronic and thermal Enthalpies= -988.710069 a.u.			
0; 1				0; 1			
6	6.224507000	0.396937000	-0.528892000	6	6.222718000	0.343787000	-0.589839000
6	5.036613000	1.074793000	-0.795717000	6	5.041042000	1.041865000	-0.840750000
6	6.224921000	-0.871737000	0.071322000	6	6.211151000	-0.917436000	0.028247000
1	5.035783000	2.054437000	-1.258850000	1	5.054552000	2.015802000	-1.316846000
6	3.832882000	0.458341000	-0.450049000	6	3.832979000	0.451762000	-0.460713000
6	5.032397000	-1.505685000	0.423273000	6	5.013521000	-1.523577000	0.414885000
1	5.033838000	-2.486507000	0.885219000	1	5.002160000	-2.496708000	0.891512000
6	3.852969000	-0.822810000	0.153409000	6	3.841616000	-0.821042000	0.160004000
6	1.793445000	-0.064385000	-0.104147000	6	1.786214000	-0.036146000	-0.061815000
7	2.524618000	0.905778000	-0.595616000	7	2.527982000	0.918174000	-0.585946000
7	2.513304000	-1.134983000	0.357120000	7	2.503101000	-1.105681000	0.399384000
1	2.104448000	-1.935594000	0.812228000	1	2.101837000	-1.910180000	0.857033000
7	0.418522000	-0.055893000	-0.072822000	7	0.415370000	-0.008887000	-0.011754000
7	-0.197476000	-0.994508000	0.687739000	7	-0.197588000	-0.954618000	0.760167000

6	-1.477354000	-1.011099000	0.825732000	6	-1.480233000	-0.978413000	0.871356000
1	-1.828999000	-1.867973000	1.389851000	1	-1.835113000	-1.826884000	1.447582000
1	-0.020087000	0.850373000	-0.210659000	1	-0.023196000	0.904886000	-0.114156000
1	7.167755000	-1.370470000	0.264349000	1	7.148032000	-1.431906000	0.208442000
6	-2.550131000	-0.152146000	0.280379000	6	-2.545737000	-0.136393000	0.292102000
6	-3.737165000	-0.800985000	-0.141707000	6	-3.711972000	-0.804725000	-0.160321000
6	-2.529273000	1.256050000	0.223836000	6	-2.536477000	1.273055000	0.237956000
6	-4.831449000	-0.080054000	-0.622459000	6	-4.802979000	-0.096077000	-0.666545000
6	-3.619766000	1.985210000	-0.258996000	6	-3.624111000	1.988100000	-0.270844000
6	-4.757495000	1.307981000	-0.678243000	6	-4.742504000	1.293662000	-0.717311000
1	7.170612000	0.857788000	-0.789794000	1	7.171297000	0.783500000	-0.876974000
8	-1.390843000	1.855145000	0.689114000	8	-1.418983000	1.882345000	0.736179000
6	-1.330525000	3.279177000	0.788482000	6	-1.381011000	3.314714000	0.834132000
1	-1.412032000	3.750413000	-0.195177000	1	-1.433750000	3.777269000	-0.153899000
1	-2.115651000	3.655051000	1.450197000	1	-2.195118000	3.677840000	1.464710000
1	-0.353666000	3.499211000	1.214362000	1	-0.424752000	3.547702000	1.296870000
8	-3.719845000	-2.159212000	-0.051846000	8	-3.673084000	-2.161349000	-0.078630000
6	-4.880180000	-2.893729000	-0.425773000	6	-4.832204000	-2.914284000	-0.451883000
1	-5.743842000	-2.613972000	0.185945000	1	-5.696202000	-2.633483000	0.155864000
1	-5.116361000	-2.750118000	-1.484854000	1	-5.062784000	-2.779377000	-1.511794000
1	-4.634375000	-3.939427000	-0.249818000	1	-4.576330000	-3.954960000	-0.264940000
1	-3.590147000	3.064351000	-0.299638000	1	-3.609340000	3.067452000	-0.309307000
1	-5.603912000	1.871481000	-1.053665000	1	-5.586876000	1.846981000	-1.111729000
1	-5.727023000	-0.584422000	-0.955491000	1	-5.684211000	-0.609962000	-1.022087000

5h_A1, optimization in gas phase B3LYP/6-311++G**, E= -988.470422798 a.u. Sum of electronic and thermal Enthalpies= -988.164000 a.u.			
-1; 1			
6	6.898911000	-0.125775000	0.002238000
6	5.993003000	-1.186408000	0.002034000
6	6.455600000	1.212233000	0.001062000
1	6.335966000	-2.217020000	0.002914000
6	4.623240000	-0.893118000	0.000607000
6	5.095316000	1.522635000	-0.000357000
1	4.754814000	2.553893000	-0.001226000
6	4.170681000	0.471277000	-0.000605000
6	2.518038000	-0.820023000	-0.001444000
7	3.524365000	-1.715698000	0.000000000
7	2.794087000	0.486209000	-0.001837000
7	1.220659000	-1.352123000	-0.002758000
7	0.112183000	-0.645269000	-0.001680000
6	-1.031453000	-1.253419000	-0.001282000
1	-1.089722000	-2.349587000	-0.001557000
1	1.189275000	-2.369876000	-0.001832000
1	7.188627000	2.014126000	0.001272000
6	-2.283692000	-0.512330000	-0.000560000
6	-2.295584000	0.894624000	-0.000441000
6	-3.501777000	-1.217146000	0.000006000
1	-1.345390000	1.408497000	-0.000893000
1	-3.481123000	-2.298953000	-0.000098000
6	-3.511179000	1.570466000	0.000239000
6	-4.708543000	-0.514954000	0.000668000
6	-4.726527000	0.877126000	0.000794000
8	-5.946025000	-1.119898000	0.001248000
6	-6.002015000	-2.534374000	0.001164000
1	-5.528255000	-2.959189000	-0.891716000
1	-5.527357000	-2.959329000	0.893499000
1	-7.061304000	-2.792354000	0.001677000
8	-3.621409000	2.938242000	0.000411000
6	-2.423686000	3.704150000	-0.000047000
1	-1.818821000	3.505177000	0.890593000
1	-1.819644000	3.505408000	-0.891298000
1	-2.739049000	4.747432000	0.000231000
1	7.965739000	-0.331440000	0.003317000
1	-5.665336000	1.414853000	0.001320000

5h_A2, optimization in gas phase B3LYP/6-311++G**, E= -988.476517961 a.u. Sum of electronic and thermal Enthalpies= -988.170654 a.u.			
-1; 1			
6	-6.684810000	0.154028000	-0.000770000
6	-5.919718000	-1.016060000	-0.000862000
6	-6.084656000	1.420428000	-0.000265000
1	-6.388032000	-1.994462000	-0.001257000
6	-4.523825000	-0.911782000	-0.000451000
6	-4.688145000	1.552268000	0.000206000
1	-4.221543000	2.532583000	0.000638000
6	-3.932601000	0.387552000	0.000076000
6	-2.390135000	-1.245142000	0.000015000
7	-3.561397000	-1.890570000	-0.000491000
7	-2.577872000	0.140297000	0.000610000
1	-1.804008000	0.783431000	-0.000122000
7	-1.178011000	-1.838224000	-0.000148000
7	-0.185363000	-0.943485000	-0.000053000
6	1.029253000	-1.419672000	-0.000030000
1	1.176876000	-2.503064000	-0.000080000
1	-6.705055000	2.310736000	-0.000213000
6	2.201722000	-0.570864000	0.000075000
6	2.118282000	0.839126000	0.000135000
6	3.479791000	-1.172180000	0.000096000
1	1.135742000	1.286157000	0.000112000
1	3.540414000	-2.252353000	0.000040000
6	3.278868000	1.603290000	0.000227000
6	4.627730000	-0.382251000	0.000182000
6	4.545389000	1.009348000	0.000254000
8	5.908987000	-0.893937000	0.000210000
6	6.067536000	-2.300040000	0.000228000
1	5.624693000	-2.758613000	0.892276000
1	5.624808000	-2.758624000	-0.891872000
1	7.143059000	-2.480645000	0.000297000
8	3.286134000	2.981571000	0.000288000
6	2.039500000	3.654266000	0.000316000
1	1.449732000	3.413160000	-0.891517000
1	1.449696000	3.413019000	0.892086000
1	2.273868000	4.719270000	0.000403000
1	-7.768258000	0.081521000	-0.001108000
1	5.440467000	1.616798000	0.000324000

5h_Aw1, optimization in solv.water B3LYP/6-311++G**, E= -988.557159759 a.u. Sum of electronic and thermal Enthalpies= -988.250193 a.u.			
-1; 1			
6	6.911726000	-0.088911000	0.004504000
6	6.018216000	-1.163195000	0.002024000
6	6.451691000	1.241466000	0.005114000
1	6.380053000	-2.187162000	0.001555000
6	4.645558000	-0.885538000	0.000159000
6	5.084890000	1.533726000	0.003291000
1	4.736501000	2.562351000	0.003770000
6	4.177338000	0.468158000	0.000770000
6	2.523732000	-0.853375000	-0.003199000
7	3.552275000	-1.725726000	-0.002378000
7	2.795336000	0.459999000	-0.001467000

5h_Aw2, optimization in solv.water B3LYP/6-311++G**, E= -988.559374404 a.u. Sum of electronic and thermal Enthalpies= -988.252972 a.u.			
-1; 1			
6	-6.708022000	0.139605000	0.000304000
6	-5.936619000	-1.027472000	-0.000112000
6	-6.112464000	1.408826000	0.000705000
1	-6.406265000	-2.005526000	-0.000435000
6	-4.542208000	-0.909909000	-0.000120000
6	-4.717511000	1.550041000	0.000725000
1	-4.254234000	2.530595000	0.001053000
6	-3.957969000	0.387299000	0.000308000
6	-2.393976000	-1.223154000	-0.000254000
7	-3.563399000	-1.883878000	-0.000544000
7	-2.595524000	0.153021000	0.000361000

7	1.233311000	-1.376846000	-0.006442000	1	-1.842178000	0.822017000	-0.000254000
7	0.129643000	-0.622283000	-0.004165000	7	-1.187866000	-1.823498000	-0.000703000
6	-1.014560000	-1.216455000	-0.003424000	7	-0.176028000	-0.926884000	-0.000664000
1	-1.080540000	-2.309340000	-0.004050000	6	1.029068000	-1.405265000	-0.000453000
1	1.160310000	-2.390534000	-0.005131000	1	1.183988000	-2.488384000	-0.000330000
1	7.172247000	2.053004000	0.007041000	1	-6.737039000	2.295169000	0.001008000
6	-2.277244000	-0.478175000	-0.001757000	6	2.215399000	-0.557147000	-0.000213000
6	-2.313701000	0.926528000	-0.002217000	6	2.132069000	0.849019000	-0.000326000
6	-3.471083000	-1.216869000	0.000322000	6	3.478320000	-1.178854000	0.000082000
1	-1.383435000	1.474620000	-0.003889000	1	1.156279000	1.311048000	-0.000571000
1	-3.424253000	-2.297205000	0.000679000	1	3.531174000	-2.259162000	0.000156000
6	-3.547709000	1.576092000	-0.000574000	6	3.301335000	1.607285000	-0.000137000
6	-4.698733000	-0.545965000	0.001979000	6	4.638341000	-0.399324000	0.000260000
6	-4.741750000	0.847360000	0.001519000	6	4.558736000	0.993367000	0.000159000
8	-5.912273000	-1.174113000	0.004126000	8	5.906179000	-0.916131000	0.000544000
6	-5.945885000	-2.603113000	0.004817000	6	6.067815000	-2.335202000	0.000730000
1	-5.467221000	-3.011395000	-0.889904000	1	5.625944000	-2.785306000	0.894484000
1	-5.464398000	-3.010582000	0.898391000	1	5.626328000	-2.785497000	-0.893118000
1	-7.000002000	-2.873408000	0.006599000	1	7.142018000	-2.510522000	0.000979000
8	-3.695564000	2.934722000	-0.000882000	8	3.323690000	2.976451000	-0.000250000
6	-2.521789000	3.750282000	-0.002998000	6	2.080775000	3.679759000	-0.000533000
1	-1.915693000	3.573316000	0.889998000	1	1.493894000	3.448218000	-0.894215000
1	-1.918366000	3.572541000	-0.897649000	1	1.493553000	3.448338000	0.892956000
1	-2.876863000	4.778965000	-0.002915000	1	2.338867000	4.737182000	-0.000555000
1	7.979740000	-0.281663000	0.005961000	1	-7.790060000	0.061341000	0.000301000
1	-5.693530000	1.363515000	0.002775000	1	5.459957000	1.593355000	0.000298000
5h_R1, optimization in gas phase B3LYP/6-311++G**, E= -988.367473394 a.u. Sum of electronic and thermal Enthalpies= -988.060115 a.u.				**5h_R2,** optimization in gas phase B3LYP/6-311++G**, E= -988.385058312 a.u. Sum of electronic and thermal Enthalpies= -988.077845 a.u.			
0; 2				0; 2			
6	-6.869442000	-0.156871000	-0.000005000	6	-6.749187000	0.020150000	-0.000224000
6	-5.990583000	-1.209686000	-0.000061000	6	-5.935277000	-1.098510000	-0.000152000
6	-6.422309000	1.209900000	0.000071000	6	-6.206900000	1.325508000	-0.000165000
1	-6.326908000	-2.239490000	-0.000093000	1	-6.340740000	-2.102873000	-0.000136000
6	-4.605073000	-0.904551000	-0.000052000	6	-4.541721000	-0.903609000	-0.000013000
6	-5.089290000	1.546477000	0.000085000	6	-4.834719000	1.550430000	-0.000017000
1	-4.758355000	2.577935000	0.000111000	1	-4.430300000	2.555791000	0.000004000
6	-4.150062000	0.490729000	0.000031000	6	-4.013226000	0.424308000	0.000044000
6	-2.505415000	-0.797433000	-0.000008000	6	-2.405121000	-1.112775000	0.000086000
7	-3.537277000	-1.706695000	-0.000033000	7	-3.539394000	-1.825207000	0.000234000
7	-2.804717000	0.519560000	-0.000049000	7	-2.652931000	0.256001000	0.000145000
7	-1.249555000	-1.304824000	-0.000016000	1	-1.922302000	0.949473000	-0.000227000
7	-0.137951000	-0.552433000	0.000023000	7	-1.184851000	-1.675311000	0.000113000
6	0.987779000	-1.179731000	0.000027000	7	-0.200049000	-0.762016000	0.000126000
1	1.023537000	-2.276170000	-0.000013000	6	0.992136000	-1.297787000	0.000149000
1	-1.194261000	-2.323522000	0.000000000	1	1.074814000	-2.386414000	0.000118000
1	-7.172204000	1.993179000	0.000106000	1	-6.880971000	2.174452000	-0.000234000
6	2.261616000	-0.473540000	0.000012000	6	2.209814000	-0.514770000	0.000068000
6	2.304833000	0.928569000	-0.000002000	6	2.186092000	0.891534000	0.000071000
6	3.441764000	-1.232469000	0.000013000	6	3.433366000	-1.207937000	-0.000013000
1	1.374366000	1.476607000	-0.000003000	1	1.231469000	1.394543000	0.000137000
1	3.380639000	-2.312296000	0.000022000	1	3.425409000	-2.289151000	-0.000013000
6	3.545247000	1.564691000	-0.000014000	6	3.391139000	1.589956000	-0.000005000
6	4.676036000	-0.574809000	0.000004000	6	4.630977000	-0.489144000	-0.000083000
6	4.727512000	0.817341000	-0.000009000	6	4.610553000	0.905113000	-0.000080000
8	5.883218000	-1.208087000	0.000006000	8	5.868904000	-1.057329000	-0.000159000

6	5.910814000	-2.629611000	0.000033000	6	5.970274000	-2.476609000	-0.000125000
1	5.430270000	-3.039368000	0.894994000	1	5.511223000	-2.909872000	0.894710000
1	5.430271000	-3.039403000	-0.894912000	1	5.511136000	-2.909922000	-0.894891000
1	6.964022000	-2.904853000	0.000039000	1	7.036397000	-2.696150000	-0.000172000
8	3.711071000	2.914985000	-0.000025000	8	3.491841000	2.948954000	-0.000004000
6	2.551160000	3.742975000	-0.000031000	6	2.297331000	3.720838000	0.000089000
1	1.942282000	3.574383000	-0.893730000	1	1.696783000	3.525725000	-0.894687000
1	1.942286000	3.574401000	0.893674000	1	1.696903000	3.525694000	0.894940000
1	2.920923000	4.766692000	-0.000042000	1	2.617733000	4.761208000	0.000085000
1	-7.936896000	-0.346748000	-0.000013000	1	-7.826343000	-0.099091000	-0.000304000
1	5.684707000	1.322323000	-0.000017000	1	5.540231000	1.459140000	-0.000133000
5h_Rw1, optimization in solv. water B3LYP/6-311++G**, E= -988.387825423 a.u. Sum of electronic and thermal Enthalpies= -988.080286 a.u.				**5h_Rw2,** optimization in solv. water B3LYP/6-311++G**, E= -988.403478431 a.u. Sum of electronic and thermal Enthalpies= -988.096242 a.u.			
0; 2				0; 2			
6	-6.876310000	-0.142600000	0.000054000	6	-6.740652000	0.024411000	-0.000257000
6	-5.999051000	-1.199513000	0.000058000	6	-5.933611000	-1.099429000	-0.000248000
6	-6.424017000	1.220194000	0.000015000	6	-6.190653000	1.329104000	-0.000094000
1	-6.343462000	-2.226920000	0.000079000	1	-6.350617000	-2.099453000	-0.000284000
6	-4.613478000	-0.899026000	0.000021000	6	-4.538293000	-0.909343000	-0.000061000
6	-5.086888000	1.549369000	-0.000019000	6	-4.818293000	1.547657000	0.000096000
1	-4.755783000	2.581141000	-0.000039000	1	-4.403744000	2.548091000	0.000179000
6	-4.154570000	0.488655000	-0.000019000	6	-4.003404000	0.415385000	0.000099000
6	-2.504817000	-0.812500000	-0.000002000	6	-2.396115000	-1.115410000	-0.000006000
7	-3.545510000	-1.709153000	-0.000008000	7	-3.533198000	-1.831658000	0.000223000
7	-2.804582000	0.508120000	-0.000030000	7	-2.643743000	0.246085000	0.000157000
7	-1.249083000	-1.311299000	-0.000025000	1	-1.922750000	0.952404000	-0.000026000
7	-0.146709000	-0.537995000	-0.000051000	7	-1.180227000	-1.691007000	0.000035000
6	0.983999000	-1.163010000	-0.000088000	7	-0.186009000	-0.787584000	0.000160000
1	1.022913000	-2.255653000	-0.000071000	6	1.006735000	-1.321567000	0.000245000
1	-1.169018000	-2.328654000	-0.000031000	1	1.104193000	-2.408786000	0.000094000
1	-7.169167000	2.007498000	0.000014000	1	-6.860975000	2.180694000	-0.000116000
6	2.256575000	-0.456767000	-0.000043000	6	2.215513000	-0.524900000	0.000114000
6	2.315089000	0.946728000	-0.000027000	6	2.170032000	0.882096000	0.000083000
6	3.427174000	-1.231086000	-0.000018000	6	3.445999000	-1.206541000	0.000019000
1	1.395843000	1.512675000	-0.000047000	1	1.210194000	1.375621000	0.000151000
1	3.351263000	-2.309426000	-0.000029000	1	3.451304000	-2.287482000	0.000038000
6	3.563193000	1.567607000	0.000010000	6	3.366246000	1.595871000	-0.000024000
6	4.669746000	-0.589246000	0.000016000	6	4.634361000	-0.472109000	-0.000076000
6	4.736263000	0.803883000	0.000031000	6	4.594296000	0.923198000	-0.000101000
8	5.866614000	-1.237785000	0.000036000	8	5.878540000	-1.024656000	-0.000152000
6	5.873471000	-2.669084000	0.000039000	6	5.996828000	-2.450937000	-0.000109000
1	5.386038000	-3.065694000	0.894897000	1	5.541584000	-2.884080000	0.894747000
1	5.386086000	-3.065698000	-0.894843000	1	5.541468000	-2.884144000	-0.894874000
1	6.922342000	-2.957623000	0.000068000	1	7.064985000	-2.656921000	-0.000171000
8	3.747569000	2.916417000	0.000026000	8	3.449255000	2.954939000	-0.000053000
6	2.595257000	3.765195000	0.000004000	6	2.236814000	3.715030000	0.000030000
1	1.987699000	3.603441000	-0.894511000	1	1.642962000	3.508530000	-0.894574000
1	1.987655000	3.603426000	0.894485000	1	1.643100000	3.508554000	0.894731000
1	2.979742000	4.782836000	0.000021000	1	2.544054000	4.758616000	-0.000008000
1	-7.943995000	-0.329082000	0.000076000	1	-7.818338000	-0.088861000	-0.000351000
1	5.699744000	1.298182000	0.000057000	1	5.517642000	1.489006000	-0.000177000
5h_RC, optimization in gas phase B3LYP/6-311++G**, E= -988.769863921 a.u. Sum of electronic and thermal Enthalpies= -988.448967 a.u.				**5h_RCw,** optimization in solv. water B3LYP/6-311++G**, E= -988.838908593 a.u. Sum of electronic and thermal Enthalpies= -988.518036 a.u.			
1; 2				1; 2			

6	-6.853201000	-0.106686000	-0.000186000	6	6.803783000	-0.053884000	0.000020000
6	-5.978904000	-1.170376000	-0.000048000	6	5.961796000	-1.142158000	-0.000044000
6	-6.388939000	1.235326000	-0.000241000	6	6.300745000	1.277691000	0.000087000
1	-6.317281000	-2.198536000	0.000013000	1	6.333371000	-2.158815000	-0.000101000
6	-4.597133000	-0.877510000	0.000022000	6	4.570604000	-0.889568000	-0.000035000
6	-5.032712000	1.556846000	-0.000144000	6	4.939195000	1.560345000	0.000086000
1	-4.699017000	2.586781000	-0.000162000	1	4.568917000	2.576932000	0.000132000
6	-4.151439000	0.487636000	-0.000036000	6	4.086635000	0.464668000	0.000033000
6	-2.470791000	-0.928090000	0.000158000	6	2.444324000	-0.987693000	-0.000054000
7	-3.539159000	-1.725863000	0.000145000	7	3.537901000	-1.764263000	-0.000085000
7	-2.769112000	0.405107000	0.000202000	7	2.715578000	0.349157000	-0.000034000
1	-2.093543000	1.154790000	-0.000488000	1	2.025634000	1.088308000	0.000285000
7	-1.215166000	-1.415973000	0.000209000	7	1.201198000	-1.491741000	-0.000064000
7	-0.145562000	-0.605116000	0.000130000	7	0.134546000	-0.677187000	0.000022000
6	1.016188000	-1.191581000	0.000139000	6	-1.027831000	-1.255812000	0.000047000
1	1.075850000	-2.284336000	0.000186000	1	-1.107938000	-2.344941000	-0.000059000
1	-1.131369000	-2.434520000	0.000237000	1	1.110431000	-2.509730000	-0.000097000
1	-7.117050000	2.037655000	-0.000340000	1	7.007100000	2.099010000	0.000133000
6	2.260120000	-0.469878000	0.000065000	6	-2.255489000	-0.494869000	0.000018000
6	2.294976000	0.940136000	0.000074000	6	-2.243643000	0.913215000	-0.000011000
6	3.444939000	-1.233459000	-0.000019000	6	-3.462007000	-1.217921000	0.000026000
1	1.368353000	1.493091000	0.000155000	1	-1.298599000	1.434529000	-0.000024000
1	3.385118000	-2.313033000	-0.000019000	1	-3.434191000	-2.298205000	0.000052000
6	3.531143000	1.579238000	-0.000005000	6	-3.458900000	1.591685000	-0.000023000
6	4.677088000	-0.577773000	-0.000102000	6	-4.670647000	-0.518913000	0.000018000
6	4.714108000	0.822433000	-0.000095000	6	-4.665780000	0.878485000	-0.000009000
8	5.878477000	-1.185677000	-0.000194000	8	-5.896077000	-1.100606000	0.000035000
6	5.942669000	-2.614450000	-0.000152000	6	-5.980125000	-2.531102000	0.000043000
1	5.473234000	-3.027853000	0.897454000	1	-5.514388000	-2.951026000	-0.895387000
1	5.473141000	-3.027910000	-0.897683000	1	-5.514390000	-2.951016000	0.895480000
1	7.002195000	-2.857992000	-0.000199000	1	-7.042951000	-2.761476000	0.000044000
8	3.712902000	2.915322000	0.000001000	8	-3.585934000	2.942629000	-0.000045000
6	2.572330000	3.774433000	0.000146000	6	-2.398121000	3.743600000	-0.000053000
1	1.965522000	3.619804000	-0.897380000	1	-1.799613000	3.555523000	0.895165000
1	1.965675000	3.619705000	0.897757000	1	-1.799601000	3.555490000	-0.895255000
1	2.969061000	4.786806000	0.000165000	1	-2.740851000	4.775716000	-0.000074000
1	-7.921009000	-0.286483000	-0.000248000	1	7.876358000	-0.202450000	0.000018000
1	5.670441000	1.330335000	-0.000153000	1	-5.604993000	1.417591000	-0.000017000
5h_M, optimization in gas phase B3LYP/6-311++G**, E= -989.019600506 a.u. Sum of electronic and thermal Enthalpies= -988.698884 a.u.				**5h_Mw,** optimization in solv. water B3LYP/6-311++G**, E= -989.038043185 a.u. Sum of electronic and thermal Enthalpies= -988.717509 a.u.			
0; 1				0; 1			
6	6.814565000	0.031703000	0.005426000	6	6.791944000	0.060973000	0.003859000
6	5.982488000	-1.085556000	0.004449000	6	5.975775000	-1.070524000	0.002497000
6	6.292554000	1.334543000	0.003170000	6	6.248750000	1.356155000	0.003309000
1	6.384209000	-2.091719000	0.006146000	1	6.398721000	-2.068671000	0.002917000
6	4.602273000	-0.878167000	0.001157000	6	4.591333000	-0.883767000	0.000553000
6	4.915917000	1.562830000	-0.000174000	6	4.867180000	1.562681000	0.001353000
1	4.514410000	2.569815000	-0.001976000	1	4.445918000	2.561001000	0.000915000
6	4.094157000	0.442934000	-0.001063000	6	4.062435000	0.429706000	0.000015000
6	2.478493000	-1.063203000	-0.003454000	6	2.461752000	-1.093451000	-0.002487000
7	3.560120000	-1.799361000	-0.000337000	7	3.560697000	-1.819094000	-0.001036000
7	2.710069000	0.287081000	-0.004438000	7	2.683197000	0.255953000	-0.002142000
1	1.992042000	0.992925000	-0.004690000	1	1.962438000	0.961778000	-0.001966000
7	1.205233000	-1.574028000	-0.006534000	7	1.198283000	-1.613810000	-0.004895000
7	0.132863000	-0.755323000	-0.004328000	7	0.126086000	-0.788343000	-0.003292000

6	-1.035616000	-1.288942000	-0.002850000	6	-1.043023000	-1.320291000	-0.002428000
1	-1.148783000	-2.378819000	-0.002862000	1	-1.166594000	-2.406828000	-0.002611000
1	1.114155000	-2.585290000	-0.002830000	1	1.098171000	-2.624534000	-0.002473000
1	6.970138000	2.180457000	0.003985000	1	6.912633000	2.212941000	0.004408000
6	-2.268494000	-0.502827000	-0.001201000	6	-2.265111000	-0.513595000	-0.001210000
6	-2.248288000	0.899185000	-0.001154000	6	-2.220973000	0.889127000	-0.001423000
6	-3.486285000	-1.197110000	0.000272000	6	-3.492311000	-1.191452000	0.000181000
1	-1.296921000	1.408999000	-0.002275000	1	-1.262691000	1.386427000	-0.002550000
1	-3.480337000	-2.278657000	0.000158000	1	-3.501559000	-2.272607000	0.000313000
6	-3.456647000	1.595716000	0.000425000	6	-3.418401000	1.604554000	-0.000210000
6	-4.688232000	-0.479998000	0.001856000	6	-4.683140000	-0.455482000	0.001390000
6	-4.674993000	0.911772000	0.001929000	6	-4.647910000	0.937606000	0.001190000
8	-5.924011000	-1.057270000	0.003390000	8	-5.927221000	-1.015223000	0.002820000
6	-6.018239000	-2.475525000	0.003158000	6	-6.040053000	-2.440855000	0.003134000
1	-5.558632000	-2.907690000	-0.892289000	1	-5.584423000	-2.873905000	-0.891787000
1	-5.556445000	-2.908131000	0.897267000	1	-5.582498000	-2.873664000	0.897190000
1	-7.083304000	-2.701032000	0.004401000	1	-7.107506000	-2.651584000	0.004310000
8	-3.555819000	2.955816000	0.000598000	8	-3.495100000	2.966739000	-0.000276000
6	-2.361986000	3.727569000	-0.001009000	6	-2.280609000	3.721526000	-0.001593000
1	-1.759776000	3.533399000	0.892976000	1	-1.685606000	3.513645000	0.892142000
1	-1.761964000	3.533086000	-0.896393000	1	-1.687444000	3.513503000	-0.896516000
1	-2.682391000	4.768058000	-0.000780000	1	-2.583132000	4.766711000	-0.001369000
1	7.889918000	-0.105583000	0.007962000	1	7.869313000	-0.060584000	0.005366000
1	-5.605687000	1.463677000	0.003128000	1	-5.570851000	1.503833000	0.002130000

5i_A1, optimization in gas phase B3LYP/6-311++G**, E= -1103.01453577 a.u. Sum of electronic and thermal Enthalpies= -1102.673201 a.u.			
-1; 1			
6	7.479076000	0.152108000	0.089948000
6	6.642173000	-0.963925000	0.101642000
6	6.952227000	1.458469000	0.041493000
1	7.049495000	-1.970159000	0.138774000
6	5.257088000	-0.758869000	0.063981000
6	5.575266000	1.681203000	0.003657000
1	5.170383000	2.688258000	-0.033631000
6	4.719345000	0.573406000	0.014674000
6	3.151778000	-0.820301000	0.017318000
7	4.212376000	-1.649569000	0.064679000
7	3.344818000	0.500410000	-0.014901000
7	1.890306000	-1.432425000	0.005040000
7	0.740780000	-0.793548000	-0.033249000
6	-0.364843000	-1.466697000	-0.034376000
1	-0.361977000	-2.564030000	-0.002456000
1	1.920311000	-2.449570000	0.034452000
1	7.632951000	2.305203000	0.033461000
6	-1.657097000	-0.797327000	-0.076287000
6	-1.748155000	0.604126000	-0.128471000
6	-2.835942000	-1.561117000	-0.061194000
1	-0.827886000	1.170238000	-0.138151000
1	-2.760186000	-2.639792000	-0.018758000
6	-2.992686000	1.221487000	-0.168269000
6	-4.084100000	-0.935845000	-0.094760000
6	-4.178389000	0.461103000	-0.153656000
8	-5.279902000	-1.608798000	-0.071951000
6	-5.249063000	-3.023967000	-0.053452000
1	-4.745966000	-3.429515000	-0.938931000
1	-4.754186000	-3.408313000	0.846430000
1	-6.291080000	-3.344311000	-0.054556000
8	-3.171063000	2.577680000	-0.219752000
6	-2.010341000	3.397852000	-0.279106000
1	-1.385989000	3.277115000	0.612049000
1	-1.409429000	3.177173000	-1.166906000
1	-2.376128000	4.423020000	-0.332418000
1	8.556502000	0.014957000	0.118201000
8	-5.409559000	1.066863000	-0.264905000
6	-5.926872000	1.593474000	0.955296000
1	-6.061541000	0.798412000	1.697957000
1	-5.268223000	2.368639000	1.359550000
1	-6.897617000	2.031563000	0.716190000

5i_A2, optimization in gas phase B3LYP/6-311++G**, E= -1103.02037650 a.u. Sum of electronic and thermal Enthalpies= -1102.679602 a.u.			
-1; 1			
6	7.229953000	0.457598000	0.070923000
6	6.547107000	-0.762052000	0.103577000
6	6.544568000	1.678163000	0.007387000
1	7.081615000	-1.704654000	0.152909000
6	5.147639000	-0.755379000	0.071693000
6	5.142417000	1.712254000	-0.025631000
1	4.609517000	2.656905000	-0.075305000
6	4.468960000	0.498859000	0.007045000
6	3.042026000	-1.236107000	0.043397000
7	4.255072000	-1.797890000	0.092667000
7	3.134612000	0.158379000	-0.009377000
1	2.319024000	0.746013000	-0.051965000
7	1.874435000	-1.911367000	0.043499000
7	0.821532000	-1.088074000	-0.010197000
6	-0.356296000	-1.646765000	-0.015179000
1	-0.431028000	-2.737064000	0.023480000
1	7.102083000	2.608820000	-0.017181000
6	-1.584396000	-0.880389000	-0.067863000
6	-1.597730000	0.529144000	-0.120028000
6	-2.819436000	-1.560848000	-0.061974000
1	-0.648186000	1.043098000	-0.120940000
1	-2.812154000	-2.641943000	-0.018861000
6	-2.800492000	1.222590000	-0.167672000
6	-4.022891000	-0.858849000	-0.105877000
6	-4.032416000	0.542106000	-0.165086000
8	-5.261221000	-1.455052000	-0.091719000
6	-5.318434000	-2.869230000	-0.073365000
1	-4.833149000	-3.305578000	-0.954081000
1	-4.855018000	-3.283821000	0.829827000
1	-6.378486000	-3.124678000	-0.083350000
8	-2.895529000	2.592523000	-0.214226000
6	-1.691741000	3.339354000	-0.255984000
1	-1.084841000	3.179007000	0.642412000
1	-1.093329000	3.089490000	-1.139128000
1	-1.992347000	4.386149000	-0.307564000
1	8.315567000	0.460528000	0.095015000
8	-5.221723000	1.230448000	-0.284799000
6	-5.756321000	1.701211000	0.948862000
1	-5.966768000	0.867385000	1.628775000
1	-5.069599000	2.405006000	1.431717000
1	-6.689768000	2.214684000	0.708697000

5i_Aw1, optimization in solv.water B3LYP/6-311++G**, E= -1103.10436088 a.u. Sum of electronic and thermal Enthalpies= -1102.762476 a.u.			
-1; 1			
6	7.503125000	0.159248000	0.052396000
6	6.670862000	-0.963161000	0.076358000
6	6.969483000	1.461103000	0.012786000
1	7.089521000	-1.964761000	0.106797000
6	5.284901000	-0.763332000	0.059610000
6	5.588295000	1.675860000	-0.004274000
1	5.183199000	2.683053000	-0.035096000

5i_Aw2, optimization in solv.water B3LYP/6-311++G**, E= -1102.765016 a.u. Sum of electronic and thermal Enthalpies= -909.706017 a.u.			
-1; 1			
6	7.263610000	0.430334000	0.095517000
6	6.569207000	-0.784340000	0.111494000
6	6.587891000	1.657263000	0.040184000
1	7.100848000	-1.729142000	0.154894000
6	5.170644000	-0.758427000	0.070918000
6	5.186912000	1.706708000	-0.001372000
1	4.661301000	2.654383000	-0.044315000

6	4.741706000	0.561555000	0.018962000	6	4.504403000	0.497539000	0.014952000
6	3.164329000	-0.850547000	0.042883000	6	3.047180000	-1.211130000	0.026136000
7	4.240387000	-1.663260000	0.074407000	7	4.257401000	-1.793521000	0.076679000
7	3.362188000	0.475946000	0.009022000	7	3.160259000	0.175157000	-0.013166000
7	1.905359000	-1.444225000	0.050237000	1	2.365696000	0.793282000	-0.052369000
7	0.762447000	-0.749648000	-0.003662000	7	1.883869000	-1.888061000	0.016629000
6	-0.348950000	-1.402087000	-0.012498000	7	0.814312000	-1.058423000	-0.032839000
1	-0.360088000	-2.496544000	0.020669000	6	-0.355271000	-1.615576000	-0.039377000
1	1.887154000	-2.460112000	0.067344000	1	-0.438479000	-2.706342000	-0.005029000
1	7.643440000	2.311554000	-0.004998000	1	7.153611000	2.582224000	0.029033000
6	-1.646880000	-0.729908000	-0.067261000	6	-1.597079000	-0.851058000	-0.086892000
6	-1.755889000	0.668539000	-0.114204000	6	-1.613675000	0.554329000	-0.146010000
6	-2.804222000	-1.521575000	-0.073974000	6	-2.814593000	-1.553100000	-0.071757000
1	-0.854663000	1.263298000	-0.108906000	1	-0.673393000	1.085209000	-0.159390000
1	-2.708367000	-2.598352000	-0.040030000	1	-2.796877000	-2.633734000	-0.027733000
6	-3.013670000	1.266247000	-0.164872000	6	-2.826172000	1.238840000	-0.187005000
6	-4.065710000	-0.921975000	-0.126733000	6	-4.030009000	-0.865388000	-0.109700000
6	-4.179907000	0.476216000	-0.171545000	6	-4.047137000	0.537033000	-0.167793000
8	-5.242107000	-1.610153000	-0.142064000	8	-5.253674000	-1.470147000	-0.095757000
6	-5.198418000	-3.037895000	-0.082510000	6	-5.308112000	-2.896416000	-0.032355000
1	-4.670763000	-3.454517000	-0.945080000	1	-4.826741000	-3.351428000	-0.902808000
1	-4.723963000	-3.381021000	0.841245000	1	-4.841335000	-3.271234000	0.883143000
1	-6.236315000	-3.364350000	-0.100377000	1	-6.366376000	-3.150588000	-0.029931000
8	-3.220261000	2.612164000	-0.212692000	8	-2.937446000	2.598108000	-0.249289000
6	-2.080330000	3.474905000	-0.211553000	6	-1.740066000	3.377272000	-0.260039000
1	-1.492285000	3.352063000	0.702281000	1	-1.155988000	3.218091000	0.650938000
1	-1.446372000	3.293535000	-1.083968000	1	-1.125093000	3.147148000	-1.134791000
1	-2.477848000	4.486971000	-0.255164000	1	-2.064237000	4.415183000	-0.307293000
1	8.580216000	0.026661000	0.064559000	1	8.348030000	0.422779000	0.126615000
8	-5.413423000	1.070905000	-0.285899000	8	-5.241535000	1.214304000	-0.266920000
6	-6.081080000	1.317805000	0.963646000	6	-5.801578000	1.625172000	0.991105000
1	-6.261555000	0.380690000	1.496869000	1	-6.006670000	0.757057000	1.624085000
1	-5.490582000	1.993561000	1.588860000	1	-5.125300000	2.310572000	1.509595000
1	-7.032927000	1.787250000	0.716905000	1	-6.735579000	2.138039000	0.761924000
5i_R1, optimization in gas phase B3LYP/6-311++G**, E= -1102.91285223 a.u. Sum of electronic and thermal Enthalpies= -1102.570518 a.u.				**5i_R2,** optimization in gas phase B3LYP/6-311++G**, E= -1102.93074299 a.u. Sum of electronic and thermal Enthalpies= -1102.588487 a.u.			
0; 2				0; 2			
6	7.475166000	0.063865000	0.074989000	6	7.330160000	0.269170000	0.065659000
6	6.647048000	-1.029805000	0.087955000	6	6.578958000	-0.892858000	0.098214000
6	6.963639000	1.406427000	0.033399000	6	6.717086000	1.540567000	0.003119000
1	7.032231000	-2.041905000	0.119067000	1	7.039946000	-1.871825000	0.146096000
6	5.249121000	-0.791893000	0.058626000	6	5.177620000	-0.776861000	0.067341000
6	5.615875000	1.677990000	0.004151000	6	5.334457000	1.687244000	-0.028550000
1	5.236160000	2.692054000	-0.027146000	1	4.874792000	2.667465000	-0.076647000
6	4.728318000	0.578685000	0.016173000	6	4.576930000	0.517610000	0.004396000
6	3.146844000	-0.786610000	0.022848000	6	3.056286000	-1.105856000	0.041215000
7	4.220416000	-1.644708000	0.062103000	7	4.226748000	-1.753018000	0.088565000
7	3.382821000	0.542625000	-0.005579000	7	3.227839000	0.273316000	-0.010436000
7	1.916533000	-1.353763000	0.015847000	1	2.460211000	0.924155000	-0.051258000
7	0.770246000	-0.657629000	-0.022003000	7	1.867027000	-1.734954000	0.044120000
6	-0.324288000	-1.340166000	-0.022592000	7	0.835330000	-0.878418000	-0.005812000
1	-0.305483000	-2.436774000	0.007138000	6	-0.327836000	-1.477894000	-0.007495000
1	1.911127000	-2.373710000	0.040310000	1	-0.352076000	-2.568899000	0.027868000
1	7.674854000	2.224996000	0.025126000	1	7.342612000	2.425595000	-0.020921000
6	-1.628487000	-0.700499000	-0.062991000	6	-1.581885000	-0.763898000	-0.053720000

6	-1.746020000	0.696197000	-0.107528000	6	-1.638496000	0.640378000	-0.096777000
6	-2.773539000	-1.510366000	-0.056281000	6	-2.770849000	-1.514215000	-0.054145000
1	-0.844158000	1.290519000	-0.108121000	1	-0.712553000	1.194915000	-0.092065000
1	-2.663616000	-2.586162000	-0.025057000	1	-2.710567000	-2.593652000	-0.027145000
6	-3.008127000	1.281251000	-0.143526000	6	-2.869874000	1.284265000	-0.134994000
6	-4.038890000	-0.924316000	-0.097798000	6	-4.005209000	-0.870786000	-0.100302000
6	-4.167751000	0.475327000	-0.141950000	6	-4.068237000	0.535539000	-0.136541000
8	-5.210104000	-1.619118000	-0.103984000	8	-5.207217000	-1.509491000	-0.121990000
6	-5.158818000	-3.040094000	-0.132530000	6	-5.221813000	-2.932590000	-0.158280000
1	-4.634912000	-3.401377000	-1.023597000	1	-4.705566000	-3.312241000	-1.045803000
1	-4.677565000	-3.442368000	0.765470000	1	-4.768792000	-3.360743000	0.742060000
1	-6.195072000	-3.371961000	-0.164881000	1	-6.272100000	-3.214976000	-0.203154000
8	-3.231160000	2.618398000	-0.179880000	8	-3.031993000	2.632206000	-0.169643000
6	-2.104909000	3.490107000	-0.228955000	6	-1.870557000	3.451568000	-0.210595000
1	-1.481674000	3.388245000	0.665198000	1	-1.256281000	3.319801000	0.686706000
1	-1.497508000	3.304033000	-1.120079000	1	-1.268120000	3.243632000	-1.101110000
1	-2.516435000	4.496785000	-0.272971000	1	-2.235277000	4.476394000	-0.251947000
1	8.550267000	-0.075025000	0.096211000	1	8.412085000	0.209949000	0.088051000
8	-5.389290000	1.062820000	-0.265261000	8	-5.253920000	1.189105000	-0.259115000
6	-6.176949000	1.139880000	0.930590000	6	-6.093115000	1.222115000	0.904450000
1	-6.397459000	0.142325000	1.318490000	1	-6.380518000	0.213924000	1.209887000
1	-5.661593000	1.735749000	1.690394000	1	-5.584033000	1.736171000	1.725773000
1	-7.104242000	1.636229000	0.647400000	1	-6.979089000	1.786316000	0.616572000
5i_Rw1, optimization in solv. water B3LYP/6-311++G**, E= -1102.93619929 a.u. Sum of electronic and thermal Enthalpies= -1102.593719 a.u.				**5i_Rw2,** optimization in solv. water B3LYP/6-311++G**, E= -1102.95209726a.u. Sum of electronic and thermal Enthalpies= -1102.609868 a.u.			
0; 2				0; 2			
6	7.481942000	0.070558000	0.079871000	6	7.319665000	0.275885000	0.083684000
6	6.652913000	-1.025319000	0.100478000	6	6.575138000	-0.891129000	0.102188000
6	6.968470000	1.409286000	0.026731000	6	6.699365000	1.546579000	0.031261000
1	7.043781000	-2.035243000	0.140466000	1	7.047199000	-1.865605000	0.142461000
6	5.255906000	-0.789341000	0.066947000	6	5.172579000	-0.779580000	0.067090000
6	5.617311000	1.675581000	-0.006640000	6	5.316935000	1.687255000	-0.004324000
1	5.239556000	2.690484000	-0.046695000	1	4.848079000	2.662733000	-0.044546000
6	4.734612000	0.573654000	0.012852000	6	4.565868000	0.511703000	0.014181000
6	3.145783000	-0.801380000	0.027052000	6	3.045736000	-1.106098000	0.029142000
7	4.225208000	-1.648218000	0.075232000	7	4.218755000	-1.757200000	0.075340000
7	3.384519000	0.530475000	-0.011399000	7	3.217170000	0.266206000	-0.008939000
7	1.913610000	-1.357767000	0.020170000	1	2.457572000	0.929990000	-0.045878000
7	0.777310000	-0.639578000	-0.024980000	7	1.861358000	-1.748307000	0.022722000
6	-0.323680000	-1.319387000	-0.032612000	7	0.820711000	-0.903414000	-0.025310000
1	-0.308502000	-2.412641000	-0.006350000	6	-0.342747000	-1.502998000	-0.027714000
1	1.882025000	-2.377336000	0.051407000	1	-0.379447000	-2.593393000	0.008400000
1	7.676262000	2.230268000	0.012815000	1	7.321134000	2.434182000	0.018506000
6	-1.624680000	-0.677676000	-0.076835000	6	-1.590261000	-0.778965000	-0.074783000
6	-1.754265000	0.720062000	-0.118394000	6	-1.629844000	0.627169000	-0.124513000
6	-2.761421000	-1.500482000	-0.078943000	6	-2.783523000	-1.523762000	-0.071257000
1	-0.863626000	1.330142000	-0.115616000	1	-0.700405000	1.176286000	-0.125747000
1	-2.639624000	-2.574479000	-0.054221000	1	-2.731983000	-2.603286000	-0.042042000
6	-3.021967000	1.292205000	-0.154787000	6	-2.855898000	1.281346000	-0.162634000
6	-4.032843000	-0.928367000	-0.121295000	6	-4.012436000	-0.869529000	-0.114535000
6	-4.171832000	0.471882000	-0.151904000	6	-4.058145000	0.538368000	-0.152287000
8	-5.193510000	-1.633335000	-0.145032000	8	-5.218638000	-1.493288000	-0.132990000
6	-5.127561000	-3.063083000	-0.105513000	6	-5.250166000	-2.924264000	-0.092114000
1	-4.592177000	-3.456154000	-0.973888000	1	-4.744495000	-3.353584000	-0.961165000
1	-4.649465000	-3.409291000	0.814743000	1	-4.794613000	-3.301498000	0.827391000

1	-6.160226000	-3.403940000	-0.129977000	1	-6.303716000	-3.193972000	-0.114068000
8	-3.260087000	2.627735000	-0.194150000	8	-3.006747000	2.629691000	-0.209451000
6	-2.139660000	3.518607000	-0.202967000	6	-1.830320000	3.444847000	-0.217119000
1	-1.540573000	3.406632000	0.704764000	1	-1.241852000	3.294367000	0.692035000
1	-1.513008000	3.353470000	-1.083499000	1	-1.214125000	3.237671000	-1.096196000
1	-2.562910000	4.520056000	-0.239319000	1	-2.186440000	4.472025000	-0.255344000
1	8.556758000	-0.067291000	0.103852000	1	8.401706000	0.222162000	0.109606000
8	-5.404237000	1.049891000	-0.252439000	8	-5.248271000	1.196476000	-0.253436000
6	-6.177078000	1.092326000	0.964897000	6	-6.028308000	1.277756000	0.958041000
1	-6.367994000	0.084137000	1.336879000	1	-6.287411000	0.280973000	1.318644000
1	-5.655707000	1.682136000	1.723473000	1	-5.476471000	1.825982000	1.726091000
1	-7.118109000	1.575587000	0.707343000	1	-6.933281000	1.823456000	0.696331000
5i_RC, optimization in gas phase B3LYP/6-311++G**, E= -1103.32569437 a.u. Sum of electronic and thermal Enthalpies= -1102.969109a.u.				**5i_RCw,** optimization in solv. water B3LYP/6-311++G**, E= -1103.39202027a.u. Sum of electronic and thermal Enthalpies= -1103.035621 a.u.			
1; 2				1; 2			
6	7.467730000	0.096016000	-0.000189000	6	7.392530000	0.202923000	0.000143000
6	6.637576000	-1.007990000	0.000031000	6	6.609012000	-0.940661000	0.000104000
6	6.948230000	1.412299000	-0.000355000	6	6.816460000	1.492851000	0.000113000
1	7.024072000	-2.019143000	0.000163000	1	7.047679000	-1.931058000	0.000133000
6	5.249738000	-0.778739000	0.000080000	6	5.215186000	-0.777238000	0.000034000
6	5.579456000	1.667894000	-0.000298000	6	5.437659000	1.680393000	0.000050000
1	5.196546000	2.680827000	-0.000418000	1	4.999649000	2.670564000	0.000040000
6	4.746647000	0.557436000	-0.000087000	6	4.654343000	0.530211000	0.000009000
6	3.128971000	-0.930997000	0.000216000	6	3.099495000	-1.020797000	-0.000076000
7	4.219208000	-1.678618000	0.000270000	7	4.216508000	-1.725891000	-0.000021000
7	3.366204000	0.414650000	0.000067000	7	3.285535000	0.330403000	-0.000014000
1	2.660857000	1.134978000	-0.000268000	1	2.552784000	1.025679000	-0.000142000
7	1.882816000	-1.474485000	0.000344000	7	1.860215000	-1.593454000	-0.000139000
7	0.783882000	-0.722936000	0.000234000	7	0.768606000	-0.843983000	-0.000173000
6	-0.359020000	-1.354763000	0.000252000	6	-0.382747000	-1.462679000	-0.000101000
1	-0.379245000	-2.448506000	0.000268000	1	-0.428978000	-2.552638000	-0.000036000
1	1.847976000	-2.495146000	0.000445000	1	1.821738000	-2.613734000	-0.000055000
1	7.638483000	2.247338000	-0.000524000	1	7.466631000	2.359659000	0.000148000
6	-1.616040000	-0.674892000	0.000037000	6	-1.612484000	-0.736621000	-0.000126000
6	-1.707660000	0.734503000	0.000033000	6	-1.641977000	0.678082000	-0.000336000
6	-2.791048000	-1.457569000	-0.000227000	6	-2.816734000	-1.473198000	0.000065000
1	-0.800500000	1.318948000	0.000081000	1	-0.709431000	1.221300000	-0.000498000
1	-2.704270000	-2.535240000	-0.000332000	1	-2.770140000	-2.552703000	0.000266000
6	-2.943323000	1.345499000	-0.000103000	6	-2.848786000	1.337855000	-0.000297000
6	-4.042914000	-0.867292000	-0.000413000	6	-4.041233000	-0.832087000	0.000040000
6	-4.149823000	0.557526000	-0.000049000	6	-4.086706000	0.599570000	-0.000104000
8	-5.208841000	-1.549925000	-0.000872000	8	-5.231466000	-1.462359000	0.000217000
6	-5.183235000	-2.982145000	0.000147000	6	-5.261742000	-2.898116000	0.000111000
1	-4.688274000	-3.363295000	-0.897284000	1	-4.779212000	-3.294111000	-0.896393000
1	-4.688171000	-3.362032000	0.898053000	1	-4.779347000	-3.294258000	0.896622000
1	-6.225698000	-3.291049000	0.000392000	1	-6.315814000	-3.163205000	0.000014000
8	-3.155547000	2.669207000	-0.000268000	8	-3.002250000	2.673797000	-0.000426000
6	-2.031082000	3.552123000	0.000382000	6	-1.826488000	3.497091000	0.000353000
1	-1.422784000	3.407630000	0.898077000	1	-1.227954000	3.315403000	0.896152000
1	-1.422218000	3.408268000	-0.897036000	1	-1.227704000	3.316721000	-0.895552000
1	-2.450835000	4.554943000	0.000590000	1	-2.190759000	4.521235000	0.001045000
1	8.542117000	-0.040356000	-0.000238000	1	8.472166000	0.111243000	0.000201000
8	-5.256742000	1.274240000	0.000502000	8	-5.166284000	1.359287000	-0.000073000
6	-6.616026000	0.772286000	0.000033000	6	-6.543778000	0.900845000	0.000285000
1	-6.804292000	0.181835000	-0.894169000	1	-6.748523000	0.316678000	-0.893572000

1	-6.804652000	0.181035000	0.893627000	1	-6.748057000	0.316827000	0.894356000
1	-7.223908000	1.673343000	0.000323000	1	-7.122831000	1.820538000	0.000357000
5i_M, optimization in gas phase B3LYP/6-311++G**, E= -1103.56432825 a.u. Sum of electronic and thermal Enthalpies= -1103.208628 a.u.				**5i_Mw,** optimization in solv. water B3LYP/6-311++G**, E= -1103.58564596 a.u. Sum of electronic and thermal Enthalpies= -1103.230076 a.u.			
0; 1				0; 1			
6	7.396811000	0.284968000	0.038055000	6	7.370386000	0.319442000	0.060083000
6	6.628397000	-0.876387000	0.080238000	6	6.618736000	-0.855616000	0.091523000
6	6.803036000	1.555246000	-0.020596000	6	6.755815000	1.580973000	0.005115000
1	7.086020000	-1.857363000	0.125473000	1	7.097215000	-1.827467000	0.133985000
6	5.238807000	-0.747469000	0.062835000	6	5.226136000	-0.747887000	0.066719000
6	5.415707000	1.705245000	-0.038679000	6	5.364869000	1.708702000	-0.020317000
1	4.958359000	2.687118000	-0.084138000	1	4.888612000	2.681141000	-0.062992000
6	4.657860000	0.541972000	0.003847000	6	4.624726000	0.532863000	0.011309000
6	3.128450000	-1.051330000	0.057289000	6	3.111624000	-1.077814000	0.046300000
7	4.249876000	-1.724950000	0.095009000	7	4.249878000	-1.739485000	0.087425000
7	3.284750000	0.308844000	0.002409000	7	3.257389000	0.281349000	-0.000281000
1	2.528510000	0.972398000	-0.036473000	1	2.497763000	0.944312000	-0.037191000
7	1.885904000	-1.631110000	0.073079000	7	1.879818000	-1.667476000	0.050307000
7	0.769425000	-0.872913000	0.015970000	7	0.762393000	-0.903078000	-0.005192000
6	-0.367300000	-1.471443000	0.009726000	6	-0.373536000	-1.502677000	-0.014491000
1	-0.419516000	-2.565522000	0.046033000	1	-0.432781000	-2.594089000	0.019553000
1	1.850393000	-2.645454000	0.095694000	1	1.835267000	-2.681855000	0.074862000
1	7.432150000	2.437225000	-0.052620000	1	7.370502000	2.473404000	-0.018296000
6	-1.641117000	-0.758814000	-0.045249000	6	-1.641213000	-0.774792000	-0.069655000
6	-1.704917000	0.640165000	-0.084962000	6	-1.689079000	0.625759000	-0.115970000
6	-2.819888000	-1.515445000	-0.056343000	6	-2.825107000	-1.523458000	-0.075540000
1	-0.784895000	1.204986000	-0.071051000	1	-0.764997000	1.184547000	-0.110653000
1	-2.757362000	-2.595021000	-0.025818000	1	-2.770765000	-2.602966000	-0.043344000
6	-2.943126000	1.276813000	-0.135886000	6	-2.922083000	1.273583000	-0.164127000
6	-4.061563000	-0.877695000	-0.112931000	6	-4.061839000	-0.874466000	-0.126396000
6	-4.134095000	0.523359000	-0.155970000	6	-4.117913000	0.527731000	-0.168967000
8	-5.259148000	-1.526488000	-0.131981000	8	-5.263698000	-1.512475000	-0.141985000
6	-5.264148000	-2.948038000	-0.156319000	6	-5.280105000	-2.942011000	-0.089481000
1	-4.745832000	-3.333551000	-1.040566000	1	-4.771129000	-3.375190000	-0.954953000
1	-4.808909000	-3.367196000	0.747630000	1	-4.820215000	-3.308653000	0.832438000
1	-6.312540000	-3.238387000	-0.198776000	1	-6.330840000	-3.223685000	-0.108199000
8	-3.110742000	2.625611000	-0.168103000	8	-3.076676000	2.624465000	-0.210234000
6	-1.954281000	3.451516000	-0.197996000	6	-1.904377000	3.443769000	-0.206691000
1	-1.346436000	3.322828000	0.704216000	1	-1.322349000	3.295635000	0.707155000
1	-1.342661000	3.248773000	-1.083507000	1	-1.278623000	3.240840000	-1.080182000
1	-2.324271000	4.474488000	-0.241347000	1	-2.263647000	4.469983000	-0.247168000
1	8.478127000	0.208227000	0.050431000	1	8.452758000	0.258758000	0.078303000
8	-5.333644000	1.158509000	-0.295551000	8	-5.323337000	1.171814000	-0.280806000
6	-6.094360000	1.319485000	0.907534000	6	-6.012384000	1.391146000	0.963913000
1	-6.345539000	0.348785000	1.343658000	1	-6.236756000	0.440447000	1.453622000
1	-5.544080000	1.926819000	1.633370000	1	-5.413664000	2.020976000	1.627809000
1	-7.008577000	1.837800000	0.620042000	1	-6.940929000	1.902796000	0.713681000

5j_A1, optimization in gas phase B3LYP/6-311++G**, E= -949.176724656 a.u. Sum of electronic and thermal Enthalpies= -948.900427 a.u.			
-1; 1			
6	-5.497006000	1.664221000	0.330248000
6	-4.277510000	1.628408000	1.014171000
6	-5.876269000	0.637779000	-0.544089000
1	-3.988266000	2.424840000	1.691017000
6	-3.422088000	0.539189000	0.815735000
6	-5.036643000	-0.465307000	-0.760753000
1	-5.328385000	-1.262531000	-1.437723000
6	-3.828049000	-0.495339000	-0.079429000
6	-1.812036000	-0.901886000	0.832686000
7	-2.188881000	0.268338000	1.359107000
7	-2.783811000	-1.394534000	-0.045948000
1	-6.828867000	0.693388000	-1.060633000
1	-2.688202000	-2.263354000	-0.543772000
7	-0.709537000	-1.652941000	0.990601000
7	0.171521000	-1.126361000	1.850537000
6	1.280556000	-1.771891000	2.063346000
1	1.471851000	-2.717612000	1.548153000
6	2.282532000	-1.257663000	2.978196000
6	3.472003000	-1.974794000	3.203377000
6	2.084201000	-0.033335000	3.677469000
6	4.445878000	-1.512165000	4.079689000
6	3.087474000	0.434879000	4.545510000
6	4.254001000	-0.301275000	4.747016000
1	-6.165768000	2.506353000	0.480249000
8	2.924681000	1.594774000	5.280280000
6	2.750528000	2.797230000	4.527961000
1	3.612702000	2.966156000	3.869746000
1	1.835275000	2.766170000	3.935260000
1	2.694202000	3.604990000	5.259915000
1	3.615954000	-2.912037000	2.674157000
1	4.992831000	0.091482000	5.436452000
8	0.955700000	0.686272000	3.534453000
1	0.367362000	0.203775000	2.873214000
1	5.353361000	-2.084169000	4.241431000

5j_A2, optimization in gas phase B3LYP/6-311++G**, E= -949.176410234 a.u. Sum of electronic and thermal Enthalpies= -948.899964 a.u.			
-1; 1			
6	-5.514121000	1.584563000	0.596881000
6	-4.309272000	1.475637000	1.306142000
6	-5.810583000	0.702560000	-0.451303000
1	-4.075559000	2.158592000	2.116833000
6	-3.434579000	0.465558000	0.931470000
6	-4.925163000	-0.312440000	-0.823938000
1	-5.158921000	-0.993940000	-1.634692000
6	-3.717211000	-0.444115000	-0.128250000
6	-1.782406000	-1.033158000	0.637046000
7	-2.192540000	0.076323000	1.391297000
7	-2.696375000	-1.346811000	-0.287236000
1	-6.750140000	0.811119000	-0.984647000
1	-1.702077000	0.434508000	2.192306000
7	-0.630066000	-1.706086000	0.818852000
7	0.165452000	-1.154706000	1.742891000
6	1.268884000	-1.789404000	2.048336000
1	1.481764000	-2.745125000	1.565856000
6	2.223694000	-1.260797000	3.001268000
6	3.368082000	-2.005118000	3.348379000
6	2.039798000	0.008462000	3.616559000
6	4.297136000	-1.525672000	4.263126000
6	2.993766000	0.493424000	4.523210000
6	4.112651000	-0.272680000	4.849927000
1	-6.222430000	2.361865000	0.863875000
8	2.822881000	1.705147000	5.168271000
6	2.815955000	2.859235000	4.326981000
1	3.761503000	2.938916000	3.775459000
1	1.981531000	2.833993000	3.623714000
1	2.714034000	3.718867000	4.991672000
1	3.510813000	-2.976712000	2.885788000
1	4.818028000	0.129736000	5.567892000
8	0.947145000	0.757010000	3.333883000
1	0.425929000	0.222159000	2.660944000
1	5.166878000	-2.121251000	4.519307000

5j_A3, optimization in gas phase B3LYP/6-311++G**, E= -949.153449564 a.u. Sum of electronic and thermal Enthalpies= -948.877114 a.u.			
-1; 1			
6	-5.400568000	1.658773000	0.464946000
6	-4.155077000	1.537027000	1.102414000
6	-5.846484000	0.696981000	-0.438663000
1	-3.809232000	2.284992000	1.805830000
6	-3.376739000	0.427616000	0.806870000
6	-5.061362000	-0.428810000	-0.741678000
1	-5.408526000	-1.177542000	-1.445215000
6	-3.832616000	-0.550316000	-0.113524000
6	-1.777897000	-1.182594000	0.652318000
7	-2.135740000	0.017596000	1.248793000
7	-2.838255000	-1.515655000	-0.188656000
1	-6.812171000	0.813882000	-0.917678000
1	-1.482938000	0.430367000	1.910630000
1	-2.842051000	-2.353804000	-0.742893000

5j_Aw1, optimization in solv.water B3LYP/6-311++G**, E= -949.254582285 a.u. Sum of electronic and thermal Enthalpies= -948.977974 a.u.			
-1; 1			
6	-5.495809000	1.653616000	0.382454000
6	-4.271026000	1.598800000	1.056510000
6	-5.882648000	0.645343000	-0.511519000
1	-3.979474000	2.383129000	1.747060000
6	-3.425705000	0.508919000	0.823900000
6	-5.051221000	-0.455232000	-0.760369000
1	-5.347680000	-1.236391000	-1.451600000
6	-3.836923000	-0.502031000	-0.087296000
6	-1.818075000	-0.947998000	0.790398000
7	-2.181819000	0.214769000	1.352403000
7	-2.795952000	-1.410432000	-0.085892000
1	-6.838158000	0.715500000	-1.019183000
1	-2.727913000	-2.265113000	-0.615633000
7	-0.707294000	-1.695477000	0.936720000

7	-0.696221000	-1.859074000	0.829414000
7	0.087158000	-1.153054000	1.754020000
6	1.209249000	-1.702848000	2.068529000
1	1.471870000	-2.664348000	1.605256000
6	2.171230000	-1.152723000	2.994461000
6	3.334455000	-1.919809000	3.226021000
6	1.962241000	0.117313000	3.691338000
6	4.332676000	-1.516806000	4.093410000
6	3.066428000	0.502052000	4.566727000
6	4.182249000	-0.281759000	4.757816000
1	-6.023446000	2.519102000	0.683295000
8	2.973054000	1.665876000	5.320495000
6	2.800295000	2.867892000	4.574587000
1	3.674390000	3.051467000	3.932160000
1	1.895524000	2.817167000	3.966218000
1	2.722954000	3.675317000	5.307696000
1	3.433337000	-2.865036000	2.695335000
1	4.942589000	0.075521000	5.447317000
8	0.936031000	0.839820000	3.577833000
1	5.214335000	-2.126925000	4.257150000

5j_Aw2, optimization in solv.water
B3LYP/6-311++G**, E= -949.253960816 a.u.
Sum of electronic and thermal Enthalpies= -948.977025 a.u.

-1; 1

6	-5.489790000	1.668845000	0.368008000
6	-4.258401000	1.628223000	1.036645000
6	-5.882357000	0.625375000	-0.482490000
1	-3.952136000	2.433457000	1.695245000
6	-3.452631000	0.518272000	0.820586000
6	-5.064514000	-0.488926000	-0.694841000
1	-5.376231000	-1.291598000	-1.354777000
6	-3.830418000	-0.549510000	-0.037111000
6	-1.872997000	-1.079469000	0.744473000
7	-2.208114000	0.151726000	1.304008000
7	-2.848184000	-1.517764000	-0.068941000
1	-6.841169000	0.684372000	-0.986506000
1	-1.627097000	0.683612000	1.929066000
7	-0.735848000	-1.764541000	0.962084000
7	0.107458000	-1.162605000	1.830889000
6	1.240691000	-1.763081000	2.065508000
1	1.463681000	-2.704551000	1.559012000
6	2.234194000	-1.233933000	2.984047000
6	3.439267000	-1.933140000	3.191633000
6	2.025108000	-0.028105000	3.699984000
6	4.405891000	-1.461989000	4.070753000
6	3.012082000	0.448792000	4.576250000
6	4.192775000	-0.266565000	4.761913000
1	-6.145608000	2.520093000	0.512176000
8	2.793628000	1.596279000	5.313551000
6	2.885315000	2.823596000	4.570929000
1	3.889689000	2.940850000	4.151535000
1	2.143014000	2.853971000	3.770483000
1	2.692025000	3.627188000	5.280840000
1	3.602292000	-2.858791000	2.649631000
1	4.931366000	0.123547000	5.452702000
8	0.873507000	0.674913000	3.560185000

7	0.169720000	-1.161955000	1.809173000
6	1.287012000	-1.788032000	2.031624000
1	1.509240000	-2.728281000	1.520668000
6	2.265085000	-1.254790000	2.965959000
6	3.464860000	-1.949315000	3.209608000
6	2.032171000	-0.037465000	3.660697000
6	4.410028000	-1.467631000	4.106731000
6	3.000461000	0.446382000	4.556391000
6	4.176903000	-0.265351000	4.779193000
1	-6.160198000	2.493667000	0.554806000
8	2.765761000	1.601401000	5.278466000
6	2.872069000	2.821207000	4.526520000
1	3.885007000	2.935578000	4.127009000
1	2.146639000	2.843203000	3.710550000
1	2.663708000	3.631728000	5.224368000
1	3.641527000	-2.880877000	2.681727000
1	4.897053000	0.133477000	5.484500000
8	0.889239000	0.665765000	3.485582000
1	0.338773000	0.154180000	2.812216000
1	5.325931000	-2.019248000	4.283886000

5j_Aw3, optimization in solv.water
B3LYP/6-311++G**, E= -949.243339981 a.u.
Sum of electronic and thermal Enthalpies= -948.966092 a.u.

-1; 1

6	-5.768631000	1.448606000	0.224548000
6	-4.561937000	1.478235000	0.937943000
6	-6.055428000	0.415138000	-0.670539000
1	-4.338824000	2.279437000	1.631920000
6	-3.664758000	0.443048000	0.722463000
6	-5.147818000	-0.630914000	-0.887897000
1	-5.369467000	-1.432819000	-1.581656000
6	-3.954986000	-0.600101000	-0.180915000
6	-1.902718000	-0.997687000	0.719633000
7	-2.407315000	0.170588000	1.252203000
7	-2.862261000	-1.460276000	-0.160489000
1	-6.996022000	0.418226000	-1.208731000
1	-1.887427000	0.700207000	1.934152000
1	-2.754386000	-2.307010000	-0.695543000
7	-0.771254000	-1.590759000	0.955103000
7	-0.012942000	-0.874225000	1.888553000
6	1.115958000	-1.443326000	2.161632000
1	1.335120000	-2.389944000	1.651875000
6	2.154818000	-0.994296000	3.070639000
6	3.266938000	-1.860919000	3.191817000
6	2.103160000	0.239242000	3.840087000
6	4.339462000	-1.592073000	4.023950000
6	3.263374000	0.478225000	4.678909000
6	4.324680000	-0.399130000	4.769691000
1	-6.489372000	2.244128000	0.373025000
8	3.281064000	1.607654000	5.490601000
6	3.452742000	2.844013000	4.788633000
1	4.434562000	2.874507000	4.301273000
1	2.664287000	2.979553000	4.045817000
1	3.397906000	3.638837000	5.533922000
1	3.265720000	-2.775794000	2.604618000
1	5.146616000	-0.149268000	5.434273000

1	0.323271000	0.168140000	2.901226000	8	1.135440000	1.065396000	3.812280000
1	5.324725000	-2.017023000	4.219404000	1	5.174442000	-2.278841000	4.098785000
5j_R1, optimization in gas phase B3LYP/6-311++G**, E= -949.080881210 a.u. Sum of electronic and thermal Enthalpies= -948.802892 a.u.				**5j_R2,** optimization in gas phase B3LYP/6-311++G**, E= -949.078772212 a.u. Sum of electronic and thermal Enthalpies= -948.800797 a.u.			
0; 2				0; 2			
6	-5.519818000	1.620551000	0.305952000	6	-5.620779000	1.510480000	0.418683000
6	-4.317155000	1.613363000	0.989485000	6	-4.438586000	1.516199000	1.151356000
6	-5.879661000	0.568546000	-0.567633000	6	-5.888818000	0.525807000	-0.559767000
1	-4.035039000	2.414961000	1.660903000	1	-4.243851000	2.276384000	1.898524000
6	-3.450820000	0.522454000	0.793268000	6	-3.525771000	0.500648000	0.875333000
6	-5.046174000	-0.521865000	-0.782657000	6	-4.983372000	-0.482971000	-0.833601000
1	-5.330529000	-1.323687000	-1.453796000	1	-5.178737000	-1.242696000	-1.580330000
6	-3.833335000	-0.530459000	-0.094005000	6	-3.777708000	-0.504707000	-0.107109000
6	-1.838204000	-0.891963000	0.822556000	6	-1.845126000	-0.954675000	0.722282000
7	-2.226219000	0.277102000	1.340768000	7	-2.287231000	0.191893000	1.380871000
7	-2.785960000	-1.412154000	-0.052643000	7	-2.741324000	-1.381451000	-0.180897000
1	-6.832117000	0.615283000	-1.082820000	1	-6.825903000	0.568695000	-1.102285000
1	-2.683135000	-2.285671000	-0.544744000	1	-1.796179000	0.659689000	2.124233000
7	-0.713567000	-1.604468000	1.016065000	7	-0.684658000	-1.590362000	0.928926000
7	0.136962000	-1.038030000	1.873456000	7	0.109172000	-0.996977000	1.837890000
6	1.247123000	-1.705857000	2.078251000	6	1.212046000	-1.663961000	2.091832000
1	1.409011000	-2.651613000	1.557322000	1	1.368603000	-2.616505000	1.584357000
6	2.252884000	-1.217759000	2.974999000	6	2.213713000	-1.194109000	3.007871000
6	3.424816000	-1.983449000	3.177491000	6	3.340484000	-2.007257000	3.266053000
6	2.088688000	0.011445000	3.680294000	6	2.097744000	0.058900000	3.669902000
6	4.408034000	-1.555954000	4.044577000	6	4.318129000	-1.600313000	4.151876000
6	3.116082000	0.445480000	4.547417000	6	3.111247000	0.473007000	4.555504000
6	4.248249000	-0.338764000	4.722648000	6	4.199079000	-0.359452000	4.790797000
1	-6.206873000	2.448091000	0.438795000	1	-6.358383000	2.283247000	0.602225000
8	2.992240000	1.583479000	5.297493000	8	3.012485000	1.642426000	5.261079000
6	2.866745000	2.826268000	4.589464000	6	3.037333000	2.859389000	4.500775000
1	3.722913000	2.970825000	3.921432000	1	3.965025000	2.927966000	3.922391000
1	1.937340000	2.867493000	4.021205000	1	2.175995000	2.929266000	3.834885000
1	2.870014000	3.601860000	5.354294000	1	3.005889000	3.666188000	5.231842000
1	3.532676000	-2.918052000	2.638071000	1	3.419570000	-2.961844000	2.757968000
1	5.005299000	0.019508000	5.410510000	1	4.951371000	-0.018292000	5.492370000
8	0.992454000	0.768642000	3.564253000	8	1.035423000	0.862356000	3.477934000
1	0.367300000	0.333790000	2.923908000	1	0.441996000	0.403529000	2.832560000
1	5.301068000	-2.148345000	4.201048000	1	5.175604000	-2.230838000	4.351769000
5j_R3, optimization in gas phase B3LYP/6-311++G**, E= -949.068741869 a.u. Sum of electronic and thermal Enthalpies= -948.790662 a.u.				**5j_Rw1,** optimization in solv. water B3LYP/6-311++G**, E= -949.095893215 a.u. Sum of electronic and thermal Enthalpies= -948.818199 a.u.			
0; 2				0; 2			
6	-5.333789000	1.738684000	0.350820000	6	-5.559935000	1.591543000	0.317778000
6	-4.096336000	1.645494000	0.995496000	6	-4.360349000	1.590519000	1.006205000
6	-5.795259000	0.719709000	-0.486810000	6	-5.904988000	0.544751000	-0.572763000
1	-3.739817000	2.435644000	1.644924000	1	-4.095257000	2.389972000	1.687624000
6	-3.343005000	0.502064000	0.772997000	6	-3.480919000	0.510221000	0.797739000
6	-5.036927000	-0.433701000	-0.711834000	6	-5.059730000	-0.532527000	-0.799901000
1	-5.396472000	-1.223158000	-1.360973000	1	-5.327477000	-1.330260000	-1.481511000
6	-3.810260000	-0.525706000	-0.071600000	6	-3.848091000	-0.535215000	-0.105648000
6	-1.780586000	-1.135900000	0.734014000	6	-1.855131000	-0.896047000	0.805664000
7	-2.100918000	0.095311000	1.244323000	7	-2.254691000	0.266579000	1.344227000
7	-2.826456000	-1.512085000	-0.072006000	7	-2.795355000	-1.406259000	-0.076152000
1	-6.758403000	0.821991000	-0.972133000	1	-6.856220000	0.588658000	-1.090088000

1	-1.463601000	0.555364000	1.882319000
1	-2.836384000	-2.388088000	-0.568159000
7	-0.707672000	-1.857348000	0.948424000
7	0.123914000	-1.168952000	1.782757000
6	1.209886000	-1.787545000	2.118063000
1	1.398018000	-2.788907000	1.718130000
6	2.217658000	-1.236464000	2.987498000
6	3.364062000	-2.000236000	3.214822000
6	2.080903000	0.079669000	3.650086000
6	4.403188000	-1.542984000	4.023258000
6	3.247396000	0.537584000	4.434230000
6	4.347034000	-0.281161000	4.623938000
1	-5.945033000	2.619684000	0.505567000
8	3.275202000	1.722071000	5.076017000
6	2.459075000	2.843556000	4.695147000
1	2.468982000	2.986500000	3.613614000
1	1.432041000	2.714564000	5.030149000
1	2.923253000	3.696746000	5.189800000
1	3.444333000	-2.973519000	2.742369000
1	5.160758000	0.082744000	5.239895000
8	1.048657000	0.771260000	3.600523000
1	5.277300000	-2.165225000	4.176912000

1	-2.695663000	-2.270681000	-0.588470000
7	-0.723458000	-1.596948000	0.995170000
7	0.121190000	-1.035187000	1.866690000
6	1.236998000	-1.695705000	2.065812000
1	1.416275000	-2.630834000	1.533692000
6	2.232229000	-1.206837000	2.977325000
6	3.415515000	-1.955159000	3.175253000
6	2.050299000	0.010064000	3.695810000
6	4.390793000	-1.521279000	4.051353000
6	3.061708000	0.445781000	4.574157000
6	4.209168000	-0.316884000	4.746676000
1	-6.257271000	2.409073000	0.458017000
8	2.887578000	1.587108000	5.321137000
6	3.023643000	2.825174000	4.597833000
1	4.031610000	2.911255000	4.181198000
1	2.282079000	2.895876000	3.799899000
1	2.859325000	3.620043000	5.323772000
1	3.541249000	-2.881180000	2.625767000
1	4.961955000	0.042171000	5.439040000
8	0.941124000	0.757432000	3.574471000
1	0.340336000	0.306934000	2.917865000
1	5.292754000	-2.101103000	4.201990000

5j_Rw2, optimization in solv. water
B3LYP/6-311++G**, E= -949.095677464 a.u.
Sum of electronic and thermal Enthalpies= -948.817703 a.u.

0; 2

6	-5.646373000	1.520930000	0.309575000
6	-4.459816000	1.565018000	1.032084000
6	-5.935108000	0.469165000	-0.593622000
1	-4.246080000	2.372797000	1.720813000
6	-3.562071000	0.518377000	0.824648000
6	-5.045200000	-0.569181000	-0.799908000
1	-5.261560000	-1.376221000	-1.489543000
6	-3.833544000	-0.551489000	-0.081124000
6	-1.894565000	-0.950979000	0.772662000
7	-2.326073000	0.234153000	1.347143000
7	-2.800757000	-1.438320000	-0.096958000
1	-6.875803000	0.484797000	-1.131137000
1	-1.821043000	0.776087000	2.029940000
7	-0.739269000	-1.590111000	1.002975000
7	0.071516000	-0.984361000	1.889811000
6	1.189748000	-1.638835000	2.107721000
1	1.357641000	-2.578276000	1.580443000
6	2.204822000	-1.173548000	3.010239000
6	3.365293000	-1.960887000	3.194009000
6	2.077476000	0.046228000	3.728881000
6	4.365847000	-1.559077000	4.057155000
6	3.110916000	0.451660000	4.593420000
6	4.234614000	-0.349090000	4.752890000
1	-6.373075000	2.314240000	0.440097000
8	2.981832000	1.599829000	5.338022000
6	3.160725000	2.830276000	4.610386000
1	4.170045000	2.878778000	4.191228000
1	2.420391000	2.924961000	3.813712000
1	3.026390000	3.632600000	5.334176000
1	3.453382000	-2.891163000	2.644677000

5j_Rw3, optimization in solv. water
B3LYP/6-311++G**, E= -949.085932406 a.u.
Sum of electronic and thermal Enthalpies= -948.807862 a.u.

0; 2

6	-5.616228000	1.574217000	0.197365000
6	-4.414681000	1.587377000	0.907272000
6	-5.955086000	0.509136000	-0.650335000
1	-4.152166000	2.408847000	1.561724000
6	-3.568444000	0.498287000	0.738029000
6	-5.105532000	-0.584584000	-0.820489000
1	-5.364462000	-1.407850000	-1.474208000
6	-3.909615000	-0.570970000	-0.112859000
6	-1.894087000	-1.011657000	0.798640000
7	-2.324568000	0.189749000	1.277424000
7	-2.857118000	-1.475830000	-0.047713000
1	-6.896692000	0.534586000	-1.185352000
1	-1.778410000	0.730260000	1.932445000
1	-2.783282000	-2.354679000	-0.538604000
7	-0.773200000	-1.669995000	1.057226000
7	0.008734000	-0.990159000	1.923115000
6	1.137063000	-1.602674000	2.193975000
1	1.330556000	-2.554944000	1.692531000
6	2.161222000	-1.134033000	3.066027000
6	3.336151000	-1.919395000	3.147456000
6	2.062746000	0.095018000	3.882504000
6	4.409355000	-1.546701000	3.926607000
6	3.273900000	0.471864000	4.632857000
6	4.377185000	-0.336640000	4.665528000
1	-6.301382000	2.406477000	0.304509000
8	3.249105000	1.593100000	5.415994000
6	3.102825000	2.853666000	4.732318000
1	3.963529000	3.024245000	4.078571000
1	2.178366000	2.881606000	4.156354000
1	3.080284000	3.615481000	5.510031000

1	5.007852000	-0.014772000	5.434942000	1	3.386133000	-2.834833000	2.567656000
8	0.989708000	0.829943000	3.616903000	1	5.228551000	-0.038513000	5.267059000
1	0.377306000	0.395390000	2.975129000	8	1.024195000	0.775559000	3.983791000
1	5.249314000	-2.169264000	4.196706000	1	5.295798000	-2.168359000	3.965125000
5j_RC, optimization in gas phase B3LYP/6-311++G**, E= -949.469256573 a.u. Sum of electronic and thermal Enthalpies= -949.176968 a.u.				**5j_RCw,** optimization in solv. water B3LYP/6-311++G**, E= -949.539399194 a.u. Sum of electronic and thermal Enthalpies= -949.247283 a.u.			
1; 2				1; 2			
6	-5.708163000	1.489426000	0.287399000	6	-5.710793000	1.490744000	0.250037000
6	-4.528503000	1.539352000	1.018308000	6	-4.534847000	1.552514000	0.982350000
6	-5.968576000	0.454258000	-0.634082000	6	-5.974349000	0.435284000	-0.653222000
1	-4.333124000	2.336170000	1.724635000	1	-4.332060000	2.360145000	1.672890000
6	-3.613216000	0.514311000	0.795885000	6	-3.622055000	0.517631000	0.782738000
6	-5.059304000	-0.569526000	-0.858078000	6	-5.071302000	-0.595843000	-0.855631000
1	-5.261581000	-1.363705000	-1.565422000	1	-5.269632000	-1.404984000	-1.545834000
6	-3.874111000	-0.523192000	-0.126287000	6	-3.885699000	-0.539129000	-0.121046000
6	-1.852471000	-0.889099000	0.794503000	6	-1.875417000	-0.885399000	0.807497000
7	-2.361426000	0.251272000	1.336459000	7	-2.379591000	0.264316000	1.328382000
7	-2.771273000	-1.357807000	-0.092704000	7	-2.791695000	-1.371153000	-0.071821000
1	-6.903626000	0.459704000	-1.180076000	1	-6.908589000	0.435059000	-1.200636000
1	-1.883363000	0.791698000	2.041816000	1	-1.903773000	0.831458000	2.015584000
1	-2.621297000	-2.201246000	-0.629933000	1	-2.652419000	-2.226052000	-0.595608000
7	-0.705375000	-1.527478000	1.006908000	7	-0.727189000	-1.523395000	1.028442000
7	0.104189000	-0.931374000	1.884359000	7	0.081728000	-0.928981000	1.909857000
6	1.220328000	-1.612419000	2.110481000	6	1.202427000	-1.599607000	2.112577000
1	1.353995000	-2.561424000	1.591814000	1	1.353797000	-2.533598000	1.572468000
6	2.232795000	-1.168995000	2.994886000	6	2.217858000	-1.155407000	3.005238000
6	3.367360000	-2.003488000	3.201763000	6	3.374504000	-1.962424000	3.169471000
6	2.144713000	0.078932000	3.701039000	6	2.109941000	0.062726000	3.743461000
6	4.358019000	-1.625194000	4.071163000	6	4.380887000	-1.582927000	4.027121000
6	3.183191000	0.461510000	4.577172000	6	3.157486000	0.443496000	4.605285000
6	4.260156000	-0.394111000	4.754083000	6	4.267567000	-0.376185000	4.741162000
1	-6.449334000	2.266268000	0.428063000	1	-6.450001000	2.272668000	0.371775000
8	3.100262000	1.593016000	5.323806000	8	3.047963000	1.577960000	5.366943000
6	3.169004000	2.855751000	4.631343000	6	3.240070000	2.821969000	4.662324000
1	4.108834000	2.931076000	4.076867000	1	4.247700000	2.864144000	4.239545000
1	2.319917000	2.984167000	3.958710000	1	2.496432000	2.942826000	3.872602000
1	3.142269000	3.615874000	5.409062000	1	3.120190000	3.609274000	5.404390000
1	3.427709000	-2.943070000	2.665581000	1	3.445583000	-2.885844000	2.607321000
1	5.033072000	-0.088400000	5.449716000	1	5.051411000	-0.063174000	5.421110000
8	1.095680000	0.891606000	3.564727000	8	1.040360000	0.861035000	3.655979000
1	0.468423000	0.472037000	2.933571000	1	0.407190000	0.457798000	3.017966000
1	5.217774000	-2.261344000	4.237811000	1	5.259264000	-2.202390000	4.154626000
5j_M, optimization in gas phase B3LYP/6-311++G**, E= -949.714148124 a.u. Sum of electronic and thermal Enthalpies= -949.422671 a.u.				**5j_Mw,** optimization in solv. water B3LYP/6-311++G**, E= -949.730217212 a.u. Sum of electronic and thermal Enthalpies= -949.439204 a.u.			
0; 1				0; 1			
6	-5.668724000	1.481903000	0.488971000	6	-5.631918000	1.570015000	0.313329000
6	-4.459650000	1.447510000	1.193964000	6	-4.420933000	1.565775000	1.015577000
6	-5.942792000	0.559246000	-0.521994000	6	-5.955207000	0.546372000	-0.583321000
1	-4.247114000	2.164603000	1.977762000	1	-4.169384000	2.357990000	1.709777000
6	-3.547973000	0.462144000	0.851263000	6	-3.556839000	0.505498000	0.785940000
6	-5.020670000	-0.435716000	-0.867050000	6	-5.081118000	-0.521999000	-0.813813000
1	-5.236387000	-1.151243000	-1.651471000	1	-5.329888000	-1.315073000	-1.508059000
6	-3.824936000	-0.469667000	-0.166538000	6	-3.881513000	-0.523617000	-0.116338000
6	-1.761920000	-0.942385000	0.678066000	6	-1.836614000	-0.978760000	0.762334000

7	-2.278011000	0.153315000	1.339115000	7	-2.299614000	0.195539000	1.305155000
7	-2.716942000	-1.308061000	-0.247624000	7	-2.810159000	-1.410609000	-0.106098000
1	-6.886456000	0.611133000	-1.051620000	1	-6.900499000	0.578191000	-1.111918000
1	-1.808346000	0.583506000	2.117716000	1	-1.788745000	0.733059000	1.985354000
1	-2.581535000	-2.085103000	-0.872754000	1	-2.724352000	-2.258804000	-0.644077000
7	-0.636822000	-1.573636000	0.823565000	7	-0.723597000	-1.637722000	0.956298000
7	0.176195000	-0.998510000	1.776718000	7	0.118753000	-1.036794000	1.862801000
6	1.246721000	-1.665314000	2.062221000	6	1.227970000	-1.667791000	2.080609000
1	1.424928000	-2.622385000	1.568170000	1	1.424175000	-2.604692000	1.555964000
6	2.233926000	-1.193902000	3.018445000	6	2.243089000	-1.185353000	3.003118000
6	3.333287000	-2.013979000	3.332343000	6	3.413497000	-1.943428000	3.194994000
6	2.113136000	0.067426000	3.651010000	6	2.085322000	0.022725000	3.723741000
6	4.287558000	-1.605912000	4.250066000	6	4.402730000	-1.523988000	4.072245000
6	3.096783000	0.484031000	4.566712000	6	3.098357000	0.448193000	4.600429000
6	4.165387000	-0.355900000	4.862037000	6	4.242219000	-0.324473000	4.771803000
1	-6.402434000	2.240063000	0.734715000	1	-6.329817000	2.383876000	0.469829000
8	2.986673000	1.673363000	5.243568000	8	2.935410000	1.594594000	5.348017000
6	3.070962000	2.865941000	4.453409000	6	3.089839000	2.826510000	4.620947000
1	4.031004000	2.907992000	3.926652000	1	4.100855000	2.899894000	4.208448000
1	2.250404000	2.926162000	3.736444000	1	2.353844000	2.902424000	3.817957000
1	3.008350000	3.695608000	5.157063000	1	2.931114000	3.628102000	5.341148000
1	3.418835000	-2.979598000	2.845558000	1	3.529408000	-2.870196000	2.643678000
1	4.894644000	-0.011315000	5.585913000	1	5.000383000	0.025431000	5.462992000
8	1.066353000	0.884043000	3.399109000	8	0.972478000	0.781369000	3.597801000
1	0.502203000	0.416897000	2.732772000	1	0.386978000	0.321164000	2.944200000
1	5.126309000	-2.247705000	4.491049000	1	5.296723000	-2.118872000	4.214484000

5k_A1, optimization in gas phase B3LYP/6-311++G**, E= -949.180735477 a.u. Sum of electronic and thermal Enthalpies= -948.904412 a.u.			
-1; 1			
6	-5.345139000	1.787280000	0.208444000
6	-4.087167000	1.760764000	0.820434000
6	-5.857241000	0.668876000	-0.460662000
1	-3.694998000	2.629566000	1.337762000
6	-3.328210000	0.586849000	0.758948000
6	-5.115851000	-0.520797000	-0.537402000
1	-5.510143000	-1.389702000	-1.055780000
6	-3.869116000	-0.541185000	0.071118000
6	-1.828512000	-0.961777000	0.924910000
7	-2.084375000	0.306343000	1.270465000
7	-2.892455000	-1.506075000	0.193672000
1	-6.836386000	0.719111000	-0.925679000
1	-2.896174000	-2.449570000	-0.154839000
7	-0.779487000	-1.766637000	1.147017000
7	0.200517000	-1.180077000	1.854075000
6	1.260994000	-1.880336000	2.123774000
1	1.338667000	-2.915741000	1.778213000
6	2.356643000	-1.308405000	2.884808000
6	3.507234000	-2.059420000	3.181055000
6	2.314335000	0.029943000	3.362809000
6	4.572859000	-1.544519000	3.907522000
6	3.386256000	0.556697000	4.097080000
6	4.507170000	-0.225495000	4.367275000
1	-5.938588000	2.695581000	0.253125000
1	3.556920000	-3.084178000	2.824094000
8	1.259997000	0.828477000	3.132143000
1	0.586667000	0.301481000	2.598870000
1	5.451494000	-2.139299000	4.126262000
8	5.600720000	0.221354000	5.082877000
6	5.576688000	1.547996000	5.571574000
1	5.505656000	2.279536000	4.757383000
1	4.742953000	1.709663000	6.265642000
1	6.518760000	1.691772000	6.102085000
1	3.296752000	1.580466000	4.434333000

5k_A2, optimization in gas phase B3LYP/6-311++G**, E= -949.180395135 a.u. Sum of electronic and thermal Enthalpies= -948.904030 a.u.			
-1; 1			
6	-5.171166000	1.898768000	0.177960000
6	-3.886850000	1.832473000	0.739418000
6	-5.771948000	0.757405000	-0.369558000
1	-3.419330000	2.714118000	1.166846000
6	-3.244001000	0.603162000	0.726967000
6	-5.119003000	-0.478731000	-0.378563000
1	-5.587834000	-1.359559000	-0.803904000
6	-3.835230000	-0.570059000	0.173518000
6	-1.888924000	-1.188250000	0.889390000
7	-2.012442000	0.179021000	1.183763000
7	-2.992142000	-1.645690000	0.283650000
1	-6.767417000	0.836153000	-0.796268000
1	-1.281110000	0.746420000	1.574974000
7	-0.811250000	-1.941991000	1.166098000
7	0.143238000	-1.279792000	1.840115000
6	1.257957000	-1.916902000	2.085158000
1	1.377063000	-2.938779000	1.719154000
6	2.338864000	-1.312251000	2.839050000
6	3.547017000	-1.999632000	3.059409000
6	2.232359000	-0.012530000	3.399765000
6	4.597955000	-1.452027000	3.782414000
6	3.283137000	0.549169000	4.131634000
6	4.463732000	-0.168644000	4.321053000
1	-5.702582000	2.844754000	0.170198000
1	3.654038000	-2.997166000	2.643962000
8	1.102762000	0.711778000	3.240662000
1	0.483577000	0.127488000	2.706252000
1	5.520821000	-1.997170000	3.939753000
8	5.549184000	0.310280000	5.026269000
6	5.451810000	1.598980000	5.600252000
1	5.300848000	2.372719000	4.837550000
1	4.635200000	1.656879000	6.330240000
1	6.400484000	1.776208000	6.108007000
1	3.135852000	1.542823000	4.532734000

5k_A3, optimization in gas phase B3LYP/6-311++G**, E= -949.158035722 a.u. Sum of electronic and thermal Enthalpies= -948.881560 a.u.			
-1; 1			
6	-5.259454000	1.794775000	0.253349000
6	-3.981197000	1.700807000	0.828556000
6	-5.830766000	0.715660000	-0.416539000
1	-3.538043000	2.540315000	1.350816000
6	-3.299431000	0.498580000	0.711415000
6	-5.143170000	-0.504519000	-0.539455000
1	-5.587660000	-1.344470000	-1.062015000
6	-3.882663000	-0.599000000	0.027503000
6	-1.826752000	-1.234467000	0.790844000
7	-2.059605000	0.085462000	1.152716000
7	-2.959191000	-1.633203000	0.079766000
1	-6.819275000	0.812933000	-0.851448000
1	-1.341624000	0.561375000	1.692381000
1	-3.075350000	-2.571178000	-0.261430000

5k_Aw1, optimization in solv.water B3LYP/6-311++G**, E= -949.261306587 a.u. Sum of electronic and thermal Enthalpies= -948.984636 a.u.			
-1; 1			
6	-5.308409000	1.809027000	0.244167000
6	-4.048937000	1.758394000	0.853062000
6	-5.833070000	0.704111000	-0.439577000
1	-3.651000000	2.618770000	1.380880000
6	-3.309408000	0.574199000	0.769281000
6	-5.109014000	-0.493064000	-0.536632000
1	-5.512237000	-1.349820000	-1.065266000
6	-3.860443000	-0.535064000	0.070034000
6	-1.827104000	-1.007555000	0.906216000
7	-2.060564000	0.263641000	1.275154000
7	-2.897029000	-1.519767000	0.173861000
1	-6.811872000	0.772682000	-0.901059000
1	-2.934956000	-2.455225000	-0.198952000
7	-0.777881000	-1.816926000	1.125122000

7	-0.791137000	-1.952087000	1.050189000	7	0.204571000	-1.222804000	1.842418000
7	0.100443000	-1.157464000	1.788526000	6	1.268407000	-1.912691000	2.122925000
6	1.199440000	-1.740437000	2.131704000	1	1.362617000	-2.949129000	1.787514000
1	1.352298000	-2.785712000	1.827240000	6	2.356446000	-1.325202000	2.886365000
6	2.261696000	-1.135535000	2.892211000	6	3.512005000	-2.068520000	3.192044000
6	3.386772000	-1.938866000	3.168894000	6	2.302567000	0.013382000	3.352156000
6	2.227514000	0.247433000	3.384799000	6	4.564557000	-1.533915000	3.917336000
6	4.484529000	-1.504629000	3.887979000	6	3.359288000	0.563897000	4.085526000
6	3.403344000	0.660072000	4.136176000	6	4.487657000	-0.207115000	4.367911000
6	4.470609000	-0.177307000	4.370580000	1	-5.890782000	2.722434000	0.303309000
1	-5.807991000	2.726590000	0.335435000	1	3.575030000	-3.095194000	2.845311000
1	3.383368000	-2.960069000	2.791552000	8	1.225749000	0.793703000	3.098524000
8	1.278918000	1.049040000	3.197540000	1	0.579286000	0.229712000	2.566035000
1	5.337439000	-2.141254000	4.087902000	1	5.446717000	-2.120310000	4.143569000
8	5.603390000	0.190017000	5.083256000	8	5.564877000	0.247916000	5.076434000
6	5.661487000	1.504100000	5.595250000	6	5.547053000	1.591046000	5.561713000
1	5.616313000	2.254316000	4.795914000	1	5.480188000	2.308672000	4.738638000
1	4.847098000	1.701087000	6.303601000	1	4.716279000	1.750372000	6.255444000
1	6.618678000	1.586706000	6.113909000	1	6.489841000	1.729494000	6.087462000
1	3.379213000	1.679406000	4.500193000	1	3.267011000	1.589388000	4.416476000
5k_Aw2, optimization in solv.water B3LYP/6-311++G**, E= -949.260860767 a.u. Sum of electronic and thermal Enthalpies= -948.983861 a.u.				**5k_Aw3,** optimization in solv.water B3LYP/6-311++G**, E= -949.250834284 a.u. Sum of electronic and thermal Enthalpies= -948.973552 a.u.			
-1; 1				-1; 1			
6	-5.239435000	1.861828000	0.136074000	6	-5.523066000	1.660415000	0.000026000
6	-3.959040000	1.822587000	0.707686000	6	-4.278014000	1.705860000	0.643990000
6	-5.817447000	0.708352000	-0.411767000	6	-5.970655000	0.496085000	-0.628314000
1	-3.508888000	2.712598000	1.133626000	1	-3.930071000	2.608281000	1.131902000
6	-3.296054000	0.603216000	0.704703000	6	-3.508008000	0.552678000	0.632428000
6	-5.142178000	-0.517055000	-0.410843000	6	-5.191115000	-0.669441000	-0.640061000
1	-5.597881000	-1.404151000	-0.838102000	1	-5.537484000	-1.572521000	-1.127969000
6	-3.861978000	-0.577962000	0.152303000	6	-3.959586000	-0.622285000	-0.003957000
6	-1.898963000	-1.150643000	0.893684000	6	-1.904147000	-1.044798000	0.880790000
7	-2.055578000	0.206627000	1.175233000	7	-2.255667000	0.260342000	1.162493000
7	-2.991253000	-1.639867000	0.278061000	7	-2.961441000	-1.575905000	0.164345000
1	-6.809870000	0.767370000	-0.846101000	1	-6.937618000	0.489317000	-1.117579000
1	-1.347626000	0.798692000	1.574878000	1	-1.637093000	0.865463000	1.679058000
7	-0.818921000	-1.893486000	1.178997000	1	-2.977044000	-2.526195000	-0.169319000
7	0.143651000	-1.216911000	1.860208000	7	-0.823664000	-1.691397000	1.194150000
6	1.250418000	-1.857182000	2.104663000	7	0.051850000	-0.879721000	1.930367000
1	1.370242000	-2.880806000	1.741816000	6	1.152495000	-1.483451000	2.245892000
6	2.345032000	-1.270964000	2.857665000	1	1.269795000	-2.519609000	1.903095000
6	3.538686000	-1.990648000	3.062442000	6	2.276669000	-0.969380000	2.999107000
6	2.267563000	0.022696000	3.427036000	6	3.371938000	-1.851380000	3.143946000
6	4.600544000	-1.470213000	3.782980000	6	2.358139000	0.352446000	3.606716000
6	3.329590000	0.560639000	4.158942000	6	4.532861000	-1.530676000	3.821195000
6	4.496501000	-0.184376000	4.336104000	6	3.587207000	0.654115000	4.301194000
1	-5.786877000	2.797577000	0.119963000	6	4.630350000	-0.248262000	4.402596000
1	3.623180000	-2.986211000	2.638722000	1	-6.146310000	2.546941000	-0.007687000
8	1.147872000	0.774699000	3.278166000	1	3.292352000	-2.837136000	2.692307000
1	0.514245000	0.225443000	2.738547000	8	1.424301000	1.218045000	3.555380000
1	5.511610000	-2.037347000	3.929415000	1	5.355567000	-2.229208000	3.911416000
8	5.585737000	0.257509000	5.032119000	8	5.812551000	0.008303000	5.053632000
6	5.538714000	1.556017000	5.625955000	6	5.996424000	1.289083000	5.653157000
1	5.406835000	2.333284000	4.867571000	1	5.944597000	2.088048000	4.907130000
1	4.735045000	1.623646000	6.364990000	1	5.252286000	1.473973000	6.433883000

1	6.498586000	1.691117000	6.120575000	1	6.990525000	1.271619000	6.097106000
1	3.212605000	1.553351000	4.571610000	1	3.650318000	1.638825000	4.746895000
5k_R1, optimization in gas phase B3LYP/6-311++G**, E= -949.091932410 a.u. Sum of electronic and thermal Enthalpies= -948.813731 a.u.				**5k_R2,** optimization in gas phase B3LYP/6-311++G**, E= -949.089877607 a.u. Sum of electronic and thermal Enthalpies= -948.811759 a.u.			
0; 2				0; 2			
6	-5.364047000	1.748675000	0.181873000	6	-5.367988000	1.748194000	0.144613000
6	-4.124492000	1.752799000	0.798713000	6	-4.124899000	1.790789000	0.767980000
6	-5.852224000	0.603665000	-0.486420000	6	-5.841104000	0.580942000	-0.495166000
1	-3.744300000	2.627044000	1.312801000	1	-3.771739000	2.691483000	1.256169000
6	-3.353673000	0.578562000	0.744277000	6	-3.364705000	0.623974000	0.731701000
6	-5.113532000	-0.571409000	-0.557423000	6	-5.085498000	-0.578039000	-0.531408000
1	-5.495215000	-1.445350000	-1.072189000	1	-5.439063000	-1.477910000	-1.019595000
6	-3.864833000	-0.567542000	0.063513000	6	-3.823649000	-0.565069000	0.090201000
6	-1.847114000	-0.937548000	0.927131000	6	-1.877230000	-1.029719000	0.878232000
7	-2.116175000	0.324941000	1.264250000	7	-2.124851000	0.297502000	1.224904000
7	-2.881934000	-1.513548000	0.198203000	7	-2.898976000	-1.559410000	0.191986000
1	-6.828403000	0.643730000	-0.955833000	1	-6.817162000	0.600508000	-0.965711000
1	-2.871807000	-2.459751000	-0.148308000	1	-1.492806000	0.892493000	1.733332000
7	-0.765738000	-1.702244000	1.179830000	7	-0.772633000	-1.733123000	1.169991000
7	0.176821000	-1.078454000	1.882539000	7	0.144067000	-1.049465000	1.873220000
6	1.245375000	-1.797597000	2.147101000	6	1.229279000	-1.745776000	2.142275000
1	1.300755000	-2.828047000	1.789888000	1	1.286034000	-2.772046000	1.777215000
6	2.330690000	-1.252038000	2.893664000	6	2.324488000	-1.213312000	2.889130000
6	3.473572000	-2.043721000	3.168533000	6	3.465959000	-2.014619000	3.137462000
6	2.313350000	0.088788000	3.388258000	6	2.322178000	0.111201000	3.411263000
6	4.540181000	-1.560076000	3.884011000	6	4.540790000	-1.546913000	3.853247000
6	3.400970000	0.582091000	4.118262000	6	3.410678000	0.592988000	4.140652000
6	4.502794000	-0.231373000	4.364347000	6	4.513885000	-0.229824000	4.360811000
1	-5.978767000	2.640934000	0.208776000	1	-5.991446000	2.634917000	0.149909000
1	3.494733000	-3.062761000	2.796944000	1	3.481130000	-3.026125000	2.746165000
8	1.284471000	0.912871000	3.182621000	8	1.277438000	0.932938000	3.220259000
1	0.588264000	0.434342000	2.655090000	1	0.607258000	0.428708000	2.692670000
1	5.412198000	-2.165674000	4.093217000	1	5.412264000	-2.159913000	4.042068000
8	5.595963000	0.161364000	5.059515000	8	5.613389000	0.145843000	5.053925000
6	5.645190000	1.487355000	5.581636000	6	5.671734000	1.459657000	5.605282000
1	5.597189000	2.229450000	4.778971000	1	5.618887000	2.219858000	4.820021000
1	4.832937000	1.661359000	6.293803000	1	4.867357000	1.619611000	6.329634000
1	6.602074000	1.566202000	6.093868000	1	6.633728000	1.524054000	6.109710000
1	3.342165000	1.601502000	4.471939000	1	3.357875000	1.605029000	4.515775000
5k_R3, optimization in gas phase B3LYP/6-311++G**, E= -949.074511888 a.u. Sum of electronic and thermal Enthalpies= -948.796225 a.u.				**5k_Rw1,** optimization in solv. water B3LYP/6-311++G**, E= -949.107727214 a.u. Sum of electronic and thermal Enthalpies= -948.829778 a.u.			
0; 2				0; 2			
6	-5.231066000	1.811053000	0.256706000	6	-5.376692000	1.746427000	0.171641000
6	-3.969547000	1.723134000	0.850344000	6	-4.139947000	1.758109000	0.795181000
6	-5.793820000	0.725941000	-0.423463000	6	-5.856682000	0.596608000	-0.498873000
1	-3.534352000	2.563404000	1.377027000	1	-3.772133000	2.638495000	1.308738000
6	-3.294376000	0.515413000	0.739261000	6	-3.363842000	0.585842000	0.744722000
6	-5.115633000	-0.490473000	-0.536631000	6	-5.112986000	-0.574761000	-0.565154000
1	-5.552652000	-1.330016000	-1.063805000	1	-5.483153000	-1.453023000	-1.079633000
6	-3.862690000	-0.577443000	0.053047000	6	-3.866367000	-0.563055000	0.063162000
6	-1.832699000	-1.202927000	0.830972000	6	-1.854109000	-0.933937000	0.929711000
7	-2.054134000	0.093963000	1.200003000	7	-2.125483000	0.332571000	1.269110000
7	-2.935044000	-1.614135000	0.130598000	7	-2.884168000	-1.506346000	0.200537000
1	-6.774485000	0.828068000	-0.872255000	1	-6.830587000	0.632536000	-0.972945000

1	-1.348831000	0.589678000	1.735023000	1	-2.884204000	-2.452364000	-0.152015000
1	-3.017709000	-2.542349000	-0.251503000	7	-0.769188000	-1.693620000	1.186277000
7	-0.776794000	-1.952314000	1.079628000	7	0.175223000	-1.070380000	1.891763000
7	0.105307000	-1.215694000	1.792312000	6	1.245612000	-1.791708000	2.153724000
6	1.215687000	-1.822091000	2.120571000	1	1.303089000	-2.820215000	1.794563000
1	1.362288000	-2.860710000	1.807610000	6	2.332607000	-1.249725000	2.899438000
6	2.252024000	-1.203592000	2.868161000	6	3.475267000	-2.045607000	3.168430000
6	3.404669000	-1.978800000	3.154673000	6	2.321304000	0.088644000	3.398505000
6	2.201681000	0.200722000	3.367852000	6	4.542954000	-1.561782000	3.882228000
6	4.464919000	-1.487707000	3.868525000	6	3.405379000	0.583962000	4.125483000
6	3.359249000	0.664758000	4.120955000	6	4.509964000	-0.233058000	4.366617000
6	4.436317000	-0.140387000	4.358445000	1	-5.995915000	2.635592000	0.194465000
1	-5.783589000	2.740342000	0.325837000	1	3.495196000	-3.063426000	2.795112000
1	3.440084000	-3.000826000	2.790862000	8	1.278931000	0.908335000	3.188309000
8	1.241884000	0.960981000	3.171643000	1	0.596049000	0.407531000	2.659207000
1	5.338850000	-2.090977000	4.080084000	1	5.413558000	-2.171894000	4.085361000
8	5.552133000	0.213066000	5.049226000	8	5.601822000	0.157377000	5.056367000
6	5.625563000	1.532471000	5.579505000	6	5.659686000	1.489803000	5.585023000
1	5.579498000	2.280534000	4.781713000	1	5.605972000	2.229056000	4.782322000
1	4.818453000	1.714134000	6.296235000	1	4.854507000	1.657809000	6.304099000
1	6.586794000	1.596262000	6.086291000	1	6.621303000	1.562685000	6.087308000
1	3.301261000	1.684996000	4.473857000	1	3.354472000	1.602058000	4.484618000
5k_Rw2, optimization in solv. water B3LYP/6-311++G**, E=-949.107644832 a.u. Sum of electronic and thermal Enthalpies= -948.829473 a.u.				**5k_Rw3,** optimization in solv. water B3LYP/6-311++G**, E= -949.096009447 a.u. Sum of electronic and thermal Enthalpies= -948.817428 a.u.			
0; 2				0; 2			
6	-5.377623000	1.745983000	0.085500000	6	-5.483720000	1.676400000	0.035957000
6	-4.131831000	1.803923000	0.701049000	6	-4.245726000	1.727244000	0.676946000
6	-5.860996000	0.557668000	-0.510012000	6	-5.932407000	0.509583000	-0.601941000
1	-3.767090000	2.716599000	1.156088000	1	-3.898488000	2.626505000	1.169692000
6	-3.378861000	0.630344000	0.702723000	6	-3.475799000	0.570194000	0.655416000
6	-5.112283000	-0.607330000	-0.508592000	6	-5.160171000	-0.651570000	-0.624080000
1	-5.479307000	-1.519173000	-0.964565000	1	-5.503827000	-1.552651000	-1.116100000
6	-3.846938000	-0.577265000	0.106429000	6	-3.926492000	-0.600496000	0.014530000
6	-1.892248000	-1.011189000	0.905813000	6	-1.891749000	-1.015128000	0.889545000
7	-2.138490000	0.319305000	1.203222000	7	-2.223540000	0.273135000	1.179759000
7	-2.918330000	-1.569079000	0.241348000	7	-2.925388000	-1.549266000	0.181148000
1	-6.839237000	0.565748000	-0.976202000	1	-6.900126000	0.509469000	-1.088745000
1	-1.502889000	0.942813000	1.674488000	1	-1.606037000	0.876957000	1.703359000
7	-0.787847000	-1.714807000	1.210202000	1	-2.931145000	-2.501056000	-0.155374000
7	0.135489000	-1.031753000	1.904156000	7	-0.791577000	-1.691023000	1.200910000
6	1.230122000	-1.724009000	2.152395000	7	0.064516000	-0.931772000	1.910511000
1	1.299051000	-2.743577000	1.771795000	6	1.178403000	-1.567170000	2.225022000
6	2.327013000	-1.198153000	2.895654000	1	1.282862000	-2.597002000	1.872254000
6	3.481463000	-1.997206000	3.099700000	6	2.260840000	-1.045422000	2.968449000
6	2.321328000	0.110398000	3.460256000	6	3.382772000	-1.908948000	3.145334000
6	4.563279000	-1.538797000	3.809002000	6	2.318161000	0.311421000	3.568931000
6	3.416357000	0.582409000	4.183371000	6	4.504989000	-1.530130000	3.823843000
6	4.533665000	-0.235331000	4.356936000	6	3.538534000	0.664398000	4.266658000
1	-5.996610000	2.635276000	0.061426000	6	4.581828000	-0.214292000	4.390871000
1	3.499712000	-2.995799000	2.677820000	1	-6.112227000	2.558721000	0.031430000
8	1.262571000	0.927594000	3.317180000	1	3.335016000	-2.904012000	2.715590000
1	0.582827000	0.445516000	2.784119000	8	1.374086000	1.127053000	3.496958000
1	5.442919000	-2.150814000	3.960779000	1	5.349090000	-2.197176000	3.945782000
8	5.639284000	0.131829000	5.036107000	8	5.747539000	0.039936000	5.031425000
6	5.701838000	1.439288000	5.624070000	6	5.933698000	1.327185000	5.631881000

1	5.620308000	2.213840000	4.857894000	1	5.883612000	2.117868000	4.878842000
1	4.915902000	1.566883000	6.372119000	1	5.184528000	1.506305000	6.407354000
1	6.676519000	1.497238000	6.102454000	1	6.925948000	1.304513000	6.076639000
1	3.365604000	1.581052000	4.593201000	1	3.571238000	1.658705000	4.690511000
5k_RC, optimization in gas phase B3LYP/6-311++G**, E= -949.489319243 a.u. Sum of electronic and thermal Enthalpies= -949.196583 a.u.				**5k_RCw,** optimization in solv. water B3LYP/6-311++G**, E= -949.554972706 a.u. Sum of electronic and thermal Enthalpies= -949.262492 a.u.			
1; 2				1; 2			
6	-5.480486000	1.693313000	0.079762000	6	-5.483670000	1.686799000	0.086373000
6	-4.246371000	1.769170000	0.714786000	6	-4.255635000	1.764375000	0.730792000
6	-5.915297000	0.514533000	-0.555527000	6	-5.907819000	0.510499000	-0.566639000
1	-3.915886000	2.677602000	1.202284000	1	-3.930246000	2.665888000	1.232902000
6	-3.460272000	0.621526000	0.691775000	6	-3.461407000	0.620405000	0.699949000
6	-5.132403000	-0.632444000	-0.580306000	6	-5.119592000	-0.631496000	-0.598815000
1	-5.468733000	-1.537700000	-1.069641000	1	-5.441617000	-1.535483000	-1.098809000
6	-3.895323000	-0.559072000	0.054937000	6	-3.886353000	-0.557249000	0.047221000
6	-1.851709000	-0.939902000	0.924710000	6	-1.855489000	-0.929778000	0.925818000
7	-2.200754000	0.343934000	1.213200000	7	-2.209625000	0.347154000	1.225010000
7	-2.879621000	-1.487292000	0.221814000	7	-2.872519000	-1.478534000	0.211686000
1	-6.885062000	0.502790000	-1.037081000	1	-6.874180000	0.499432000	-1.055267000
1	-1.608232000	0.977400000	1.727700000	1	-1.631137000	0.987254000	1.749371000
1	-2.858303000	-2.442165000	-0.108564000	1	-2.853945000	-2.430349000	-0.130355000
7	-0.757770000	-1.639250000	1.212067000	7	-0.757217000	-1.630127000	1.214042000
7	0.157263000	-0.969644000	1.912855000	7	0.156153000	-0.965680000	1.920846000
6	1.243623000	-1.687597000	2.181444000	6	1.236984000	-1.687502000	2.187853000
1	1.282992000	-2.712433000	1.813182000	1	1.278690000	-2.712300000	1.820542000
6	2.333615000	-1.181387000	2.916072000	6	2.330280000	-1.182021000	2.924806000
6	3.463992000	-2.019872000	3.156688000	6	3.454296000	-2.024388000	3.166320000
6	2.367542000	0.157619000	3.448313000	6	2.371499000	0.153129000	3.451087000
6	4.542291000	-1.579067000	3.862991000	6	4.539117000	-1.587541000	3.871305000
6	3.466312000	0.608164000	4.169467000	6	3.475882000	0.600296000	4.169807000
6	4.550161000	-0.248313000	4.379166000	6	4.555206000	-0.259533000	4.380444000
1	-6.125013000	2.563440000	0.073267000	1	-6.134112000	2.552661000	0.084933000
1	3.451364000	-3.029394000	2.762291000	1	3.434493000	-3.034694000	2.774961000
8	1.348487000	0.997720000	3.264778000	8	1.356695000	1.004430000	3.269070000
1	0.658502000	0.527060000	2.741932000	1	0.657040000	0.544062000	2.746820000
1	5.403608000	-2.206367000	4.050444000	1	5.393899000	-2.224758000	4.055662000
8	5.647917000	0.079761000	5.052249000	8	5.660714000	0.074924000	5.054391000
6	5.786662000	1.391675000	5.626302000	6	5.787323000	1.396182000	5.611126000
1	5.759314000	2.155353000	4.845999000	1	5.749260000	2.149591000	4.822046000
1	5.003605000	1.569947000	6.366468000	1	5.003679000	1.577652000	6.349094000
1	6.759818000	1.390663000	6.109573000	1	6.761121000	1.413325000	6.093080000
1	3.446965000	1.619131000	4.550005000	1	3.465034000	1.612277000	4.547929000
5k_M, optimization in gas phase B3LYP/6-311++G**, E= -949.722771010 a.u. Sum of electronic and thermal Enthalpies= -949.431296 a.u.				**5k_Mw,** optimization in solv. water B3LYP/6-311++G**, E= -949.738914396 a.u. Sum of electronic and thermal Enthalpies= -949.447789 a.u.			
0; 1				0; 1			
6	-5.362590000	1.785470000	0.097598000	6	-5.358001000	1.790225000	0.066187000
6	-4.103392000	1.781665000	0.710715000	6	-4.097868000	1.792973000	0.677222000
6	-5.875777000	0.636763000	-0.506095000	6	-5.880002000	0.630583000	-0.515229000
1	-3.706353000	2.673831000	1.180037000	1	-3.692207000	2.690285000	1.128277000
6	-3.387001000	0.596032000	0.694337000	6	-3.390072000	0.600421000	0.680954000
6	-5.150516000	-0.560882000	-0.522166000	6	-5.163050000	-0.571957000	-0.510631000
1	-5.550850000	-1.451307000	-0.992084000	1	-5.565878000	-1.470324000	-0.961861000
6	-3.904050000	-0.562748000	0.084139000	6	-3.914389000	-0.566144000	0.094273000
6	-1.846406000	-1.069131000	0.926788000	6	-1.863238000	-1.064671000	0.937900000

7	-2.134158000	0.253498000	1.201964000	7	-2.137842000	0.259295000	1.191600000
7	-2.943272000	-1.556141000	0.242730000	7	-2.958529000	-1.561276000	0.268939000
1	-6.853260000	0.668528000	-0.972222000	1	-6.858474000	0.659716000	-0.979804000
1	-1.484638000	0.860362000	1.671998000	1	-1.488088000	0.881480000	1.642607000
1	-2.991869000	-2.510522000	-0.072521000	1	-3.024775000	-2.520385000	-0.033760000
7	-0.806154000	-1.791061000	1.202433000	7	-0.817398000	-1.791546000	1.223168000
7	0.157183000	-1.100123000	1.911613000	7	0.150903000	-1.102282000	1.925297000
6	1.238507000	-1.770207000	2.151818000	6	1.239020000	-1.767333000	2.151708000
1	1.319997000	-2.793956000	1.780607000	1	1.331657000	-2.787699000	1.773699000
6	2.351093000	-1.222921000	2.899058000	6	2.354494000	-1.219314000	2.897763000
6	3.511638000	-1.994688000	3.106822000	6	3.524904000	-1.983493000	3.078875000
6	2.323021000	0.080420000	3.450785000	6	2.321419000	0.072035000	3.475317000
6	4.593298000	-1.514931000	3.816321000	6	4.609897000	-1.504720000	3.786957000
6	3.411293000	0.577342000	4.173208000	6	3.410587000	0.568333000	4.196467000
6	4.541878000	-0.217056000	4.354056000	6	4.553072000	-0.217444000	4.350637000
1	-5.946080000	2.698249000	0.094455000	1	-5.936931000	2.705876000	0.045873000
1	3.548487000	-2.996837000	2.692148000	1	3.568633000	-2.976987000	2.645255000
8	1.246025000	0.878881000	3.298581000	8	1.231024000	0.864035000	3.349378000
1	0.583560000	0.360425000	2.776092000	1	0.566211000	0.357564000	2.815968000
1	5.482682000	-2.111621000	3.972018000	1	5.504805000	-2.099812000	3.918409000
8	5.648445000	0.179427000	5.039960000	8	5.661692000	0.179412000	5.031110000
6	5.667777000	1.479173000	5.617430000	6	5.676423000	1.477829000	5.632026000
1	5.571860000	2.256499000	4.852202000	1	5.561318000	2.261339000	4.878081000
1	4.871531000	1.596809000	6.359855000	1	4.890006000	1.571104000	6.385965000
1	6.635652000	1.571226000	6.107317000	1	6.650054000	1.571160000	6.108346000
1	3.335239000	1.578435000	4.573404000	1	3.333423000	1.560625000	4.618428000

5l_A1, optimization in gas phase B3LYP/6-311++G**, E= -949.152785641 a.u. Sum of electronic and thermal Enthalpies= -948.876089 a.u.			
-1; 1			
6	-6.937616000	0.297220000	0.105937000
6	-6.080237000	-0.802267000	0.145528000
6	-6.435635000	1.610804000	0.007894000
1	-6.468389000	-1.813938000	0.220884000
6	-4.699543000	-0.573217000	0.085341000
6	-5.063809000	1.857424000	-0.052941000
1	-4.677875000	2.869685000	-0.128360000
6	-4.187279000	0.766316000	-0.014609000
6	-2.594253000	-0.596620000	0.016833000
7	-3.638526000	-1.443894000	0.104080000
7	-2.812219000	0.717830000	-0.057283000
7	-1.323117000	-1.188818000	0.010646000
7	-0.180899000	-0.541072000	-0.056941000
6	0.927080000	-1.212051000	-0.042495000
1	0.921485000	-2.308155000	0.026854000
1	-1.340579000	-2.204829000	0.076640000
1	-7.132136000	2.444135000	-0.020758000
6	2.220428000	-0.551708000	-0.114980000
6	2.352783000	0.846941000	-0.222261000
6	3.397971000	-1.319682000	-0.078665000
6	3.610740000	1.428254000	-0.278754000
6	4.657654000	-0.731150000	-0.146931000
6	4.777178000	0.660644000	-0.237838000
1	-8.011961000	0.141553000	0.150863000
8	6.007507000	1.279564000	-0.358636000
6	6.814908000	1.258837000	0.818184000
1	6.302702000	1.759663000	1.648813000
1	7.068862000	0.235544000	1.108286000
1	7.727604000	1.805086000	0.574527000
1	3.326827000	-2.403269000	-0.004025000
1	3.718259000	2.504107000	-0.366384000
1	1.457102000	1.453886000	-0.257002000
8	5.815290000	-1.481909000	-0.129521000
1	5.572945000	-2.412676000	-0.096041000

5l_A2, optimization in gas phase B3LYP/6-311++G**, E= -949.160110959 a.u. Sum of electronic and thermal Enthalpies= -948.883849 a.u.			
-1; 1			
6	-6.714960000	0.615924000	0.089398000
6	-6.025358000	-0.599607000	0.129339000
6	-6.036466000	1.839247000	0.005519000
1	-6.554228000	-1.544433000	0.194532000
6	-4.626389000	-0.585640000	0.084070000
6	-4.635117000	1.880571000	-0.041252000
1	-4.107607000	2.827186000	-0.106671000
6	-3.954851000	0.671049000	-0.001235000
6	-2.519061000	-1.055047000	0.041698000
7	-3.727785000	-1.623242000	0.108627000
7	-2.618989000	0.337642000	-0.026427000
1	-1.806757000	0.929283000	-0.082448000
7	-1.346962000	-1.724525000	0.039152000
7	-0.301059000	-0.896065000	-0.034060000
6	0.880646000	-1.447752000	-0.041953000
1	0.961170000	-2.537516000	0.009868000
1	-6.599178000	2.766626000	-0.024281000
6	2.101736000	-0.674367000	-0.114514000
6	2.132785000	0.736754000	-0.191062000
6	3.346224000	-1.339677000	-0.110077000
6	3.338637000	1.418857000	-0.247555000
6	4.552405000	-0.651066000	-0.178752000
6	4.564129000	0.747725000	-0.238269000
1	-7.800299000	0.613573000	0.123721000
8	5.743061000	1.465820000	-0.358872000
6	6.556025000	1.487797000	0.812436000
1	6.012105000	1.931948000	1.655654000
1	6.890236000	0.482242000	1.083782000
1	7.423393000	2.107212000	0.575751000
1	3.362979000	-2.426841000	-0.059279000
1	3.358518000	2.502089000	-0.311336000
1	1.195432000	1.277228000	-0.202993000
8	5.766818000	-1.310382000	-0.190243000
1	5.592736000	-2.256808000	-0.173328000

5l_A3, optimization in gas phase B3LYP/6-311++G**, E= -949.164281253 a.u. Sum of electronic and thermal Enthalpies= -948.887462 a.u.			
-1; 1			
6	-6.880458000	0.399399000	0.178249000
6	-6.094132000	-0.753374000	0.214424000
6	-6.309706000	1.670288000	0.022361000
1	-6.537015000	-1.735281000	0.335906000
6	-4.709917000	-0.618882000	0.090530000
6	-4.925659000	1.827581000	-0.104154000
1	-4.481994000	2.809726000	-0.225271000
6	-4.150962000	0.676770000	-0.067641000
6	-2.596719000	-0.900105000	-0.053297000
7	-3.714471000	-1.583448000	0.096823000
7	-2.783306000	0.456347000	-0.160948000
1	-2.023202000	1.113225000	-0.247853000
7	-1.350704000	-1.432597000	-0.129260000
7	-0.260716000	-0.587512000	-0.155251000

5l_Aw1, optimization in solv.water B3LYP/6-311++G**, E= -949.242408434 a.u. Sum of electronic and thermal Enthalpies= -948.965094 a.u.			
-1; 1			
6	-6.935316000	0.328462000	0.053483000
6	-6.098855000	-0.789624000	0.109449000
6	-6.406711000	1.630522000	-0.026878000
1	-6.513660000	-1.791382000	0.171274000
6	-4.713664000	-0.585243000	0.083334000
6	-5.026423000	1.849789000	-0.053814000
1	-4.625107000	2.857028000	-0.116152000
6	-4.175677000	0.739797000	0.001126000
6	-2.592930000	-0.664925000	0.064163000
7	-3.665729000	-1.480358000	0.122812000
7	-2.795839000	0.659090000	-0.009663000
7	-1.331659000	-1.253640000	0.087720000
7	-0.191553000	-0.557903000	0.003983000
6	0.921013000	-1.208618000	0.001270000

6	0.896449000	-1.147592000	-0.079265000
1	0.961279000	-2.240284000	0.014567000
1	-1.248787000	-2.419470000	0.084130000
1	-6.948667000	2.546056000	-0.001573000
6	2.166564000	-0.444451000	-0.106257000
6	2.256402000	0.951924000	-0.251434000
6	3.333313000	-1.214456000	0.014950000
6	3.525309000	1.529571000	-0.255835000
6	4.661845000	-0.674586000	-0.023303000
6	4.686382000	0.772811000	-0.135630000
1	-7.957653000	0.311332000	0.272925000
8	5.883533000	1.461944000	-0.223576000
6	6.845260000	1.178686000	0.793840000
1	6.473551000	1.514838000	1.772779000
1	7.064174000	0.110015000	0.826204000
1	7.737895000	1.753775000	0.535698000
1	3.261782000	-2.295899000	0.103074000
1	3.640146000	2.604869000	-0.362169000
1	1.364183000	1.556685000	-0.350524000
8	5.707249000	-1.393817000	0.024493000

1	0.933412000	-2.302087000	0.061222000
1	-1.310249000	-2.268900000	0.127419000
1	-7.083944000	2.477507000	-0.068849000
6	2.215909000	-0.535024000	-0.083429000
6	2.346049000	0.862105000	-0.159479000
6	3.381507000	-1.318222000	-0.094848000
6	3.606414000	1.441131000	-0.236315000
6	4.644267000	-0.735849000	-0.182075000
6	4.763705000	0.661757000	-0.245431000
1	-8.011874000	0.192333000	0.072244000
8	5.992347000	1.267898000	-0.388219000
6	6.814394000	1.279770000	0.792919000
1	6.317185000	1.832456000	1.595940000
1	7.039255000	0.263813000	1.124042000
1	7.737268000	1.788470000	0.517176000
1	3.303297000	-2.400616000	-0.045939000
1	3.716873000	2.518181000	-0.295799000
1	1.460156000	1.483739000	-0.155258000
8	5.795714000	-1.474711000	-0.221106000
1	5.583677000	-2.414510000	-0.169433000

5l_Aw2, optimization in solv.water
B3LYP/6-311++G**, E= -949.244506817 a.u.
Sum of electronic and thermal Enthalpies= -948.967713 a.u.

-1; 1			
6	-6.733795000	0.604700000	0.098727000
6	-6.037941000	-0.608717000	0.133352000
6	-6.059802000	1.831084000	0.016312000
1	-6.568213000	-1.553094000	0.197640000
6	-4.639702000	-0.581992000	0.083766000
6	-4.659215000	1.881293000	-0.034642000
1	-4.134970000	2.828524000	-0.098733000
6	-3.975264000	0.673296000	0.000239000
6	-2.516221000	-1.033225000	0.033604000
7	-3.725123000	-1.615936000	0.102694000
7	-2.630960000	0.351852000	-0.030203000
1	-1.837398000	0.969880000	-0.087607000
7	-1.351872000	-1.709219000	0.027750000
7	-0.284372000	-0.879308000	-0.042625000
6	0.885976000	-1.435256000	-0.052755000
1	0.970498000	-2.525640000	-0.006321000
1	-6.626699000	2.755044000	-0.009015000
6	2.124209000	-0.667714000	-0.122317000
6	2.160111000	0.738657000	-0.191354000
6	3.350057000	-1.359050000	-0.123409000
6	3.375877000	1.408368000	-0.250980000
6	4.567334000	-0.685568000	-0.191164000
6	4.587806000	0.716700000	-0.249319000
1	-7.817999000	0.596655000	0.136395000
8	5.775468000	1.408784000	-0.374021000
6	6.550947000	1.509075000	0.832734000
1	5.989019000	2.045164000	1.604038000
1	6.832948000	0.519693000	1.200192000
1	7.447099000	2.073312000	0.576439000
1	3.352139000	-2.444720000	-0.079067000
1	3.407438000	2.491242000	-0.305558000
1	1.231861000	1.295284000	-0.196018000

5l_Aw3, optimization in solv.water
B3LYP/6-311++G**, E= -949.249053038 a.u.
Sum of electronic and thermal Enthalpies= -948.971730 a.u.

-1; 1			
6	-6.871915000	0.427461000	0.000721000
6	-6.096955000	-0.731776000	0.064250000
6	-6.282332000	1.700116000	-0.059122000
1	-6.556881000	-1.712493000	0.110116000
6	-4.706539000	-0.596878000	0.067206000
6	-4.893219000	1.855082000	-0.057367000
1	-4.435665000	2.836349000	-0.103855000
6	-4.130334000	0.695699000	0.006291000
6	-2.583858000	-0.883945000	0.094766000
7	-3.711780000	-1.567938000	0.121319000
7	-2.758344000	0.472043000	0.026607000
1	-2.010560000	1.148289000	-0.007916000
7	-1.342385000	-1.442027000	0.140869000
7	-0.235729000	-0.648471000	0.052249000
6	0.907329000	-1.236457000	0.036998000
1	0.966344000	-2.328941000	0.087385000
1	-1.272784000	-2.454984000	0.140153000
1	-6.913932000	2.579660000	-0.107830000
6	2.178085000	-0.518685000	-0.049236000
6	2.252752000	0.883949000	-0.113757000
6	3.355237000	-1.279403000	-0.076217000
6	3.511424000	1.478971000	-0.196116000
6	4.663754000	-0.715188000	-0.184403000
6	4.680852000	0.725306000	-0.225447000
1	-7.953030000	0.344434000	-0.002684000
8	5.881739000	1.404846000	-0.381466000
6	6.790204000	1.290491000	0.721811000
1	6.357636000	1.746172000	1.620328000
1	7.032578000	0.243935000	0.914137000
1	7.691744000	1.836594000	0.441266000
1	3.290840000	-2.364122000	-0.040852000
1	3.602625000	2.560175000	-0.245301000

8	5.771184000	-1.340521000	-0.212934000	1	1.353931000	1.486633000	-0.095153000
1	5.623538000	-2.292845000	-0.166899000	8	5.730419000	-1.430818000	-0.252033000
5l_R1, optimization in gas phase B3LYP/6-311++G**, E= -949.050711786 a.u. Sum of electronic and thermal Enthalpies= -948.772983 a.u.				**5l_R2,** optimization in gas phase B3LYP/6-311++G**, E= -949.069761142 a.u. Sum of electronic and thermal Enthalpies= -948.792074 a.u.			
0; 2				0; 2			
6	-6.922168000	0.217915000	0.052684000	6	-6.812732000	0.429609000	0.016793000
6	-6.083043000	-0.865224000	0.116220000	6	-6.052796000	-0.724153000	0.095801000
6	-6.424761000	1.563132000	-0.050050000	6	-6.209208000	1.703225000	-0.086999000
1	-6.457602000	-1.878829000	0.193433000	1	-6.506129000	-1.704628000	0.175521000
6	-4.687503000	-0.613983000	0.076874000	6	-4.652006000	-0.597667000	0.070181000
6	-5.080330000	1.847738000	-0.090879000	6	-4.827834000	1.860417000	-0.114581000
1	-4.710959000	2.863086000	-0.168403000	1	-4.375469000	2.841888000	-0.194656000
6	-4.181193000	0.759388000	-0.028008000	6	-4.061164000	0.698941000	-0.034811000
6	-2.585597000	-0.586784000	0.041817000	6	-2.528141000	-0.909163000	0.069638000
7	-3.649890000	-1.454255000	0.119985000	7	-3.693869000	-1.564293000	0.132261000
7	-2.835887000	0.736929000	-0.047623000	7	-2.710306000	0.465743000	-0.032099000
7	-1.349415000	-1.140826000	0.060604000	1	-1.947800000	1.121578000	-0.091353000
7	-0.209579000	-0.436381000	-0.009496000	7	-1.334217000	-1.527847000	0.102162000
6	0.889441000	-1.110077000	0.018450000	7	-0.310227000	-0.664082000	0.028648000
1	0.876913000	-2.204846000	0.096259000	6	0.858331000	-1.251478000	0.053839000
1	-1.334106000	-2.158547000	0.130878000	1	0.893062000	-2.340762000	0.126533000
1	-7.144933000	2.372529000	-0.096198000	1	-6.841773000	2.581505000	-0.146909000
6	2.189343000	-0.464930000	-0.052724000	6	2.102425000	-0.523405000	-0.011551000
6	2.326688000	0.928667000	-0.161551000	6	2.165722000	0.880316000	-0.103842000
6	3.346778000	-1.258947000	-0.018631000	6	3.310555000	-1.244191000	0.011198000
6	3.590585000	1.492168000	-0.219180000	6	3.391953000	1.517071000	-0.152127000
6	4.614136000	-0.692740000	-0.092977000	6	4.542158000	-0.607230000	-0.057295000
6	4.747004000	0.706633000	-0.176731000	6	4.595568000	0.800567000	-0.118150000
1	-7.995809000	0.069083000	0.079529000	1	-7.894294000	0.362553000	0.034024000
8	5.950550000	1.333702000	-0.305851000	8	5.742807000	1.521705000	-0.223733000
6	6.938052000	1.120728000	0.715987000	6	6.863979000	1.208522000	0.619884000
1	6.531066000	1.389658000	1.696126000	1	6.534994000	1.055861000	1.651820000
1	7.286022000	0.087905000	0.726502000	1	7.393098000	0.324344000	0.267769000
1	7.761228000	1.789509000	0.469420000	1	7.512943000	2.081755000	0.570116000
1	3.255708000	-2.340397000	0.048217000	1	3.280905000	-2.329589000	0.061669000
1	3.718994000	2.564813000	-0.301952000	1	3.459844000	2.596536000	-0.215434000
1	1.440329000	1.548785000	-0.192754000	1	1.247892000	1.451961000	-0.126187000
8	5.756184000	-1.449209000	-0.108673000	8	5.723186000	-1.302088000	-0.092643000
1	5.527006000	-2.384156000	-0.084417000	1	5.542510000	-2.247713000	-0.066547000
5l_R3, optimization in gas phase B3LYP/6-311++G**, E= -949.071114204 a.u. Sum of electronic and thermal Enthalpies= -948.792628 a.u.				**5l_Rw1,** optimization in solv. water B3LYP/6-311++G**, E= -949.073988121 a.u. Sum of electronic and thermal Enthalpies= -948.796008 a.u.			
0; 2				0; 2			
6	-6.884075000	0.422668000	-0.124938000	6	-6.912425000	0.237839000	0.069767000
6	-6.108470000	-0.732172000	-0.062660000	6	-6.078476000	-0.852123000	0.137810000
6	-6.298974000	1.698683000	-0.151223000	6	-6.405330000	1.575592000	-0.043414000
1	-6.558394000	-1.717437000	-0.042276000	1	-6.464577000	-1.861047000	0.223038000
6	-4.720238000	-0.590344000	-0.026466000	6	-4.682488000	-0.611279000	0.091888000
6	-4.914042000	1.861547000	-0.115902000	6	-5.055712000	1.846703000	-0.090363000
1	-4.464183000	2.847573000	-0.136456000	1	-4.682897000	2.860592000	-0.175877000
6	-4.148318000	0.703964000	-0.053750000	6	-4.167695000	0.750838000	-0.023222000
6	-2.609726000	-0.876043000	0.045383000	6	-2.572354000	-0.614696000	0.049343000
7	-3.724660000	-1.559362000	0.035798000	7	-3.647959000	-1.463837000	0.136605000
7	-2.774037000	0.482684000	-0.005685000	7	-2.817776000	0.713124000	-0.047565000
1	-2.024848000	1.155435000	-0.006702000	7	-1.337876000	-1.164847000	0.064339000

7	-1.363850000	-1.451787000	0.101749000	7	-0.204935000	-0.443069000	-0.014312000
7	-0.252889000	-0.694373000	0.104946000	6	0.898314000	-1.118328000	-0.003020000
6	0.887820000	-1.288035000	0.154473000	1	0.886887000	-2.210116000	0.063363000
1	0.952075000	-2.380380000	0.192486000	1	-1.300884000	-2.182101000	0.137098000
1	-1.328370000	-2.466417000	0.134743000	1	-7.117174000	2.391679000	-0.092728000
1	-6.934436000	2.575266000	-0.199979000	6	2.195674000	-0.472380000	-0.079822000
6	2.146392000	-0.554434000	0.161719000	6	2.340100000	0.923343000	-0.168752000
6	2.173605000	0.875990000	0.114625000	6	3.345053000	-1.281284000	-0.071161000
6	3.337840000	-1.240618000	0.213496000	6	3.607519000	1.480168000	-0.233663000
6	3.365737000	1.562812000	0.120079000	6	4.615110000	-0.721436000	-0.150020000
6	4.624242000	-0.583862000	0.222483000	6	4.752767000	0.679355000	-0.216989000
6	4.595618000	0.885098000	0.171805000	1	-7.986556000	0.096272000	0.101247000
1	-7.964343000	0.337362000	-0.153765000	8	5.976181000	1.276488000	-0.346147000
8	5.677593000	1.665487000	0.170618000	6	6.869712000	1.170093000	0.782594000
6	7.031236000	1.165406000	0.218011000	1	6.419611000	1.642530000	1.660005000
1	7.201773000	0.595350000	1.129655000	1	7.109756000	0.128435000	0.997024000
1	7.240991000	0.533435000	-0.643247000	1	7.772150000	1.708475000	0.498907000
1	7.645713000	2.063915000	0.200285000	1	3.244702000	-2.360900000	-0.017534000
1	3.365848000	-2.324241000	0.249926000	1	3.740074000	2.553652000	-0.298371000
1	3.386479000	2.645661000	0.084364000	1	1.462481000	1.555897000	-0.179414000
1	1.236355000	1.415035000	0.073942000	8	5.754550000	-1.471102000	-0.186116000
8	5.695784000	-1.229781000	0.270176000	1	5.537724000	-2.410294000	-0.137655000
5l_Rw2, optimization in solv. water B3LYP/6-311++G**, E= -949.089925922 a.u. Sum of electronic and thermal Enthalpies= -948.812205 a.u.				**5l_Rw3,** optimization in solv. water B3LYP/6-311++G**, E= -949.089581322 a.u. Sum of electronic and thermal Enthalpies= -948.811150 a.u.			
0; 2				0; 2			
6	-6.781297000	0.466929000	0.074175000	6	-6.858082000	0.468615000	-0.119628000
6	-6.035961000	-0.698344000	0.126402000	6	-6.104617000	-0.703931000	-0.074825000
6	-6.162082000	1.735866000	-0.020668000	6	-6.246120000	1.733321000	-0.128796000
1	-6.507107000	-1.671361000	0.199217000	1	-6.580097000	-1.678047000	-0.067882000
6	-4.633471000	-0.587030000	0.082178000	6	-4.712441000	-0.590394000	-0.038858000
6	-4.780025000	1.876487000	-0.066114000	6	-4.856694000	1.866942000	-0.093354000
1	-4.312195000	2.850548000	-0.138970000	1	-4.383103000	2.841477000	-0.100384000
6	-4.027881000	0.702605000	-0.013570000	6	-4.113878000	0.692757000	-0.048623000
6	-2.506504000	-0.912869000	0.045736000	6	-2.599454000	-0.912248000	0.026320000
7	-3.679229000	-1.563074000	0.116904000	7	-3.734007000	-1.578583000	0.008334000
7	-2.679330000	0.457569000	-0.034347000	7	-2.746642000	0.446251000	-0.005420000
1	-1.920343000	1.120325000	-0.095331000	1	-1.989683000	1.113480000	0.000796000
7	-1.322182000	-1.554006000	0.053851000	7	-1.365553000	-1.502436000	0.073186000
7	-0.282242000	-0.708847000	-0.023382000	7	-0.253999000	-0.741788000	0.090040000
6	0.881005000	-1.307679000	-0.016182000	6	0.886270000	-1.336682000	0.139302000
1	0.918049000	-2.396975000	0.048487000	1	0.957058000	-2.426798000	0.167835000
1	-6.784658000	2.622165000	-0.058999000	1	-1.323941000	-2.517555000	0.095858000
6	2.126521000	-0.582090000	-0.089509000	1	-6.863182000	2.623679000	-0.164150000
6	2.183247000	0.823281000	-0.174550000	6	2.134620000	-0.585497000	0.157116000
6	3.330164000	-1.313505000	-0.079847000	6	2.140792000	0.847038000	0.117916000
6	3.411238000	1.460880000	-0.232252000	6	3.334874000	-1.256435000	0.210454000
6	4.560100000	-0.672936000	-0.150084000	6	3.322880000	1.547963000	0.130997000
6	4.606839000	0.735799000	-0.210983000	6	4.610033000	-0.583197000	0.227770000
1	-7.863178000	0.413463000	0.106027000	6	4.563351000	0.885793000	0.182600000
8	5.786376000	1.414514000	-0.331424000	1	-7.939987000	0.404793000	-0.147845000
6	6.699661000	1.339913000	0.784660000	8	5.630082000	1.684546000	0.187392000
1	6.226476000	1.751712000	1.680191000	6	6.999415000	1.220235000	0.224874000
1	7.018070000	0.313160000	0.964495000	1	7.188353000	0.656072000	1.135955000
1	7.555744000	1.952340000	0.507862000	1	7.218844000	0.603124000	-0.644161000
1	3.298377000	-2.397561000	-0.032577000	1	7.590281000	2.133483000	0.207756000

1	3.474962000	2.540880000	-0.292911000	1	3.367953000	-2.340009000	0.241744000
1	1.266170000	1.396823000	-0.186574000	1	3.326598000	2.631040000	0.100495000
8	5.746647000	-1.345805000	-0.184904000	1	1.197759000	1.376011000	0.076365000
1	5.592008000	-2.297375000	-0.138068000	8	5.693564000	-1.218937000	0.278534000
5l_RC, optimization in gas phase B3LYP/6-311++G**, E= -949.460100553 a.u. Sum of electronic and thermal Enthalpies= -949.168378 a.u.				**5l_RCw,** optimization in solv. water B3LYP/6-311++G**, E= -949.528117095 a.u. Sum of electronic and thermal Enthalpies= -949.236519 a.u.			
1; 2				1; 2			
6	-6.931860000	0.271340000	-0.113881000	6	-6.886211000	0.357969000	-0.115858000
6	-6.103907000	-0.829640000	-0.052774000	6	-6.095494000	-0.775086000	-0.062643000
6	-6.410866000	1.589575000	-0.147680000	6	-6.320246000	1.656126000	-0.139862000
1	-6.488554000	-1.841078000	-0.026373000	1	-6.522661000	-1.770013000	-0.043726000
6	-4.713739000	-0.597689000	-0.024870000	6	-4.700477000	-0.596112000	-0.032819000
6	-5.042785000	1.849706000	-0.121438000	6	-4.945342000	1.861642000	-0.111438000
1	-4.661989000	2.862904000	-0.148043000	1	-4.518806000	2.856328000	-0.129877000
6	-4.209844000	0.742384000	-0.059937000	6	-4.150713000	0.721040000	-0.057870000
6	-2.593345000	-0.742680000	0.035469000	6	-2.583765000	-0.812305000	0.028598000
7	-3.688994000	-1.492693000	0.033985000	7	-3.700198000	-1.529756000	0.020827000
7	-2.831744000	0.601399000	-0.019090000	7	-2.783580000	0.536281000	-0.017218000
1	-2.125666000	1.322035000	-0.026567000	1	-2.057610000	1.239172000	-0.020102000
7	-1.353822000	-1.283351000	0.086696000	7	-1.349019000	-1.373981000	0.079046000
7	-0.255909000	-0.522696000	0.086833000	7	-0.259282000	-0.615693000	0.089440000
6	0.887568000	-1.149916000	0.135684000	6	0.890165000	-1.237042000	0.141211000
1	0.910514000	-2.243564000	0.173468000	1	0.930129000	-2.327306000	0.174280000
1	-1.315766000	-2.303683000	0.123358000	1	-1.305573000	-2.394468000	0.109019000
1	-7.102082000	2.422478000	-0.195583000	1	-6.980140000	2.514397000	-0.181510000
6	2.140504000	-0.463297000	0.141309000	6	2.122056000	-0.517020000	0.152267000
6	2.234163000	0.949985000	0.096097000	6	2.172066000	0.901143000	0.107862000
6	3.332240000	-1.216466000	0.192285000	6	3.332011000	-1.238541000	0.204827000
6	3.463426000	1.556475000	0.102156000	6	3.383874000	1.540559000	0.113205000
6	4.577255000	-0.615474000	0.198692000	6	4.559488000	-0.602802000	0.209383000
6	4.663170000	0.808629000	0.152528000	6	4.602517000	0.823674000	0.160686000
1	-8.006035000	0.135962000	-0.136915000	1	-7.964633000	0.258299000	-0.139688000
8	5.768140000	1.544125000	0.151087000	8	5.690363000	1.592462000	0.155704000
6	7.125144000	1.036534000	0.195252000	6	7.056766000	1.111261000	0.173735000
1	7.294091000	0.476357000	1.112895000	1	7.253638000	0.553884000	1.087059000
1	7.328887000	0.413686000	-0.673594000	1	7.255932000	0.494077000	-0.699812000
1	7.741008000	1.931791000	0.175940000	1	7.657133000	2.016889000	0.144265000
1	3.277603000	-2.300779000	0.226902000	1	3.305775000	-2.322635000	0.241202000
1	3.561417000	2.634225000	0.068320000	1	3.448438000	2.620743000	0.078516000
1	1.332028000	1.544956000	0.056723000	1	1.252796000	1.469372000	0.068224000
8	5.736184000	-1.323702000	0.246773000	8	5.733541000	-1.281858000	0.258946000
1	5.559707000	-2.271305000	0.275893000	1	5.573211000	-2.234167000	0.275720000
5l_M, optimization in gas phase B3LYP/6-311++G**, E= -949.703436941 a.u. Sum of electronic and thermal Enthalpies= -949.412308 a.u.				**5l_Mw,** optimization in solv. water B3LYP/6-311++G**, E= -949.723661233 a.u. Sum of electronic and thermal Enthalpies= -949.432602 a.u.			
0; 1				0; 1			
6	-6.860538000	0.447491000	0.080473000	6	-6.831614000	0.490277000	0.066962000
6	-6.088604000	-0.711019000	0.131648000	6	-6.080011000	-0.684131000	0.117112000
6	-6.271259000	1.717312000	-0.020713000	6	-6.217177000	1.750355000	-0.015883000
1	-6.542585000	-1.691618000	0.209820000	1	-6.558425000	-1.654834000	0.181114000
6	-4.700097000	-0.579501000	0.079487000	6	-4.687541000	-0.577256000	0.082596000
6	-4.885257000	1.869851000	-0.073919000	6	-4.826403000	1.877238000	-0.051399000
1	-4.431352000	2.851191000	-0.152233000	1	-4.350218000	2.848520000	-0.115701000
6	-4.123736000	0.709243000	-0.022175000	6	-4.086301000	0.702024000	-0.000926000
6	-2.590006000	-0.878672000	0.034044000	6	-2.573339000	-0.907956000	0.056886000

7	-3.708005000	-1.553923000	0.112392000	7	-3.711254000	-1.568494000	0.117046000
7	-2.750402000	0.479157000	-0.049523000	7	-2.719107000	0.450037000	-0.015207000
1	-1.997106000	1.144297000	-0.115285000	1	-1.959486000	1.111867000	-0.069139000
7	-1.345764000	-1.457160000	0.031195000	7	-1.341184000	-1.497468000	0.065635000
7	-0.233121000	-0.697365000	-0.033090000	7	-0.225400000	-0.733426000	-0.012722000
6	0.907376000	-1.288411000	-0.018443000	6	0.911714000	-1.330746000	-0.019224000
1	0.966803000	-2.381123000	0.045639000	1	0.973696000	-2.421368000	0.034823000
1	-1.307820000	-2.469271000	0.102661000	1	-1.296145000	-2.511304000	0.107404000
1	-6.903174000	2.597043000	-0.058593000	1	-6.831858000	2.642308000	-0.053401000
6	2.173134000	-0.563484000	-0.084166000	6	2.174731000	-0.597677000	-0.097876000
6	2.245303000	0.834152000	-0.175324000	6	2.237211000	0.802612000	-0.170313000
6	3.369576000	-1.295438000	-0.058075000	6	3.370464000	-1.331776000	-0.104232000
6	3.480429000	1.463402000	-0.225149000	6	3.470383000	1.437535000	-0.236870000
6	4.608601000	-0.664568000	-0.123682000	6	4.606343000	-0.693768000	-0.180887000
6	4.673173000	0.737743000	-0.193086000	6	4.660791000	0.709231000	-0.238311000
1	-7.941106000	0.369032000	0.119124000	1	-7.913880000	0.430253000	0.092225000
8	5.854513000	1.415535000	-0.316473000	8	5.857298000	1.372126000	-0.369844000
6	6.788593000	1.303098000	0.767362000	6	6.693774000	1.386846000	0.803011000
1	6.333144000	1.656205000	1.698775000	1	6.181587000	1.894715000	1.625570000
1	7.137096000	0.276466000	0.887940000	1	6.967514000	0.373406000	1.101747000
1	7.625195000	1.949275000	0.505041000	1	7.588356000	1.944396000	0.529701000
1	3.334345000	-2.380775000	-0.001410000	1	3.338005000	-2.416357000	-0.060234000
1	3.552968000	2.542282000	-0.297331000	1	3.534414000	2.518209000	-0.292343000
1	1.333422000	1.415853000	-0.201569000	1	1.324213000	1.383695000	-0.170042000
8	5.787509000	-1.362217000	-0.137649000	8	5.789782000	-1.376476000	-0.216654000
1	5.604898000	-2.307549000	-0.126112000	1	5.625215000	-2.326082000	-0.169023000

•OCH_3, optimization in gas phase UB3LYP/6-311++G**, E= -115.092242725 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.013156 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -115.0304048 a.u.	•OCH_3, optimization in solv. water UB3LYP/6-311++G**, E= -115.096964810 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.012967 a.u. SP at UM06-2X/6-311++G** (water), E = -115.0348749 a.u.
0; 2 O,0,-0.542701254,1.1647992475,-0.7684676273 C,0,-0.542701254,-0.0546902007,-0.1535274307 H,0,-1.4535259344,-0.6392046442,-0.3494952988 H,0,0.3681234264,-0.6392046442,-0.3494952988 H,0,-0.542701254,0.1683002417,0.9336731406	0; 2 O,0,-0.542701254,1.1647009955,-0.7699088199 C,0,-0.542701254,-0.0562420061,-0.154940791 H,0,-1.4547521288,-0.6372187769,-0.3480744033 H,0,0.3693496208,-0.6372187769,-0.3480744033 H,0,-0.542701254,0.1659785644,0.9336859026

•OCH_3, optimization in solv. benzene UB3LYP/6-311++G**, E= -115.094393078 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.013101 a.u. SP at UM06-2X/6-311++G** (benzene), E = -115.0324574 a.u.	•OOH, optimization in gas phase UB3LYP/6-311++G**, E= -150.958068504 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = -0.008105 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -150.8901994 a.u.
0; 2 O,0,-0.542701254,1.1645078135,-0.7689092564 C,0,-0.542701254,-0.0559561974,-0.153989909 H,0,-1.4542696344,-0.6380800889,-0.349026855 H,0,0.3688671264,-0.6380800889,-0.3490268551 H,0,-0.542701254,0.1676085617,0.9336403605	0; 2 O,0,-0.306139169,1.1388043421,-2.1424755632 O,0,-0.306139169,-0.0270805258,-1.5060352389 H,0,-0.306139169,0.1884605977,-0.5528209269

•OOH, optimization in solv. water UB3LYP/6-311++G**, E= -150.964780698 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = -0.008053 a.u. SP at UM06-2X/6-311++G** (water), E = -150.8969992 a.u.	•OOH, optimization in solv. benzene UB3LYP/6-311++G**, E= -150.961129474 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = -0.008069 a.u. SP at UM06-2X/6-311++G** (benzene), E = -150.8933064 a.u.
0; 2 O,0,-0.306139,1.1379239837,-2.1444397586 O,0,-0.306139,-0.0237597154,-1.5065192542 H,0,-0.306139,0.1860197317,-0.5503729872	0; 2 O,0,-0.306139,1.1383564014,-2.1432686227 O,0,-0.306139,-0.0255806399,-1.50619998 H,0,-0.306139,0.1874082384,-0.5518633973

•$OOCH_3$, optimization in gas phase UB3LYP/6-311++G**, E= -190.278586116 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.016992 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -190.1876185 a.u.	•$OOCH_3$, optimization in solv. water UB3LYP/6-311++G**, E= -190.284326005 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.016975 a.u. SP at UM06-2X/6-311++G** (water), E = -190.1932773 a.u.
0; 2 O,0,-0.6287934329,0.9734939662,-2.2828435942 O,0,-0.0261013982,0.1151060603,-1.48545576 C,0,-0.2603648628,0.4264572346,-0.0888044033 H,0,0.2785957037,-0.3368319596,0.4708498691 H,0,0.1310086065,1.4215918002,0.1237133536 H,0,-1.3311786562,0.3795584683,0.1107204548	0; 2 O,0,-0.6250065868,0.9717067375,-2.2914105693 O,0,-0.027489238,0.1189456043,-1.4862760211 C,0,-0.2622260287,0.4281603262,-0.0827591648 H,0,0.2801712921,-0.3365914913,0.4692502908 H,0,0.1302631174,1.4224474636,0.1267339751 H,0,-1.332546596,0.3747069296,0.1126414093

•$OOCH_3$, optimization in solv. benzene UB3LYP/6-311++G**, E= -190.281233643 a.u.	

Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.017005 a.u. SP at UM06-2X/6-311++G** (benzene), E = -190.1902317 a.u.	
0; 2 O,0,-0.6284086333,0.971514086,-2.2872628741 O,0,-0.0258190063,0.1177872607,-1.4861079328 C,0,-0.2611078928,0.4275051996,-0.0854612127 H,0,0.279045421,-0.3372566968,0.4700466162 H,0,0.1313524153,1.4218784278,0.1261972282 H,0,-1.3318963439,0.3779472926,0.1107680951	

CH_3OH, optimization in gas phase B3LYP/6-311++G**, E= -115.765000516 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.028256 a.u. SP at M06-2X/6-311++G** (gas phase), E = -115.7042429 a.u.	**CH_3OH,** optimization in solv. water B3LYP/6-311++G**, E= -115.770994501 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.028208 a.u. SP at M06-2X/6-311++G** (water), E = -115.710319 a.u.
0; 1 C,0,-0.5427011111,-0.0404122452,-0.1311789776 H,0,-1.4355853596,-0.6313198453,-0.3696508423 H,0,0.3501828757,-0.6313203446,-0.3696505627 H,0,-0.5427012085,0.1667074575,0.9391595874 O,0,-0.5427006807,1.2209524696,-0.792318007 H,0,-0.5426993458,1.0735888879,-1.7422916478	0; 1 C,0,-0.5427011139,-0.0417572885,-0.1269825989 H,0,-1.4344450825,-0.6280011846,-0.3726430335 H,0,0.3490426038,-0.6280016675,-0.372642766 H,0,-0.5427012125,0.1632030739,0.9436275165 O,0,-0.5427006851,1.224581695,-0.793618674 H,0,-0.54269934,1.0681717516,-1.7436708941

CH_3OH, optimization in solv.benzene B3LYP/6-311++G**, E= -115.767636667 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.028212 a.u. SP at M06-2X/6-311++G** (gas phase), E = -115.706921 a.u.	**H_2O_2,** optimization in gas phase B3LYP/6-311++G**, E= -151.602167214 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.004783 a.u. SP at M06-2X/6-311++G** (gas phase), E = -151.5348367 a.u.
0; 1 C,0,-0.5427011152,-0.0410652154,-0.1293715439 H,0,-1.4352155203,-0.6298000895,-0.3708595429 H,0,0.3498130337,-0.6298005749,-0.3708592807 H,0,-0.542701206,0.1650601607,0.9410611871 O,0,-0.5427006941,1.2224883817,-0.7929450679 H,0,-0.542699328,1.0713137173,-1.7429562016	0; 1 O,0,1.1977831272,0.6138362017,0.2166830546 H,0,2.0532615739,0.7290136674,-0.2195686027 O,0,0.7145279581,1.9851163877,0.2167643944 H,0,-0.1085067895,1.8814278349,-0.2805154243

H_2O_2, optimization in solv. water B3LYP/6-311++G**, E= -151.610319710 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.004694 a.u. SP at M06-2X/6-311++G** (water), E = -151.5432771 a.u.	**H_2O_2,** optimization in solv. benzene B3LYP/6-311++G**, E= -151.605785476 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.004746 a.u. SP at M06-2X/6-311++G** (benzene), E = -151.5385802 a.u.
0; 1 O,0,0.0245439665,0.7244644118,-0.2778637938 H,0,0.8043110446,0.885846646,0.2746485821 O,0,-0.0395000429,-0.7244644117,-0.2760932712 H,0,-0.7875505982,-0.885846646,0.3186562462	0; 1 O,0,1.2267234342,0.6249348576,0.223525939 H,0,2.0123763705,0.7168579489,-0.3346021732 O,0,0.7279243628,1.9890099431,0.2244850231 H,0,-0.1193597549,1.8752621127,-0.2298039112

CH_3OOH, optimization in gas phase	**CH_3OOH,** optimization in solv. water

B3LYP/6-311++G**, E= -190.919207443 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.028790 a.u. SP at M06-2X/6-311++G** (gas phase), E = -190.8290719 a.u.	B3LYP/6-311++G**, E= -190.925863161 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.029054 a.u. SP at M06-2X/6-311++G** (water), E = -190.8359915 a.u.
0; 1 O,0,0.0282667429,0.6784258573,0.0354538367 O,0,-0.048571578,-0.7782656166,-0.0247019925 H,0,-0.9585437975,-0.9110112107,0.2747217621 C,0,1.2636719094,0.979206533,0.6602844449 H,0,2.1023633772,0.5664965646,0.0913723084 H,0,1.313420543,2.0704221029,0.6502394175 H,0,1.2902321529,0.6105840694,1.690778093	0; 1 O,0,0.0347411443,0.7149521414,-0.055395327 O,0,-0.1112454623,-0.7265025134,-0.1772081846 H,0,-0.7997650422,-0.909672444,0.4807951865 C,0,1.2453046049,0.9655704905,0.6540050666 H,0,2.1025693845,0.5391182127,0.1271331243 H,0,1.3267058735,2.0544792844,0.6735356528 H,0,1.1925288472,0.5779131285,1.6752823513

CH_3OOH, optimization in solv. benzene B3LYP/6-311++G**, E= -190.922064314 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.028906 a.u. SP at M06-2X/6-311++G** (benzene), E = -190.832056 a.u.	
0; 1 O,0,0.0330058263,0.693947587,-0.0103686244 O,0,-0.0723705599,-0.7555103266,-0.1064558048 H,0,-0.8940244968,-0.9097529047,0.3820124412 C,0,1.2557790102,0.9730505219,0.6573673812 H,0,2.1054653467,0.5567104443,0.1092739027 H,0,1.3182381143,2.0635657715,0.6623768678 H,0,1.2447461093,0.5938472065,1.6839417063	

TS H10(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.49694585 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.225226 a.u. 1 imaginary frequency = 1294.5591 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.0626285 a.u.	**TS H10 (•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.52048224 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.226011 a.u. 1 imaginary frequency = 823.4067 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.0887791 a.u.
0, 2 C,0,6.8829721045,0.0412450749,0.10035088 C,0,5.9889237179,-1.0044928128,-0.0411731804 C,0,6.4442248034,1.382107242,0.2525821051 H,0,6.3218965087,-2.0284848297,-0.1589605121 C,0,4.6173012908,-0.7008904527,-0.0283915865 C,0,5.0988482421,1.70997987,0.2687202345 H,0,4.7682917334,2.73518549,0.3814460225 C,0,4.183519037,0.6587405004,0.1297677683 C,0,2.5035238727,-0.683343083,-0.0648830448 N,0,3.5328648921,-1.522303163,-0.149351397 N,0,1.2223164533,-1.1371511136,-0.1421304467 N,0,0.1853861726,-0.2959268062,-0.0638406627 C,0,-1.0068957416,-0.7768129913,-0.1484714299 H,0,-1.1795647185,-1.8500824046,-0.2946089394 H,0,1.1056226602,-2.1439912097,-0.2490554973 H,0,7.1846186351,2.1669594429,0.3561960674 C,0,-2.1718757571,0.0850137699,-0.0541686082 C,0,-3.4501774474,-0.481876443,-0.172173903 C,0,-2.0347624753,1.4720644113,0.1539635681 H,0,-3.559419222,-1.5487044625,-0.3314906292 H,0,-1.0483882595,1.9192879887,0.2484814903 C,0,-4.5837343713,0.3201586896,-0.0874981374 C,0,-3.1629595845,2.2670482705,0.2371593791 C,0,-4.4423226036,1.6871251472,0.1159172827 H,0,7.9480486148,-0.1608451011,0.0938284491 O,0,-3.0382842108,3.6066168985,0.4390563385 H,0,-3.9200653188,3.9990505755,0.4745259349 O,0,-5.4903455717,2.5661560947,0.2155587742 H,0,-6.3322028667,2.1077568248,0.1272995874 H,0,-5.5744901718,-0.1140064203,-0.1790383093 N,0,2.8147242609,0.639738603,0.1022738662 H,0,2.09095385,1.5243699994,0.2441622175 O,0,1.2334640589,2.5664016806,0.4427367035 C,0,1.7559526385,3.7307084781,0.9677314161 H,0,2.6723564593,3.565617933,1.5625803989 H,0,2.0311067942,4.4334690059,0.1558921263 H,0,1.0205291402,4.2581295928,1.5937286032	0, 2 C,0,6.8800720052,0.0399014841,0.0598802174 C,0,5.9815908691,-1.0094633927,-0.0469350822 C,0,6.4429661471,1.3814449105,0.181483812 H,0,6.3171047275,-2.0355035084,-0.140771084 C,0,4.6105489161,-0.7035810367,-0.0298178212 C,0,5.0938564796,1.7095418552,0.2002650562 H,0,4.7651706875,2.7372164143,0.2918818183 C,0,4.1829613316,0.654494645,0.0956933226 C,0,2.4842074363,-0.6981022525,-0.0497246977 N,0,3.5211708926,-1.5307012507,-0.1202165695 N,0,1.2028248281,-1.1464523551,-0.1003517214 N,0,0.1732970137,-0.2917228708,-0.0357542971 C,0,-1.0220332609,-0.7834738866,-0.102065134 H,0,-1.1866415035,-1.8572021103,-0.2259770399 H,0,1.0663710117,-2.1540141576,-0.1737828867 H,0,7.1821920219,2.1700141017,0.2603325939 C,0,-2.1868104132,0.0716248403,-0.0207651268 C,0,-3.4636472375,-0.5059871425,-0.1355424481 C,0,-2.0664294439,1.4650967476,0.1664921201 H,0,-3.5626304341,-1.5756927451,-0.2775147983 H,0,-1.0865513727,1.9229954247,0.2615204018 C,0,-4.6038398797,0.2862022637,-0.0732882016 C,0,-3.1992149261,2.2511732248,0.2269331211 C,0,-4.4778056165,1.6609794122,0.1048716904 H,0,7.9444795825,-0.1644430438,0.0497184844 O,0,-3.0843243341,3.5977002759,0.4076397014 H,0,-3.9685173464,3.9898691442,0.4296174321 O,0,-5.5217819197,2.5299142587,0.1786786503 H,0,-6.3682883849,2.075994066,0.0819394873 H,0,-5.5898732262,-0.1559860822,-0.1631970534 N,0,2.8076943105,0.6251613101,0.0779338087 H,0,2.1414211524,1.4749717581,0.1910534043 O,0,1.2804155618,2.7217166616,0.3744313171 C,0,1.849287678,3.8084563432,1.010382389 H,0,2.6659305762,3.5285491928,1.6998045953 H,0,2.2993061327,4.503251848,0.272549851 H,0,1.1074789372,4.4000786524,1.571322687

TS H10 (•OCH_3), optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.50622653 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.225292 a.u. 1 imaginary frequency = 1191.1177 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1025.0712722 a.u.	**TS H24(•OCH_3),** optimization in gas phase UB3LYP/6-311++G**, E= -1025.50769495 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228393 a.u. 1 imaginary frequency = 173.0861 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.0789289 a.u.
0, 2 C,0,6.881790599,0.0437599597,0.0923535591	0, 2 C,0,6.3936622592,0.1118391658,0.1425366473

C,0,5.9867495325,-1.0036061884,-0.0376102195	C,0,5.5736061888,-0.9941872707,-0.0416977722
C,0,6.44309891,1.3854974036,0.2299705097	C,0,5.8608648287,1.408176135,0.2711869559
H,0,6.3213848009,-2.0284764513,-0.1439663453	H,0,5.9799643219,-1.9931488831,-0.1436554733
C,0,4.6149863766,-0.6991760686,-0.0279495775	C,0,4.1898783548,-0.7869823705,-0.0961838675
C,0,5.0965651438,1.7133944391,0.2426280343	C,0,4.4874405333,1.6394180162,0.2185454623
H,0,4.7662282769,2.7396817886,0.3446393205	H,0,4.0819693181,2.6396036727,0.3171707807
C,0,4.1826000009,0.6604708362,0.1152997939	C,0,3.6712075917,0.5288560119,0.0377156363
C,0,2.4966866691,-0.6835882909,-0.0645794592	C,0,2.0656506671,-0.9645528114,-0.2505713503
N,0,3.5291652103,-1.522260217,-0.1401480752	N,0,3.1678888779,-1.695111004,-0.2799284319
N,0,1.2157773272,-1.1349879037,-0.134354979	N,0,2.298225027,0.3761440297,-0.0620528649
N,0,0.1819610292,-0.2880059187,-0.0634260098	H,0,1.5728626545,1.0732577476,-0.0068572809
C,0,-1.0112999919,-0.7738728972,-0.1396039704	N,0,-0.2257183482,-0.6086583669,-0.2718779611
H,0,-1.1807272507,-1.8477709207,-0.2745989254	C,0,-1.4027525397,-1.1309464288,-0.182269831
H,0,1.0905529852,-2.1423859491,-0.2264932729	H,0,-1.526481573,-2.2152634203,-0.1501720074
H,0,7.1829450158,2.1718490186,0.3252347448	H,0,6.533289572,2.2460502604,0.414134006
C,0,-2.1764976942,0.0848998941,-0.0508229298	C,0,-2.6066440012,-0.3187208837,-0.0977938105
C,0,-3.4536869989,-0.4881609473,-0.1638807729	C,0,-3.8420047804,-0.9639947745,0.0598604889
C,0,-2.0466423402,1.4751019117,0.1463518702	C,0,-2.5725992252,1.0855480326,-0.1726580612
H,0,-3.5578212172,-1.5566572895,-0.3139212226	H,0,-3.8815143859,-2.0454614492,0.1178209571
H,0,-1.0628844312,1.9277357464,0.2377316804	H,0,-1.6321242013,1.6047328834,-0.3010400059
C,0,-4.590680664,0.308759045,-0.0867556987	C,0,-5.0193291319,-0.2258383088,0.1459778157
C,0,-3.1778317337,2.2651176396,0.2221457716	C,0,-3.7393174808,1.8219411918,-0.0868152819
C,0,-4.4563197553,1.6792513864,0.1045131406	C,0,-4.9713786043,1.1598436284,0.0737133428
H,0,7.9467003415,-0.1589719414,0.0880607034	H,0,7.4683271964,-0.0218378548,0.1878751237
O,0,-3.0590650522,3.6079186537,0.4138181759	O,0,-3.6918439491,3.1808608943,-0.1597972191
H,0,-3.9423571675,3.9990150959,0.4441927879	H,0,-4.5912218011,3.5264449493,-0.0899479217
O,0,-5.504395664,2.5523713482,0.1952217304	O,0,-6.0675256005,1.9822175702,0.1469845017
H,0,-6.3474777982,2.0939929497,0.1056282333	H,0,-6.8752701641,1.4684581235,0.2480298833
H,0,-5.579551911,-0.1293630278,-0.1737092248	H,0,-5.973847668,-0.7279293169,0.2699646833
N,0,2.8121204641,0.6393191606,0.0872886286	N,0,0.8130986699,-1.4712790972,-0.4024627706
H,0,2.1060209257,1.5175225641,0.2219290659	H,0,0.6756915949,-2.531721372,-0.2908868787
O,0,1.2546173952,2.6081754556,0.4192867402	O,0,0.4054948686,-3.8817313393,0.3300487855
C,0,1.793034581,3.7351387549,1.00857314	C,0,1.5036202863,-4.5744328197,0.7894712696
H,0,2.6796008094,3.5177691351,1.6311579976	H,0,1.3334270049,-5.0490815756,1.7652717991
H,0,2.1240237922,4.4592204301,0.2372461325	H,0,1.8014511771,-5.3468602759,0.0561903932
H,0,1.0525884835,4.2653443946,1.6272709221	H,0,2.3825383813,-3.9028863494,0.8477321375

TS H24 (•OCH_3), optimization in solv.water UB3LYP/6-311++G**, E= -1025.52509441 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.225579 a.u. 1 imaginary frequency = 121.2110 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.0804992 a.u.	**TS H22 (•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.52826868 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.224340 a.u. 1 imaginary frequency = 323.9673 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.1065882 a.u.
0, 2	0, 2
C,0,6.4457321943,0.394779433,0.0091904311	C,0,6.4734441426,0.3168289926,-0.0297277599
C,0,5.6497749987,-0.7414649875,0.1347864372	C,0,5.6669176672,-0.8124832072,0.0945582794
C,0,5.8805907825,1.6742759164,-0.1390302347	C,0,5.9204307247,1.600887333,-0.1803258559
H,0,6.0879711773,-1.7262901972,0.2490238504	H,0,6.0959346437,-1.8010885319,0.2104826524
C,0,4.2602515228,-0.5787912397,0.1097005365	C,0,4.2798041971,-0.6367072528,0.0657821551
C,0,4.4971941934,1.8585746903,-0.1659781984	C,0,4.5387125887,1.7974702649,-0.2111661104
H,0,4.0610560705,2.8438072528,-0.2799994526	H,0,4.1113309539,2.7862615189,-0.3270248153
C,0,3.7092828063,0.7201151534,-0.0403298555	C,0,3.7412487794,0.6659656609,-0.0865650974
C,0,2.1326999941,-0.8207168398,0.1284421715	C,0,2.1530481508,-0.8584844346,0.078174425
N,0,3.2506836496,-1.5221029533,0.213667475	N,0,3.258993282,-1.5718170295,0.1662860068

N,0,2.3366109105,0.5252713156,-0.0240055321	N,0,2.3647880082,0.4835975513,-0.0742860671
H,0,1.6032090478,1.213597551,-0.1033094355	H,0,1.639029168,1.1797450507,-0.1568212974
N,0,-0.1840562243,-0.5266113566,0.0989118165	N,0,0.8968985183,-1.3868918101,0.1313149769
C,0,-1.3549697697,-1.0649339207,0.1335356714	N,0,-0.1820595648,-0.5794550402,0.034264367
H,0,-1.4723812422,-2.1473775463,0.2190467852	C,0,-1.34700666,-1.1294499584,0.0876726828
H,0,6.5316110514,2.5355353208,-0.2343134552	H,0,-1.4508149244,-2.2115205203,0.2067933206
C,0,-2.5751380739,-0.2734142797,0.063540875	H,0,0.8082355877,-2.3932036007,0.244215615
C,0,-3.8103963582,-0.9378995546,0.0982431627	H,0,6.579232453,2.4563122733,-0.2743537649
C,0,-2.556871146,1.1310367982,-0.0343852044	C,0,-2.5740221363,-0.3562437783,-0.0053611336
H,0,-3.8398771319,-2.0187016132,0.1726367528	C,0,-3.8042275947,-1.036178014,0.0659188516
H,0,-1.616610861,1.6670851367,-0.0620757975	C,0,-2.5699280947,1.0427344537,-0.1639448757
C,0,-5.0042120163,-0.2229808047,0.0376520858	H,0,-3.815643222,-2.1132229017,0.1866801141
C,0,-3.740357787,1.8429809586,-0.0941027379	H,0,-1.6315910092,1.5799223386,-0.2215057851
C,0,-4.9748517887,1.1632354817,-0.0568426375	C,0,-5.0056362898,-0.3427006836,-0.0168906
H,0,7.5249521251,0.2933407067,0.02553286	C,0,-3.765227144,1.7387022021,-0.2472580264
O,0,-3.7094159317,3.2048051123,-0.1875378045	C,0,-4.9942692891,1.0400449875,-0.1726738771
H,0,-4.6177079864,3.5372200964,-0.2091640427	H,0,7.5516173276,0.2055140963,-0.010424075
O,0,-6.0794939365,1.9645172864,-0.1200876878	O,0,-6.160855318,1.7272972316,-0.2537863373
H,0,-6.8922687074,1.4472341343,-0.0657891343	H,0,-5.9478377568,2.6679213392,-0.3566484012
H,0,-5.9565554965,-0.7411334457,0.0640428684	H,0,-5.9560731581,-0.8595906698,0.037885641
N,0,0.8846948364,-1.3596187043,0.1825115527	O,0,-3.8779656717,3.0784635826,-0.3999672389
H,0,0.7806763522,-2.3843602762,0.2951402111	H,0,-2.9896775596,3.5397792305,-0.4427174516
O,0,0.3979790677,-4.0940072916,0.4788555367	O,0,-1.5752233695,4.2942064276,-0.4959735097
C,0,1.3312979939,-5.0989415308,0.5410878321	C,0,-1.5237224171,5.6519083127,-0.7101641905
H,0,0.9396127695,-6.0572374889,0.1721057356	H,0,-0.7915025847,6.1246931534,-0.0359031237
H,0,2.2792570342,-4.8370523186,0.0504429149	H,0,-1.1171601161,5.8253249268,-1.7263404732
H,0,1.5701916595,-5.2585746751,1.6132322882	H,0,-2.4984433121,6.150095505,-0.6383102205

TS H23 (•OCH_3), optimization in solv. water UB3LYP/6-311++G**, E= -1025.52844593 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.224829 a.u. 1 imaginary frequency = 321.3565 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.1069931 a.u.	**TS H25(•OCH_3),** optimization in gas phase UB3LYP/6-311++G**, E= -1025.48772589 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.226004 a.u. 1 imaginary frequency = 1532.1620 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.0621222 a.u.
0, 2	0, 2
C,0,6.3111788419,0.4868061672,0.1851373495	C,0,6.2892636226,0.4230871483,-0.0555373797
C,0,5.6056277826,-0.6222163865,-0.2798378251	C,0,5.5355895659,-0.6916617175,-0.4114580474
C,0,5.6482242886,1.627928243,0.6678444713	C,0,5.6811614166,1.6054693361,0.3976456717
H,0,6.1201833964,-1.500905944,-0.6515286596	H,0,6.0021245834,-1.6048303241,-0.7608149103
C,0,4.2089703276,-0.5721553046,-0.2545045807	C,0,4.1452854931,-0.6067906645,-0.3064578437
C,0,4.2538168175,1.6972233348,0.7009022641	C,0,4.2948688038,1.7111910644,0.5095954133
H,0,3.7413591971,2.5763967677,1.0728276795	H,0,3.8279155047,2.624763233,0.8593853334
C,0,3.5586043433,0.5874803381,0.2354427291	C,0,3.5501154455,0.5936917985,0.1529046108
C,0,2.1089203801,-0.9503371984,-0.4070791001	C,0,2.0423327372,-0.9516213326,-0.3148735281
N,0,3.2727351452,-1.5197868476,-0.6502740057	N,0,3.1715523362,-1.5528507284,-0.5944833475
N,0,2.2024515414,0.307449429,0.121527622	N,0,2.1831152608,0.337388876,0.1340788658
H,0,1.4177920262,0.8910793819,0.3698918699	H,0,1.4240754238,0.9413937945,0.4058968217
N,0,0.9025311352,-1.5398063897,-0.649435553	N,0,0.8093619989,-1.5315892412,-0.4584854246
N,0,-0.2443482381,-0.8793146354,-0.3668479753	N,0,-0.3018614886,-0.8471735997,-0.1336317938
C,0,-1.3556373947,-1.4874870373,-0.6000475724	H,0,0.7355215449,-2.5241489448,-0.6947265688
H,0,-1.3636932192,-2.5020105784,-1.0080910695	H,0,6.3004191738,2.453522538,0.6660476921
H,0,0.9001977288,-2.4792456703,-1.0367878602	C,0,-2.7219139723,-0.8282641583,-0.0082413716
H,0,6.2290179368,2.4717606412,1.0219030583	C,0,-3.8170670493,-1.5477123139,0.4965417502
C,0,-2.6492286427,-0.8742630322,-0.340962137	C,0,-2.9191559894,0.4828436623,-0.4841695226

C,0,-3.812778169,-1.6120126184,-0.619397269	H,0,-3.6732789501,-2.558624101,0.8578331155
C,0,-2.7741006951,0.4286310407,0.1778367742	H,0,-2.0919707181,1.0477039369,-0.8943761588
H,0,-3.7290931488,-2.6168502342,-1.0175960486	C,0,-5.0783377311,-0.9640925813,0.5457828388
H,0,-1.8936919607,1.0181285466,0.4007586473	C,0,-4.1716809265,1.0678949467,-0.4278578118
C,0,-5.0730482571,-1.0707145197,-0.389479837	C,0,-5.2571305871,0.3366935184,0.0892994675
C,0,-4.0248460671,0.9685898201,0.4068395851	H,0,7.3700240994,0.3808156803,-0.128410285
C,0,-5.1923903268,0.2209291739,0.1233067664	O,0,-4.3472607913,2.3396862438,-0.8789934061
H,0,7.3951536673,0.4702114246,0.1749701025	H,0,-5.2758769575,2.5830527262,-0.7704257811
O,0,-4.1430880888,2.2311440699,0.9087898745	O,0,-6.4553006901,1.0027056193,0.0929776737
H,0,-5.0864795001,2.4327250952,0.9964275263	H,0,-7.1558555703,0.4487408021,0.4524137652
H,0,-5.967173142,-1.6437600211,-0.6053099756	H,0,-5.9241352101,-1.5177414994,0.9414642982
O,0,-6.3589459274,0.8477884684,0.3841027977	C,0,-1.4176148516,-1.4617626253,-0.0409437921
H,0,-7.1638502578,0.3048900969,0.1540624433	H,0,-1.3221330804,-2.7476555772,-0.1460871681
O,0,-8.5325395821,-0.4898877573,-0.2129172873	O,0,-0.9116811114,-3.8616642422,-0.5324559513
C,0,-9.7519008045,0.0342407233,0.1424908097	C,0,-1.6335118324,-4.2930125161,-1.6611937205
H,0,-9.7122380581,1.0937587725,0.4223958791	H,0,-1.3050039334,-5.3175856079,-1.8762552936
H,0,-10.505241,-0.1513622614,-0.6373690993	H,0,-2.7172354237,-4.3185841683,-1.484810908
H,0,-10.1086930761,-0.5377890984,1.0234946057	H,0,-1.4312581459,-3.6868059811,-2.5551773033

TS H25 (•OCH_3), optimization in solv. water UB3LYP/6-311++G**, E= -1025.50823718 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.225738 a.u. 1 imaginary frequency = 1470.0196 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.0829009 a.u.	**TS H25 (•OCH_3),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.49640801 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.226106 a.u. 1 imaginary frequency = 1510.4232 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1025.0711391 a.u.
0, 2	0, 2
C,0,6.2998685633,0.3921038748,-0.0499264093	C,0,6.2937787388,0.4119458539,-0.0526781525
C,0,5.5353056008,-0.7117331847,-0.4231268621	C,0,5.5371769756,-0.7003830671,-0.4130647336
C,0,5.701179594,1.5740430588,0.4197979322	C,0,5.6879813362,1.5942469066,0.4046477953
H,0,5.9996626969,-1.6219691684,-0.7846958407	H,0,6.0042249706,-1.6123844333,-0.7654282564
C,0,4.1447114459,-0.6141532005,-0.3185309246	C,0,4.1466940247,-0.6123391429,-0.3083534062
C,0,4.3147595689,1.6908575399,0.5315329262	C,0,4.3013828802,1.7024563026,0.5162549806
H,0,3.8519417973,2.6010941542,0.8936027773	H,0,3.8350030891,2.6148891601,0.8692273754
C,0,3.559928283,0.5849986624,0.1570300072	C,0,3.5541321285,0.5877819315,0.1548463383
C,0,2.030010131,-0.9301963383,-0.3315782505	C,0,2.0392793343,-0.9487084448,-0.3177359166
N,0,3.1579868525,-1.5452642824,-0.6201125573	N,0,3.1688287189,-1.5545082874,-0.5996042284
N,0,2.1917993285,0.3450503787,0.1353360658	N,0,2.1869412254,0.3362508297,0.1354426658
H,0,1.4455525345,0.9685600833,0.4050466022	H,0,1.4324938557,0.947481752,0.4066003742
N,0,0.7946674103,-1.4933393008,-0.4883075136	N,0,0.8055687756,-1.522926918,-0.4660121053
N,0,-0.3125389272,-0.8119505294,-0.1321404511	N,0,-0.3044184603,-0.8372925255,-0.1317386057
H,0,0.7062201511,-2.4785742199,-0.7499079977	H,0,0.7267984663,-2.5144396445,-0.7043312395
H,0,6.3276509977,2.4124873656,0.7013320145	H,0,6.3089156757,2.4399570407,0.6766410489
C,0,-2.7310739051,-0.8175629916,-0.0024568996	C,0,-2.724880466,-0.8251319871,-0.0015925022
C,0,-3.815936317,-1.5358062866,0.5305386011	C,0,-3.8126337631,-1.5394947459,0.5273687027
C,0,-2.9454910184,0.4817240259,-0.5090267162	C,0,-2.9317567663,0.476488582,-0.5010444874
H,0,-3.663001468,-2.5387950755,0.9093823045	H,0,-3.662760501,-2.5433925295,0.9052216826
H,0,-2.1266257794,1.0437667189,-0.9401433744	H,0,-2.1105680043,1.0364743315,-0.9299047236
C,0,-5.0815814911,-0.9647852892,0.5824261903	C,0,-5.0756579543,-0.9607355334,0.5788523435
C,0,-4.2028929698,1.0524370636,-0.4530013451	C,0,-4.1864855781,1.0555186556,-0.4446742664
C,0,-5.2796524819,0.3244330258,0.0950868759	C,0,-5.2656131128,0.3301800919,0.0967466025
H,0,7.380289851,0.3401246798,-0.1224055205	H,0,7.3744875353,0.3669825091,-0.125435319
O,0,-4.3990121119,2.3130487742,-0.9334850921	O,0,-4.373136513,2.318267402,-0.919580241
H,0,-5.3294172144,2.552372191,-0.8181996495	H,0,-5.3027692378,2.5595682217,-0.8093592214
O,0,-6.4745011497,0.9766314223,0.0944664815	O,0,-6.463105298,0.9894460417,0.0964143529

H,0,-7.1773075751,0.4292815228,0.4663854021	H,0,-7.1663607683,0.4360280809,0.4544054069
H,0,-5.9175356289,-1.5152309449,0.9994244232	H,0,-5.9145935011,-1.5085966485,0.9953162007
C,0,-1.4243723791,-1.4366928775,-0.0406890124	C,0,-1.4193432503,-1.4530533571,-0.0388135687
H,0,-1.3122444652,-2.7137395412,-0.1433429938	H,0,-1.3235014186,-2.7346429567,-0.1421412459
O,0,-0.8837863644,-3.8496353088,-0.5141113058	O,0,-0.9171774209,-3.8617444482,-0.5220628009
C,0,-1.5969123746,-4.2769440146,-1.656064479	C,0,-1.6199152303,-4.2712447423,-1.6734424169
H,0,-1.2583038739,-5.2942232694,-1.8894627082	H,0,-1.2978524232,-5.2960550861,-1.896751665
H,0,-2.6797152011,-4.3142497259,-1.4827987581	H,0,-2.7067301143,-4.286406285,-1.5195317591
H,0,-1.3961711106,-3.6516949925,-2.5358729427	H,0,-1.390966949,-3.6540089102,-2.5527040083

TS H10 (•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.35229195 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.203186 a.u. 1 imaginary frequency = 1735.8365 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9128108 a.u.	**TS H10 (•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.37860937 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.202645 a.u. 1 imaginary frequency = 1547.4211 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9439811 a.u.
0, 2 C,0,6.930512194,-0.1170615069,-0.0314622155 C,0,6.0099208514,-1.1438894225,-0.1132745738 C,0,6.5310307746,1.2434637793,0.0941002049 H,0,6.3148626439,-2.1788319096,-0.2090291666 C,0,4.6459305045,-0.8033943384,-0.0679275581 C,0,5.1992749712,1.6105066303,0.1416229087 H,0,4.885903516,2.6426803289,0.2373708561 C,0,4.2532543152,0.5774345132,0.0604076062 C,0,2.5374556303,-0.7119127657,-0.0344409312 N,0,3.5371762828,-1.5928896816,-0.1258562357 N,0,1.2413888117,-1.1229986849,-0.0552930477 N,0,0.2308383293,-0.2469498839,0.0413282259 C,0,-0.9732911703,-0.7043945957,0.0140523113 H,0,-1.1682995025,-1.7789392457,-0.0861151741 H,0,1.0852384636,-2.1258849376,-0.1449906245 H,0,7.2974345749,2.0077663288,0.1536168663 C,0,-2.1261137005,0.1741185906,0.1146416634 C,0,-3.4113713431,-0.3870555743,0.0749197579 C,0,-1.9771830355,1.5679873349,0.2511970402 H,0,-3.5329011428,-1.4592722985,-0.0294935767 H,0,-0.9900138621,2.0167387807,0.2827525308 C,0,-4.5368722072,0.4257201719,0.1694503472 C,0,-3.0960299774,2.3746712963,0.345760657 C,0,-4.3818541196,1.7993067774,0.3043544274 H,0,7.9898757092,-0.3456633646,-0.0633801341 O,0,-2.9538938713,3.72142444,0.4785381275 H,0,-3.8309559604,4.1225139742,0.5321841708 O,0,-5.419844073,2.6899141459,0.405986697 H,0,-6.2674983698,2.234844408,0.3736051728 H,0,-5.5322730534,-0.0062579794,0.1388062914 N,0,2.8902974766,0.6034462473,0.0791059411 H,0,2.1517698573,1.5651456875,0.1803649009 O,0,1.3967600576,2.574976622,0.2897089364 O,0,2.321757334,3.6431305426,0.3735586773 H,0,1.7355871814,4.4064308296,0.4684529995	0, 2 C,0,6.9281323858,-0.1254369955,-0.036639867 C,0,6.0000907156,-1.1461180748,-0.1247027696 C,0,6.5345895666,1.2330282285,0.1047327221 H,0,6.301887767,-2.1810156938,-0.2328719227 C,0,4.6369987812,-0.7976821705,-0.0694419626 C,0,5.2012143082,1.6054747429,0.1621781928 H,0,4.8961644376,2.6387619015,0.2698072013 C,0,4.2537879563,0.5783477538,0.0738116854 C,0,2.5172248767,-0.7092962228,-0.0267092038 N,0,3.5246252394,-1.5846364436,-0.1303880442 N,0,1.2242724618,-1.1129168899,-0.0477642512 N,0,0.222408682,-0.2283480947,0.057183507 C,0,-0.9852506663,-0.6977529055,0.0191314091 H,0,-1.169167415,-1.7690807988,-0.0953791936 H,0,1.0516447208,-2.1132420211,-0.1496541933 H,0,7.3028876809,1.9946950624,0.1692712635 C,0,-2.1354385438,0.1700595164,0.1232007242 C,0,-3.4198689681,-0.4011714721,0.06755476 C,0,-2.0006188839,1.5665532906,0.2754432317 H,0,-3.5301753254,-1.4727496081,-0.048900599 H,0,-1.0175416545,2.0220618611,0.3185401614 C,0,-4.5513982426,0.3990543525,0.1592515374 C,0,-3.1244315123,2.3615249893,0.3671987623 C,0,-4.4103982235,1.776346624,0.307220969 H,0,7.9857273822,-0.3592335255,-0.0756830426 O,0,-2.9942330852,3.7096442286,0.5144853278 H,0,-3.8739883828,4.1101298119,0.5574508943 O,0,-5.4444011522,2.6522213657,0.4041511828 H,0,-6.2973718615,2.2036578851,0.3444614941 H,0,-5.5427828115,-0.0377805766,0.1157917497 N,0,2.8848639651,0.5998776047,0.0999577301 H,0,2.2134233824,1.5110698193,0.1844429144 O,0,1.4403576211,2.6754026729,0.2761426169 O,0,2.4442777226,3.6964778205,0.3733146323 H,0,1.9203620749,4.5088969615,0.3380343799

TS H10 (•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.36282196 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.203087 a.u. 1 imaginary frequency = 1749.0927 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9260779 a.u.	**TS H24 (•OOH),** optimization in gas phase UB3LYP/6-311++G**, E= -1061.36127939 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.205130 a.u. 1 imaginary frequency = 2122.3876 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9246629 a.u.
0, 2 C,0,6.9323140331,-0.1251373173,-0.029568532 C,0,6.0076011393,-1.1488212415,-0.1111796752 C,0,6.5368754005,1.2358503362,0.0958225501 H,0,6.3107022613,-2.1844350694,-0.2068843348 C,0,4.6442281609,-0.8033826497,-0.0658615678	0, 2 C,0,6.3141987427,-0.1567928631,0.2412294437 C,0,5.4550436816,-1.2435218165,0.1608617148 C,0,5.8314352398,1.1666012422,0.2208567967 H,0,5.8238246314,-2.2618746407,0.1737543552 C,0,4.0811078203,-0.9887334336,0.0588577458

C,0,5.205028339,1.6066680836,0.1432237869	C,0,4.4707426745,1.4445182348,0.1198685655
H,0,4.8957899053,2.6400059618,0.238946474	H,0,4.1044544865,2.464198879,0.1052376732
C,0,4.2566039463,0.576883862,0.061974188	C,0,3.6114230408,0.3534252707,0.0453290968
C,0,2.5313761407,-0.7074685239,-0.0329404633	C,0,1.9410028866,-1.0925512873,-0.1168281148
N,0,3.532725296,-1.5900263697,-0.1238767795	N,0,3.0243131431,-1.8620759913,-0.0533024128
N,0,1.2360214221,-1.1132022594,-0.054177458	N,0,2.2361865792,0.2464320368,-0.0567728231
N,0,0.2290418436,-0.2318108009,0.0428884318	H,0,1.5409195382,0.9753834299,-0.0880062994
C,0,-0.9757502118,-0.6943244134,0.0120847983	N,0,-0.3143030587,-0.7035981868,-0.1675040702
H,0,-1.1655924277,-1.7681030352,-0.0918198734	C,0,-1.5018608928,-1.1851821727,0.0100411194
H,0,1.0710753737,-2.1151145418,-0.1430666836	H,0,-1.6387654836,-2.2575740573,0.1710391352
H,0,7.3049722446,1.9983494241,0.1553515748	H,0,6.5355380469,1.9877612142,0.2866230993
C,0,-2.1299304409,0.1780202215,0.1135168544	C,0,-2.6914827416,-0.3535466711,0.0166415766
C,0,-3.4128655328,-0.3911671417,0.0705508463	C,0,-3.9347651509,-0.9594698624,0.2555131237
C,0,-1.9907621754,1.5733459888,0.2548954796	C,0,-2.6384653044,1.0338460291,-0.2142036258
H,0,-3.5268860415,-1.4636478802,-0.0376528463	H,0,-3.9888169272,-2.0270167692,0.4340414906
H,0,-1.0067887784,2.0283885191,0.2885361603	H,0,-1.6915625277,1.5216580787,-0.4034273982
C,0,-4.543434698,0.4130558599,0.1666204731	C,0,-5.1004875765,-0.1997770173,0.2659777669
C,0,-3.1144115441,2.3716958336,0.3512326542	C,0,-3.7939172809,1.7917545045,-0.2034011331
C,0,-4.3982317187,1.7884024498,0.3064677657	C,0,-5.0338608126,1.1688389236,0.0384618331
H,0,7.9907681497,-0.3574246947,-0.0615895989	H,0,7.3818236252,-0.3252890343,0.3202060624
O,0,-2.9810664637,3.7196783372,0.4892228317	O,0,-3.7284233065,3.1327738212,-0.4261623935
H,0,-3.8603368825,4.1174573875,0.5432242163	H,0,-4.6217347529,3.498559508,-0.3877497505
O,0,-5.4382201054,2.6693399218,0.4095465249	O,0,-6.116692057,2.0093979539,0.027831352
H,0,-6.2863689018,2.2128183129,0.3742610731	H,0,-6.9310312942,1.5236486739,0.1945188785
H,0,-5.5359167553,-0.0240536408,0.1339843677	H,0,-6.0607882213,-0.6706870401,0.4515254001
N,0,2.8919289636,0.6051057015,0.0803519253	N,0,0.6899008555,-1.6074791353,-0.2325939217
H,0,2.1752848361,1.5576561417,0.1762818506	H,0,0.6382993984,-2.7189850284,0.3206120411
O,0,1.4229689881,2.6057333291,0.2826761069	O,0,0.8171978432,-3.8036480712,0.8846905386
O,0,2.3733287088,3.6590739789,0.3611696688	O,0,1.7531444118,-4.41022402,0.0583440091
H,0,1.8058025253,4.4374149287,0.4504112098	H,0,2.4800538731,-3.7378531019,0.0216570647

TS H24 (•OOH), optimization in solv. water UB3LYP/6-311++G**, E= -1061.38533093 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.205314 a.u. 1 imaginary frequency = 1918.2111 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.94792 a.u.	**TS H24 (•OOH),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.37116526 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.205046 a.u. 1 imaginary frequency = 2107.4097 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.934233 a.u.
0, 2	0, 2
C,0,6.3238180221,-0.1598743383,0.204048244	C,0,6.3189739281,-0.1577706342,0.2275454584
C,0,5.464237273,-1.2474048546,0.1593726431	C,0,5.4605105763,-1.2447733153,0.1505017974
C,0,5.8394731957,1.1663386842,0.1718139434	C,0,5.8346064163,1.1666689561,0.2131506053
H,0,5.8346249445,-2.2651539112,0.1817107416	H,0,5.8302695874,-2.2628615131,0.1590263345
C,0,4.0872551777,-0.9896037242,0.0812479551	C,0,4.0851680551,-0.9889594323,0.0581013698
C,0,4.4785649003,1.4465157811,0.0938656758	C,0,4.4738275901,1.4454393034,0.1216186707
H,0,4.1098350218,2.4643321498,0.0692696791	H,0,4.1066584719,2.4646063947,0.1111503253
C,0,3.6173876818,0.3534595706,0.0538487646	C,0,3.6143573586,0.3533166605,0.0500294385
C,0,1.9458199235,-1.0842346886,-0.0469022329	C,0,1.9455147432,-1.0904836254,-0.1030505842
N,0,3.0261491111,-1.8612755584,0.0073774844	N,0,3.0280542486,-1.8620436305,-0.0491934017
N,0,2.2422421883,0.2497766204,-0.0205505309	N,0,2.2395297277,0.2468825549,-0.0441510101
H,0,1.55791468,0.9917056358,-0.0507532278	H,0,1.5479300148,0.9805483422,-0.0699392556
N,0,-0.3239692776,-0.6979950378,-0.0981265897	N,0,-0.315321432,-0.7000858946,-0.1491704337
C,0,-1.5153095347,-1.1879546537,0.0562602661	C,0,-1.5033861151,-1.1839657061,0.0277001129
H,0,-1.6564160728,-2.2591381236,0.2149179033	H,0,-1.6410819266,-2.2554450258,0.1908905463
H,0,6.5464537639,1.9866737381,0.2093576964	H,0,6.5392749909,1.9875547944,0.2761023182

C,0,-2.698526441,-0.3581498163,0.038138278	C,0,-2.6913228606,-0.3535736427,0.0290672634
C,0,-3.9513289182,-0.9684727518,0.2288810591	C,0,-3.9364886351,-0.9619032263,0.2571742709
C,0,-2.6345611483,1.0353862176,-0.1701158305	C,0,-2.6365713022,1.0352545859,-0.1992466735
H,0,-4.011117532,-2.0385845062,0.387964403	H,0,-3.9909122211,-2.0296733167,0.4338586313
H,0,-1.6802672711,1.5245349285,-0.3172631058	H,0,-1.6880736593,1.5242196182,-0.3782994251
C,0,-5.1160944405,-0.2111226712,0.2139261165	C,0,-5.1029817763,-0.2045084522,0.2576951747
C,0,-3.789629543,1.7899982214,-0.1840946265	C,0,-3.793109687,1.7902083689,-0.1986707042
C,0,-5.0416647673,1.1640770367,0.0101293577	C,0,-5.0362955867,1.1652258484,0.0301187748
H,0,7.3928885432,-0.3264135933,0.2637974355	H,0,7.3872460099,-0.3252447975,0.299220312
O,0,-3.7205320187,3.1359465777,-0.3830591368	O,0,-3.7284890391,3.1324907934,-0.4193253985
H,0,-4.6146939942,3.5050378766,-0.3624379661	H,0,-4.6229175139,3.4981715914,-0.3908569124
O,0,-6.1120738364,2.0013799219,-0.0195096673	O,0,-6.1164783195,2.0015299103,0.0080021385
H,0,-6.9391757306,1.5264693315,0.129807251	H,0,-6.9360796379,1.516338366,0.1562249095
H,0,-6.0819974296,-0.6817780828,0.3601281941	H,0,-6.0647358543,-0.6750055589,0.4338170082
N,0,0.687206704,-1.5916364741,-0.1372635612	N,0,0.6904924231,-1.6022744923,-0.2137342179
H,0,0.5984992567,-2.6375152266,0.2938702599	H,0,0.618593613,-2.6810180604,0.2972737916
O,0,0.8338231485,-3.8781171797,0.9096001972	O,0,0.8141401975,-3.8078393019,0.8989863166
O,0,1.7608690254,-4.4086437184,-0.01410869	O,0,1.734374294,-4.4093105152,0.0355302391
H,0,2.4839503946,-3.7356453812,-0.0013793834	H,0,2.4783783202,-3.7587979473,0.0266212091

TS H22 (•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.36513306 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.204108 a.u. 1 imaginary frequency = 1354.0120 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.919492 a.u.	**TS H22 (•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.38668987 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.203767 a.u. 1 imaginary frequency = 1324.9552 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9448315 a.u.
0, 2	0, 2
C,0,6.112979486,0.7864994619,0.2269048812	C,0,6.0963036225,0.7919200854,0.2821606196
C,0,5.3834678817,-0.3975939024,0.2355220049	C,0,5.3708687857,-0.3910672116,0.1901689883
C,0,5.4785884999,2.0396121555,0.1688895019	C,0,5.4558072288,2.0449047516,0.3427434508
H,0,5.869822627,-1.3645000366,0.2793941867	H,0,5.8646648126,-1.3545297793,0.1434110324
C,0,3.9894322167,-0.3107756945,0.1853330713	C,0,3.9737680908,-0.3035137013,0.1588663309
C,0,4.0895403731,2.1489516674,0.1184256577	C,0,4.0662253077,2.155037312,0.3131349267
H,0,3.6033917029,3.1164263271,0.0712857626	H,0,3.5741509018,3.1188881885,0.3597405059
C,0,3.3673683662,0.9619449874,0.1286736423	C,0,3.3468177172,0.9684516629,0.2207557467
C,0,1.8926533028,-0.6767344357,0.1232558075	C,0,1.8704502368,-0.6613077575,0.0802218271
N,0,3.035152864,-1.316949424,0.1801437321	N,0,3.0220938306,-1.305177966,0.0716746105
N,0,2.0046888829,0.6872725934,0.0903873903	N,0,1.9880375016,0.6969845664,0.1670692757
H,0,1.2277669363,1.3279630164,0.0394292367	H,0,1.216840028,1.3482343469,0.1883267483
N,0,0.6718142301,-1.2980822055,0.0961409481	N,0,0.6561099534,-1.2794616149,0.0084549437
N,0,-0.4562872342,-0.5726850028,0.0511200191	N,0,-0.4713630721,-0.5541677607,0.0208701738
C,0,-1.5859184491,-1.1950618268,0.0012983236	C,0,-1.5965383594,-1.1907526767,-0.0633434699
H,0,-1.620224602,-2.2897066453,-0.0134102895	H,0,-1.6178973683,-2.2798048545,-0.1462334723
H,0,0.670252793,-2.3147513782,0.1064036862	H,0,0.6464347607,-2.2955390626,-0.0549889921
H,0,6.0809867086,2.9404716728,0.1622040248	H,0,6.0562402169,2.9442334999,0.414154295
C,0,-2.8524966901,-0.4911208466,-0.0417836752	C,0,-2.8645584872,-0.498399735,-0.0511245198
C,0,-4.0404555376,-1.2569550135,-0.1540735103	C,0,-4.046122051,-1.273000499,-0.1650777581
C,0,-2.9316998598,0.9050290734,0.0184583503	C,0,-2.957800912,0.898892694,0.0684285843
H,0,-3.9727375921,-2.3383531377,-0.1993472434	H,0,-3.9698798097,-2.3499995555,-0.2581168408
H,0,-2.034241275,1.500626339,0.1165583828	H,0,-2.0624632009,1.5001676344,0.1576348584
C,0,-5.2832614471,-0.6489123193,-0.208458938	C,0,-5.2929300075,-0.6723579524,-0.1598736265
C,0,-4.1717804934,1.5390779929,-0.0377569328	C,0,-4.2011905179,1.5157288922,0.0760074793
C,0,-5.3595527547,0.7409102439,-0.1490576394	C,0,-5.3802677266,0.7141935928,-0.0390591282
H,0,7.1954497403,0.7457662422,0.2646176117	H,0,7.1791582394,0.752426414,0.3078233522

O,0,-6.5416312741,1.3692968508,-0.1932178651	O,0,-6.5783945649,1.3219289711,-0.0272217896
H,0,-6.3521599578,2.322909057,-0.1271079989	H,0,-6.4224670823,2.2778408853,0.0668785721
H,0,-6.1957696255,-1.2257459153,-0.2919392333	H,0,-6.2013978519,-1.2553008284,-0.2457324464
O,0,-4.3853566772,2.8395106064,-0.0068377412	O,0,-4.4266099015,2.8239982795,0.1827648868
H,0,-3.5402729973,3.5057656581,0.2781002818	H,0,-3.5697381204,3.4379115879,0.3312130792
O,0,-2.694636447,4.4028680179,0.6842122311	O,0,-2.5801555633,4.3987239571,0.5692865513
O,0,-1.4790837272,3.7449075302,0.9105651168	O,0,-1.3348654882,3.7673751004,0.3945491188
H,0,-1.0108930201,4.3724685005,1.4805188757	H,0,-0.7027145495,4.445134773,0.6791862059

TS H22 (•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.37412048 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.204241 a.u. 1 imaginary frequency = 1305.5142 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9289446 a.u.	**TS H23 (•OOH),** optimization in gas phase UB3LYP/6-311++G**, E= -1061.36661035 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.203324 a.u. 1 imaginary frequency = 1127.0302 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9212728 a.u.
0, 2	0, 2
C,0,6.1206203014,0.7740897157,0.2208515673	C,0,6.311667608,0.4605925808,0.1574945572
C,0,5.3868047725,-0.4075302537,0.2382128985	C,0,5.5944168781,-0.7195391813,-0.0069537183
C,0,5.4900031766,2.0297990192,0.1586148416	C,0,5.6643321351,1.7018112749,0.2853016634
H,0,5.8717897124,-1.3751457354,0.2854139159	H,0,6.0906282703,-1.6773180013,-0.1058500112
C,0,3.9921660706,-0.3153843991,0.1923084636	C,0,4.199465405,-0.6406278627,-0.0424558465
C,0,4.1010392335,2.1442237315,0.1126141193	C,0,4.2742014079,1.8031281531,0.2526893541
H,0,3.6172594459,3.1124855348,0.0627916312	H,0,3.7780207192,2.7615242795,0.3517664354
C,0,3.3743818918,0.9595895647,0.1311907517	C,0,3.5646384091,0.6199316951,0.0880516503
C,0,1.8905033455,-0.6707681434,0.13757596	C,0,2.1060239689,-1.0160356247,-0.1545122047
N,0,3.0335601176,-1.3169021088,0.1946859475	N,0,3.2554181871,-1.6451459818,-0.1930021033
N,0,2.0116795583,0.6911279581,0.09835834	N,0,2.2043638473,0.3392396721,0.0106835006
H,0,1.2406667322,1.3395543708,0.0461875172	H,0,1.4224245443,0.9726651665,0.0618254365
N,0,0.6691340089,-1.2865625109,0.1146463917	N,0,0.8941446453,-1.6445938326,-0.2681715041
N,0,-0.4561704212,-0.5568330647,0.063967389	N,0,-0.2508371301,-0.9463202306,-0.2180582377
C,0,-1.5842831806,-1.1839519369,0.0014933054	C,0,-1.3614703044,-1.6014526492,-0.3272190503
H,0,-1.6138306594,-2.2773911533,-0.023106141	H,0,-1.3515515198,-2.6893710889,-0.4529252716
H,0,0.6587689783,-2.3036044026,0.127737976	H,0,0.9118785543,-2.6544125772,-0.3868958419
H,0,6.0957214263,2.928369589,0.1452806234	H,0,6.257402333,2.5999330813,0.4119769246
C,0,-2.8517516451,-0.4847158471,-0.0438009152	C,0,-2.6536521174,-0.9595728691,-0.2907275836
C,0,-4.0341032365,-1.2578363308,-0.1699305179	C,0,-3.8097353031,-1.767104157,-0.4006850558
C,0,-2.940915651,0.9118173313,0.0272208446	C,0,-2.7972894259,0.4348765909,-0.1410858348
H,0,-3.9590016157,-2.3380359015,-0.2243197554	H,0,-3.6987683902,-2.8405713705,-0.5080718782
H,0,-2.0477786773,1.5127194416,0.1342887908	H,0,-1.9266250761,1.0715453451,-0.0584361054
C,0,-5.2795936367,-0.6566518293,-0.2261935708	C,0,-5.0745958466,-1.2136470261,-0.3571353246
C,0,-4.1840330974,1.5366127285,-0.0282953611	C,0,-4.0541614801,0.9965297609,-0.1075029802
C,0,-5.3649998103,0.7325376775,-0.1540870883	C,0,-5.2239298591,0.1791789933,-0.2156948002
H,0,7.2030827362,0.7295727247,0.2549118957	H,0,7.3945650046,0.4261212729,0.1880214076
O,0,-6.5540364192,1.3501290339,-0.1988719727	O,0,-4.2167646673,2.3311890608,0.0248988443
H,0,-6.3812217279,2.3057780364,-0.1223880226	H,0,-5.171883542,2.5050154365,0.0063108636
H,0,-6.1873964202,-1.2392478249,-0.320372428	H,0,-5.9625352226,-1.8296968586,-0.4309017976
O,0,-4.4068783364,2.8388398716,0.0166417436	O,0,-6.3762927895,0.8141558108,-0.1629557487
H,0,-3.5700231051,3.4920892549,0.2983589883	H,0,-7.211667632,0.2537151275,-0.5894199622
O,0,-2.7083948536,4.4120450041,0.7052233408	O,0,-8.1755768419,-0.3714106446,-1.2584327697
O,0,-1.4760896902,3.769096893,0.8922918709	O,0,-9.3418796532,-0.0891537904,-0.5542985286
H,0,-0.9917823739,4.4004341712,1.4453483191	H,0,-10.0276578064,-0.1765029355,-1.2341129287

TS H23 (•OOH), optimization in solv. water UB3LYP/6-311++G**, -1061.38795996 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.202911 a.u. 1 imaginary frequency = 1301.4163 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9434599 a.u.	**TS H23 (•OOH),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.37578851 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.203398 a.u. 1 imaginary frequency = 1049.5746 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9324934 a.u.
0, 2 C,0,6.2942404491,0.492388237,0.1809250409 C,0,5.5952918235,-0.6995292471,0.0135167313 C,0,5.626158745,1.7250684323,0.3029688069 H,0,6.1113689491,-1.6478547203,-0.0805435614 C,0,4.1978903468,-0.640785591,-0.0307294533 C,0,4.2342234238,1.8057196019,0.261250585 H,0,3.7198869929,2.7544887416,0.3554968544 C,0,3.5428033061,0.6110065674,0.0936558486 C,0,2.1033415984,-1.0403197092,-0.1549460442 N,0,3.2680431956,-1.6574457297,-0.1854106492 N,0,2.1900845913,0.3132855311,0.0083385142 H,0,1.4048260646,0.9456199964,0.055752875 N,0,0.9024455806,-1.6795104338,-0.2741871793 N,0,-0.2430328541,-0.9811775808,-0.2339992052 C,0,-1.351506008,-1.6406340946,-0.3480832228 H,0,-1.3457379027,-2.7263957305,-0.4700205788 H,0,0.9154006863,-2.6909168062,-0.3862078983 H,0,6.2050156436,2.6320931886,0.4323217016 C,0,-2.637888129,-0.9841531539,-0.3178724794 C,0,-3.8014371808,-1.7787932304,-0.4238297701 C,0,-2.7673656041,0.4136128241,-0.176776234 H,0,-3.7048785726,-2.8536152571,-0.5247863723 H,0,-1.888609539,1.0405776919,-0.0974213309 C,0,-5.060130303,-1.2057888805,-0.3836992074 C,0,-4.0183446971,0.9898407271,-0.1465714985 C,0,-5.1908461905,0.1855106586,-0.2489029655 H,0,7.3773913118,0.4739389057,0.2182324208 O,0,-4.1561104702,2.3344850565,-0.0213500551 H,0,-5.1037648964,2.5404058021,-0.0472842138 H,0,-5.9527710957,-1.815706401,-0.4511627765 O,0,-6.3485862574,0.8373404858,-0.1964757328 H,0,-7.1564090339,0.2880316291,-0.5744133635 O,0,-8.251586169,-0.3580512243,-1.2335798967 O,0,-9.3646458156,-0.0458762123,-0.4619532063 H,0,-10.1080446796,-0.1481834546,-1.0787369334	0, 2 C,0,6.30900995,0.4700811681,0.1499291003 C,0,5.5954503145,-0.7138337653,-0.0064061986 C,0,5.6568886366,1.7099096351,0.2741525247 H,0,6.0968924726,-1.6693447897,-0.1026804106 C,0,4.1994414442,-0.6398925768,-0.0373248144 C,0,4.2660175763,1.8059096751,0.245901808 H,0,3.7655568396,2.7621470106,0.3419412042 C,0,3.5599791547,0.6190125959,0.0895360244 C,0,2.103843846,-1.0204142993,-0.1424578246 N,0,3.2579309533,-1.6475218694,-0.1811122881 N,0,2.2015152028,0.334427246,0.0175229897 H,0,1.420585375,0.970308354,0.0675713687 N,0,0.8951825035,-1.6519412818,-0.2528800828 N,0,-0.2500799914,-0.9539620096,-0.2091379764 C,0,-1.3581090632,-1.612683592,-0.329741451 H,0,-1.3453615942,-2.6985240753,-0.4638769324 H,0,0.9094862177,-2.6625292597,-0.3673731915 H,0,6.2470375199,2.6108660303,0.394345944 C,0,-2.6497332636,-0.9692274427,-0.2944212497 C,0,-3.8062748267,-1.7738014365,-0.416594376 C,0,-2.7924133644,0.4244418573,-0.1327020616 H,0,-3.6975852649,-2.8462508106,-0.533729077 H,0,-1.9207706097,1.0587184126,-0.0403484754 C,0,-5.0702756146,-1.2168334639,-0.3724771812 C,0,-4.0485332589,0.9878932925,-0.098897616 C,0,-5.2169282283,0.1735546024,-0.2179145699 H,0,7.392161143,0.4397099501,0.1766567096 O,0,-4.2055498909,2.3245759158,0.0453510308 H,0,-5.1582944537,2.5090862881,0.0230388809 H,0,-5.9580923513,-1.8319951722,-0.4538240466 O,0,-6.3731527523,0.8104393318,-0.1609032213 H,0,-7.19325383,0.261571914,-0.5874286618 O,0,-8.1953706704,-0.3555346587,-1.277761827 O,0,-9.3503779102,-0.080957074,-0.5513946838 H,0,-10.0501049012,-0.1387290821,-1.2210438174

TS H25(•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.33359627 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.201580 a.u. 1 imaginary frequency = 1492.6485 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9019405 a.u.	**TS H25(•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.35746006 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.201373 a.u. 1 imaginary frequency = 1497.9276 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9256896 a.u.
0, 2 C,0,6.3285247775,0.489232231,-0.0640152507 C,0,5.5850698289,-0.6178633781,-0.4635527534 C,0,5.7108343796,1.6407133286,0.4506803221 H,0,6.059451291,-1.5073522181,-0.8601925214 C,0,4.1955670376,-0.5562317413,-0.339377135	0, 2 C,0,6.3174779782,0.4627186195,-0.0560433453 C,0,5.569737389,-0.6389753313,-0.4681002672 C,0,5.7022125902,1.6099436908,0.4739724665 H,0,6.0469207323,-1.5224846311,-0.8762125255 C,0,4.1794344615,-0.5746372401,-0.3402044907

C,0,4.3246803283,1.7224995386,0.582488798	C,0,4.315507653,1.6929735959,0.6096953487
H,0,3.8499235406,2.6121731154,0.9800336816	H,0,3.8398869036,2.5765037423,1.0182995264
C,0,3.5907051745,0.6130266529,0.1815430736	C,0,3.5778669121,0.5894755541,0.1962537437
C,0,2.0977769619,-0.9274952788,-0.340978908	C,0,2.072500219,-0.9330664941,-0.3386746514
N,0,3.2290546096,-1.5012361219,-0.6604047638	N,0,3.2063711049,-1.5120705968,-0.6693834441
N,0,2.22572829,0.3398638994,0.1659979055	N,0,2.2140191944,0.322415659,0.182811862
H,0,1.4627828191,0.9221390194,0.4721792973	H,0,1.4593786006,0.9192659656,0.4872771157
N,0,0.8697955707,-1.5198686325,-0.4970455492	N,0,0.8448592157,-1.5168404776,-0.4986172576
N,0,-0.2532696919,-0.8604623176,-0.1518549643	N,0,-0.2725943121,-0.8602193246,-0.1279167324
H,0,0.831972601,-2.487742648,-0.8074796492	H,0,0.7925940921,-2.4703352575,-0.8493715363
H,0,6.3221398357,2.4834097877,0.7520168291	H,0,6.315700126,2.4478229528,0.7842759081
C,0,-2.6773780356,-0.8379771146,-0.040765683	C,0,-2.6917932379,-0.8408163355,-0.009103002
C,0,-3.7714798323,-1.5740850389,0.4434472432	C,0,-3.7682125029,-1.5270111126,0.582339249
C,0,-2.879981489,0.476033149,-0.5100952951	C,0,-2.9141586036,0.4280144754,-0.5869071853
H,0,-3.6264846647,-2.5932487493,0.7781899695	H,0,-3.6096020166,-2.5081693775,1.0119133159
H,0,-2.0530460196,1.0517749872,-0.9054746658	H,0,-2.102222271,0.9631199341,-1.0630696434
C,0,-5.0368754631,-1.000505799,0.4843773564	C,0,-5.0306525401,-0.9501151625,0.6268888896
C,0,-4.1375010596,1.049405133,-0.4618691988	C,0,-4.1696276199,1.0031462946,-0.5409151165
C,0,-5.2214266424,0.3033250808,0.0385179108	C,0,-5.2363204343,0.3097184827,0.0695413855
H,0,7.4088043869,0.4645833875,-0.1505092897	H,0,7.3975578759,0.4361494258,-0.1453047162
O,0,-4.320211145,2.324023021,-0.9024996396	O,0,-4.3737415476,2.2344384775,-1.0880437427
H,0,-5.252119713,2.5577826186,-0.8013156893	H,0,-5.2999914224,2.4850834511,-0.9634381781
O,0,-6.4246761907,0.9582536329,0.035824194	O,0,-6.4293423399,0.9628324519,0.0548415562
H,0,-7.1251114396,0.3924902976,0.3769776333	H,0,-7.1237969978,0.4431813723,0.478802427
H,0,-5.8830916107,-1.5669076188,0.8603877791	H,0,-5.859540339,-1.4734361723,1.0902481436
C,0,-1.370850431,-1.4592939927,-0.0723123789	C,0,-1.3894875157,-1.4637482149,-0.0429335284
H,0,-1.3142718435,-2.8580824504,-0.134271723	H,0,-1.3295115866,-2.8424446693,-0.1245709855
O,0,-1.0688453289,-3.9721976233,-0.3280028471	O,0,-1.0801847543,-3.977850653,-0.3261940649
O,0,-2.1749356361,-4.47170493,-1.0732993566	O,0,-2.0006061588,-4.3997474116,-1.3321700229
H,0,-1.799691166,-4.5774095375,-1.9592632712	H,0,-1.4690738479,-4.3637726836,-2.1419065018

TS H25(•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.34372737 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.201372 a.u. 1 imaginary frequency = 1508.2529 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9121184 a.u.	
0, 2 C,0,6.3257585877,0.4793640363,-0.0605421586 C,0,5.5807397932,-0.6258990725,-0.4647078459 C,0,5.7091105955,1.62847576,0.4616792285 H,0,6.056368689,-1.5124461129,-0.8669826629 C,0,4.1910793512,-0.5642276839,-0.3372903183 C,0,4.322788793,1.7096805087,0.596645503 H,0,3.8476392599,2.5964055143,0.9997812097 C,0,3.5875759608,0.602382432,0.1909385678 C,0,2.0895498282,-0.9314943671,-0.3351967531 N,0,3.2218828433,-1.5065950944,-0.6607779736 N,0,2.2231151053,0.3311785152,0.177697167 H,0,1.4640600049,0.9187252643,0.4859232182 N,0,0.8615012897,-1.5199762798,-0.4930254037 N,0,-0.2590677003,-0.8606816896,-0.1361442961 H,0,0.8176361645,-2.4852062957,-0.8110398534 H,0,6.3211327966,2.4694330313,0.7664926526	

C,0,-2.6817867093,-0.8381541821,-0.0210242137 C,0,-3.7650651809,-1.5490621161,0.5234803559 C,0,-2.8961708054,0.4516438364,-0.550515304 H,0,-3.6115028713,-2.5484766869,0.9100999028 H,0,-2.0784273742,1.0067122128,-0.9922210108 C,0,-5.0295232128,-0.9748870568,0.566594595 C,0,-4.1534120119,1.0246420369,-0.5038921421 C,0,-5.2268852343,0.3047932398,0.0573735523 H,0,7.4058756918,0.4545292138,-0.1495504839 O,0,-4.3488743329,2.2758965194,-1.0046457362 H,0,-5.2797453477,2.5138729232,-0.8974974369 O,0,-6.4270080926,0.9568389183,0.0463768638 H,0,-7.1271744706,0.4058073225,0.4143118556 H,0,-5.8656386221,-1.5193338524,0.9928671381 C,0,-1.3769126306,-1.4599206656,-0.0561167277 H,0,-1.3245447046,-2.8497807495,-0.138932949 O,0,-1.0819980721,-3.9709839724,-0.3476000812 O,0,-2.118176138,-4.4263912252,-1.2130232183 H,0,-1.6723362432,-4.4758011822,-2.071455241	

TS H10 (•$OOCH_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.67027246 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228478 a.u. 1 imaginary frequency = 1780.9127 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2088107 a.u.	**TS H10 (•$OOCH_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.69471184 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228270 a.u. 1 imaginary frequency = 1880.3217 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2388648 a.u.
0, 2 C,0,6.9339184376,-0.0473475356,0.1751920241 C,0,6.027237068,-1.0600785961,-0.0736068615 C,0,6.5162402519,1.2862566274,0.4436459591 H,0,6.3460339504,-2.0750102068,-0.2777430769 C,0,4.6597549201,-0.7324192135,-0.0539713425 C,0,5.1799557829,1.6397034122,0.4700433531 H,0,4.8530870179,2.6518989528,0.6733250295 C,0,4.2475250799,0.6213263392,0.2196050107 C,0,2.5515739189,-0.6511538787,-0.1120122659 N,0,3.5620964218,-1.5127682956,-0.2596734543 N,0,1.2623406829,-1.0658902338,-0.245625877 N,0,0.2341517129,-0.2184630454,-0.0959253889 C,0,-0.9590697741,-0.6844379358,-0.2329264245 H,0,-1.1298997415,-1.7425403067,-0.465392966 H,0,1.1252498241,-2.0523584641,-0.4602504099 H,0,7.2716503079,2.0406851219,0.6318168722 C,0,-2.1322437096,0.1609729683,-0.0865455381 C,0,-3.4039049739,-0.4095006154,-0.2449853343 C,0,-2.0159591519,1.5325383389,0.2107358704 H,0,-3.5010539592,-1.4646655017,-0.4741243074 H,0,-1.0395255118,1.9875055451,0.3367168577 C,0,-4.5475917893,0.3720650269,-0.1097859049 C,0,-3.1525440314,2.3084028385,0.3447417508 C,0,-4.4243612933,1.7238409961,0.1833433831 H,0,7.9956492684,-0.2670485405,0.1674012736 O,0,-3.0416638633,3.6341972764,0.6323036661 H,0,-3.9280452077,4.0139946953,0.6879916783 O,0,-5.4825061025,2.5835776452,0.3376253229 H,0,-6.3189302099,2.1246332915,0.2098262794 H,0,-5.532486046,-0.067859757,-0.2319172683 N,0,2.8845907347,0.6419219799,0.1754862073 H,0,2.1259179619,1.6052066494,0.3522434765 O,0,1.3787805319,2.5824489537,0.5308693943 O,0,2.283000703,3.6281172311,0.7737562442 C,0,1.5340600885,4.8146597104,0.9888751046 H,0,2.2728347502,5.5976587308,1.1700472304 H,0,0.935239249,5.051763661,0.1045559641 H,0,0.8794706103,4.6990799948,1.8577885281	0, 2 C,0,6.9311207878,-0.1419695001,-0.0678319164 C,0,5.9956838524,-1.1560498829,-0.1547203722 C,0,6.5474703959,1.2188187426,0.0807983604 H,0,6.290224673,-2.1925491344,-0.268075057 C,0,4.6351823399,-0.798740429,-0.0907873622 C,0,5.2171625603,1.5998048362,0.1466735246 H,0,4.91972377,2.6346374367,0.2607218455 C,0,4.2606061757,0.5798116754,0.0599293929 C,0,2.517138923,-0.6918265972,-0.036388172 N,0,3.5172749872,-1.5767731333,-0.1489557523 N,0,1.2227708774,-1.0923935698,-0.0519879996 N,0,0.218211603,-0.2104562879,0.0580535979 C,0,-0.9866044279,-0.6867005355,0.0277110243 H,0,-1.1641219171,-1.7595977031,-0.0835627255 H,0,1.0498047492,-2.092569955,-0.1533680337 H,0,7.3214121702,1.9749353134,0.143881829 C,0,-2.1440896343,0.1721306808,0.1357874098 C,0,-3.4236055991,-0.4097321266,0.0871103264 C,0,-2.0213146695,1.5697126088,0.2851013488 H,0,-3.5255384459,-1.4824698605,-0.0265302615 H,0,-1.0423495767,2.0334832291,0.323742751 C,0,-4.5618438818,0.381161529,0.182738895 C,0,-3.1514603079,2.3556001485,0.3805851113 C,0,-4.432321984,1.7596819274,0.3274242435 H,0,7.986934812,-0.3827438833,-0.1135469772 O,0,-3.0316864441,3.7052665444,0.524611483 H,0,-3.9147133543,4.0981430159,0.5705593137 O,0,-5.4736954957,2.6275076899,0.4271650991 H,0,-6.3228752905,2.1717879805,0.3690408564 H,0,-5.549524408,-0.0646490204,0.1447683044 N,0,2.8925130146,0.6144545562,0.091667472 H,0,2.2188095151,1.5571516963,0.2086703646 O,0,1.4901170375,2.6847710791,0.3486590592 O,0,2.4936852899,3.6873839852,0.4550644353 C,0,1.8551079853,4.9442470464,0.6155708261 H,0,2.6596071716,5.6786142997,0.6921679427 H,0,1.2235220924,5.1699638712,-0.2497121516 H,0,1.2493388233,4.9562917564,1.5274340541

TS H10 (•$OOCH_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.67995384 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228966 a.u. 1 imaginary frequency = 1852.6734 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2212464 a.u.	**TS H24 (•$OOCH_3$),** optimization in gas phase UB3LYP/6-311++G**, E= -1100.67755355 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.229154 a.u. 1 imaginary frequency = 1721.8738 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2173357 a.u.
0, 2	0, 2

C,0,6.8021924222,0.0542112558,0.0546196805	C,0,6.2928056463,-0.0007349482,-0.2848274958
C,0,5.9160812933,-1.0052005639,-0.0034370912	C,0,5.4751994338,-1.0171648757,0.1860268117
C,0,6.355644038,1.4037863048,0.1002290467	C,0,5.7616002946,1.233771718,-0.7116829669
H,0,6.2579721685,-2.0326567027,-0.0383133347	H,0,5.8791794937,-1.9661261109,0.5170104542
C,0,4.5410339331,-0.7079927073,-0.0163050873	C,0,4.0925307307,-0.7851600966,0.229690726
C,0,5.0103354082,1.7270873022,0.0893396445	C,0,4.3935263289,1.4891522559,-0.6804072355
H,0,4.6630411917,2.7521352724,0.1238563179	H,0,3.9911708246,2.4393865206,-1.011343811
C,0,4.1000790344,0.6614588029,0.0308334149	C,0,3.5753830784,0.4665602532,-0.2098470405
C,0,2.4265868982,-0.686035086,-0.0532333935	C,0,1.972431665,-0.895391362,0.4816667938
N,0,3.459963364,-1.5364802581,-0.0691040146	N,0,3.0771594809,-1.6061287893,0.6540419447
N,0,1.1484071186,-1.1443924438,-0.0939919587	N,0,2.2100654949,0.3554400455,-0.0460361645
N,0,0.1017328355,-0.3048647514,-0.0780064153	H,0,1.4867945763,1.0320597964,-0.231733868
C,0,-1.0791782377,-0.8246471915,-0.1107256442	N,0,-0.28006859,-0.4817714173,0.4942712607
H,0,-1.2161034998,-1.9109179493,-0.1496142376	C,0,-1.4802541386,-0.9617434884,0.5836083345
H,0,1.027218208,-2.1554488346,-0.1337470614	H,0,-1.6344004507,-2.0118388475,0.8376993816
H,0,7.0941400197,2.1960728584,0.1445654596	H,0,6.434849613,2.0018611531,-1.0742320012
C,0,-2.2766746494,-0.0056144753,-0.0957743278	C,0,-2.6575869215,-0.1493167285,0.3369758371
C,0,-3.5287702627,-0.6396621385,-0.1285359463	C,0,-3.9203849857,-0.7571908686,0.4165394793
C,0,-2.2096530228,1.4009955884,-0.046579892	C,0,-2.5754269807,1.2212138692,0.0272568345
H,0,-3.5878391406,-1.7213255007,-0.1656597609	H,0,-3.9958344952,-1.8118007131,0.6540327987
H,0,-1.2498128196,1.9048603882,-0.0194995041	H,0,-1.6132199423,1.7113585498,-0.0374337833
C,0,-4.6993871952,0.1115522384,-0.1121773056	C,0,-5.0764570857,-0.0166037601,0.1906216682
C,0,-3.3729073092,2.1469729078,-0.0307256768	C,0,-3.7212678266,1.9600347594,-0.1975707403
C,0,-4.6252005588,1.4984668459,-0.0628182562	C,0,-4.9807241223,1.3349420017,-0.1152541089
H,0,7.8685791711,-0.1409814618,0.0658378521	H,0,7.3650290764,-0.1532064663,-0.3270927139
O,0,-3.3093181575,3.5065775512,0.0168759368	O,0,-3.6279740154,3.2846063706,-0.4973942412
H,0,-4.2085287025,3.8610005843,0.0244033895	H,0,-4.5183237735,3.6390152262,-0.6194947408
O,0,-5.7093955936,2.3316287715,-0.0417826754	O,0,-6.0521831366,2.1556245237,-0.356864723
H,0,-6.5333621941,1.8317772368,-0.0538608277	H,0,-6.8804329622,1.6705573928,-0.2823382814
H,0,-5.6678820781,-0.3770989731,-0.1360414561	H,0,-6.0518861604,-0.4891227057,0.2513664339
N,0,2.7348828175,0.6426743698,0.0058470577	N,0,0.7269252538,-1.3301630129,0.815426271
H,0,1.9705173286,1.5953722353,0.0356196314	H,0,0.5116250672,-2.4953783042,0.7766024549
O,0,1.2019125992,2.598980099,0.0695633583	O,0,0.2241501328,-3.7362468276,0.5807362327
O,0,2.1036899406,3.6789316377,0.1234907506	O,0,0.6184793282,-4.3302210819,1.7764761945
C,0,1.3513340819,4.8827322969,0.1701783267	C,0,1.8548070618,-5.0172029472,1.575369683
H,0,2.0883234446,5.6870189552,0.2087423552	H,0,2.6376699386,-4.3021118013,1.3096271176
H,0,0.7302574716,4.9788221289,-0.7252221416	H,0,2.0764882824,-5.4951445498,2.53158366
H,0,0.719236643,4.903089546,1.0628330968	H,0,1.7399131953,-5.7680156328,0.7887471636

TS H24 (•OOCH$_3$), optimization in solv. water UB3LYP/6-311++G**, E= -1100.70026786 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.227356 a.u. 1 imaginary frequency = 1413.1037 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2392994 a.u.	**TS H24 (•OOCH$_3$),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.68668922 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228959 a.u. 1 imaginary frequency = 1631.2332 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2259634 a.u.
0, 2	0, 2
C,0,6.3696591625,0.1986493222,-0.0951034827	C,0,6.2961863815,0.011499088,-0.2680992149
C,0,5.5714118282,-0.7538808319,0.5204178903	C,0,5.4777744936,-1.0086366092,0.1934645194
C,0,5.8109035827,1.3242494761,-0.7400966526	C,0,5.7650379022,1.2485951575,-0.6905175903
H,0,5.9985079267,-1.61762036,1.0158997439	H,0,5.8824913589,-1.9589391019,0.5200338294
C,0,4.1799038509,-0.5679843574,0.4845084319	C,0,4.0942885319,-0.777136129,0.2320085855
C,0,4.4354206406,1.5322292252,-0.7884754101	C,0,4.3967385584,1.5031385082,-0.6638241245
H,0,4.0102832162,2.3964725136,-1.2837030713	H,0,3.9941248724,2.4542413782,-0.9912033928
C,0,3.6362927424,0.5729012978,-0.1721446429	C,0,3.5775612974,0.4768518034,-0.2019234761

C,0,2.0537036455,-0.7067426103,0.6856089947	C,0,1.9723163894,-0.8881733894,0.4710380109
N,0,3.1753575482,-1.3416777603,1.0134322035	N,0,3.0765073329,-1.6012657095,0.645779578
N,0,2.2713771528,0.4469972224,-0.0249841826	N,0,2.2119106171,0.3650878535,-0.0445322611
H,0,1.5426910434,1.0604484802,-0.3592468296	H,0,1.4924439568,1.0458992839,-0.2335037504
N,0,-0.218383644,-0.3718493057,0.6059399392	N,0,-0.2841393244,-0.4795191342,0.4771989737
C,0,-1.4073787388,-0.8141405128,0.8831684173	C,0,-1.4849312007,-0.9567353214,0.585827832
H,0,-1.5408195462,-1.7531493993,1.4229294519	H,0,-1.6395653879,-2.0015404176,0.8592848561
H,0,6.4709660105,2.0441974494,-1.2095461588	H,0,6.4393179818,2.0190991837,-1.0458677282
C,0,-2.6018315683,-0.0965073745,0.4963115445	C,0,-2.6610111546,-0.1461168152,0.3383058433
C,0,-3.851887957,-0.6362826493,0.8482368377	C,0,-3.925867706,-0.7454041846,0.4554979562
C,0,-2.5526551341,1.1232983046,-0.2101691681	C,0,-2.5764007645,1.2162458529,-0.0091053135
H,0,-3.9009827831,-1.5739295909,1.3889269689	H,0,-4.0027164871,-1.7929853726,0.7217397459
H,0,-1.6012683083,1.554261214,-0.4943045337	H,0,-1.6123732892,1.6978934511,-0.1057943324
C,0,-5.0276921248,0.0222527037,0.5096386383	C,0,-5.0821446496,-0.0053250774,0.2319324228
C,0,-3.7189766782,1.7803693056,-0.5458450218	C,0,-3.7225616094,1.9540271376,-0.2313741393
C,0,-4.967650718,1.2278481192,-0.1833385492	C,0,-4.9853676004,1.338578201,-0.1100806518
H,0,7.446965331,0.0816173191,-0.0839328389	H,0,7.3687164424,-0.1395918546,-0.3068447753
O,0,-3.6640075304,2.9592370626,-1.2275035865	O,0,-3.6291690162,3.2707678403,-0.5677848247
H,0,-4.5647926264,3.2771284833,-1.3815164956	H,0,-4.5198961042,3.6271355257,-0.6865741899
O,0,-6.051252818,1.956181157,-0.5644029085	O,0,-6.0525632308,2.1575180209,-0.3523312759
H,0,-6.8755189018,1.5346505382,-0.2905973124	H,0,-6.8858891455,1.6823001861,-0.2587784572
H,0,-5.9911622536,-0.3947779308,0.7805548481	H,0,-6.0584101601,-0.470156205,0.3220596307
N,0,0.8141000088,-1.1349219255,1.0360472958	N,0,0.7251593141,-1.3264639109,0.7944217005
H,0,0.6429611381,-2.2226232232,1.2841386289	H,0,0.518303141,-2.4682098606,0.7770312437
O,0,0.2279309894,-3.5615470638,1.2844432805	O,0,0.2234322145,-3.752863709,0.5879052596
O,0,1.2808400248,-4.3582118009,1.7584311591	O,0,0.6483940241,-4.3337059466,1.7844716675
C,0,1.4421643122,-5.479818854,0.8942445965	C,0,1.8548987772,-5.0633093243,1.5544485153
H,0,1.7016514108,-5.1493225657,-0.1155711077	H,0,2.6459036814,-4.3817910986,1.2319200945
H,0,2.2590579621,-6.0641954603,1.3212681692	H,0,2.1064037048,-5.516279435,2.5153142551
H,0,0.5254688033,-6.0760066174,0.868156913	H,0,1.6864528565,-5.8369308653,0.8002769781

TS H22 (•$OOCH_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.68299572 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.227880 a.u. 1 imaginary frequency = 1646.4684 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2135965 a.u.	**TS H22 (•$OOCH_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.70331898 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.227485 a.u. 1 imaginary frequency = 1888.7453 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.240045 a.u.
0, 2	0, 2
C,0,5.9281545935,0.392308202,0.6955101182	C,0,5.9184232486,0.3968752778,0.6987880222
C,0,5.2557390143,-0.6625531148,0.0875196898	C,0,5.2491425722,-0.6559842842,0.0845448484
C,0,5.2371205328,1.4954704133,1.2260033832	C,0,5.22257377,1.4971653272,1.2366116005
H,0,5.7857819838,-1.5137442294,-0.3222459076	H,0,5.7851101072,-1.5020373058,-0.3291614194
C,0,3.8614074372,-0.5985976888,0.0159283568	C,0,3.8520222712,-0.5931838691,0.0139169977
C,0,3.8466353988,1.5792821113,1.1654168943	C,0,3.832066022,1.5797862003,1.1774337427
H,0,3.3161747652,2.43094035,1.5749893293	H,0,3.2975468192,2.4261710634,1.5909532922
C,0,3.1819843053,0.5219104947,0.5567611945	C,0,3.1687984321,0.5237981201,0.5620166188
C,0,1.7869090894,-0.9414116458,-0.3228137638	C,0,1.7712441739,-0.9310070483,-0.3235445508
N,0,2.9563733769,-1.4975025136,-0.5279996603	N,0,2.9489525108,-1.4877479253,-0.5338109017
N,0,1.8356840594,0.2663496076,0.3195462014	N,0,1.8262679972,0.269682562,0.325240661
H,0,1.0319410729,0.8271390986,0.5554038513	H,0,1.0282507621,0.8375569749,0.5698439326
N,0,0.5996491877,-1.5035804045,-0.7111373201	N,0,0.5900607631,-1.4915547962,-0.7142416421
N,0,-0.5635350342,-0.8785945252,-0.4680038719	N,0,-0.5699090792,-0.8682093874,-0.4670839578
C,0,-1.6545740091,-1.4476821807,-0.8594815807	C,0,-1.6581817831,-1.4484672744,-0.8662463441
H,0,-1.6232905407,-2.4127735554,-1.3766154492	H,0,-1.6197176346,-2.4092261077,-1.3849171104

H,0,0.6490442441,-2.4012683379,-1.1859613859	H,0,0.6312730301,-2.3873162568,-1.1966587733
H,0,5.7959535205,2.2985496609,1.6921120835	H,0,5.7803017437,2.2983171452,1.7072437983
C,0,-2.9600673318,-0.8577140252,-0.6430917275	C,0,-2.9593155034,-0.8624787343,-0.6477857811
C,0,-4.0955560201,-1.5624289436,-1.1190240348	C,0,-4.0921197627,-1.5708414702,-1.1239800721
C,0,-3.1305854874,0.3675084879,0.0130428865	C,0,-3.1351000249,0.3666708166,0.0124905963
H,0,-3.9577836854,-2.5110511853,-1.6259812318	H,0,-3.9528112676,-2.5176408034,-1.6321073592
H,0,-2.2703596448,0.9118982816,0.3803797481	H,0,-2.274440679,0.9120944563,0.3781760917
C,0,-5.3735646354,-1.0594660441,-0.9465113988	C,0,-5.3688855214,-1.0689259289,-0.9472791104
C,0,-4.4081460149,0.8959453504,0.199322015	C,0,-4.4102157115,0.885515382,0.1988946675
C,0,-5.5387433908,0.1604182164,-0.2928464955	C,0,-5.5361597759,0.1507330982,-0.2906249361
H,0,7.0096397342,0.3663638179,0.7632225729	H,0,6.9999046468,0.3736908171,0.7667131015
O,0,-6.7564067749,0.6850162931,-0.1028048486	O,0,-6.7638639487,0.6624738956,-0.1037324313
H,0,-6.6185371902,1.527322934,0.3694289081	H,0,-6.6550609115,1.5072657066,0.3684295606
H,0,-6.2466961688,-1.5896235985,-1.3059408155	H,0,-6.2403835957,-1.6017676327,-1.3068144082
O,0,-4.7018974448,2.0294004733,0.795782592	O,0,-4.7071116861,2.0294629606,0.804110684
H,0,-3.8193386534,2.6584664929,1.1934826546	H,0,-3.846030351,2.6007530068,1.1709020095
O,0,-2.8451249015,3.3136185375,1.6042830751	O,0,-2.7963630337,3.2970528511,1.6135789655
O,0,-3.3879885737,4.440149181,2.2102461305	O,0,-3.3436910582,4.4457399527,2.2017260339
C,0,-2.3220451067,5.2511035031,2.6880205976	C,0,-2.2833040248,5.2648574152,2.6852175017
H,0,-2.8026811065,6.1140804088,3.1507215485	H,0,-2.7677359475,6.1357923705,3.128658455
H,0,-1.7303907162,4.7013794084,3.4256037055	H,0,-1.7028800977,4.7279678038,3.4407359707
H,0,-1.6858228847,5.567384668,1.8564929554	H,0,-1.6335992419,5.5709803508,1.8605187857

TS H22 (•OOCH$_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.69150841 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.226967 a.u. 1 imaginary frequency = 1702.2347 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2219105 a.u.	**TS H23 (•OOCH$_3$),** optimization in gas phase UB3LYP/6-311++G**, E= -1100.68566689 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228713 a.u. 1 imaginary frequency = 1419.2708 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.217935 a.u.
0, 2	0, 2
C,0,5.9269529652,0.3921687298,0.6942977879	C,0,6.328257476,0.5170937187,0.1430485728
C,0,5.2556487551,-0.664093331,0.0870666152	C,0,5.6162124602,-0.6095649425,-0.2550005293
C,0,5.234061694,1.4950248474,1.2253053927	C,0,5.6746995099,1.6857566664,0.5703414771
H,0,5.7884811644,-1.5138068426,-0.3225763074	H,0,6.1172985097,-1.5115265528,-0.584796357
C,0,3.8603303145,-0.6017314253,0.0168822895	C,0,4.2204148815,-0.550870121,-0.2194678689
C,0,3.8432824617,1.5770055781,1.1661005291	C,0,4.2833415118,1.7656897629,0.6133191029
H,0,3.3107764939,2.4273923742,1.575103279	H,0,3.7822319384,2.6681954269,0.9433738626
C,0,3.1794211449,0.5181107502,0.5582292486	C,0,3.5792003503,0.636388268,0.2141598541
C,0,1.7827028115,-0.9441664177,-0.3195249047	C,0,2.1277175023,-0.930793938,-0.3343912646
N,0,2.955445684,-1.5007343168,-0.5260763236	N,0,3.2806343044,-1.5138337407,-0.5560372785
N,0,1.8343323921,0.262138796,0.3227303657	N,0,2.2196765239,0.3547606906,0.1268882279
H,0,1.0332722477,0.8266257023,0.5616147377	H,0,1.4338697063,0.9453156689,0.348334939
N,0,0.5973605476,-1.5061404167,-0.7074449335	N,0,0.9179701834,-1.5397136708,-0.5397478097
N,0,-0.5643837032,-0.8795936222,-0.4647401825	N,0,-0.2308241538,-0.8893756462,-0.2936543311
C,0,-1.6542499788,-1.4494086109,-0.8632045167	C,0,-1.3384934228,-1.5250868874,-0.5016347637
H,0,-1.6211276491,-2.4108469559,-1.3846911006	H,0,-1.3225249136,-2.5590541413,-0.8627642006
H,0,0.6420720842,-2.4034158244,-1.1844187357	H,0,0.9392637613,-2.4977545054,-0.8797924129
H,0,5.7922468839,2.2990880568,1.6905094935	H,0,6.2635886427,2.543653702,0.8731559786
C,0,-2.957806306,-0.8586904761,-0.6456842445	C,0,-2.63513215,-0.9318643225,-0.2787328596
C,0,-4.0932043763,-1.56079045,-1.1267440626	C,0,-3.7855737459,-1.7187555474,-0.5199083932
C,0,-3.128974916,0.3644501149,0.0172872781	C,0,-2.7891491521,0.394277689,0.1750164701
H,0,-3.9557000283,-2.5067895124,-1.6379658497	H,0,-3.6663428057,-2.7409499779,-0.8622704489
H,0,-2.2683149846,0.9056370587,0.3884238593	H,0,-1.9232092732,1.0147663979,0.3634307194
C,0,-5.3702192492,-1.0571180212,-0.9523829277	C,0,-5.0542174888,-1.2133176954,-0.3131233069

C,0,-4.4052479732,0.8916986308,0.2042373411	C,0,-4.0500840481,0.9097285988,0.3741670178
C,0,-5.5349394783,0.1601115711,-0.292488841	C,0,-5.2164180657,0.1134383278,0.132913523
H,0,7.0085532949,0.3679418834,0.7610033752	H,0,7.4118138325,0.4966763719,0.1245491289
O,0,-6.7554464243,0.681673881,-0.1031628855	O,0,-4.2257082589,2.1797059916,0.8005177988
H,0,-6.6272090237,1.5229145632,0.3728275407	H,0,-5.1842259798,2.327430987,0.8558097721
H,0,-6.2429073694,-1.5854241194,-1.3156395793	H,0,-5.9363493989,-1.8174300395,-0.4873017494
O,0,-4.6983513203,2.0255486947,0.808251541	O,0,-6.3698004893,0.6978496449,0.3632191619
H,0,-3.8203264398,2.6410332299,1.1924693888	H,0,-7.2457567366,0.2162456878,-0.1378589372
O,0,-2.8303507785,3.3144998154,1.6024536633	O,0,-8.2234473428,-0.255351652,-0.8358448686
O,0,-3.3815638172,4.4295333358,2.2304857423	O,0,-9.3294158241,-0.1436792712,-0.0127832983
C,0,-2.3225417668,5.264323842,2.6864939245	C,0,-10.5024375951,-0.1126442176,-0.8216950921
H,0,-2.8115089123,6.1137423463,3.1649890527	H,0,-10.5738660673,-1.029281369,-1.4131076968
H,0,-1.7005667931,4.7263123165,3.4072986269	H,0,-11.3345485999,-0.0424425093,-0.1201178043
H,0,-1.7149426516,5.5997882245,1.8414453219	H,0,-10.4794411222,0.7585400264,-1.4816546952

TS H23 (•OOCH$_3$), optimization in solv. water UB3LYP/6-311++G**, E= -1100.70567790 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228506 a.u. 1 imaginary frequency = 1746.6597 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2403714 a.u.	**TS H23 (•OOCH$_3$),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.70567789 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228502 a.u. 1 imaginary frequency = 1746.4979 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2321484 a.u.
0, 2	0, 2
C,0,6.3104578905,0.5635041445,0.1631414473	C,0,6.3091802231,0.5639662251,0.163458055
C,0,5.6198368983,-0.5808345816,-0.2255635695	C,0,5.618790822,-0.580511808,-0.2252520885
C,0,5.6327521165,1.7279646296,0.569587362	C,0,5.6312365529,1.7283550417,0.5697084226
H,0,6.1430731999,-1.4768100228,-0.5385760932	H,0,6.1422110288,-1.4764319801,-0.5381157759
C,0,4.2213309425,-0.5437473136,-0.2015725	C,0,4.220276617,-0.5436391227,-0.2014664885
C,0,4.2393889944,1.785723607,0.6006831611	C,0,4.2378594595,1.7859000636,0.6005974283
H,0,3.7177390608,2.6821690434,0.9133397298	H,0,3.7160272181,2.6822929716,0.9131009466
C,0,3.556368844,0.6388198914,0.2113423695	C,0,3.5550726385,0.6388583499,0.2112546874
C,0,2.1285694503,-0.952825459,-0.3258018479	C,0,2.1275958346,-0.9530510127,-0.3259699075
N,0,3.2983722929,-1.5243681502,-0.5322634289	N,0,3.2975157288,-1.5244303383,-0.5322132609
N,0,2.2049859619,0.3368832314,0.1181252032	N,0,2.2037489136,0.3367051986,0.1178652037
H,0,1.4145553568,0.9280487785,0.3288105788	H,0,1.4131963587,0.9277623732,0.328395909
N,0,0.9320098034,-1.57870262,-0.5316373609	N,0,0.9311597539,-1.5791204646,-0.5319466839
N,0,-0.2204007222,-0.9330948508,-0.2960434126	N,0,-0.2213811706,-0.9336704597,-0.2965507416
C,0,-1.3227840079,-1.5796657867,-0.5072315023	C,0,-1.3236391227,-1.5804024919,-0.5078783873
H,0,-1.3046955035,-2.6129952455,-0.8619657415	H,0,-1.3053536944,-2.6137359244,-0.8625905353
H,0,0.954529055,-2.5404331948,-0.8636617176	H,0,0.9538706126,-2.5408847311,-0.8638587541
H,0,6.2050713429,2.5995690558,0.8650756431	H,0,6.2033774587,2.6000734612,0.8652059809
C,0,-2.6167045252,-0.9773750672,-0.2899649597	C,0,-2.6176795278,-0.9782890318,-0.290803335
C,0,-3.7705813828,-1.7574044162,-0.5337922696	C,0,-3.7714121633,-1.7584811303,-0.5347955163
C,0,-2.7646943969,0.3522868292,0.1593839045	C,0,-2.7659199663,0.3513513825,0.1585157053
H,0,-3.6586371042,-2.7808555981,-0.8726209231	H,0,-3.6592751784,-2.7819161241,-0.8736077367
H,0,-1.8942858553,0.967003261,0.3495126468	H,0,-1.8956254776,0.9661900038,0.3487705756
C,0,-5.0362351956,-1.2383393966,-0.3334991139	C,0,-5.0371672041,-1.2395932456,-0.3346863433
C,0,-4.0232693155,0.876994015,0.35140277	C,0,-4.0245987715,0.8758855915,0.350345691
C,0,-5.1885100174,0.0877478319,0.1086426247	C,0,-5.1896911453,0.0864714769,0.1074322554
H,0,7.3943702892,0.5605837261,0.1534467775	H,0,7.3930945035,0.5612118343,0.1539192782
O,0,-4.1836421081,2.1559484761,0.7748867333	O,0,-4.1852058658,2.1548200296,0.7737988678
H,0,-5.1370799635,2.331596324,0.823170755	H,0,-5.1386736475,2.3303390622,0.8219562863
H,0,-5.9199427738,-1.8396465236,-0.5087821576	H,0,-5.9207630766,-1.8410286396,-0.5100928058
O,0,-6.3504360525,0.6799510292,0.3376529918	O,0,-6.3517355017,0.6785089895,0.3362923271
H,0,-7.1842062282,0.2208648727,-0.1648441599	H,0,-7.1853799903,0.2193382513,-0.166303508

O,0,-8.2407043977,-0.2319222708,-0.9037494026	O,0,-8.2417826845,-0.2334656163,-0.9053114234
O,0,-9.3144315379,-0.1832508478,-0.02847439	O,0,-9.31556759,-0.1849356577,-0.0301219248
C,0,-10.5285348799,-0.037873892,-0.7695571044	C,0,-10.5295932806,-0.0391288657,-0.7712475743
H,0,-10.6554397078,-0.8848032626,-1.4480798755	H,0,-10.65654612,-0.8857872464,-1.4500981702
H,0,-11.3226368657,-0.0240677663,-0.0228633272	H,0,-11.3237549078,-0.0255069396,-0.0246142706
H,0,-10.5133438077,0.8992501993,-1.3311949605	H,0,-10.5142431775,0.8982034045,-1.3325327482

TS H25(•$OOCH_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.65057474 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.226590 a.u. 1 imaginary frequency = 1464.7177 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9019405 a.u.	**TS H25(•$OOCH_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.67282438 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.226757 a.u. 1 imaginary frequency = 1509.2090 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2197288 a.u.
0, 2	0, 2
C,0,6.3760938988,0.4988949456,0.0009764903	C,0,6.3580949753,0.5011646712,-0.0411170254
C,0,5.6537168538,-0.6507192345,-0.3078228558	C,0,5.6385392042,-0.6500423471,-0.3582241137
C,0,5.7341916863,1.6879591554,0.3827979248	C,0,5.713112424,1.6752100477,0.3836732878
H,0,6.1471013673,-1.5692931309,-0.6017947847	H,0,6.1389090211,-1.5542283563,-0.6853492288
C,0,4.260971131,-0.5935401235,-0.2281861543	C,0,4.246513669,-0.608132318,-0.2424002666
C,0,4.3439906458,1.7658965423,0.4679330354	C,0,4.3237414404,1.7364185519,0.5056712907
H,0,3.8502478556,2.684824192,0.762612877	H,0,3.8251799387,2.6408970011,0.8332000793
C,0,3.6315167599,0.6140152563,0.1584761169	C,0,3.6147597656,0.5837475078,0.1875059508
C,0,2.1671634822,-0.9882271837,-0.2489526203	C,0,2.1480838933,-1.0153708834,-0.2187714174
N,0,3.3120307546,-1.5772115406,-0.4796045038	N,0,3.2974004356,-1.5940025809,-0.4921481277
N,0,2.2697963275,0.3246808166,0.1328284043	N,0,2.2573939607,0.2839386974,0.1916811851
H,0,1.4938190299,0.9241848708,0.3636312571	H,0,1.486891468,0.8872343089,0.4379652413
N,0,0.9491288673,-1.6067322096,-0.3797546105	N,0,0.9353722388,-1.6397781125,-0.3276976176
N,0,-0.1886193312,-0.9326006649,-0.1137116297	N,0,-0.2014821555,-0.9656087249,-0.0515953857
H,0,0.9281645211,-2.6026168975,-0.5841479117	H,0,0.9053490559,-2.6106063123,-0.6275653458
H,0,6.3290942984,2.5633809089,0.6160317843	H,0,6.3046923569,2.551637293,0.6216709748
C,0,-2.6167117825,-0.9262897509,-0.0300931578	C,0,-2.6238246412,-0.9493030851,0.0101796005
C,0,-3.7048927692,-1.6362604193,0.5030319876	C,0,-3.7082567918,-1.5930271273,0.6324913303
C,0,-2.8319525697,0.3448397933,-0.6003603736	C,0,-2.8402492515,0.2690762664,-0.6687549234
H,0,-3.550074329,-2.6246000843,0.9166160265	H,0,-3.5550218224,-2.5374550097,1.1391639844
H,0,-2.009544576,0.898612352,-1.0346948159	H,0,-2.0219115526,0.769076908,-1.171460912
C,0,-4.9774411788,-1.0765616591,0.4928645335	C,0,-4.9736579053,-1.0201608662,0.6091613487
C,0,-4.0967507573,0.9047871694,-0.60303243	C,0,-4.0986513516,0.8401770744,-0.6901641555
C,0,-5.1748092154,0.1867302057,-0.0524972222	C,0,-5.1734088849,0.1924706893,-0.0457718164
H,0,7.4585820358,0.478117565,-0.053254498	H,0,7.439057352,0.4923150654,-0.1232216859
O,0,-4.2916549009,2.1393745219,-1.142138039	O,0,-4.2964288501,2.0237523348,-1.3369005908
H,0,-5.2268938331,2.3685231179,-1.0637604376	H,0,-5.2266082567,2.2767659162,-1.253447689
O,0,-6.3862650371,0.824915615,-0.1121244186	O,0,-6.3684176813,0.8383271418,-0.1304165327
H,0,-7.0809890433,0.2795690543,0.2711753703	H,0,-7.0664694198,0.3540816388,0.3278665833
H,0,-5.8191028467,-1.6226681381,0.9073011956	H,0,-5.8089082296,-1.5115772639,1.0956933811
C,0,-1.3016334158,-1.5317576865,-0.0069066435	C,0,-1.3167985427,-1.5654553057,0.0472773629
H,0,-1.2389810574,-2.9511433019,0.0445143265	H,0,-1.2670469834,-2.9665025165,0.0802258677
O,0,-0.9966598135,-4.066652777,-0.0340274797	O,0,-1.0580867876,-4.1105604003,0.0065787912
O,0,-2.0524721595,-4.6283739312,-0.7936761614	O,0,-2.053159479,-4.6301568905,-0.8630671352
C,0,-1.5721009806,-4.9013028124,-2.1053266127	C,0,-1.490486874,-4.7946408353,-2.1654905787
H,0,-0.7080791575,-5.5700288102,-2.0695669091	H,0,-0.6229345348,-5.4580173656,-2.1301897149
H,0,-2.4049350326,-5.3915684102,-2.6138973322	H,0,-2.2856998568,-5.2483429357,-2.7599742953
H,0,-1.3110233684,-3.9754240061,-2.6293160878	H,0,-1.2115583469,-3.8275878772,-2.5941347016

TS H25(•$OOCH_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.66005613 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.226872 a.u. 1 imaginary frequency = 1492.5967 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2071483 a.u.	
0, 2 C,0,6.3626038121,0.4844262531,-0.0206393944 C,0,5.6395001945,-0.6678224309,-0.3211518636 C,0,5.7212964319,1.6725608999,0.3663572583 H,0,6.1343580532,-1.5846144871,-0.6189575403 C,0,4.2470488853,-0.61354855,-0.2277470719 C,0,4.3313209001,1.7469756663,0.4652647654 H,0,3.8371205707,2.6641099555,0.7640740165 C,0,3.6184124368,0.5928443768,0.1639218637 C,0,2.1503378852,-1.0097931769,-0.2272952592 N,0,3.2963937511,-1.5989606171,-0.4689165902 N,0,2.2577891934,0.3016403909,0.1527434293 H,0,1.485185085,0.9061218148,0.3851288099 N,0,0.9331403509,-1.6285578542,-0.3460778386 N,0,-0.2029228481,-0.9494274034,-0.0800410413 H,0,0.9063384449,-2.6210908666,-0.5654813472 H,0,6.3162008319,2.5497937896,0.5928068741 C,0,-2.6294586011,-0.9343154247,-0.002898072 C,0,-3.7144734701,-1.6098268609,0.5805400959 C,0,-2.8462231888,0.3088562579,-0.632833613 H,0,-3.5596753133,-2.5755731119,1.0444665447 H,0,-2.0269461922,0.8347840753,-1.1063013136 C,0,-4.983597522,-1.0436845873,0.5634235714 C,0,-4.1079246605,0.8746513094,-0.6446264905 C,0,-5.183146896,0.1927063064,-0.0420121344 H,0,7.444580306,0.4658200082,-0.0856970094 O,0,-4.3048002729,2.0826390468,-1.2425992473 H,0,-5.2375720822,2.3233371432,-1.161470272 O,0,-6.3878615939,0.8337216224,-0.1147936893 H,0,-7.0836421178,0.3163626201,0.3063777736 H,0,-5.8216760316,-1.5616470271,1.0179041738 C,0,-1.3180754348,-1.5453015748,0.0267798068 H,0,-1.2639530753,-2.9583288688,0.0695827776 O,0,-1.0314515344,-4.0835053019,-0.0097359282 O,0,-2.0348169242,-4.6222659922,-0.8536116625 C,0,-1.4813337146,-4.8247144367,-2.151635874 H,0,-0.612754143,-5.4862192398,-2.102719769 H,0,-2.280048882,-5.2959521479,-2.7278427276 H,0,-1.2052496342,-3.8704675766,-2.6121430118	

TS R1_imino(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.50337119 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.227178 a.u. 1 imaginary frequency = 125.6210 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.071427 a.u.	**TS R1_imino(•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.52276427 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.226022 a.u. 1 imaginary frequency = 107.4441 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.1036863 a.u.
0, 2 C,0,-5.9317161122,1.621691039,0.0514238106 C,0,-4.5494918359,1.7992626983,0.0749307682 C,0,-6.5034120608,0.3441866017,-0.0369207082 H,0,-4.1071580784,2.7846437532,0.1490193776 C,0,-3.7517691975,0.6597313179,0.0043944838 C,0,-5.7114578925,-0.8025984431,-0.1045762271 H,0,-6.1548362651,-1.7888203614,-0.1724640066 C,0,-4.3335443568,-0.6246969996,-0.0829858963 C,0,-2.0833280103,-0.825376377,-0.0813332644 N,0,-3.2754016274,-1.5152242548,-0.1329172397 H,0,-7.5821510288,0.2438324496,-0.0515692329 H,0,-3.313876217,-2.5190838241,-0.2026073341 N,0,-0.9254927982,-1.4510805114,-0.1323170522 N,0,0.1102517508,-0.5806921618,-0.0580791077 C,0,1.2832708037,-1.1259570637,-0.0212828148 H,0,1.3784785959,-2.2155804112,-0.0124778753 C,0,2.4941883792,-0.3277910546,0.0158651939 C,0,3.7376004121,-0.9810373449,0.0503910616 C,0,2.4494891781,1.0815540438,0.0164620854 C,0,4.9189785816,-0.2476568622,0.0832935321 C,0,3.6246653473,1.8089463582,0.049809005 C,0,4.8643585088,1.1406736179,0.0820927483 H,0,-6.57849793,2.4893121086,0.105332336 H,0,3.7777069704,-2.0643309811,0.052814409 H,0,1.4941383304,1.5978406963,-0.0023758898 O,0,5.9683312341,1.9578665872,0.1105591813 H,0,6.7767998559,1.436074906,0.1323500009 H,0,5.8806957426,-0.7510970564,0.109929125 O,0,3.5849733287,3.1716121329,0.0480727488 H,0,4.4905188056,3.5056661379,0.0774293371 N,0,-2.3767564952,0.5040669854,0.0109458677 H,0,-1.656819592,1.2999711336,0.0019433621 O,0,-0.7039186386,2.5097876568,-0.0553477334 C,0,-0.9953306243,3.7091898805,-0.6587705799 H,0,-1.9963084788,3.7513010809,-1.1229138835 H,0,-0.9344133814,4.5281151496,0.0842135241 H,0,-0.2410091042,3.9631651921,-1.4247473024	0, 2 C,0,-6.1239491365,1.3501478185,-0.6436774809 C,0,-4.744221537,1.568883849,-0.581538667 C,0,-6.6675103086,0.0710881824,-0.470952673 H,0,-4.3241632106,2.5583493146,-0.7122779197 C,0,-3.9327730574,0.4661100916,-0.3442151247 C,0,-5.8523029709,-1.0391307564,-0.2287827262 H,0,-6.2714811483,-2.0285424266,-0.0938424203 C,0,-4.48254254,-0.8198562919,-0.1686566941 C,0,-2.2294465009,-0.9710843682,0.0155720202 N,0,-3.4104148824,-1.6740365769,0.05172178 H,0,-7.7413350857,-0.0636937982,-0.5237769679 H,0,-3.4526752097,-2.6696342771,0.2048043632 N,0,-1.0592136482,-1.5408791388,0.1832574093 N,0,-0.0295925097,-0.6414629426,0.0644718458 C,0,1.1405180404,-1.1132951185,0.3301485126 H,0,1.2461784245,-2.146908772,0.6710500621 C,0,2.3599490268,-0.3244069879,0.1995112998 C,0,3.5786880892,-0.8844027141,0.6133087953 C,0,2.3586406272,0.9788055658,-0.334225137 C,0,4.766889196,-0.1640396468,0.5094449117 C,0,3.5370360734,1.6960516768,-0.4375103677 C,0,4.7513513618,1.1234759167,-0.013730003 H,0,-6.7842546955,2.1895106071,-0.8269252961 H,0,3.5985543827,-1.8876956005,1.0233612829 H,0,1.4335844973,1.4281696135,-0.6731522993 O,0,5.855773435,1.9179878727,-0.1672491113 H,0,6.657067556,1.45906652,0.1120685578 H,0,5.7053377994,-0.6012618346,0.8335896698 O,0,3.5190884265,2.9589292324,-0.9615331422 H,0,4.4226605375,3.3041714653,-0.9715655549 N,0,-2.5537084835,0.3386698077,-0.2238844919 H,0,-1.8696060317,1.1010344707,-0.2795402747 O,0,-0.9524680355,2.7167040247,-0.3440464332 C,0,-0.6708259509,3.3355903655,0.8477573969 H,0,-0.6223904102,2.6367432191,1.695136519 H,0,0.2251271594,3.9689500089,0.7958381773 H,0,-1.5202178798,4.0185699784,1.0588991317

TS R2_imino(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.50443287 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.225167 a.u. 1 imaginary frequency = 86.3334 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.0694046 a.u.	**TS R5_imino(•OCH_3),** optimization in gas phase UB3LYP/6-311++G**, E= -1025.48629459 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.224527 a.u. 1 imaginary frequency = 1410.2122 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.0602682 a.u.
0, 2 C,0,-5.8305888464,1.67159506,0.0223049739 C,0,-4.4451883492,1.8328364942,-0.016072421 C,0,-6.4154756744,0.4021293227,0.1425919621	0, 2 C,0,5.4232154015,1.7568459147,0.1332798285 C,0,4.023624233,1.7755041872,0.158387898 C,0,6.1279208045,0.5644125172,-0.0396180052

H,0,-3.9955788517,2.8139781156,-0.109691701	H,0,3.4779263297,2.7016266299,0.2933319202
C,0,-3.6686286157,0.6838938187,0.070346238	C,0,3.3650671104,0.5660309559,0.0053986074
C,0,-5.6375646742,-0.7502230909,0.228782283	C,0,5.4617088349,-0.6568501808,-0.1948132607
H,0,-6.0888677428,-1.730168688,0.3200274822	H,0,6.010815736,-1.5810916558,-0.3293842348
C,0,-4.2527996431,-0.5979645611,0.1924517737	C,0,4.0760714097,-0.6368040393,-0.1695884402
C,0,-2.033918132,-0.868489992,0.1775175282	C,0,1.8532123046,-1.1224163738,-0.1957963483
N,0,-2.3009407452,0.4789724813,0.0634235742	N,0,2.0117513298,0.2333588765,-0.0166487063
H,0,-7.4952307916,0.3160954342,0.1679265513	N,0,3.1238504067,-1.6455902231,-0.2940116345
H,0,-1.5563359807,1.1542965244,-0.0070655876	H,0,7.211051466,0.5807253854,-0.0545308026
N,0,-0.8615478886,-1.4616256092,0.2126789922	H,0,1.2177541342,0.8443944274,0.084335027
N,0,0.1558999574,-0.5588078764,0.1162207174	H,0,3.2888277789,-2.6317782814,-0.409411562
C,0,1.3329399954,-1.0977035932,0.1428546722	N,0,0.7724976245,-1.8417741227,-0.2672762449
H,0,1.4185856571,-2.1828210007,0.2334571625	N,0,-0.3580612021,-1.0724297871,-0.1447945666
C,0,2.5579579899,-0.3227026893,0.0580078261	C,0,-2.7728456836,-0.8719465571,-0.0087378596
C,0,3.7887005143,-0.997590905,0.0966107026	C,0,-3.9623848573,-1.5980661951,0.1385783755
C,0,2.5546746479,1.0801801578,-0.0602978166	C,0,-2.8277226817,0.5324466922,-0.078805393
C,0,4.9864778261,-0.2930566587,0.0201351301	C,0,-5.1836834752,-0.9328280231,0.2213581072
C,0,3.7421077455,1.7834039907,-0.1364060558	C,0,-4.0403438152,1.1928701632,0.0055813501
C,0,4.9667583352,1.0908413198,-0.0957479033	C,0,-5.2255524561,0.4530461175,0.1574837509
H,0,-6.4669782289,2.5460837631,-0.0429702887	H,0,5.9662591412,2.6868119291,0.2510560942
H,0,3.8067387414,-2.0774537678,0.1867231422	H,0,-3.920522677,-2.6791003413,0.1839415601
H,0,1.6188311272,1.6217800847,-0.0922027488	H,0,-1.9218560591,1.1116511065,-0.2001534399
O,0,6.0864485912,1.8816026949,-0.1779451074	O,0,-6.3765097655,1.2030003972,0.2293529311
H,0,6.8857879659,1.3467454384,-0.1394557577	H,0,-7.1451616177,0.6334717336,0.3342293953
H,0,5.9358436109,-0.8190211136,0.050464133	H,0,-6.1053150168,-1.4954883694,0.3366878627
O,0,3.7224129081,3.1412974389,-0.2500498882	O,0,-4.0791340524,2.5555646704,-0.0611955366
H,0,4.6330057292,3.461260785,-0.2880701538	H,0,-4.9998822695,2.838945156,0.0086897744
N,0,-3.2300958144,-1.5241031625,0.2550312981	C,0,-1.5068705157,-1.5963036329,-0.0828449945
H,0,-3.3500894325,-2.5848667175,0.3503844691	H,0,-1.6209378873,-2.8598763251,-0.0695716601
O,0,-3.5519566614,-4.0957058302,0.4822594461	O,0,-1.8694615892,-4.1061488488,-0.1321428849
C,0,-4.7339523841,-4.7593091014,0.6912873332	C,0,-1.3172979551,-4.6353033583,-1.308216044
H,0,-4.9480017384,-5.4324782871,-0.1609626011	H,0,-1.5523146685,-5.708876001,-1.3052657578
H,0,-4.655968914,-5.4279284842,1.5680681535	H,0,-1.7597924133,-4.2060225522,-2.2189565195
H,0,-5.6099977335,-4.1021463157,0.832425286	H,0,-0.2272713872,-4.5213809913,-1.3505745866

TS R5_imino(•OCH_3), optimization in solv. water UB3LYP/6-311++G**, E= -1025.50979263 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.225116 a.u. 1 imaginary frequency = 1135.0200 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.0828028 a.u.	**TS R5_imino(•OCH_3),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.49595095 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.225727 a.u. 1 imaginary frequency = 1318.2490 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1025.069771 a.u.
0, 2	0, 2
C,0,5.435463654,1.8345744585,0.3404801267	C,0,5.4215339824,1.7792697633,0.1474851908
C,0,4.0377165183,1.8132033621,0.38815311	C,0,4.0223224067,1.7883916362,0.1822042935
C,0,6.1706829388,0.6853555157,0.0280097564	C,0,6.134514144,0.5914771196,-0.0340574236
H,0,3.466954532,2.7011143897,0.6301650576	H,0,3.4695428785,2.7091352544,0.3236873124
C,0,3.4121831472,0.6058347232,0.1127297124	C,0,3.3729703223,0.573281812,0.0294393776
C,0,5.5381432934,-0.5304549042,-0.2505042378	C,0,5.4774303646,-0.6344011547,-0.1889350929
H,0,6.106324432,-1.4199708647,-0.4926396381	H,0,6.0310909546,-1.5547181563,-0.3298799147
C,0,4.1510963148,-0.5488105289,-0.203670037	C,0,4.0912134578,-0.6231667783,-0.1545636486
C,0,1.9521680297,-1.0858996196,-0.2542711313	C,0,1.8756865089,-1.1234267249,-0.1709302787
N,0,2.0680849043,0.2374163719,0.0750248528	N,0,2.0218159707,0.2301491313,0.0145898273
N,0,3.2233381233,-1.563491055,-0.4253842361	N,0,3.1455661435,-1.6382008196,-0.2769409766
H,0,7.2526141755,0.7354987884,0.0002086351	H,0,7.217410186,0.6163737274,-0.0560184947
H,0,1.2670990702,0.8270096262,0.2425188029	H,0,1.2280534277,0.8412619439,0.1218603684
H,0,3.4229803678,-2.5211791685,-0.670725834	H,0,3.3219542092,-2.6220541623,-0.402338671

N,0,0.877272708,-1.8289968884,-0.3998836763	N,0,0.7960621953,-1.8533791087,-0.2450738562
N,0,-0.2653259871,-1.1247181402,-0.1844512791	N,0,-0.3392388449,-1.1005483322,-0.1150127481
C,0,-2.6722855065,-0.937043318,-0.0103524691	C,0,-2.7530727196,-0.8961346178,0.0116183584
C,0,-3.8481343477,-1.6375691314,0.2951942222	C,0,-3.9425769492,-1.6117142994,0.2051712132
C,0,-2.7469518295,0.4456469481,-0.2719603855	C,0,-2.8079190561,0.5044245969,-0.1213761017
C,0,-5.0727537197,-0.9755111462,0.3510699478	C,0,-5.1630216905,-0.9428444822,0.2738164374
C,0,-3.9618459415,1.104428879,-0.2110742048	C,0,-4.0193676398,1.1685831302,-0.050637925
C,0,-5.1342692656,0.3903916207,0.1026059045	C,0,-5.2051196958,0.4393935359,0.1488726558
H,0,5.9567065011,2.7608423576,0.5506310085	H,0,5.9589367244,2.7126589091,0.2644533159
H,0,-3.7991235938,-2.7020891953,0.4875257456	H,0,-3.9038755572,-2.6897176782,0.2989419841
H,0,-1.853421481,1.0060328211,-0.5172821479	H,0,-1.9025827869,1.0758544946,-0.2801642093
O,0,-6.2790104302,1.1377316823,0.1325163039	O,0,-6.3513210585,1.1925651572,0.2013009962
H,0,-7.0446011326,0.5949462434,0.3564463155	H,0,-7.1232916981,0.6319534928,0.3352812067
H,0,-5.9806519678,-1.5195807417,0.5879759786	H,0,-6.0837655276,-1.4974399494,0.4249497743
O,0,-4.0192361676,2.446955414,-0.4593431323	O,0,-4.057855469,2.5280789131,-0.1778787253
H,0,-4.937267847,2.74009649,-0.3747011644	H,0,-4.9774039767,2.8177309853,-0.108958991
C,0,-1.4052506412,-1.6609874873,-0.052222597	C,0,-1.4882498596,-1.6240466368,-0.045961799
H,0,-1.4869924326,-2.9070301368,0.0223727107	H,0,-1.5930970884,-2.8796248197,-0.0262480221
O,0,-1.6604643961,-4.2167123455,0.0128418161	O,0,-1.8093547338,-4.1502668541,-0.0966308305
C,0,-1.8407747498,-4.6513547725,-1.311049588	C,0,-1.4268372296,-4.6130104333,-1.3656419594
H,0,-2.0229423781,-5.7348308585,-1.2811240538	H,0,-1.6372757618,-5.6914768058,-1.385107648
H,0,-2.7125879225,-4.1882624228,-1.795684279	H,0,-2.0054907922,-4.1526584132,-2.1794922209
H,0,-0.9563079725,-4.4819549661,-1.9407929159	H,0,-0.3567567414,-4.4711213761,-1.5624697746

TS R1(•OOH)_imino, optimization in gas phase UB3LYP/6-311++G**, E= -1061.36150420 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.203581 a.u. 1 imaginary frequency = 1267.6060 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9202508 a.u.	**TS R1(•OOH)_imino,** optimization in solv. water UB3LYP/6-311++G**, E= -1061.38599903 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.204219 a.u. 1 imaginary frequency = 721.0044 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9479114 a.u.
0, 2 C,0,-5.9216156764,1.596049351,-0.1138064337 C,0,-4.5429567531,1.7787053751,-0.1033680458 C,0,-6.4939685803,0.3120899054,-0.0889655118 H,0,-4.0882068357,2.7611091033,-0.1222435098 C,0,-3.744730314,0.633541195,-0.0671267673 C,0,-5.7062388551,-0.8370642383,-0.052794143 H,0,-6.1513834323,-1.8246336475,-0.0336425787 C,0,-4.3271688872,-0.6563997473,-0.0423037405 C,0,-2.0839006402,-0.8313951425,-0.0135287298 N,0,-3.2662122192,-1.5408542971,-0.009426897 H,0,-7.5730033805,0.2124774469,-0.0980867561 H,0,-3.2971926978,-2.5473996353,0.0139008931 N,0,-0.9157970208,-1.45705707,0.0146669465 N,0,0.1140367172,-0.584856906,0.0055487192 C,0,1.2885059003,-1.138195418,0.0328897427 H,0,1.3741275765,-2.2280165095,0.0604465762 C,0,2.5041923674,-0.3517497965,0.0283108514 C,0,3.7421443391,-1.0172585756,0.0608222105 C,0,2.475856644,1.0580663208,-0.0077870148 C,0,4.9309685075,-0.2964454948,0.0578860178 C,0,3.6580492635,1.7736074328,-0.0107775567 C,0,4.8911021584,1.0923097019,0.0223115198 H,0,-6.5717490075,2.4625110688,-0.1417378719 H,0,3.770741909,-2.100482551,0.0882161036 H,0,1.5288445352,1.5863198191,-0.0333040389 O,0,6.0025558102,1.8975148273,0.0162304494 H,0,6.8067445538,1.3692153539,0.0433302133 H,0,5.8875693859,-0.8094246456,0.0831480472 O,0,3.6320929017,3.1355797561,-0.0455672253 H,0,4.541099217,3.4615653389,-0.0413449613 N,0,-2.3732769866,0.4933848553,-0.0487148424 H,0,-1.5998562922,1.3487393882,-0.0622259364 O,0,-0.7378889677,2.3865096514,-0.0801913839 O,0,-1.5702265437,3.5273215735,-0.1202063909 H,0,-0.9257097863,4.2484178501,-0.1349671246	0, 2 C,0,-5.9440799802,1.5743981044,-0.1094046285 C,0,-4.5662457015,1.7714066838,-0.0948827287 C,0,-6.5030905012,0.2831239006,-0.0904455882 H,0,-4.1264241639,2.7604611339,-0.1097250805 C,0,-3.7610743269,0.6326986692,-0.0606765673 C,0,-5.7046636757,-0.8581620425,-0.055987685 H,0,-6.1348945142,-1.8515294532,-0.0416312858 C,0,-4.3267408916,-0.6624349298,-0.0411790972 C,0,-2.0839156265,-0.8396165472,-0.0081584511 N,0,-3.2622777112,-1.5421603337,-0.0082440591 H,0,-7.5808433814,0.1729920432,-0.1027663924 H,0,-3.3061798424,-2.5502259873,0.0103299624 N,0,-0.9090316274,-1.4487874348,0.0179377714 N,0,0.120880238,-0.568802371,0.011349444 C,0,1.2965100389,-1.1245346606,0.0312834836 H,0,1.3802794281,-2.2138015183,0.0511009846 C,0,2.5183733558,-0.350767415,0.0279861246 C,0,3.749623741,-1.0311022553,0.0529476642 C,0,2.5123774087,1.0604412372,0.0003772759 C,0,4.9488649633,-0.3282182699,0.0511161828 C,0,3.7030022466,1.7591743452,-0.0009847253 C,0,4.9317653693,1.063094601,0.0245969295 H,0,-6.6023934845,2.4344806185,-0.1359227374 H,0,3.7649958326,-2.114452922,0.0734812941 H,0,1.574002358,1.6028112932,-0.0204994496 O,0,6.0420987581,1.8522768338,0.0207434413 H,0,6.8508481506,1.3256782443,0.0427682161 H,0,5.8966568196,-0.8546816913,0.0703195327 O,0,3.691708034,3.1236575611,-0.0269347152 H,0,4.6039348906,3.4457203261,-0.0221083444 N,0,-2.386260023,0.4890190452,-0.0387971768 H,0,-1.675227342,1.2895175222,-0.0551203016 O,0,-0.7585028682,2.5504736607,-0.0953686106 O,0,-1.6440346643,3.6480980726,-0.125870264 H,0,-1.0524923074,4.4135529356,-0.1860404185

TS R1(•OOH)_imino, optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.37134407 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.203672 a.u. 1 imaginary frequency = 1084.2853 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9319845 a.u.	**TS R2(•OOH),** optimization in gas phase UB3LYP/6-311++G**, E= -1061.36050144 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.201551 a.u. 1 imaginary frequency = 1431.3047 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9162948 a.u.
0, 2 C,0,-5.9341597737,1.5855925059,-0.117892419 C,0,-4.5567005996,1.7765628003,-0.1047440395 C,0,-6.4991545205,0.2972665321,-0.093488392	0, 2 C,0,-5.9062539875,1.8644704773,-0.0626561034 C,0,-4.51916035,1.9964123662,-0.0805612484 C,0,-6.5240552304,0.6045722298,0.0302285083

H,0,-4.1090720958,2.7620857,-0.1234468619	H,0,-4.0469974856,2.968823126,-0.1521095037
C,0,-3.7530371039,0.6352620032,-0.0660806597	C,0,-3.7712511648,0.8261761158,-0.0021752188
C,0,-5.7057124941,-0.8473155889,-0.0548011475	C,0,-5.7779430024,-0.5656836661,0.1079088935
H,0,-6.1440300585,-1.8376977679,-0.0365533808	H,0,-6.2485622082,-1.5383251472,0.1799708848
C,0,-4.3270830188,-0.6579996294,-0.0412681837	C,0,-4.3864805317,-0.4457210502,0.0909310153
C,0,-2.0850026877,-0.8261508794,-0.0086757863	C,0,-2.1984212782,-0.7757310148,0.1020313458
N,0,-3.2630708824,-1.5375990026,-0.0055516473	N,0,-2.4120196892,0.583154246,0.0071672334
H,0,-7.5775626211,0.1918518935,-0.1050487304	H,0,-7.6059798335,0.5466919166,0.0411451106
H,0,-3.2960405823,-2.5448772143,0.0185943518	H,0,-1.6467540195,1.2372558967,-0.0395387723
N,0,-0.9121241945,-1.4446200122,0.0205729981	N,0,-1.0343654137,-1.4059571228,0.141052011
N,0,0.1166084301,-0.5701677248,0.0108070747	N,0,0.0053319235,-0.5373537275,0.0818767649
C,0,1.2915322924,-1.1260517723,0.0354616973	C,0,1.1671810928,-1.1171461288,0.1165025843
H,0,1.3747573763,-2.2158390931,0.0612410574	H,0,1.2130793717,-2.2060012412,0.1860379936
C,0,2.5102388976,-0.3469257083,0.0295542126	C,0,2.4149457923,-0.3819882003,0.0674838287
C,0,3.7440215226,-1.0216333964,0.058410381	C,0,3.6233401799,-1.0976212833,0.1089876621
C,0,2.493206207,1.0637109599,-0.0045783326	C,0,2.4577496729,1.0232553202,-0.0194056084
C,0,4.9383660634,-0.3107627791,0.0538348032	C,0,4.8433886626,-0.4307800896,0.0651914718
C,0,3.6806609767,1.7695200582,-0.0087401589	C,0,3.6677667551,1.6889702217,-0.0629984978
C,0,4.9103618937,1.0791302191,0.0206336283	C,0,4.8690832675,0.955655585,-0.0204325828
H,0,-6.5893492327,2.4481074155,-0.1477587269	H,0,-6.5226460298,2.7537276824,-0.1218711704
H,0,3.7646225216,-2.1049508801,0.0841404493	H,0,3.6050782673,-2.1791423515,0.1753258755
H,0,1.5501194009,1.5988023045,-0.0278863848	H,0,1.5400753229,1.5949220344,-0.0522304376
O,0,6.0239294879,1.8739844095,0.0134883176	O,0,6.0135320092,1.7109682764,-0.069181831
H,0,6.8282165749,1.3434403324,0.0369936297	H,0,6.7955909411,1.1509911615,-0.0307999363
H,0,5.8907162473,-0.8306010787,0.0756859516	H,0,5.7751118379,-0.9871645129,0.0974297054
O,0,3.6648177504,3.1324699502,-0.0413415089	O,0,3.6935373392,3.0483378665,-0.146320214
H,0,4.576010592,3.4543760187,-0.0382170868	H,0,4.6140811769,3.3405431911,-0.1628618611
N,0,-2.3805802792,0.4984740953,-0.0451928234	N,0,-3.399896873,-1.4052201475,0.1500999449
H,0,-1.62891434,1.3420263443,-0.0590362709	H,0,-3.5904344008,-2.5519442547,0.2692884439
O,0,-0.7558743715,2.4288194046,-0.0793597078	O,0,-4.0205824916,-3.7933410524,0.4285262871
O,0,-1.6069017212,3.5609025918,-0.1171406911	O,0,-2.882121284,-4.613705243,0.4869521184
H,0,-0.9762666575,4.2946059886,-0.1370256124	H,0,-3.2688808991,-5.4782250698,0.6868132026

TS R2(•OOH)_imino, optimization in solv. water UB3LYP/6-311++G**, E= -1061.38632971 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.203134 a.u. 1 imaginary frequency = 818.4330 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9457501 a.u.	**TS R2(•OOH)_imino,** optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.37112528 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.202851 a.u. 1 imaginary frequency = 1188.0968 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9290742 a.u.
0, 2	0, 2
C,0,-5.9235141905,1.8940840308,-0.0970742432	C,0,-5.9119251208,1.8660565704,-0.0681797692
C,0,-4.5358939771,2.0192619796,-0.1098973333	C,0,-4.5253751534,1.9986960601,-0.0868789522
C,0,-6.5491837039,0.6375371883,-0.0004998794	C,0,-6.5304545042,0.6050568217,0.0194476853
H,0,-4.0545923284,2.9862139768,-0.1842079094	H,0,-4.0520167379,2.9705253322,-0.1538187082
C,0,-3.7952307189,0.8444711923,-0.0226044899	C,0,-3.7778205979,0.8271633094,-0.0149163039
C,0,-5.8096950401,-0.5379709692,0.085983185	C,0,-5.7850357024,-0.5659559323,0.0905783408
H,0,-6.2905129384,-1.505118755,0.1601764634	H,0,-6.2572570926,-1.5379141504,0.1585892735
C,0,-4.4196881199,-0.4202071358,0.0735114764	C,0,-4.3938290447,-0.4440755651,0.0723558084
C,0,-2.2114117268,-0.7463861629,0.0926698426	C,0,-2.2003202911,-0.7691361124,0.0784861167
N,0,-2.4336729597,0.6023147011,-0.0071233066	N,0,-2.4180096702,0.5865119527,-0.0083899987
H,0,-7.6312109513,0.5847311252,0.0063029778	H,0,-7.6123011481,0.5474115991,0.031366069
H,0,-1.6804814924,1.2727009115,-0.0563087113	H,0,-1.6589413975,1.2490502277,-0.0520375307
N,0,-1.0566183798,-1.3912695866,0.1370318876	N,0,-1.0371086325,-1.4032325092,0.1114252756
N,0,-0.0020347945,-0.5351440787,0.0839504551	N,0,0.0056399503,-0.5376363759,0.0636930531

C,0,1.156821367,-1.1218469861,0.114012405	C,0,1.1675568675,-1.1204562023,0.0860725335
H,0,1.206105953,-2.2113716775,0.1725553282	H,0,1.2146612968,-2.2102705605,0.1353526997
C,0,2.4055172599,-0.3916256076,0.0746185411	C,0,2.4142038955,-0.3856508423,0.0499089719
C,0,3.6115086659,-1.1147234047,0.1050307616	C,0,3.6226784962,-1.1035546286,0.0686834016
C,0,2.4533320577,1.0166869097,0.0099639854	C,0,2.4568261321,1.022322323,-0.0005032595
C,0,4.8354426007,-0.4559983321,0.0722933429	C,0,4.842998981,-0.4374352348,0.0378302247
C,0,3.6675171647,1.6733166116,-0.0213714961	C,0,3.667239632,1.6867822593,-0.0302902768
C,0,4.8694736389,0.9337796382,0.0101288513	C,0,4.869791531,0.9517288262,-0.0107891471
H,0,-6.5349730167,2.7859715012,-0.163196143	H,0,-6.528626407,2.7553364482,-0.1224048746
H,0,3.5882245481,-2.1969986001,0.1539594428	H,0,3.604040103,-2.186342859,0.1068789008
H,0,1.5378158717,1.5936176797,-0.0138515984	H,0,1.5390865925,1.5950195398,-0.0144263797
O,0,6.0077223854,1.6817032559,-0.0247379888	O,0,6.0107129683,1.7051337353,-0.0424892458
H,0,6.7966364292,1.127004819,0.0149523292	H,0,6.7959245732,1.1469394116,-0.0144843748
H,0,5.7636452138,-1.0161521264,0.0954105898	H,0,5.7747329412,-0.9935312223,0.0518429565
O,0,3.7029147852,3.0357823987,-0.0816330518	O,0,3.6949140417,3.0487740854,-0.0771631709
H,0,4.6257195015,3.3262970679,-0.0880315895	H,0,4.6158501343,3.3422740557,-0.0860752478
N,0,-3.4211383674,-1.3725934921,0.1396797049	N,0,-3.4025351997,-1.4002500847,0.1233185029
H,0,-3.5590313202,-2.4288568058,0.2449609104	H,0,-3.5776046901,-2.5143377077,0.2556993771
O,0,-3.9435755865,-3.9264457837,0.4295796047	O,0,-4.007498281,-3.8125842555,0.4600821647
O,0,-2.7607972814,-4.6806627916,0.5043624181	O,0,-2.8572889256,-4.6240435053,0.5503345323
H,0,-3.0790715491,-5.5782266915,0.6872112375	H,0,-3.2268405396,-5.4744988093,0.8287093518

TS R3(•OOH)_imino, optimization in gas phase UB3LYP/6-311++G**, E= -1061.36589210 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.203508 a.u. 1 imaginary frequency = 1253.8959 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9180204 a.u.	**TS R3(•OOH)_imino,** optimization in solv. water UB3LYP/6-311++G**, E= -1061.38940544 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.205143 a.u. 1 imaginary frequency = 842.3080 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9482925 a.u.
0, 2	0, 2
C,0,-5.618669297,1.9695253999,0.3838595847	C,0,-5.3361040151,1.8164182476,-0.0851733807
C,0,-4.2255208432,2.0795640685,0.3638547552	C,0,-3.9478660666,1.9463060863,-0.1423003342
C,0,-6.251543439,0.7263809295,0.287703092	C,0,-5.9473471552,0.5711026641,0.1261516561
H,0,-3.7362399134,3.042954788,0.4388028922	H,0,-3.4748545132,2.9063588251,-0.3054233725
C,0,-3.4945841927,0.9064156612,0.2448630635	C,0,-3.1967922006,0.7882136518,0.0191830997
C,0,-5.5158663088,-0.4559246046,0.1678918663	C,0,-5.1942040435,-0.5921213711,0.2879710533
H,0,-6.0081714338,-1.418029733,0.0931995049	H,0,-5.6642639493,-1.5536630088,0.4506011552
C,0,-4.1330320607,-0.3464326416,0.1481890515	C,0,-3.8114047508,-0.4630714386,0.2307293699
C,0,-1.8909712222,-0.6866126388,0.0707036862	C,0,-1.574628776,-0.7698287716,0.2173258462
N,0,-2.1270838905,0.6590344981,0.1943978274	N,0,-1.8272707928,0.5584761695,0.0173017074
N,0,-3.1217766192,-1.2962428249,0.0430873228	N,0,-2.7857710064,-1.3907930771,0.3467371939
H,0,-7.3334738399,0.6758217538,0.3061184882	H,0,-7.0282209142,0.5097332418,0.1645032726
H,0,-1.3631469633,1.3169511913,0.2321814288	H,0,-1.0843220372,1.2314684222,-0.1039958925
H,0,-3.2237191289,-2.2945857269,-0.0415403225	H,0,-2.8826740332,-2.3828900901,0.5048870829
N,0,-0.7569160435,-1.3337973277,-0.0106548943	N,0,-0.4198520437,-1.4038161466,0.283776205
N,0,0.2989398008,-0.4713655839,0.044405235	N,0,0.6235849877,-0.5461335995,0.1295277086
C,0,1.462650736,-1.0340897702,-0.0345445342	C,0,1.7957672274,-1.1052129483,0.1645256116
H,0,1.527989821,-2.1198601941,-0.1363969692	H,0,1.8751910742,-2.1860836107,0.3008847276
C,0,2.6930825221,-0.2749071121,0.0055580511	C,0,3.0179862937,-0.3473971019,0.0266707894
C,0,3.9196722722,-0.9834995513,-0.0919660243	C,0,4.2487323566,-1.0387265469,0.0538349706
C,0,2.7139949882,1.1206240646,0.1437830497	C,0,3.0190335873,1.0539786564,-0.1353027218
C,0,5.134565404,-0.3220608718,-0.0603205144	C,0,5.450052149,-0.3570127506,-0.0770208987
C,0,3.9239168727,1.8064238103,0.1751286249	C,0,4.2135065676,1.7407725894,-0.2656864863
C,0,5.1462587089,1.0668062781,0.0674393726	C,0,5.4408107204,1.0271324029,-0.2353539608
H,0,-6.2181306449,2.8670842888,0.4759767911	H,0,-5.9542937807,2.6976417873,-0.2067438087

H,0,3.8983946039,-2.0630008003,-0.1909120275	H,0,4.2535117889,-2.1156362204,0.1763097187
H,0,1.7865966311,1.6717301284,0.2256004791	H,0,2.0818106546,1.5948861123,-0.159682
O,0,6.3001201101,1.7494112505,0.0926440278	O,0,6.6036727978,1.7069581528,-0.358777372
H,0,6.0595188346,2.69021218,0.1772874629	H,0,6.387365498,2.6492368228,-0.449181423
H,0,6.0749903324,-0.8534625322,-0.1376669426	H,0,6.3987236261,-0.8795349083,-0.0568458644
O,0,4.075825485,3.113226784,0.3030572909	O,0,4.3375485921,3.0739577508,-0.4238324346
H,0,3.1471758858,3.7013764026,0.1763431183	H,0,3.4522944433,3.5746704082,-0.3808056469
O,0,2.0502107769,4.3769059202,-0.0729714354	O,0,2.2221225477,4.5090595486,-0.281064674
O,0,2.287966946,5.6533065721,0.459024984	O,0,1.0678350955,3.7704541576,-0.5340744407
H,0,1.6484270793,6.1986891933,-0.0214301467	H,0,0.3493884906,4.4019965028,-0.3685203269

TS R3(•OOH)_imino, optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.37590960 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.203236 a.u. 1 imaginary frequency = 986.4250 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9297655 a.u.	**TS R4(•OOH)_imino,** optimization in gas phase UB3LYP/6-311++G**, E= -1061.36802932 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.204584 a.u. 1 imaginary frequency = 752.2540 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9218729 a.u.
0, 2	0, 2
C,0,-5.6179770517,1.9795959599,0.2821423482	C,0,-5.7133037176,1.5823673407,0.4326540704
C,0,-4.2270150833,2.0958082693,0.2517593759	C,0,-4.3254708759,1.750804154,0.4423058902
C,0,-6.2470350254,0.7281504508,0.2579607675	C,0,-6.2940956401,0.3566320589,0.0947598843
H,0,-3.7408967656,3.0632046741,0.2705432746	H,0,-3.8770091733,2.7013243639,0.7043962563
C,0,-3.4926372540,0.918592220,0.19627346440	C,0,-3.5468905475,0.6540673806,0.1033920548
C,0,-5.5094508716,-0.4558250351,0.2020652538	C,0,-5.5099448806,-0.7490934145,-0.24686917
H,0,-5.9966067106,-1.4227686957,0.1839470014	H,0,-5.9621538497,-1.6981578053,-0.5083687313
C,0,-4.1259565135,-0.3402756542,0.1712044912	C,0,-4.1329610736,-0.5815163832,-0.2373647327
C,0,-1.8890984626,-0.6729317799,0.1049515268	C,0,-1.8778426458,-0.809131697,-0.3673256811
N,0,-2.1252469074,0.6733895516,0.1546035987	N,0,-2.1700310449,0.4771292736,0.0129657816
N,0,-3.1118550687,-1.2892326063,0.1154265642	N,0,-3.0837827529,-1.4510584812,-0.51877924
H,0,-7.3287303119,0.6758233637,0.2830284246	H,0,-7.3729372378,0.2588064876,0.0968408227
H,0,-1.3677952524,1.3407861633,0.1593171393	H,0,-1.4336557961,1.1437911679,0.1850646066
H,0,-3.2149966472,-2.2917864958,0.0832715485	H,0,-3.1452080554,-2.416720899,-0.7978485315
N,0,-0.746829455,-1.3241251982,0.0551562367	N,0,-0.7201834938,-1.3818783737,-0.565049887
N,0,0.3052186363,-0.4656711574,0.057276209	N,0,0.3067489213,-0.5087409303,-0.342370579
C,0,1.4717472359,-1.0366317815,0.0074910126	C,0,1.4860922748,-1.0183841016,-0.5158415211
H,0,1.5342517957,-2.126341835,-0.0322158222	H,0,1.5751871842,-2.066199689,-0.8114720014
C,0,2.6999934675,-0.2819446148,0.0028575366	C,0,2.7004780337,-0.2602369369,-0.3340480373
C,0,3.923502679,-0.997567322,-0.0617890269	C,0,3.9401473515,-0.9152087387,-0.522813041
C,0,2.72434512,1.1241421784,0.0586008212	C,0,2.6941756732,1.1025479892,0.0314128545
C,0,5.1371354799,-0.3338850033,-0.0697977554	C,0,5.137459106,-0.2475231292,-0.3479284482
C,0,3.9328072718,1.806107292,0.0520448956	C,0,3.881778957,1.778420365,0.197166732
C,0,5.1504485797,1.0604693504,-0.012137394	C,0,5.1318654652,1.11276691,0.0097824515
H,0,-6.2220576755,2.877721948,0.3255382867	H,0,-6.3489627018,2.4201202943,0.6925930843
H,0,3.9018037058,-2.0803855493,-0.1059097287	H,0,3.9458319716,-1.964062115,-0.7979797567
H,0,1.7960015201,1.677754071,0.107831527	H,0,1.7574157923,1.6233378863,0.1765909214
O,0,6.3114110835,1.7361483212,-0.015201757	H,0,6.0885551374,-0.7485769512,-0.4820930955
H,0,6.0853083029,2.6823156271,0.0340053032	O,0,3.8972959208,3.0891070935,0.538119122
H,0,6.077325318,-0.8692624931,-0.1181782818	H,0,4.8282126017,3.3599378239,0.5804413637
O,0,4.0887295914,3.124501032,0.100102064	O,0,6.2114830831,1.8505172881,0.2035605509
H,0,3.1651092057,3.6779549915,0.1980691815	H,0,7.0947100307,1.4436430917,-0.2453627981
O,0,1.9828956347,4.3405584505,0.343725424	O,0,8.1735305748,0.9921721912,-0.9653274919
O,0,2.3260856076,5.7075185104,0.3394125432	O,0,9.2793594479,1.2393778589,-0.1569809581
H,0,1.481516791,6.1366660462,0.5393211858	H,0,10.0044043493,1.2963309765,-0.7978881253

TS R4(•OOH)_imino, optimization in solv. water UB3LYP/6-311++G**, E= -1061.38958826 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.204205 a.u. 1 imaginary frequency = 977.7658 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.945634 a.u.	**TS R4(•OOH)_imino,** optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.37752723 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.204854 a.u. 1 imaginary frequency = 516.5886 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9346891 a.u.
0, 2 C,0,-5.6972085441,1.5634410123,0.4134808093 C,0,-4.3123579598,1.7464903372,0.4138145369 C,0,-6.2701271006,0.3216396195,0.1054616935 H,0,-3.8675784623,2.7046606164,0.6513488145 C,0,-3.5278660124,0.6454735537,0.095859106 C,0,-5.4811425294,-0.7855444292,-0.2143042338 H,0,-5.9223380165,-1.7451944068,-0.4525279447 C,0,-4.1039840191,-0.6026972478,-0.2140139492 C,0,-1.8563033397,-0.8108976784,-0.3482889752 N,0,-2.1511715603,0.4779004949,0.0033176611 N,0,-3.0499195167,-1.4676355969,-0.4802050243 H,0,-7.3483130556,0.2162844033,0.1148939881 H,0,-1.4314082307,1.1675046457,0.1596527873 H,0,-3.1171410422,-2.4414908986,-0.7351067301 N,0,-0.6859342175,-1.3827654958,-0.5400913145 N,0,0.3362118058,-0.5016471316,-0.3446100693 C,0,1.5212009451,-1.0010654796,-0.5115537162 H,0,1.6303478662,-2.0538181773,-0.7826559863 C,0,2.7277606059,-0.2189530248,-0.3517675203 C,0,3.9746347018,-0.8540462189,-0.5247031384 C,0,2.7015926631,1.1535716359,-0.0215513046 C,0,5.1617935534,-0.1527318395,-0.3695407768 C,0,3.8793211143,1.8548743996,0.1262838012 C,0,5.1303936564,1.2084897147,-0.0477443111 H,0,-6.3405491539,2.4005000931,0.6566380618 H,0,4.0052773331,-1.9090223582,-0.772040573 H,0,1.7564213222,1.6638898935,0.1127073041 H,0,6.1188427165,-0.6460029002,-0.4918296074 O,0,3.85699626,3.1814485042,0.4379851606 H,0,4.7733480971,3.4954681252,0.4691200169 O,0,6.2149005961,1.9810413201,0.1260639585 H,0,7.0608786726,1.5556904536,-0.2385659869 O,0,8.3417283647,1.0152108107,-0.9213027546 O,0,9.361291067,1.2008468543,-0.0139237334 H,0,10.1718272296,1.0889663656,-0.5395123999	0, 2 C,0,-5.7145765257,1.572592824,0.4584717645 C,0,-4.3277381727,1.7428209646,0.4713211627 C,0,-6.2953320343,0.3503769863,0.1005915351 H,0,-3.8785103731,2.6888152046,0.7475125294 C,0,-3.5496666254,0.6502204077,0.1150697699 C,0,-5.5123049592,-0.7495736105,-0.2585626126 H,0,-5.9628698635,-1.6945871695,-0.5362574756 C,0,-4.1345944904,-0.5800256797,-0.2454385869 C,0,-1.8837386146,-0.8022013082,-0.379965283 N,0,-2.1732325118,0.4753732527,0.0214124773 N,0,-3.0852822336,-1.443370132,-0.5408175899 H,0,-7.3742350957,0.2529319706,0.1010658754 H,0,-1.4426292595,1.1453829689,0.2065621268 H,0,-3.1512937465,-2.4051327128,-0.8351402365 N,0,-0.721493458,-1.3730674808,-0.5911656539 N,0,0.3055971995,-0.5073968379,-0.3575428518 C,0,1.4858779999,-1.0116610932,-0.5484864404 H,0,1.5778642394,-2.0526830331,-0.8664782733 C,0,2.6991279093,-0.2537863776,-0.3576194829 C,0,3.9390635811,-0.8978570659,-0.5694232484 C,0,2.6913982124,1.1007863848,0.0399971024 C,0,5.135102784,-0.2261894025,-0.3867311888 C,0,3.8776905134,1.7774127504,0.2146545521 C,0,5.1251596677,1.1222230594,0.0030449841 H,0,-6.3514991043,2.4053229795,0.731258355 H,0,3.9498660051,-1.9398028671,-0.8688459844 H,0,1.7537827305,1.6149610737,0.2039129722 H,0,6.0864173395,-0.7217554049,-0.5386387215 O,0,3.8841513456,3.0830060069,0.5883414733 H,0,4.8103906823,3.3675142762,0.6310108488 O,0,6.2098657734,1.8635182344,0.2087345895 H,0,7.0708836429,1.4635273925,-0.2272401946 O,0,8.2185945342,1.0019458095,-0.965770952 O,0,9.3000963791,1.1811578337,-0.1119878407 H,0,10.0583649191,1.215912145,-0.7165148813

TS R5(•OOH)_imino, optimization in gas phase UB3LYP/6-311++G**, E= -1061.33273799 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.201111 a.u. 1 imaginary frequency = 1581.2403 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9001636 a.u.	**TS R5(•OOH)_imino,** optimization in solv. water UB3LYP/6-311++G**, E= -1061.36145775 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.200553 a.u. 1 imaginary frequency = 1408.1085 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9278999 a.u.
0, 2 C,0,5.4262037404,1.7983063126,0.2544201615 C,0,4.0270401017,1.7970658201,0.2971571619 C,0,6.1433796374,0.6273732043,0.002640004	0, 2 C,0,5.4112958481,1.748485723,0.5268203289 C,0,4.0150340622,1.7230643091,0.5981470832 C,0,6.1361642291,0.652166323,0.0445797542

H,0,3.4716054703,2.7065512347,0.4922380542	H,0,3.4527407471,2.5700099313,0.9710902107
C,0,3.3820912893,0.5900856375,0.0803351186	C,0,3.3800046599,0.5655920528,0.171151921
C,0,5.4908861082,-0.5912549452,-0.2163386646	C,0,5.4942228447,-0.5126232576,-0.3864029362
H,0,6.0494917304,-1.4987959428,-0.4114185396	H,0,6.0537257119,-1.361023573,-0.7602427883
C,0,4.105385573,-0.5910793096,-0.1735558158	C,0,4.1081849796,-0.5351404913,-0.3152067242
C,0,1.8898933025,-1.1030152271,-0.205469451	C,0,1.9085080614,-1.0573065635,-0.396753341
N,0,2.03215482,0.241688129,0.0528801513	N,0,2.0339364226,0.2066535938,0.1093411634
N,0,3.1646159265,-1.6033996269,-0.3435153933	N,0,3.1726004019,-1.5086317565,-0.6563298654
H,0,7.2259331475,0.6589507491,-0.0244747965	H,0,7.2175103161,0.7047040033,0.0030112043
H,0,1.2343136536,0.8371045769,0.2037580267	H,0,1.239055758,0.7695085128,0.3718800815
H,0,3.3365120505,-2.5755860968,-0.5417045524	H,0,3.3639128991,-2.4236535637,-1.0352239383
N,0,0.8217586334,-1.8366280571,-0.3144725192	N,0,0.8277356567,-1.7748998192,-0.6230051136
N,0,-0.3231518045,-1.1086141065,-0.1524805212	N,0,-0.3079963776,-1.1101346724,-0.3028598683
C,0,-2.7345985145,-0.8837143972,-0.0247920828	C,0,-2.7037316332,-0.8867141501,-0.0532023985
C,0,-3.912152617,-1.5802973745,0.2791123901	C,0,-3.8617048171,-1.5532517932,0.3740078062
C,0,-2.79618683,0.5061950432,-0.2389637659	C,0,-2.7871317664,0.4771675053,-0.4001420732
C,0,-5.124096126,-0.9009484733,0.3823891681	C,0,-5.0745482732,-0.8754033739,0.4694778164
C,0,-3.9995470311,1.181659709,-0.136334157	C,0,-3.9906714825,1.1520077752,-0.3024410747
C,0,-5.1706283434,0.4712571141,0.1781716565	C,0,-5.1435750534,0.4722793599,0.1362074483
H,0,5.9591726573,2.7267664372,0.4202222837	H,0,5.9402804783,2.6360289774,0.852683839
H,0,-3.8725077467,-2.6509409085,0.4355511542	H,0,-3.8106983346,-2.6035559293,0.6322819369
H,0,-1.9023344863,1.0619416904,-0.490577617	H,0,-1.9085285547,1.0100734681,-0.7419767612
O,0,-6.3128487684,1.2331689638,0.2535550011	O,0,-6.2782746584,1.2312606236,0.1932629242
H,0,-7.0751286093,0.682488089,0.4583262016	H,0,-7.0315998867,0.712192175,0.5001731032
H,0,-6.0345478659,-1.4414027754,0.6235349363	H,0,-5.9676714682,-1.3927576994,0.8023756407
O,0,-4.0423603256,2.5291070629,-0.3443200245	O,0,-4.0563197928,2.4750498153,-0.6357465087
H,0,-4.9558667106,2.8261760077,-0.2425558856	H,0,-4.9648493229,2.7833693009,-0.511347845
C,0,-1.4744845009,-1.6157971173,-0.1165857939	C,0,-1.448778847,-1.6248890866,-0.1401328616
H,0,-1.591606463,-2.9883091692,-0.1753990432	H,0,-1.5389858355,-2.9684570785,-0.075671043
O,0,-1.8311116501,-4.1395290844,-0.2116332879	O,0,-1.6657748355,-4.178215641,-0.0198380712
O,0,-1.5814803984,-4.5441188457,-1.5506289032	O,0,-1.8480723664,-4.6145195751,-1.3730818968
H,0,-2.47179792,-4.5734778139,-1.9294645751	H,0,-2.8119987706,-4.6594574257,-1.4572851527

TS R5(•OOH)_imino, optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.34465348 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.200484 a.u. 1 imaginary frequency = 1551.7207 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9119552 a.u.	
0, 2 C,0,5.4208833966,1.7935201015,0.3272915207 C,0,4.0223086273,1.7857015938,0.3763550439 C,0,6.142104809,0.6370603475,0.0187083045 H,0,3.4630688075,2.6819533467,0.6158436205 C,0,3.3822904064,0.5860818493,0.1064445803 C,0,5.4944283985,-0.5728828287,-0.253763214 H,0,6.0542661186,-1.4690138883,-0.4921447564 C,0,4.1084742159,-0.5784103869,-0.2054197482 C,0,1.8988177409,-1.0958869582,-0.2499937209 N,0,2.0335274739,0.2329145586,0.0700553637 N,0,3.1704526699,-1.5850666195,-0.4193483289 H,0,7.2244400545,0.6746085985,-0.0110086905 H,0,1.2376285164,0.823923874,0.2498309458 H,0,3.3512386493,-2.5465939161,-0.6606631022	

N,0,0.8276116918,-1.8303466009,-0.3877112688 N,0,-0.3169771229,-1.1201397506,-0.1829239009 C,0,-2.7260578262,-0.8911362761,-0.0257968425 C,0,-3.8961550293,-1.5741987388,0.3338286003 C,0,-2.7946224722,0.4890319035,-0.2974333537 C,0,-5.1070993684,-0.8930536423,0.4365215539 C,0,-3.9969156759,1.1663081363,-0.1947100035 C,0,-5.1611848602,0.4699805336,0.175918828 H,0,5.951578513,2.7152737856,0.5332462724 H,0,-3.8535973468,-2.6370717089,0.535748267 H,0,-1.9072200022,1.0340181291,-0.5927734067 O,0,-6.299426865,1.2324277749,0.2449605386 H,0,-7.060083028,0.6934101052,0.4882466803 H,0,-6.0106204387,-1.4229214099,0.7208024909 O,0,-4.0467948123,2.5048884438,-0.4578392786 H,0,-4.9582311627,2.8074885127,-0.3480607507 C,0,-1.4680393769,-1.6258866436,-0.1177322347 H,0,-1.5786554622,-2.9842938288,-0.1607717873 O,0,-1.7765049526,-4.1601619026,-0.1937135109 O,0,-1.6727499909,-4.5332022988,-1.564189297 H,0,-2.5981832961,-4.5593461955,-1.8482034144	

TS R1(•OOCH$_3$)_imino, optimization in gas phase UB3LYP/6-311++G**, E= -1100.67533124 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228547 a.u. 1 imaginary frequency = 1721.4289 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2140049 a.u.	**TS R1(•OOCH$_3$)_imino,** optimization in solv. water UB3LYP/6-311++G**, E= -1100.70247331 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.229194 a.u. 1 imaginary frequency = 1091.7771 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2445371 a.u.
0, 2 C,0,-5.9901529884,1.5461773221,-0.6187723457 C,0,-4.6151367455,1.7472604166,-0.5624228575 C,0,-6.5570920981,0.2763702281,-0.411509793 H,0,-4.1725350749,2.7236955323,-0.7138602954 C,0,-3.8108478444,0.6364114507,-0.2988669792 C,0,-5.76602072,-0.8379049062,-0.1390335479 H,0,-6.2059900565,-1.8146443101,0.0233395991 C,0,-4.390339322,-0.6376968356,-0.0864192533 C,0,-2.1509479676,-0.7689062953,0.0855549265 N,0,-3.3276563039,-1.4851149467,0.1549915407 H,0,-7.6334836127,0.1616336042,-0.4607299918 H,0,-3.3504957124,-2.4762398363,0.3342008633 N,0,-0.9883795322,-1.3893088209,0.2609679803 N,0,0.0578362334,-0.5589904712,0.1079315649 C,0,1.2145589776,-1.0735936618,0.3956902424 H,0,1.2762003102,-2.0910448679,0.7912212713 C,0,2.4408981606,-0.3245899074,0.2148484778 C,0,3.6657584164,-0.9073479223,0.5820790605 C,0,2.431437484,0.9790462824,-0.3210596705 C,0,4.8563908274,-0.2055925247,0.4248416917 C,0,3.6129502461,1.6789811727,-0.4699862914 C,0,4.8327705326,1.0824297808,-0.0969300876 H,0,-6.6419315483,2.3877210527,-0.8219381035 H,0,3.6835136513,-1.9096072007,0.9945417078 H,0,1.4928492221,1.4339934985,-0.613724062 O,0,5.9469833485,1.861444141,-0.2898414128 H,0,6.7440132735,1.3851991556,-0.0359993922 H,0,5.8026044641,-0.6552051402,0.7102271018 O,0,3.5945735212,2.9458837777,-0.9746705749 H,0,4.5023889912,3.2712015498,-1.0281607389 N,0,-2.4412270538,0.5249502359,-0.1847625029 H,0,-1.6930151056,1.4473372963,-0.2930439822 O,0,-1.0200691795,2.5539639993,-0.4625112067 O,0,-0.6360939739,2.9151814496,0.8321592546 C,0,0.1709577438,4.0811271047,0.7500304149 H,0,-0.3922379611,4.899027141,0.2896714891 H,0,0.4278573597,4.3297774527,1.7815667224 H,0,1.0769265074,3.8830092426,0.1697040503	0, 2 C,0,-6.0304877852,1.5743261756,-0.4145706727 C,0,-4.6548883507,1.7791030167,-0.39415823 C,0,-6.5875359417,0.2918472751,-0.2465729555 H,0,-4.2151796497,2.7597818475,-0.5228063277 C,0,-3.8464414385,0.6570714806,-0.2006296923 C,0,-5.7886123056,-0.8321057928,-0.0531519415 H,0,-6.2168639345,-1.8180809663,0.0754240846 C,0,-4.4112841524,-0.6288104546,-0.0331612089 C,0,-2.1722740956,-0.7832854712,0.0707431969 N,0,-3.3464273826,-1.4904794124,0.1315967472 H,0,-7.6646027238,0.1764263831,-0.2681517051 H,0,-3.3868975128,-2.488979675,0.2738281677 N,0,-0.9967213632,-1.3852615874,0.1974825883 N,0,0.0338419438,-0.5153469288,0.1168830399 C,0,1.2076827043,-1.0685230071,0.2265551087 H,0,1.2863342994,-2.1493648063,0.3651541834 C,0,2.4288624259,-0.2986389504,0.1739798087 C,0,3.6594397106,-0.969719848,0.3005033191 C,0,2.4224114799,1.1028796262,0.0019003478 C,0,4.857486295,-0.2669067088,0.2581954419 C,0,3.6120522876,1.8013719472,-0.0397466985 C,0,4.840015095,1.1148556849,0.0899874776 H,0,-6.6906593154,2.4206043742,-0.5623998015 H,0,3.6745650651,-2.0452638623,0.4317322987 H,0,1.4836105938,1.6356733346,-0.0982301044 O,0,5.9492428554,1.9027078582,0.0365819787 H,0,6.7568026732,1.3856857695,0.1478860326 H,0,5.8048011392,-0.785365468,0.3554586082 O,0,3.6017073195,3.1557156284,-0.2048635698 H,0,4.5133071607,3.4796269153,-0.2038001013 N,0,-2.4730891009,0.5289489611,-0.1279729283 H,0,-1.7536597206,1.3444717447,-0.2571648992 O,0,-0.879528314,2.5274210385,-0.4858968499 O,0,-1.783402841,3.5909150414,-0.6931040224 C,0,-1.0581496781,4.74328916,-1.1020326907 H,0,-0.5370098122,4.5538945162,-2.0456522423 H,0,-1.8017881148,5.5312961376,-1.2365282073 H,0,-0.3365366654,5.034999673,-0.3327833608

TS R1(•OOCH$_3$)_imino, optimization in benzene UB3LYP/6-311++G**, E= -1100.68821274 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228697 a.u. 1 imaginary frequency = 1411.8736 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2280394 a.u.	**TS R2(•OOCH$_3$)_imino,** optimization in gas phase UB3LYP/6-311++G**, E= -1100.67874124 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.227326 a.u. 1 imaginary frequency = 1568.2028 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2125598 a.u.
0, 2 C,0,-6.0397162521,1.5626498131,-0.4816605613 C,0,-4.6635439906,1.7623519833,-0.4659223842 C,0,-6.6011885363,0.2889677107,-0.2763791678 H,0,-4.2181894638,2.7366522646,-0.6217713833	0, 2 C,0,-5.8487797001,2.5433488733,-0.6243332576 C,0,-4.455707967,2.5510692388,-0.5848988718 C,0,-6.5841411301,1.3672690601,-0.3932368268 H,0,-3.8926115616,3.4592783307,-0.7632177519

C,0,-3.8558346947,0.6455852205,-0.237936759	C,0,-3.8238302505,1.3436077114,-0.3067168217
C,0,-5.8048652924,-0.8313742881,-0.048178073	C,0,-5.9536915432,0.1598859477,-0.1150843623
H,0,-6.2398587234,-1.8108474399,0.1095005075	H,0,-6.5158214242,-0.7483263613,0.0636768212
C,0,-4.4275915065,-0.6330209558,-0.0322567038	C,0,-4.5573072969,0.1548010158,-0.0727700456
C,0,-2.1871891066,-0.775897708,0.0775666591	C,0,-2.4140641734,-0.3576068838,0.1019463575
N,0,-3.3622638305,-1.4894713101,0.1595374756	N,0,-2.4949043814,0.9879552442,-0.1902855043
H,0,-7.6787255441,0.1758266178,-0.2959274022	H,0,-7.6663252773,1.4049226428,-0.4329889255
H,0,-3.3927737509,-2.4815088263,0.336194796	H,0,-1.6704539124,1.5590378286,-0.2888566726
N,0,-1.0141817319,-1.3778842738,0.2288168006	N,0,-1.3143413902,-1.0724139591,0.2907186532
N,0,0.0141542552,-0.5104316665,0.1185742343	N,0,-0.1982619589,-0.3138725381,0.1573266682
C,0,1.1883679559,-1.0514453118,0.2532600706	C,0,0.9044318087,-0.9735376445,0.3457294408
H,0,1.2724228672,-2.1261813807,0.4354235148	H,0,0.8502797175,-2.0368180668,0.5889936223
C,0,2.4059252833,-0.274061066,0.1710522294	C,0,2.2143411503,-0.3605524949,0.2496482407
C,0,3.6397739755,-0.9309502166,0.3259326543	C,0,3.3508637568,-1.1528347089,0.4831452354
C,0,2.3871072797,1.1184252456,-0.0576897589	C,0,2.3871926906,1.0005242481,-0.0691362878
C,0,4.8327546523,-0.2207845515,0.2550835266	C,0,4.6266278185,-0.6037502567,0.4027581476
C,0,3.5731336599,1.8233525651,-0.1279503682	C,0,3.6528357426,1.5492133967,-0.1502572847
C,0,4.8029195625,1.150994048,0.0291748886	C,0,4.7804540529,0.7405211274,0.0878355294
H,0,-6.696837528,2.4065610513,-0.6554428013	H,0,-6.3767669061,3.4652831616,-0.8377142313
H,0,3.661880228,-2.0001288601,0.5022914628	H,0,3.2329378654,-2.2016172276,0.7293429444
H,0,1.4441743762,1.6405643081,-0.1790540612	H,0,1.5273585254,1.6301019753,-0.2544540799
O,0,5.9144926026,1.9449543306,-0.0578468389	O,0,5.9893311814,1.3819000215,-0.0175876676
H,0,6.7193080189,1.4290505426,0.063725579	H,0,6.7156211241,0.7737613052,0.1534911591
H,0,5.7847758421,-0.7276709739,0.3748502909	H,0,5.5021927966,-1.2193459324,0.5848951735
O,0,3.5559838199,3.1688837958,-0.3486713005	O,0,3.8040891056,2.8672559292,-0.4598899609
H,0,4.4664481628,3.4924661122,-0.3641126323	H,0,4.7471662822,3.0757025202,-0.4737929748
N,0,-2.4840391204,0.5260186787,-0.1643798296	N,0,-3.6688245431,-0.8683185561,0.1745036901
H,0,-1.722934891,1.3838085082,-0.29804672	H,0,-3.9719112558,-1.9937878657,0.4010593538
O,0,-0.8813659764,2.429169683,-0.4716258637	O,0,-4.4959207337,-3.1613313414,0.6240440291
O,0,-1.7321580473,3.5274126083,-0.6901730106	O,0,-3.4346507008,-4.0389760498,0.8405072006
C,0,-0.9295115518,4.6779850682,-0.9156366309	C,0,-3.9710286833,-5.332940426,1.0704623867
H,0,-0.3039815559,4.5385421791,-1.802268618	H,0,-4.5391931663,-5.6699199817,0.1979601445
H,0,-1.6299998771,5.5009960743,-1.0717400748	H,0,-3.1081170273,-5.9806893735,1.2358688951
H,0,-0.2967495703,4.8772214201,-0.0458017465	H,0,-4.6172961549,-5.3254626601,1.9535583638

TS R2(•OOCH$_3$)_imino, optimization in solv. water UB3LYP/6-311++G**, E= -1100.70313671 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228277 a.u. 1 imaginary frequency = 1206.3537 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2424207 a.u.	**TS R2(•OOCH$_3$)_imino,** optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.68843292 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228155 a.u. 1 imaginary frequency = 1480.6215 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2251973 a.u.
0, 2	0, 2
C,0,-5.8683199624,2.5787417016,-0.6350463509	C,0,-5.8621966617,2.5489430587,-0.6486749008
C,0,-4.4761843179,2.5823124838,-0.5986129644	C,0,-4.469532508,2.5568724725,-0.6128659192
C,0,-6.6099494352,1.4054567802,-0.3978054051	C,0,-6.5991940051,1.379695567,-0.38387695
H,0,-3.9058406131,3.4843335158,-0.7807714147	H,0,-3.9045399627,3.4580654104,-0.8170053065
C,0,-3.8498537923,1.371658262,-0.3167067872	C,0,-3.8387922388,1.3557904587,-0.3034292738
C,0,-5.9855275192,0.19555894,-0.1156140738	C,0,-5.9702019064,0.1794602471,-0.0741554543
H,0,-6.5548998213,-0.7070018908,0.0671251642	H,0,-6.5342446492,-0.7219435529,0.130316898
C,0,-4.5898277189,0.1902111419,-0.0769651626	C,0,-4.5735773768,0.175568115,-0.0356124706
C,0,-2.4302664772,-0.317618056,0.0943524466	C,0,-2.425784894,-0.3301382826,0.1464333309
N,0,-2.5193133378,1.0175846877,-0.2024519873	N,0,-2.5093693283,1.0041161522,-0.1813422622
H,0,-7.6917834045,1.4478236514,-0.4360139207	H,0,-7.6813317797,1.4177490808,-0.4223360393
H,0,-1.705618396,1.6052870481,-0.3099721226	H,0,-1.6899067987,1.579388947,-0.3010357747

N,0,-1.3378993737,-1.0450926925,0.2876783196	N,0,-1.3276132546,-1.0444762328,0.3529048046
N,0,-0.2112773221,-0.3018166621,0.1540508364	N,0,-0.2072404636,-0.2974932703,0.1925464305
C,0,0.8880120489,-0.9690354933,0.3518126626	C,0,0.8929395511,-0.9575438941,0.4017016497
H,0,0.8335811596,-2.030389598,0.602930404	H,0,0.8350845518,-2.0113853963,0.6815031109
C,0,2.1972395787,-0.364017462,0.2574919445	C,0,2.2052031249,-0.3576505821,0.2825247492
C,0,3.3289832184,-1.1635450183,0.5017776902	C,0,3.3355855886,-1.1508912513,0.5450353891
C,0,2.3776109376,0.9969674744,-0.0686794237	C,0,2.3884467709,0.990022236,-0.0874327542
C,0,4.6079165139,-0.6250752199,0.425775604	C,0,4.6157013105,-0.6171615869,0.4432940806
C,0,3.6470714767,1.5337398218,-0.1459093673	C,0,3.6587987949,1.5226087371,-0.1907299632
C,0,4.7728946042,0.7187375081,0.1032296313	C,0,4.7814684791,0.7131940179,0.0755025591
H,0,-6.3934897488,3.5014148421,-0.8509672492	H,0,-6.3900451213,3.4650656037,-0.8857960131
H,0,3.2035822391,-2.2101354921,0.7529017462	H,0,3.2090126224,-2.1884911468,0.8308578351
H,0,1.5216229238,1.6307548189,-0.2613020997	H,0,1.5337803512,1.6196304144,-0.2963121178
O,0,5.9753676804,1.3491510926,0.0004984551	O,0,5.9918009915,1.3369167481,-0.0579853886
H,0,6.7076505678,0.7460552318,0.1794759145	H,0,6.7177882189,0.7261111389,0.1118458209
H,0,5.4788730342,-1.2426446811,0.6151226807	H,0,5.4860265634,-1.2317577371,0.6489310907
O,0,3.811190386,2.850135931,-0.4626311566	O,0,3.8221062123,2.8271941188,-0.5510520459
H,0,4.7565177515,3.0556868865,-0.4744149868	H,0,4.7674643469,3.0264401778,-0.5813715384
N,0,-3.6898576748,-0.8258814882,0.1724268063	N,0,-3.6814958449,-0.8381654186,0.2386183468
H,0,-3.9412311564,-1.86898454,0.3875372885	H,0,-3.969180644,-1.9391782548,0.4596962479
O,0,-4.4718657599,-3.2312125512,0.6515448576	O,0,-4.4912397841,-3.1601390441,0.6678757688
O,0,-3.3807836786,-4.0929325683,0.8561534283	O,0,-3.4126969443,-4.0270340771,0.8840181361
C,0,-3.8671423789,-5.414857131,1.0550994945	C,0,-3.9161572629,-5.3507996267,0.9886764137
H,0,-4.4192758089,-5.755702162,0.1739471342	H,0,-4.4216613416,-5.6413774301,0.0625436446
H,0,-2.9828275043,-6.0363395836,1.2078998548	H,0,-3.0429023451,-5.9837416689,1.157604481
H,0,-4.5133049185,-5.4559925294,1.9372811085	H,0,-4.6105283626,-5.4301272487,1.8308323844

TS R3(•OOCH$_3$)_imino, optimization in gas phase UB3LYP/6-311++G**, E= -1100.68427763 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228373 a.u. 1 imaginary frequency = 1495.3440 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2138449 a.u.	**TS R3(•OOCH$_3$)_imino,** optimization in solv. water UB3LYP/6-311++G**, E= -1100.70653067 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228510 a.u. 1 imaginary frequency = 1340.6666 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2449781 a.u.
0, 2	0, 2
C,0,-5.7190910057,1.7665905896,0.3473695545	C,0,-5.2787864078,1.9551306051,0.0712887277
C,0,-4.3284126751,1.9050031625,0.3187144343	C,0,-3.8907360913,2.0792978815,0.016946031
C,0,-6.3259529419,0.5086354818,0.2852804188	C,0,-5.8989019363,0.7028381607,0.207823142
H,0,-3.8592816101,2.8800594724,0.3670192482	H,0,-3.4115036843,3.0442436192,-0.0886676431
C,0,-3.5732603959,0.7449820845,0.2262242996	C,0,-3.1476407458,0.9075828409,0.1040615938
C,0,-5.5657509064,-0.6607323328,0.1922515231	C,0,-5.1548412675,-0.4730883137,0.2950104945
H,0,-6.0379021879,-1.6345650034,0.1440476672	H,0,-5.6309135523,-1.4395607419,0.4003352156
C,0,-4.1856890058,-0.5230442181,0.1638692252	C,0,-3.7709347822,-0.3499874794,0.240750185
C,0,-1.9367932251,-0.8183367984,0.0849758954	C,0,-1.5386680701,-0.6700693755,0.2018451411
N,0,-2.2010951088,0.525179803,0.1754549316	N,0,-1.7804239865,0.6682339447,0.0843670422
N,0,-3.1552128318,-1.4539334734,0.0784311125	N,0,-2.751906007,-1.2895611232,0.2968202934
H,0,-7.4065103244,0.4357918709,0.309461273	H,0,-6.9800672771,0.6476062034,0.2461159675
H,0,-1.4506423179,1.1990134607,0.19800279	H,0,-1.0330983898,1.3422889242,0.0003010067
H,0,-3.236521387,-2.4559542251,0.0193703126	H,0,-2.8549335593,-2.2893479261,0.3918386272
N,0,-0.7902995918,-1.4430677867,0.0153706066	N,0,-0.3872887477,-1.3187104206,0.2266933342
N,0,0.2483552292,-0.55717516,0.0412168824	N,0,0.6632462677,-0.4697509204,0.1173517326
C,0,1.422595965,-1.0990503457,-0.0221646488	C,0,1.8288843555,-1.0499321333,0.1325996948
H,0,1.5083912109,-2.1861463465,-0.0890125147	H,0,1.8869466956,-2.1363073398,0.2274410736
C,0,2.6395708436,-0.3171708965,-0.007509454	C,0,3.0627146675,-0.3129083894,0.0289049445
C,0,3.8773481305,-1.0095229152,-0.0803368986	C,0,4.2782447338,-1.0350958213,0.0547399377

C,0,2.6368419762,1.0829348167,0.0746454777	C,0,3.0983403638,1.0932060144,-0.0959731722
C,0,5.0810795462,-0.3274320254,-0.0709369015	C,0,5.4954993681,-0.3795314912,-0.039330904
C,0,3.8353982857,1.7914582389,0.0863462557	C,0,4.3103097749,1.7573554976,-0.1908339254
C,0,5.0695562708,1.0646663533,0.0125023933	C,0,5.5189477847,1.0092552237,-0.1613800968
H,0,-6.3368939173,2.6535290627,0.4192069757	H,0,-5.8914468379,2.8461172131,0.006332068
H,0,3.8731183714,-2.0918497204,-0.1440547703	H,0,4.254556731,-2.1144666272,0.1488455472
H,0,1.6986193784,1.6189998707,0.1302637851	H,0,2.1729440104,1.6545010449,-0.1171957629
O,0,6.2113260114,1.7674345407,0.0264483378	O,0,6.6955946909,1.6659156429,-0.2536721795
H,0,5.9499804584,2.7049399935,0.0906205019	H,0,6.4949786149,2.6139269465,-0.3287736639
H,0,6.0303554664,-0.8458686499,-0.1256557059	H,0,6.431760855,-0.9239806151,-0.0200990033
O,0,3.9685728647,3.100895242,0.1600343183	O,0,4.4664597078,3.0853465319,-0.312166227
H,0,3.0083959889,3.6942288516,0.2528183818	H,0,3.5594384636,3.5993233581,-0.3333890963
O,0,1.9068002548,4.3261269232,0.3706579594	O,0,2.2681767358,4.2833695937,-0.3591321367
O,0,2.2581414834,5.6751243838,0.39599142	O,0,2.5544553537,5.6437348459,-0.504004435
C,0,1.0790538644,6.439776385,0.594782084	C,0,1.3337415623,6.3779176597,-0.5371724881
H,0,0.6111969391,6.1762793808,1.5483118013	H,0,0.7801959369,6.2351246877,0.3952491232
H,0,1.4064832926,7.4807446513,0.6070391744	H,0,1.6224274636,7.4240365216,-0.6493870502
H,0,0.374250041,6.2722772178,-0.2255577073	H,0,0.7229678355,6.0599820064,-1.3869869889

TS R3(•$OOCH_3$)_imino, optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.69349083 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228780 a.u. 1 imaginary frequency = 1373.9264 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2260084 a.u.	**TS R4(•$OOCH_3$)_imino,** optimization in gas phase UB3LYP/6-311++G**, E= -1100.68679701 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.229382 a.u. 1 imaginary frequency = 1148.1384 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2182431 a.u.
0, 2	0, 2
C,0,-5.7043273662,1.7850582486,0.3555984467	C,0,-5.7404514836,1.790777618,0.0862623369
C,0,-4.3151980117,1.9247224876,0.3267549507	C,0,-4.3484329902,1.9014630961,0.1576277916
C,0,-6.3128176383,0.5252883037,0.290256668	C,0,-6.3596072867,0.5631212339,-0.1645492995
H,0,-3.8445876356,2.8986558371,0.377643549	H,0,-3.8702261575,2.8537359312,0.3521282384
C,0,-3.561905156,0.7623841024,0.2302326404	C,0,-3.6053280323,0.7454536704,-0.0301625473
C,0,-5.5558694498,-0.6440963623,0.1932621283	C,0,-5.6111210608,-0.6025058273,-0.3538709009
H,0,-6.0274542231,-1.6176751186,0.1434211045	H,0,-6.0930678491,-1.5530872109,-0.5482140529
C,0,-4.174627925,-0.5051282549,0.1639109213	C,0,-4.2302514951,-0.4922927349,-0.2827980092
C,0,-1.9320530668,-0.7989285628,0.0832047394	C,0,-1.9843833434,-0.82575548,-0.2620183018
N,0,-2.1906722062,0.5412463584,0.1782875802	N,0,-2.235424752,0.5032031708,-0.0249871841
N,0,-3.1451288474,-1.4350969284,0.0747957352	N,0,-3.2100352094,-1.428546002,-0.4188718176
H,0,-7.3934664141,0.4542608659,0.3153906139	H,0,-7.440505748,0.5107507871,-0.2136189275
H,0,-1.4442256675,1.2203131684,0.2034268835	H,0,-1.4782851905,1.1521262313,0.1230445264
H,0,-3.2318297811,-2.4374514429,0.0092631701	H,0,-3.302338028,-2.4136535153,-0.6061610536
N,0,-0.7797654863,-1.4284448491,0.0105464859	N,0,-0.8466870517,-1.462818274,-0.3378588455
N,0,0.2580476771,-0.5515812812,0.0394243958	N,0,0.2080412746,-0.6153212288,-0.1441061346
C,0,1.4341136818,-1.0990606201,-0.0273646742	C,0,1.3689549828,-1.189246655,-0.2037685946
H,0,1.5169672819,-2.1858380367,-0.0994096909	H,0,1.4220666714,-2.2639599645,-0.3923295692
C,0,2.6493421468,-0.3219732003,-0.0094649819	C,0,2.6083923868,-0.470865423,-0.0320623308
C,0,3.8852324574,-1.0155273623,-0.0899508765	C,0,3.8223197019,-1.1952035668,-0.0966279248
C,0,2.6494186644,1.0813740522,0.0837516081	C,0,2.6521608967,0.9201584373,0.2026107595
C,0,5.0880570824,-0.3322010119,-0.0776334487	C,0,5.041869959,-0.5683105312,0.0717272547
C,0,3.8466595878,1.7860479698,0.0978741738	C,0,3.8628318987,1.5548490468,0.3610878943
C,0,5.0773965173,1.0598989883,0.0161771193	C,0,5.0889528816,0.8206337599,0.2984217963
H,0,-6.3227433344,2.6713033748,0.4304311123	H,0,-6.3486847472,2.6757993602,0.228596934
H,0,3.8812493873,-2.0970680254,-0.1620588026	H,0,3.7884816803,-2.265050877,-0.2706089909
H,0,1.7114754128,1.6173216554,0.1455482926	H,0,1.7362007986,1.4932736987,0.2525675026
O,0,6.2247059589,1.75762199,0.0325311171	H,0,5.9720252807,-1.1221849761,0.0318899576

H,0,5.9753038613,2.6972177157,0.1035708165	O,0,3.9304848214,2.8898695716,0.5775954489
H,0,6.0368917494,-0.8508826397,-0.1383098272	H,0,4.8727834951,3.1155592123,0.6396020648
O,0,3.9802082728,3.1011195121,0.1819637064	O,0,6.1904822159,1.5228114143,0.4721734669
H,0,3.0287917779,3.6631285505,0.267004771	H,0,7.0979700652,1.0312016038,0.1027581812
O,0,1.879154415,4.2944879157,0.3759272436	O,0,8.1618508291,0.4931110607,-0.4813090111
O,0,2.2088093621,5.6547944431,0.4172165457	O,0,9.2152044495,0.7695498345,0.37361906
C,0,1.0127997809,6.4036090794,0.577496679	C,0,10.4292341815,0.7377220811,-0.3700654451
H,0,0.5172917294,6.1348800809,1.5155257364	H,0,10.412956402,1.5049424747,-1.1490142319
H,0,1.3237695497,7.4494662801,0.6004247856	H,0,11.2190212605,0.9424469547,0.3542155376
H,0,0.3371082951,6.2275746567,-0.2651709783	H,0,10.5675466321,-0.2489154824,-0.8206990987

TS R4(•OOCH$_3$)_imino, optimization in solv. water UB3LYP/6-311++G**, E= -1100.70753116 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.228899 a.u. 1 imaginary frequency = 1414.3743 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2435839 a.u.	**TS R4(•OOCH$_3$)_imino,** optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.69569890 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.229353 a.u. 1 imaginary frequency = 1026.3600 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2295426 a.u.
0, 2	0, 2
C,0,-5.6930372387,1.5707382681,0.4087114172	C,0,-5.7446175992,1.7686089906,0.2081092136
C,0,-4.3085615044,1.752864152,0.4108622744	C,0,-4.3534248675,1.8801023526,0.2774141066
C,0,-6.2669618347,0.3287064,0.1013321649	C,0,-6.3629718211,0.5570837191,-0.1215047143
H,0,-3.863151616,2.7108330378,0.6478203935	H,0,-3.8758402138,2.8179697465,0.5326902505
C,0,-3.5247844957,0.6503530082,0.0952222229	C,0,-3.6094845834,0.7402877363,0.0059210412
C,0,-5.479291226,-0.7794921123,-0.215935603	C,0,-5.614380917,-0.5905008188,-0.3948908165
H,0,-5.9209790301,-1.7390074092,-0.4535850959	H,0,-6.093608179,-1.5277200287,-0.6496343452
C,0,-4.1017379447,-0.5976443146,-0.2139126321	C,0,-4.2324642513,-0.479214806,-0.3260087372
C,0,-1.8555358651,-0.8075955276,-0.344688294	C,0,-1.9903463458,-0.8048934773,-0.3423674964
N,0,-2.1483984644,0.4811116514,0.0047286103	N,0,-2.2392804699,0.5019479581,-0.0147091173
N,0,-3.0481802209,-1.4635623659,-0.4774996119	N,0,-3.2110931439,-1.4000827599,-0.5323681898
H,0,-7.3452712416,0.2248005252,0.109507789	H,0,-7.4441140383,0.5055368378,-0.1661194791
H,0,-1.4279346716,1.1702331281,0.1610170405	H,0,-1.4877500408,1.1476822596,0.1736188192
H,0,-3.1155178084,-2.4378174218,-0.7314538086	H,0,-3.3075450429,-2.3710181809,-0.7856889269
N,0,-0.6841485206,-1.3821305396,-0.5347400012	N,0,-0.8471204325,-1.4362667407,-0.4682312597
N,0,0.3372355426,-0.5050651578,-0.339665942	N,0,0.2070595264,-0.6078334326,-0.223161859
C,0,1.5228119788,-1.0088205405,-0.5062434405	C,0,1.3697934228,-1.1760844733,-0.3255906514
H,0,1.6277428633,-2.061986967,-0.77669728	H,0,1.4256147726,-2.2354402829,-0.5861435795
C,0,2.7284330301,-0.2308072983,-0.3471119095	C,0,2.6072601967,-0.4681369044,-0.1090395618
C,0,3.9749214901,-0.8698189862,-0.523014869	C,0,3.8227637258,-1.1824534624,-0.2212319599
C,0,2.7059510346,1.1425443516,-0.0154754961	C,0,2.6485111486,0.9057735832,0.2156271487
C,0,5.1634316961,-0.1737346734,-0.3695439454	C,0,5.0406114692,-0.5617310079,-0.0127328609
C,0,3.8852827314,1.8392216121,0.1301805501	C,0,3.8575156388,1.5321347952,0.4147742722
C,0,5.1382239976,1.189982478,-0.0459713161	C,0,5.0828717451,0.8076520149,0.3040035797
H,0,-6.3361870203,2.4084822406,0.6498969926	H,0,-6.3550466893,2.6395071674,0.4141232928
H,0,4.000649607,-1.9246528914,-0.7716149152	H,0,3.7940810971,-2.238758905,-0.464249699
H,0,1.7620169915,1.6545580208,0.1207305517	H,0,1.7309086049,1.4721505586,0.3030747582
H,0,6.1191197679,-0.6685328096,-0.4945352674	H,0,5.9715665993,-1.1103822756,-0.0884841573
O,0,3.8719125135,3.1647135439,0.4423705582	O,0,3.9167524378,2.8536518334,0.7185920383
H,0,4.7920921794,3.4693402251,0.471238881	H,0,4.8558377873,3.0869543633,0.7938500443
O,0,6.2203117627,1.9541425447,0.1262472159	O,0,6.1879651881,1.5016730551,0.5250393168
H,0,7.0821138688,1.5363521999,-0.2731254072	H,0,7.075086571,1.0409038582,0.1294898582
O,0,8.288305337,1.0494919621,-0.9529952483	O,0,8.1819907401,0.5365996398,-0.5011549218
O,0,9.306407432,1.2143398565,-0.0354099817	O,0,9.2113407514,0.6955288567,0.4122812478
C,0,10.5699086501,1.2045030084,-0.7067825356	C,0,10.4542540394,0.7351741889,-0.2862310413
H,0,10.6201861291,2.0326707324,-1.4176395075	H,0,10.4729095398,1.5876641357,-0.9702626317

H,0,11.3166528843,1.3269338261,0.0778771115 H,0,10.7088860851,0.2520287723,-1.2236423856	H,0,11.2175953493,0.8455646083,0.4849983957 H,0,10.601800624,-0.194792203,-0.841574898

TS R5(•OOCH$_3$) _imino, optimization in gas phase UB3LYP/6-311++G**, E= -1100.64904885 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.226502 a.u. 1 imaginary frequency = 1577.0623 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.195043 a.u.	**TS R5(•OOCH$_3$) _imino,** optimization in solv. water UB3LYP/6-311++G**, E= -1100.67607591 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.227068 a.u. 1 imaginary frequency = 1486.6990 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2216087 a.u.
0, 2 C,0,5.4742238694,1.8729784373,0.4029866021 C,0,4.0744899271,1.8733195425,0.4255002889 C,0,6.1926813922,0.7123422956,0.1108519261 H,0,3.5180509023,2.7748473573,0.6521923083 C,0,3.4302911782,0.6785930349,0.147318518 C,0,5.5409228227,-0.4939302834,-0.1705625305 H,0,6.1006062268,-1.393535868,-0.3969226087 C,0,4.1549752005,-0.4922798121,-0.1476063803 C,0,1.9387651317,-0.9973407163,-0.2309979632 N,0,2.0803132765,0.3352121854,0.0858880053 N,0,3.2149155332,-1.4936447234,-0.375536522 H,0,7.2755866391,0.7422139369,0.1007470893 H,0,1.2816523428,0.9245484564,0.2548800589 H,0,3.3878480565,-2.4591078425,-0.6032801384 N,0,0.871585923,-1.7238933716,-0.3826470322 N,0,-0.2750885234,-1.0009756826,-0.2001793751 C,0,-2.6858294899,-0.780757339,-0.0660863418 C,0,-3.8743354434,-1.4946287902,0.1389083743 C,0,-2.7355291988,0.6240387368,-0.1446480997 C,0,-5.0850397054,-0.8193952088,0.2782017754 C,0,-3.9376033738,1.2952283028,-0.0069089659 C,0,-5.1197340557,0.5663490169,0.2077910565 H,0,6.00641806,2.7920537356,0.6167054844 H,0,-3.8456671243,-2.5756703906,0.1880531563 H,0,-1.8325576091,1.1951220542,-0.3165111086 O,0,-6.2599789849,1.3257021755,0.3292163311 H,0,-7.0282934444,0.7632442225,0.4690227547 H,0,-6.0039987495,-1.3742453799,0.4420876979 O,0,-3.9685136256,2.6571802569,-0.0832470376 H,0,-4.8829084745,2.9492618124,0.0245915446 C,0,-1.4265170013,-1.5096141521,-0.1949317593 H,0,-1.5442637752,-2.9010033667,-0.3051372973 O,0,-1.7884451531,-4.0383200462,-0.3637368229 O,0,-1.2566841373,-4.5003154192,-1.5887242726 C,0,-2.302753458,-4.5420571225,-2.5493119867 H,0,-2.679586657,-3.5361390412,-2.7654652454 H,0,-1.8480072781,-4.9662104961,-3.4476713124 H,0,-3.1222011491,-5.1814337075,-2.2070852116	0, 2 C,0,5.4507733719,1.8540125042,0.7206840895 C,0,4.0534192533,1.8102073184,0.7612312268 C,0,6.1978772714,0.7873378288,0.2077235739 H,0,3.4732019242,2.6341001314,1.1577481044 C,0,3.4409955748,0.6654957545,0.2720402942 C,0,5.5783029237,-0.3652558733,-0.2855193242 H,0,6.1556666366,-1.1905327035,-0.6832987017 C,0,4.1915775031,-0.4062045542,-0.2443158661 C,0,1.9989874873,-0.9476366156,-0.3947723897 N,0,2.1005585955,0.2960664578,0.1659541284 N,0,3.2742436289,-1.3747739944,-0.6448532579 H,0,7.2791752505,0.853210648,0.1906354595 H,0,1.2942605484,0.8392379028,0.4345481504 H,0,3.4836202826,-2.2708451913,-1.0576826688 N,0,0.9316940281,-1.6647351639,-0.6734588383 N,0,-0.217767308,-1.0199557141,-0.3503428393 C,0,-2.6168082241,-0.8016661719,-0.1378613347 C,0,-3.7888961598,-1.4909843397,0.2050329328 C,0,-2.6799421286,0.5898562869,-0.354323487 C,0,-4.9962618959,-0.8102941012,0.3442752796 C,0,-3.8783351851,1.2669180813,-0.2150016353 C,0,-5.0460380929,0.5631259135,0.1364431961 H,0,5.9624402865,2.7325746446,1.094966951 H,0,-3.7548913901,-2.561493461,0.3623291706 H,0,-1.7897936519,1.1420389337,-0.6290234163 O,0,-6.174529451,1.3271857104,0.242979594 H,0,-6.9420450004,0.7878843118,0.4688015005 H,0,-5.9003723283,-1.3459078546,0.6127137293 O,0,-3.9238563897,2.6163930381,-0.4236392014 H,0,-4.8325486303,2.9213318837,-0.2923270324 C,0,-1.3640548581,-1.5392997555,-0.2717781351 H,0,-1.4594746894,-2.8997340333,-0.3383985754 O,0,-1.5827681599,-4.0983115909,-0.3649438759 O,0,-1.3785262234,-4.5011143417,-1.7163820574 C,0,-2.6461559344,-4.6197020184,-2.3579672885 H,0,-3.1482409814,-3.6493896726,-2.4159072602 H,0,-2.4244195273,-4.9817659892,-3.3642524678 H,0,-3.2812773569,-5.3396372097,-1.8343117276

TS R5(•OOCH$_3$)_imino, optimization in benzene UB3LYP/6-311++G**, E= -1100.66023039 a.u.	

Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.226930 a.u. 1 imaginary frequency = 1573.2748 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2063655 a.u.	
0, 2 C,0,5.456831025,1.9028439797,0.3875872769 C,0,4.0574199505,1.8898335154,0.408260304 C,0,6.1886081766,0.7424853185,0.1223176125 H,0,3.4898447719,2.7891981289,0.6140337737 C,0,3.4276483337,0.6813114105,0.1549779582 C,0,5.5511478873,-0.476736743,-0.1333456273 H,0,6.1194118208,-1.3758730428,-0.3381540062 C,0,4.1645730396,-0.4874549631,-0.1130669605 C,0,1.9575506335,-1.0154398465,-0.1910814962 N,0,2.0812682619,0.3219900445,0.09864609 N,0,3.2350863014,-1.5032416297,-0.3208357967 H,0,7.2711861001,0.7839603666,0.1135037212 H,0,1.2798941783,0.9135155757,0.2493792032 H,0,3.4244916096,-2.4695416269,-0.5346974052 N,0,0.893004531,-1.7570606145,-0.3342911654 N,0,-0.2594398494,-1.0464913144,-0.1675072652 C,0,-2.6699549706,-0.8092569839,-0.0620912086 C,0,-3.8673098358,-1.5128681849,0.1269225337 C,0,-2.7075695557,0.5966054324,-0.1393470357 C,0,-5.0753037864,-0.8293548058,0.2508926924 C,0,-3.9067335598,1.2757313474,-0.0171837997 C,0,-5.0991162364,0.5571603939,0.1807216753 H,0,5.9794487582,2.8317924268,0.581571419 H,0,-3.8496755008,-2.5940287488,0.1772468953 H,0,-1.7975038692,1.1608144464,-0.2971371966 O,0,-6.2317000461,1.3245363095,0.2868852097 H,0,-7.010545495,0.7713431105,0.4115320377 H,0,-6.0005305998,-1.3762873911,0.4023685948 O,0,-3.9260892108,2.6390563354,-0.0926154923 H,0,-4.8395196592,2.9401520675,0.0037726972 C,0,-1.4141664913,-1.5469473599,-0.175537887 H,0,-1.5331059115,-2.9227464817,-0.302895148 O,0,-1.7437205642,-4.0797300167,-0.3846616438 O,0,-1.2826834625,-4.4826407489,-1.6621043546 C,0,-2.3850150253,-4.4983830542,-2.5620553248 H,0,-2.7863336541,-3.4901600793,-2.7087704474 H,0,-1.9786305574,-4.8742499431,-3.5037527696 H,0,-3.1729765381,-5.1660996302,-2.2017416639	

TS C1(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.48793140 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.230950 a.u. 1 imaginary frequency = 442.7273 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.068156 a.u.	**TS C1(•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.51041468 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231326 a.u. 1 imaginary frequency = 410.0248 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.0919231 a.u.
0, 2 C,0,5.9750756396,0.9240728127,-0.0843034908 C,0,5.1195355479,-0.1063266563,0.3483083473 C,0,5.5792758468,1.8563270042,-1.0301282508 H,0,5.4394314369,-0.8348249784,1.083113863 C,0,3.8377826103,-0.1755194767,-0.2099384578 C,0,4.2438884885,1.8809502923,-1.5534141247 H,0,4.0606714373,2.3775013242,-2.496829448 C,0,3.4426472,0.774882535,-1.1661662984 C,0,1.8463771361,-0.6894792914,-0.767114745 N,0,2.8142769263,-1.0896391318,0.0183002284 N,0,2.1519817368,0.4224707365,-1.512516723 H,0,1.5085566373,0.9144834131,-2.1128405907 N,0,0.6313726013,-1.3150115057,-0.8729815155 N,0,-0.3411052397,-0.7974899452,-1.6567051444 C,0,-1.4839276396,-1.3829579675,-1.6652449515 H,0,-1.661197133,-2.2701472165,-1.0466942898 H,0,0.4655888634,-2.1061939469,-0.2586087829 H,0,6.2661360657,2.6287223698,-1.3531624128 C,0,-2.6044163903,-0.9227327311,-2.4797437833 C,0,-3.8189385058,-1.617270999,-2.4119680654 C,0,-2.5022450375,0.1933287452,-3.3274055356 C,0,-4.9126255572,-1.2084775042,-3.1731896381 C,0,-3.5856777459,0.6020221285,-4.0846848281 C,0,-4.7996256367,-0.1047196559,-4.0058294902 H,0,6.9797225968,0.9766072768,0.3201762226 H,0,-5.8519272909,-1.7499882548,-3.11712082 H,0,-3.9141219701,-2.4808783658,-1.7635973829 O,0,-3.4706309336,1.6850940668,-4.9013731978 H,0,-4.3159344446,1.8282992769,-5.3465539577 O,0,3.409228417,3.3885078908,-0.7307216211 C,0,3.3468926114,3.309460939,0.6637979574 H,0,2.8715021261,4.2412194814,1.0020220519 H,0,2.7326867396,2.4710661204,1.0246618764 H,0,4.3370356185,3.2516406937,1.1374210983 H,0,-1.5756959661,0.7477106239,-3.3978203656 O,0,-5.8104837303,0.3842750736,-4.7980688913 H,0,-6.6133727624,-0.1345997477,-4.6869891719	0, 2 C,0,5.9826735288,0.8814301547,-0.1479388236 C,0,5.1198251975,-0.1298390062,0.3244452777 C,0,5.5743673291,1.8082323097,-1.0910129608 H,0,5.4558591111,-0.8527037809,1.0581950429 C,0,3.8222370484,-0.1863437931,-0.1962848413 C,0,4.2194242876,1.8523695055,-1.5696282794 H,0,4.0123791562,2.3384398333,-2.513501413 C,0,3.4123836062,0.7595863816,-1.152101449 C,0,1.8079099546,-0.687992263,-0.7107821939 N,0,2.794753869,-1.089256314,0.0623181493 N,0,2.1126570488,0.4196858888,-1.463046352 H,0,1.4816450026,0.8742087896,-2.1069513803 N,0,0.5883359264,-1.2918122771,-0.7940220747 N,0,-0.3688637527,-0.7720836405,-1.605225598 C,0,-1.511199738,-1.3594624041,-1.6314820936 H,0,-1.7013951359,-2.2454866742,-1.0189452275 H,0,0.4134635938,-2.1035162666,-0.2093437638 H,0,6.2664913485,2.560201138,-1.449338587 C,0,-2.6133456849,-0.8898583768,-2.4663576098 C,0,-3.8299572946,-1.5843344112,-2.4310754333 C,0,-2.4932350138,0.2359254215,-3.3014510198 C,0,-4.9086488953,-1.1689448869,-3.2105910021 C,0,-3.5623450746,0.6501412051,-4.0753699496 C,0,-4.7799667736,-0.0559677253,-4.0311883199 H,0,7.000159922,0.9175443027,0.2244864094 H,0,-5.8486313764,-1.7094617945,-3.1816628368 H,0,-3.9382321907,-2.4536232413,-1.792762765 O,0,-3.4320361257,1.7456576872,-4.8812064764 H,0,-4.2687440648,1.8930954941,-5.343860259 O,0,3.4718858521,3.3869883648,-0.7038707045 C,0,3.3832599665,3.2494594923,0.6891301507 H,0,2.6779799343,2.4655428155,1.0000208825 H,0,4.3562180035,3.0560678919,1.1619604959 H,0,3.012632024,4.2076361136,1.0792915481 H,0,-1.5643596184,0.7905271185,-3.3464524414 O,0,-5.7693911844,0.439526463,-4.8360282599 H,0,-6.5784494873,-0.0791940857,-4.752280171

TS C1(•OCH_3), optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.49759387 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231793 a.u. 1 imaginary frequency = 428.4988 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1025.0783652 a.u.	**TS C2(•OCH_3),** optimization in gas phase UB3LYP/6-311++G**, E= -1025.48816870 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231210 a.u. 1 imaginary frequency = 427.1689 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.0676247 a.u.
0, 2 C,0,5.9761031041,0.881473207,-0.0864793539	0, 2 C,0,5.8772448939,0.3303737376,0.2031206297

C,0,5.1081637238,-0.1319706488,0.3653937469	C,0,5.0253974981,-0.7350975319,0.379952635
C,0,5.5891405115,1.8017952921,-1.0463997209	C,0,5.4563248503,1.5463642189,-0.44401691
H,0,5.4237256036,-0.8509463505,1.1115905905	H,0,5.3346125697,-1.6304454314,0.90591898
C,0,3.8252346611,-0.1971073474,-0.1902623701	C,0,3.7292688246,-0.6518424627,-0.166572245
C,0,4.250782417,1.8344238088,-1.5651343481	C,0,4.1871206128,1.5792591631,-1.1020034467
H,0,4.0697647893,2.316674566,-2.5162982051	H,0,3.8962427721,2.4506049412,-1.6756310216
C,0,3.4376229878,0.7425147964,-1.1607153837	C,0,3.3477490802,0.510519889,-0.8995851258
C,0,1.8282763851,-0.7051910744,-0.745981328	C,0,1.7350686486,-0.9996980595,-0.8283018813
N,0,2.794386401,-1.1005232086,0.0492266409	N,0,2.7034051668,-1.5693548626,-0.1400528113
N,0,2.1454857979,0.3958244428,-1.5025673568	N,0,2.0440270676,0.2380200081,-1.3185530547
H,0,1.5147908035,0.8686071894,-2.1322299615	H,0,1.4149058862,0.8213888413,-1.8462823036
N,0,0.6114316123,-1.3205574611,-0.8517769608	N,0,0.5205312842,-1.5826953037,-1.0458484966
N,0,-0.351027936,-0.7942852705,-1.6472357048	N,0,-0.4414402794,-0.9321241738,-1.7394190979
C,0,-1.4967519668,-1.3742447957,-1.665552194	C,0,-1.5756189726,-1.5174823444,-1.8870470302
H,0,-1.6839818933,-2.2623193681,-1.0528009892	H,0,-1.7514891538,-2.5107558744,-1.4588581972
H,0,0.430125477,-2.109185977,-0.2383688273	H,0,0.3662087659,-2.4971811379,-0.6317041537
H,0,6.2848293935,2.5592288548,-1.385538	H,0,6.2276128541,2.2077664607,-0.8133906411
C,0,-2.6084601546,-0.8995843022,-2.4841686629	C,0,-2.6868450031,-0.916054546,-2.6160428456
C,0,-3.8229397304,-1.5967251129,-2.4431783279	C,0,-3.8953140572,-1.6186845701,-2.7073899549
C,0,-2.4996682964,0.2353404589,-3.3065173301	C,0,-2.5812724706,0.3455276204,-3.2263706636
C,0,-4.9106523659,-1.1728786048,-3.2050635628	C,0,-4.9802580139,-1.07465838,-3.3923579543
C,0,-3.5777080335,0.6594710947,-4.0626036312	C,0,-3.6559616175,0.8887055566,-3.9072119778
C,0,-4.7930468919,-0.0484424521,-4.0100702004	C,0,-4.8643784651,0.1723125501,-3.9896180155
H,0,6.9821898878,0.9277764778,0.3150068282	H,0,6.8813019864,0.2962403514,0.6080012213
H,0,-5.8484649367,-1.71804784,-3.1729724655	H,0,-5.9152702009,-1.6220712352,-3.4603567702
H,0,-3.9226645401,-2.4745867662,-1.8150224719	H,0,-3.9926424999,-2.5930860317,-2.2423322033
O,0,-3.4577990959,1.7634140662,-4.8535695103	O,0,-3.537783351,2.111421369,-4.4930671462
H,0,-4.3029077746,1.9221967978,-5.2951635439	H,0,-4.3756451243,2.3333821636,-4.9197461572
O,0,3.4572966887,3.3711144715,-0.7488077668	O,0,5.2818514625,2.7666670165,1.0254727193
C,0,3.3616454006,3.277101004,0.6446208686	C,0,4.2868744135,2.4119328202,1.9363285122
H,0,2.6893377437,2.4735185886,0.979096286	H,0,4.30628642,3.1720053428,2.7311601308
H,0,4.3371577444,3.1478797883,1.1340748959	H,0,3.275412948,2.4169953301,1.5010143937
H,0,2.9414679284,4.2314880054,0.9922576162	H,0,4.4597814643,1.4341753903,2.4108684077
H,0,-1.5736253601,0.7934029978,-3.3542414003	O,0,-5.8663851574,0.8012235907,-4.6871497253
O,0,-5.7963909834,0.4588706125,-4.7958620689	H,0,-6.6647574615,0.2638236696,-4.7002003872
H,0,-6.6151288027,-0.0331345105,-4.6706001562	H,0,-1.6582767716,0.907383164,-3.1713466219

TS C2(•OCH_3), optimization in solv. water UB3LYP/6-311++G**, E= -1025.51292772 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231890 a.u. 1 imaginary frequency = 373.4725 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.093324 a.u.	**TS C2(•OCH_3),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.49876856 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231563 a.u. 1 imaginary frequency = 405.7543 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1025.0786493 a.u.
0, 2	0, 2
C,0,5.8789770101,0.3346461974,0.172019112	C,0,5.8788923669,0.3339779851,0.1898117227
C,0,5.0346750482,-0.7349953374,0.3559787497	C,0,5.0310921818,-0.7340091145,0.3701955757
C,0,5.43903358,1.5583747063,-0.4544244126	C,0,5.4489539988,1.5523642334,-0.4492930244
H,0,5.3629619781,-1.6339372307,0.8648298187	H,0,5.3490036776,-1.6301318335,0.8899478402
C,0,3.7253931593,-0.6509501366,-0.1643753966	C,0,3.7293287327,-0.6518970664,-0.1653079425
C,0,4.1561776271,1.5900438215,-1.0915356308	C,0,4.1739460358,1.5834057742,-1.098322529
H,0,3.8507090655,2.4573928244,-1.663202668	H,0,3.8757491426,2.4528568541,-1.6709465868
C,0,3.3260027018,0.5172971997,-0.884705194	C,0,3.3394682684,0.5121716389,-0.8935697656
C,0,1.7167879757,-0.9975439211,-0.8046077013	C,0,1.7284618387,-1.0002838812,-0.8164588031
N,0,2.70765702,-1.5706574626,-0.1291958633	N,0,2.7069651126,-1.5707660313,-0.1339658828

N,0,2.0208967579,0.242681154,-1.2858790301	N,0,2.034704237,0.2383674685,-1.3035234049
H,0,1.3896453851,0.8310390142,-1.8087211163	H,0,1.4046592114,0.8226480494,-1.830484523
N,0,0.5089184271,-1.5764501893,-1.0068296503	N,0,0.5162316948,-1.5810587926,-1.0264334996
N,0,-0.4496554589,-0.9191805746,-1.7127459729	N,0,-0.443740559,-0.9272224253,-1.7263868785
C,0,-1.5807872531,-1.5112205677,-1.8637184106	C,0,-1.5768177641,-1.51468218,-1.8757746762
H,0,-1.7584660282,-2.5020361624,-1.4361004524	H,0,-1.7543029451,-2.5067174248,-1.447578395
H,0,0.3494600626,-2.4998549059,-0.6134420454	H,0,0.3598510168,-2.5001424243,-0.6228810028
H,0,6.2035858294,2.2146040505,-0.8477933199	H,0,6.2167065064,2.2131209594,-0.8276920931
C,0,-2.6847370689,-0.9096455743,-2.603223431	C,0,-2.6846731425,-0.9131995518,-2.6097809385
C,0,-3.8916670833,-1.6148562029,-2.7043528671	C,0,-3.8928138828,-1.6163131776,-2.7045018958
C,0,-2.5748833254,0.352181953,-3.2161668459	C,0,-2.5767741237,0.3478815387,-3.2220749611
C,0,-4.9718949029,-1.0767707823,-3.4014690129	C,0,-4.9755702323,-1.0748493034,-3.3949946977
C,0,-3.6453181824,0.8878612992,-3.9087675076	C,0,-3.6493650261,0.8879942364,-3.9081703892
C,0,-4.8536023284,0.1695011553,-4.0036282909	C,0,-4.858081468,0.1712380419,-3.9955045336
H,0,6.8943255125,0.2936885201,0.5477880037	H,0,6.8876171058,0.2980903198,0.5829522595
H,0,-5.9047876403,-1.6247673789,-3.4770694336	H,0,-5.9100048148,-1.6220754167,-3.4655630089
H,0,-3.9908547772,-2.5876535094,-2.2369272758	H,0,-3.9913369999,-2.5895655422,-2.2375360852
O,0,-3.5260054639,2.112898289,-4.5001827646	O,0,-3.5299421398,2.1112929584,-4.496924729
H,0,-4.3596380345,2.328862566,-4.9410677303	H,0,-4.3663395534,2.3320951825,-4.9283991374
O,0,5.3034711149,2.7646829146,1.0358834665	O,0,5.2875915258,2.766870413,1.0308817888
C,0,4.301181122,2.3986326309,1.9426597717	C,0,4.285760111,2.4060761265,1.9349675472
H,0,4.3001420914,3.1450703113,2.7501112778	H,0,4.2970320515,3.1558509047,2.739457988
H,0,3.2958431379,2.3967192159,1.495560275	H,0,3.2780523296,2.4141454101,1.4918680137
H,0,4.4763448326,1.4151418896,2.4040372412	H,0,4.4547228332,1.4227190104,2.3991594399
O,0,-5.8440339868,0.7914733447,-4.7114437067	O,0,-5.8546736971,0.7970471326,-4.6980918442
H,0,-6.6396737689,0.2472013414,-4.752386268	H,0,-6.6526711427,0.2576250612,-4.7233730678
H,0,-1.6522932663,0.9153867871,-3.1535249275	H,0,-1.6537916178,0.9099361163,-3.1643270899

TS C4(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.48685648 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231260 a.u. 1 imaginary frequency = 430.3960 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.0669138 a.u.	**TS C4(•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.51249274 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231465 a.u. 1 imaginary frequency = 378.8699 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.0932934 a.u.
0, 2	0, 2
C,0,5.9419027957,0.6031476188,0.2206334381	C,0,5.9341420633,0.6117617782,0.1932043399
C,0,5.0405034376,-0.4386900705,0.6112789398	C,0,5.0410936508,-0.4374179645,0.5907388988
C,0,5.526157561,1.6842235408,-0.5382615738	C,0,5.5023941947,1.6927368583,-0.5528172808
H,0,5.4303247475,-1.387715481,0.9504309766	H,0,5.448776291,-1.3913065973,0.896116273
C,0,3.7536967099,-0.4078047997,-0.0018366866	C,0,3.7411965992,-0.404257048,0.0004051576
C,0,4.2166358193,1.7666867292,-1.055342531	C,0,4.1803027371,1.7748941443,-1.0497613428
H,0,3.9059797288,2.6111227292,-1.6591053864	H,0,3.8571685131,2.6201125097,-1.6448372907
C,0,3.3644041574,0.706055596,-0.7737265944	C,0,3.3358910425,0.7138957451,-0.7606321564
C,0,1.7560847859,-0.7962763648,-0.6234434997	C,0,1.7257612963,-0.7868526538,-0.5923985794
N,0,2.7347550492,-1.3307712434,0.0758918819	N,0,2.7274142748,-1.3261559299,0.0936943549
N,0,2.0547058557,0.4231948626,-1.1612979193	N,0,2.0217191562,0.4319184881,-1.125016576
H,0,1.4278281244,0.9724359094,-1.7271605763	H,0,1.3924837405,0.9885060205,-1.6840706601
N,0,0.5418121581,-1.3968893235,-0.8112385542	N,0,0.5159622603,-1.3806980937,-0.7606959388
N,0,-0.4245651163,-0.7824728624,-1.5287771268	N,0,-0.4450077658,-0.7629737789,-1.4964072279
C,0,-1.5630417305,-1.3684577039,-1.6339453888	C,0,-1.578131027,-1.3589425051,-1.6104780296
H,0,-1.741186112,-2.3342846215,-1.1480001462	H,0,-1.7572134572,-2.3234699499,-1.1268447485
H,0,0.3888237756,-2.2845408131,-0.3421980516	H,0,0.3607550544,-2.284000796,-0.3223862183

H,0,6.2272061003,2.4803897878,-0.7612178304	H,0,6.197114986,2.4908178761,-0.788105846
C,0,-2.6762843688,-0.802890672,-2.3889744328	C,0,-2.6826848843,-0.7971099159,-2.3808181436
C,0,-3.8925228457,-1.4970351007,-2.4239219982	C,0,-3.8947817738,-1.4987485107,-2.4317650302
C,0,-2.5654394329,0.4163915151,-3.0789524336	C,0,-2.5683826667,0.4230210581,-3.0721113514
C,0,-4.979654129,-0.9859565679,-3.1306992813	C,0,-4.975722246,-0.9976612442,-3.155216571
C,0,-3.642182339,0.9267114454,-3.7816809092	C,0,-3.6393378015,0.9217272343,-3.7912441472
C,0,-4.8583197938,0.2196136724,-3.8064157423	C,0,-4.8530557215,0.2079757639,-3.834044023
H,0,6.9574133973,0.566060672,0.5946347397	H,0,6.9598662781,0.5712023399,0.5392639326
H,0,-5.9205508534,-1.5269924243,-3.1545802031	H,0,-5.9126023205,-1.542862081,-3.1914710025
H,0,-3.9943877727,-2.4390324102,-1.8971648573	H,0,-3.9976613203,-2.4398079795,-1.9039794914
O,0,-3.5185148221,2.1092790692,-4.4449734318	O,0,-3.5150690475,2.1065869931,-4.4591782097
H,0,-4.3587808234,2.311556956,-4.8766607046	H,0,-4.3500224767,2.3005583367,-4.9077189596
O,0,4.7572141884,-0.0029481939,2.4695360177	O,0,4.737345293,-0.0731264154,2.4742024247
C,0,3.9842399537,1.13913658,2.6717469879	C,0,4.0542686853,1.1278993585,2.6995076716
H,0,4.4146312033,2.0400872564,2.2081621257	H,0,4.5685447297,2.0000534825,2.2699893101
H,0,2.9432508358,1.0256645403,2.3323193608	H,0,3.0194667902,1.1122990407,2.3264293954
H,0,3.9656364802,1.3113786661,3.7581136926	H,0,4.0142212596,1.2777712861,3.7882432131
H,0,-1.6362291052,0.9705416619,-3.0692003978	H,0,-1.6417686132,0.9826387282,-3.0496720473
O,0,-5.861953043,0.8138956623,-4.5325109897	O,0,-5.8438050993,0.7919787995,-4.5739250866
H,0,-6.6651952972,0.2844906317,-4.5036223536	H,0,-6.646243395,0.2563420721,-4.5683604529

TS C4(•OCH_3), optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.49754886 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231357 a.u. 1 imaginary frequency = 412.0059 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1025.0779423 a.u.	**TS C6(•OCH_3),** optimization in gas phase UB3LYP/6-311++G**, E= -1025.48471068 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231760 a.u. 1 imaginary frequency = 466.3947 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.063068 a.u.
0, 2	0, 2
C,0,5.9407362533,0.6030272791,0.1986656211	C,0,6.0969654119,0.5148772793,0.067809718
C,0,5.0432872666,-0.4413307163,0.5947274889	C,0,5.2377315088,-0.5428273594,0.3163338603
C,0,5.5157451786,1.6881868143,-0.5476715294	C,0,5.673685925,1.6471007211,-0.659738688
H,0,5.4403621517,-1.3944018353,0.91422491	H,0,5.5494773668,-1.4129537209,0.8810287449
C,0,3.7465365303,-0.4039668372,0.0013626966	C,0,3.9265784684,-0.4610213827,-0.1851344892
C,0,4.1977199583,1.7752039754,-1.0467536077	C,0,4.3803923863,1.7534297471,-1.1697620743
H,0,3.8793625601,2.6225709948,-1.6420585958	H,0,4.0676128091,2.6277483356,-1.7279171411
C,0,3.348240259,0.7152757219,-0.7596418602	C,0,3.5212348022,0.6877911881,-0.9331939472
C,0,1.7366844842,-0.783299103,-0.5969853787	C,0,1.8442041968,-0.7284375134,-0.6545331301
N,0,2.7278860594,-1.3243541565,0.0887063966	N,0,2.9029911057,-1.346390129,-0.0691919403
N,0,2.0335033793,0.4374563657,-1.12988861	N,0,2.2217903588,0.4362961666,-1.3136891397
H,0,1.4044774352,0.991688823,-1.6896902652	H,0,1.5425268544,1.1203874097,-1.6088180486
N,0,0.5209845974,-1.3763496549,-0.7701051361	N,0,0.7913405717,-1.4825365045,-1.1307385244
N,0,-0.4397444916,-0.7634123394,-1.5026744094	N,0,-0.2598426196,-0.8243982462,-1.6897676396
C,0,-1.5759405669,-1.3533391357,-1.6126480076	C,0,-1.3580789783,-1.4679981427,-1.8318875754
H,0,-1.7570009653,-2.3154608425,-1.122316345	H,0,-1.4542785541,-2.5008596394,-1.4762848528
H,0,0.3691308603,-2.2749196326,-0.3216673514	H,0,0.6292092419,-2.3507871298,-0.6262849664
H,0,6.214501179,2.4844654097,-0.7773048338	H,0,6.3747655827,2.4563834492,-0.8287541045
C,0,-2.6825393648,-0.7943214589,-2.3821827582	C,0,-2.5390178425,-0.8861414725,-2.4664951286
C,0,-3.8989933595,-1.4884629995,-2.4178826951	C,0,-3.7024041875,-1.6580456945,-2.5717809704
C,0,-2.5655312376,0.416685472,-3.0867419528	C,0,-2.5405191732,0.4256378353,-2.9691436022
C,0,-4.9811245186,-0.9864572171,-3.1387564583	C,0,-4.8484366601,-1.1341355749,-3.1680612682
C,0,-3.6372866092,0.9171991762,-3.8036668419	C,0,-3.6757256322,0.9490890409,-3.5619387187
C,0,-4.8547423611,0.2109957068,-3.8292878615	C,0,-4.8375746936,0.1624940821,-3.6609817591
H,0,6.9627896985,0.5607850316,0.55437579	H,0,7.113777295,0.4802731287,0.4410369419
H,0,-5.921933361,-1.5266963557,-3.1628474959	H,0,-5.7486741316,-1.7357722081,-3.2480789323

H,0,-4.0047642947,-2.4237096714,-1.8801605779	H,0,-3.7166619432,-2.6720208666,-2.1884074979
O,0,-3.5085132753,2.0923486437,-4.4828308463	O,0,-3.6623474178,2.2224490809,-4.045734647
H,0,-4.3447197143,2.2878660429,-4.9267027603	H,0,-4.5320426032,2.4208075783,-4.4163606467
O,0,4.772460764,-0.0387387016,2.4693705897	O,0,1.1134162634,0.1411228006,0.9448435974
C,0,4.0254741434,1.1202411809,2.687704301	C,0,0.7634959324,-0.718654438,1.9764444063
H,0,4.4746519103,2.0147016927,2.2301258843	H,0,0.1637498139,-1.5829934824,1.6380206832
H,0,2.9822808572,1.0336052336,2.3479222575	H,0,1.6270753256,-1.0912657894,2.5448666675
H,0,4.0105206688,1.2851641733,3.7751612377	H,0,0.1240425412,-0.1486797646,2.6692909487
H,0,-1.6355864128,0.9700927851,-3.0774808533	H,0,-1.6533051879,1.0406003795,-2.8960335541
O,0,-5.8502588729,0.795746822,-4.5688182422	O,0,-5.9080374659,0.7776968315,-4.266117384
H,0,-6.6542575094,0.265219763,-4.5477433391	H,0,-6.6684919915,0.1886207347,-4.2942308573

TS C6(•OCH_3), optimization in solv. water UB3LYP/6-311++G**, E= -1025.50708427 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.232228 a.u. 1 imaginary frequency = 437.1980 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.0861806 a.u.	**TS C6(•OCH_3),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.49375874 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231777 a.u. 1 imaginary frequency = 460.0251 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1025.0723902 a.u.
0, 2	0, 2
C,0,6.1251338237,0.4997564101,-0.0072272778	C,0,6.1052781941,0.5117786314,0.0327951676
C,0,5.2644817853,-0.5443669478,0.2827349381	C,0,5.2482422938,-0.5438228474,0.2950757908
C,0,5.6890516674,1.6321636163,-0.7341149009	C,0,5.6719132427,1.6476936374,-0.6856764999
H,0,5.5898858341,-1.4117134166,0.8444422875	H,0,5.5691755746,-1.4151451034,0.8529125949
C,0,3.9346401955,-0.4514158277,-0.1756927078	C,0,3.9275204027,-0.4573681888,-0.1836262261
C,0,4.3807678865,1.7529310889,-1.1987494857	C,0,4.3703045987,1.7600050149,-1.1719648511
H,0,4.0577684138,2.6240389591,-1.7550868262	H,0,4.0489315516,2.6362276456,-1.7218418438
C,0,3.5163619459,0.6995273928,-0.9198391556	C,0,3.5121616237,0.6957080023,-0.9218735869
C,0,1.8299675597,-0.6991697439,-0.5847032378	C,0,1.8346067154,-0.7181442572,-0.6228510213
N,0,2.9095414289,-1.3239752004,-0.0228554537	N,0,2.9050520549,-1.3404198688,-0.0545165042
N,0,2.2035859109,0.4653539208,-1.2427971653	N,0,2.2064515601,0.4501996573,-1.2765672519
H,0,1.5434946127,1.1251534658,-1.6254013612	H,0,1.5319301044,1.1265044866,-1.5996782837
N,0,0.7773055144,-1.4469640536,-1.0491346646	N,0,0.7804344961,-1.4680828584,-1.0954438191
N,0,-0.2704809748,-0.7870600046,-1.6252446475	N,0,-0.2675044599,-0.8070318617,-1.6630037826
C,0,-1.3530486956,-1.4509884355,-1.8088315893	C,0,-1.3635333886,-1.4539025022,-1.8142893739
H,0,-1.4371743554,-2.4919901753,-1.482230473	H,0,-1.4600304044,-2.4865488678,-1.4608879698
H,0,0.6214273119,-2.3380116943,-0.5846846668	H,0,0.6166543699,-2.3437475903,-0.6046418539
H,0,6.3951596309,2.42894046,-0.93674429	H,0,6.3726820807,2.4548678409,-0.865351739
C,0,-2.5281872875,-0.8732999449,-2.4563528529	C,0,-2.5396022801,-0.8745712092,-2.459713335
C,0,-3.6740422372,-1.6656902781,-2.6045680332	C,0,-3.6995558971,-1.6507962255,-2.5745284566
C,0,-2.5450041384,0.4499961,-2.9330582885	C,0,-2.5406999792,0.4361431241,-2.9669104372
C,0,-4.817580395,-1.1541758371,-3.2161891479	C,0,-4.8416516431,-1.134042455,-3.184607526
C,0,-3.6783917007,0.9599233122,-3.5404132482	C,0,-3.6719244513,0.9518344483,-3.5735969195
C,0,-4.8242613647,0.1535188242,-3.6841121285	C,0,-4.8309309366,0.1610905812,-3.6836201734
H,0,7.1541237746,0.4573430861,0.3294272512	H,0,7.1284738401,0.474012082,0.3876664821
H,0,-5.7027558744,-1.7705562324,-3.3292953896	H,0,-5.7383215638,-1.7392215792,-3.2713895114
H,0,-3.6758913576,-2.6870597812,-2.2418859709	H,0,-3.7139875891,-2.6634165327,-2.1877959801
O,0,-3.6811305802,2.2463016134,-4.0000613206	O,0,-3.6582170902,2.2247573333,-4.0632301988
H,0,-4.5452656077,2.4353375718,-4.3917679738	H,0,-4.5242467579,2.4187129482,-4.4462035552
O,0,1.1432639076,0.160896448,1.0590640613	O,0,1.1277572367,0.1354249736,1.0024269267
C,0,0.7008610209,-0.7417698765,2.0229867734	C,0,0.7609659231,-0.7480725521,2.0102246055
H,0,0.0849322402,-1.5542905772,1.6014403266	H,0,0.1576194481,-1.597327676,1.6434699516
H,0,1.5172649988,-1.1918931139,2.6068221395	H,0,1.6167210874,-1.1443390284,2.5750332085
H,0,0.0504765642,-0.196323659,2.7254167707	H,0,0.1201613544,-0.1947579002,2.7152311404
H,0,-1.6718736376,1.0819557879,-2.8300973917	H,0,-1.6566146722,1.0552514375,-2.8875947283

O,0,-5.8863453712,0.7578695847,-4.2990267465 H,0,-6.6374377699,0.1565938877,-4.3715538127	O,0,-5.8934925657,0.7697015338,-4.3028566114 H,0,-6.6520993943,0.1777324562,-4.3499594879

TS C9(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.48622759 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.232957 a.u. 1 imaginary frequency = 437.0088 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.0682465a.u.	**TS C9(•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.50848656 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.232816 a.u. 1 imaginary frequency = 403.8532 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.0920401 a.u.
0, 2 C,0,5.7829735679,0.2071416391,-0.2968513105 C,0,4.7532283379,-0.7266187986,-0.2386653005 C,0,5.5688283914,1.5251144115,-0.7885348563 H,0,4.936301399,-1.7555624682,0.0463636596 C,0,3.4793023697,-0.3248703674,-0.6347008182 C,0,4.3241352452,1.9530098972,-1.181586774 H,0,4.1556443534,2.9485199202,-1.573014915 C,0,3.2181398452,1.0746123525,-0.9438810774 C,0,1.5049896881,-0.2349901401,-1.4127594442 N,0,2.355086624,-1.0792587074,-0.8633499158 N,0,1.995493413,1.0255103371,-1.6454498104 H,0,1.3745079608,1.8197862874,-1.7051623395 N,0,0.2428361868,-0.5927269372,-1.7678482807 N,0,-0.6193318948,0.3141887198,-2.283662697 C,0,-1.8088313495,-0.0838766785,-2.5588017155 H,0,-2.1086210009,-1.122171454,-2.3758318336 H,0,-0.0390848958,-1.5464889026,-1.5591729087 H,0,6.4168544741,2.1949701891,-0.875748306 C,0,-2.8241853057,0.7982133958,-3.1239137199 C,0,-4.1005692792,0.2828950504,-3.3833843331 C,0,-2.5565167201,2.1463687663,-3.4172150729 C,0,-5.0948490112,1.0957245565,-3.924537546 C,0,-3.5410668636,2.9560414924,-3.9545446466 C,0,-4.8191738352,2.425371247,-4.2095202185 H,0,6.7853860016,-0.0852516178,-0.0058400503 H,0,-6.0832352621,0.6934699718,-4.1242056417 H,0,-4.3215797901,-0.7552299785,-3.1626779605 O,0,-3.2678287276,4.2597072002,-4.2343413076 H,0,-4.0613095102,4.6710849644,-4.6009063295 O,0,2.5041541167,1.7821852389,0.6233233194 C,0,3.2911974739,1.7148056476,1.776344741 H,0,3.4059999615,0.6899776043,2.1579573717 H,0,4.2916756219,2.1498276204,1.631561992 H,0,2.7859777558,2.3143754,2.5464692571 O,0,-5.7214009413,3.3131464061,-4.743121399 H,0,-6.5710433224,2.8876990398,-4.8960282314 H,0,-1.5774098082,2.5656001146,-3.2265105506	0, 2 C,0,5.7698250403,0.2104753606,-0.3448164718 C,0,4.7424827127,-0.7220986967,-0.2381119058 C,0,5.5379687403,1.524598688,-0.8464510587 H,0,4.9413530266,-1.7474788078,0.0509423312 C,0,3.4542742938,-0.3254307157,-0.5963483045 C,0,4.2807577891,1.9511926588,-1.1949817917 H,0,4.0987870049,2.9393118028,-1.5992513198 C,0,3.1798042928,1.0766235074,-0.9027635198 C,0,1.4578070824,-0.2446702109,-1.3441214316 N,0,2.328741649,-1.0837005222,-0.7962883288 N,0,1.9465299578,1.0139829041,-1.5755224831 H,0,1.3433772408,1.8075934188,-1.7376156704 N,0,0.20083346,-0.5987708413,-1.6884017584 N,0,-0.6459757839,0.3204443558,-2.2280372439 C,0,-1.8249978645,-0.0850967966,-2.5411958055 H,0,-2.1221416143,-1.1252465549,-2.3804245364 H,0,-0.0902968933,-1.5575009949,-1.5158940101 H,0,6.3842977607,2.1891699427,-0.9780772666 C,0,-2.8275695596,0.7995388133,-3.1229256495 C,0,-4.0832452036,0.2701775877,-3.4502801737 C,0,-2.5726545913,2.1616889291,-3.3669261052 C,0,-5.0697135159,1.0788597497,-4.0113636503 C,0,-3.5503463809,2.9662280794,-3.9230030983 C,0,-4.8088417661,2.4225891109,-4.2486859518 H,0,6.7822609999,-0.0792399549,-0.088544577 H,0,-6.0399187403,0.666267039,-4.2652280567 H,0,-4.2929993852,-0.7773995918,-3.2680209382 O,0,-3.2912632747,4.2866743141,-4.1545291199 H,0,-4.0785059498,4.6966254399,-4.539387422 O,0,2.5314510063,1.7641580482,0.6908076254 C,0,3.3879944789,1.7250550894,1.8008125831 H,0,3.5538163552,0.7051960336,2.1767030474 H,0,4.3668351998,2.1822383752,1.5946964218 H,0,2.9182810413,2.3116674392,2.6022158032 O,0,-5.6988772746,3.3057557537,-4.7925415365 H,0,-6.5428004472,2.8791487552,-4.9846297553 H,0,-1.6106556175,2.5936739115,-3.1215578406

TS C9(•OCH_3), optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.49563997 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.233312 a.u.	**TS C13(•OCH_3),** optimization in gas phase UB3LYP/6-311++G**, E= -1025.49752253 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231499 a.u.

1 imaginary frequency = 422.5069 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1025.078266 a.u.	1 imaginary frequency = 243.6620 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.0745255 a.u.
0, 2 C,0,5.7776464018,0.2118281095,-0.3124581995 C,0,4.750014227,-0.7231429134,-0.2373971568 C,0,5.5555229902,1.5280656296,-0.8083430545 H,0,4.9402584537,-1.7503965234,0.0496802345 C,0,3.4702693664,-0.3254069067,-0.6209513642 C,0,4.3056383156,1.9533753969,-1.1862316435 H,0,4.1311289084,2.9458136241,-1.5828795787 C,0,3.2024025616,1.0746340386,-0.9292459757 C,0,1.4879641287,-0.2418021392,-1.3900922891 N,0,2.3473437075,-1.0830788951,-0.840803118 N,0,1.9765004649,1.0186611044,-1.6207108192 H,0,1.3603537247,1.812582516,-1.7207019746 N,0,0.2289244467,-0.598737404,-1.74299959 N,0,-0.6265388595,0.3142187489,-2.2685143496 C,0,-1.8142230357,-0.0841915517,-2.5527655142 H,0,-2.115972549,-1.1214128138,-2.3730250183 H,0,-0.0587531903,-1.5533345007,-1.545476448 H,0,6.4021950593,2.1973880016,-0.9112284353 C,0,-2.8243213513,0.7991502306,-3.1246080224 C,0,-4.0950287068,0.2797278388,-3.4043228569 C,0,-2.5594867583,2.1513813861,-3.4042762131 C,0,-5.0867075668,1.09095395,-3.9525299707 C,0,-3.5418111742,2.9591071095,-3.9479632704 C,0,-4.8149052399,2.4249579048,-4.2240602117 H,0,6.7840697251,-0.0779601314,-0.0330638231 H,0,-6.0698295533,0.6857409977,-4.1688019798 H,0,-4.3132965501,-0.7610524902,-3.1940766528 O,0,-3.2720720732,4.2682475646,-4.214116858 H,0,-4.0645584041,4.6803695237,-4.5835657686 O,0,2.5121372196,1.7733618077,0.6502652066 C,0,3.3270630222,1.716136967,1.7863937187 H,0,3.4619616206,0.6928640131,2.165511972 H,0,4.3197061326,2.1597900937,1.6172600762 H,0,2.8360541741,2.3101690411,2.5697545434 O,0,-5.7126707912,3.3107511046,-4.7609040787 H,0,-6.5648769894,2.8887815079,-4.9160228435 H,0,-1.5854265876,2.574759479,-3.1964776427	0, 2 C,0,5.9705375835,0.7365297297,0.1938973004 C,0,5.0722434939,-0.238029838,0.6141152901 C,0,5.6414066723,1.6486806594,-0.8243826309 H,0,5.3219203137,-0.9414751755,1.3991096135 C,0,3.8206688532,-0.2895878251,-0.0068237638 C,0,4.400250343,1.6148680798,-1.4573541315 H,0,4.1499384106,2.3193459914,-2.2420010231 C,0,3.5069170974,0.637968965,-1.0322612438 C,0,1.8394377178,-0.7488228651,-0.6362579386 N,0,2.7542590034,-1.1461050004,0.2146614368 N,0,2.216419653,0.306882418,-1.4234919342 H,0,1.6195183353,0.7594625646,-2.0979262892 N,0,0.608821186,-1.3391183499,-0.771175323 N,0,-0.3069018999,-0.7948480303,-1.5736417115 C,0,-1.4414503108,-1.4651314698,-1.6498097316 H,0,-1.4645261305,-2.5284961268,-1.4279810845 H,0,0.3095630697,-1.9829884089,-0.0387262244 H,0,6.3681720635,2.3947517768,-1.1241034325 C,0,-2.563884772,-0.9173398544,-2.4032752513 C,0,-3.5901821744,-1.7732144275,-2.8233889442 C,0,-2.6428190937,0.4513029155,-2.7091743705 C,0,-4.6677553106,-1.2774952454,-3.5535769486 C,0,-3.7095521282,0.9469696845,-3.4384966709 C,0,-4.7276464601,0.0747705645,-3.8627580994 H,0,6.9471689996,0.7980421889,0.6600960134 H,0,-5.4597976607,-1.9428159653,-3.8832117558 H,0,-3.5450162865,-2.8300220581,-2.5871526308 O,0,-3.7707736682,2.2752165225,-3.7333984671 H,0,-4.5827383863,2.4448223808,-4.2284727376 O,0,-1.7992795448,-1.4137085822,0.4742371298 C,0,-3.1123191397,-1.6355824356,0.8447154114 H,0,-3.8061547401,-0.9100029115,0.390040736 H,0,-3.4703985812,-2.6566859379,0.628795803 H,0,-3.1821505649,-1.4887990535,1.9363811008 O,0,-5.7427829383,0.6668267687,-4.5740482537 H,0,-6.4149193343,0.0206257084,-4.8127464368 H,0,-1.8726109007,1.1324874427,-2.3722344162

TS C13(•OCH_3), optimization in solv. water UB3LYP/6-311++G**, E= -1025.51877867 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.230920 a.u. 1 imaginary frequency = 228.6788 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.0971244 a.u.	**TS C13(•OCH_3),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.50619585 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231252 a.u. 1 imaginary frequency = 244.1830 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1025.084047 a.u.
0, 2 C,0,6.0290530053,0.668529261,0.1216897067 C,0,5.2000637022,-0.4146380645,0.3985841781 C,0,5.5871093461,1.7503041179,-0.6626238388 H,0,5.541739962,-1.2472406329,1.0023464518 C,0,3.9038731947,-0.4000134646,-0.1277978331 C,0,4.2994800846,1.7842787706,-1.1963767772	0, 2 C,0,5.9844720711,0.6884351279,0.2468058741 C,0,5.1336099818,-0.3665031,0.5603205891 C,0,5.5840452884,1.7233290436,-0.6174844331 H,0,5.4405098846,-1.1637397202,1.2266776628 C,0,3.8572963163,-0.372788339,-0.0109917327 C,0,4.3168188266,1.7362183378,-1.1980785306

H,0,3.9593101494,2.616599179,-1.8006095944	H,0,4.0098192304,2.5340749233,-1.8639960748
C,0,3.4765112879,0.6984287964,-0.9151020816	C,0,3.4717740283,0.6784628342,-0.8802615329
C,0,1.8900027457,-0.8149533539,-0.7012354922	C,0,1.8622945356,-0.8051304242,-0.6241104203
N,0,2.8846125002,-1.3346384476,-0.012787651	N,0,2.8250253521,-1.2885327367,0.1268889282
N,0,2.1698808861,0.3950340682,-1.2688463448	N,0,2.175125025,0.3634569903,-1.2625433222
H,0,1.5260387047,0.9421009916,-1.8211501749	H,0,1.5448017416,0.8848965139,-1.8523239762
N,0,0.6729026006,-1.4234638971,-0.8572357209	N,0,0.6450109995,-1.4127086833,-0.7926226553
N,0,-0.3011964918,-0.8227535062,-1.5356566729	N,0,-0.30790021,-0.8191536262,-1.5094950175
C,0,-1.4358047799,-1.4907514917,-1.6212104239	C,0,-1.4356927749,-1.4959342387,-1.6155249117
H,0,-1.4629879509,-2.5566985854,-1.408736314	H,0,-1.4483217838,-2.5691826138,-1.4451730307
H,0,0.5137188835,-2.2950272219,-0.3554469702	H,0,0.4211817356,-2.1954174798,-0.1805209757
H,0,6.2622041234,2.5755811352,-0.8568845159	H,0,6.2752426362,2.5286087566,-0.8375780575
C,0,-2.5533913831,-0.9332082534,-2.3746179051	C,0,-2.5628367001,-0.9253670041,-2.3455344717
C,0,-3.5867328494,-1.7838253601,-2.7896357954	C,0,-3.5820645679,-1.7724143571,-2.7995129511
C,0,-2.6214752093,0.4352605765,-2.6918532168	C,0,-2.6531716298,0.4539381957,-2.5982839064
C,0,-4.6632618615,-1.2862455974,-3.5209020687	C,0,-4.6654756091,-1.2580458155,-3.5084018811
C,0,-3.6895894868,0.9319150587,-3.4171728281	C,0,-3.726441488,0.9679331653,-3.3044679085
C,0,-4.7181183597,0.0660591776,-3.8362146061	C,0,-4.7394183176,0.1055558973,-3.762251744
H,0,7.0381607276,0.6818125801,0.5172493023	H,0,6.9790402665,0.7167092041,0.6769315876
H,0,-5.459326283,-1.9468560662,-3.8467487143	H,0,-5.4507899282,-1.9166535026,-3.8651466387
H,0,-3.5482274236,-2.8397527233,-2.5491680168	H,0,-3.5270847457,-2.8375637624,-2.6069127476
O,0,-3.7436821977,2.2625463645,-3.7202051917	O,0,-3.7995382077,2.30785398,-3.5469570178
H,0,-4.5535065317,2.4358651502,-4.2202049639	H,0,-4.6141042386,2.4911387589,-4.0340367084
O,0,-1.8825740031,-1.3387918228,0.5033203141	O,0,-1.8300845702,-1.496895768,0.5032890057
C,0,-3.233539131,-1.5201794636,0.7567762739	C,0,-3.1744211929,-1.6004268824,0.8149071557
H,0,-3.6028382921,-2.5213275953,0.4831087474	H,0,-3.6283340804,-2.558597195,0.5120546815
H,0,-3.3949643164,-1.3948702785,1.8417084778	H,0,-3.2702947609,-1.5246101031,1.9119626646
H,0,-3.8632983134,-0.7628766725,0.2627293536	H,0,-3.7708092848,-0.77492777,0.3943202756
O,0,-5.7245704057,0.6602344083,-4.5448139636	O,0,-5.7584314527,0.7166220627,-4.4459211001
H,0,-6.4017375197,0.0197354969,-4.7940094454	H,0,-6.4312273852,0.0782544574,-4.7068094595
H,0,-1.8402563444,1.1131121664,-2.3720872939	H,0,-1.8866758113,1.1283226031,-2.2394308489

TS C14(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.48003346 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231882 a.u. 1 imaginary frequency = 435.7559 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.0636994 a.u.	**TS C14(•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.50416453 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231732 a.u. 1 imaginary frequency = 406.2399 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.0891614 a.u.
0, 2	0, 2
C,0,6.0880244683,0.8232043695,-0.1946451197	C,0,6.1088555489,0.7935859931,-0.2179906033
C,0,5.3316140687,-0.2851564809,0.1799968461	C,0,5.3786433083,-0.3603373078,0.0679471071
C,0,5.5355396159,1.8636375224,-0.9575948034	C,0,5.5119812586,1.9035606833,-0.8378436444
H,0,5.7568640897,-1.0887035376,0.7693161134	H,0,5.8429902803,-1.2148111986,0.5469888884
C,0,3.9970378376,-0.3386054219,-0.224688615	C,0,4.0259914007,-0.3867743153,-0.2800027769
C,0,4.2034205883,1.8289348238,-1.371795927	C,0,4.1611151877,1.8955415078,-1.1934266411
H,0,3.7776216074,2.6335385931,-1.9604202019	H,0,3.6985070479,2.7505495223,-1.6720673671
C,0,3.4571100128,0.7200918919,-0.993525046	C,0,3.4422288621,0.741825696,-0.9044354505
C,0,1.9626200836,-0.8559949084,-0.5942392839	C,0,1.9723189916,-0.8827751372,-0.618034867
N,0,3.0307935048,-1.311974937,0.0076494859	N,0,3.0768138728,-1.3913556174,-0.1136664012
N,0,2.132908457,0.3519598637,-1.2178333684	N,0,2.1140386321,0.3856321785,-1.10880497
H,0,1.4139514712,0.8445624113,-1.7229384065	H,0,1.3764142391,0.9298009599,-1.5302272055
N,0,0.7588038306,-1.5148211457,-0.623768267	N,0,0.7730154977,-1.5376429362,-0.6583574699
N,0,-0.3124951357,-0.9506519932,-1.2222441396	N,0,-0.3058399816,-0.9328081835,-1.2103692349
C,0,-1.4185802052,-1.5905041731,-1.2135131267	C,0,-1.4049583231,-1.5847546702,-1.2547187218

H,0,-1.5208168844,-2.5721696936,-0.7437847074	H,0,-1.4909561511,-2.6033414885,-0.8706886237
H,0,0.6937926378,-2.386399923,-0.1077595603	H,0,0.7293401485,-2.481888897,-0.2872042932
H,0,6.1536394929,2.7110255283,-1.2307987504	H,0,6.1092597988,2.7839760356,-1.0450884354
C,0,-2.6438834772,-1.0280653166,-1.825814332	C,0,-2.633830935,-0.9867247023,-1.8249564235
C,0,-3.4616031318,-1.9441955501,-2.5905562244	C,0,-3.5152964089,-1.9135715197,-2.5029935972
C,0,-2.6319515492,0.3461606199,-2.2521223812	C,0,-2.5797427847,0.3582899522,-2.3427946949
C,0,-4.3325893707,-1.4830372705,-3.5515646639	C,0,-4.39823429,-1.4822782073,-3.4648871776
C,0,-3.5032585062,0.7951268984,-3.2090090223	C,0,-3.469378542,0.780091485,-3.2920662923
C,0,-4.3723083166,-0.1186985188,-3.8608693246	C,0,-4.3990599644,-0.1371345452,-3.8595811157
H,0,7.1268547194,0.8857881187,0.1090816432	H,0,7.1601283711,0.835910751,0.043805884
H,0,-4.9800640493,-2.1732725398,-4.0841603114	H,0,-5.0865782558,-2.1761733199,-3.9354478422
H,0,-3.4177349205,-2.9990705956,-2.3515621488	H,0,-3.5003962598,-2.9548071725,-2.2052114406
O,0,-3.5243798622,2.112133091,-3.5543110703	O,0,-3.4538508743,2.074377784,-3.722226228
H,0,-4.1744705952,2.2418300119,-4.2566408743	H,0,-4.1208098455,2.186839502,-4.4137766479
O,0,-3.5894710375,-1.1198151706,-0.2299353692	O,0,-3.4518807299,-0.8091397686,-0.1628988913
C,0,-4.7715942291,-0.3714421444,-0.1944744372	C,0,-4.7804727408,-0.3533785357,-0.2048864359
H,0,-4.6027535324,0.708271309,-0.3070426228	H,0,-4.8868291021,0.5911273989,-0.7573271516
H,0,-5.5063325666,-0.6960525324,-0.9476549169	H,0,-5.4758050472,-1.0894589068,-0.6313384532
H,0,-5.219033343,-0.5451073779,0.7931910261	H,0,-5.0864425793,-0.1629650518,0.8324165963
H,0,-1.9558986474,1.0435512498,-1.7770186956	H,0,-1.855562108,1.0530788867,-1.9395186932
O,0,-5.1985419655,0.4335226328,-4.7985398287	O,0,-5.2280068112,0.3879086068,-4.7947651439
H,0,-5.7484501904,-0.2397223443,-5.2134216578	H,0,-5.8233257415,-0.2800981019,-5.158567631

TS C14(•OCH_3), optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.49015464 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.232353 a.u. 1 imaginary frequency = 423.5465 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1025.0743819 a.u.	**TS C15(•OCH_3),** optimization in gas phase UB3LYP/6-311++G**, E= -1025.48804256 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231466 a.u. 1 imaginary frequency = 416.8858 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.0679367 a.u.
0, 2	0, 2
C,0,6.0849255865,0.8244629715,-0.1893024	C,0,5.8221794879,0.6740215684,0.2477438922
C,0,5.3411802827,-0.3042961237,0.1512962555	C,0,5.0354941354,-0.4575052535,0.4475980537
C,0,5.5161384421,1.8869016116,-0.9092991397	C,0,5.3372409996,1.7898609065,-0.4533259692
H,0,5.7807074351,-1.1236166332,0.7079525327	H,0,5.4082158274,-1.3191527594,0.9883495377
C,0,4.0032551363,-0.3552828287,-0.2442276046	C,0,3.7392047462,-0.4573832063,-0.0711176535
C,0,4.1802924076,1.854375611,-1.3136756807	C,0,4.0458937647,1.8093700932,-0.980472547
H,0,3.7411987795,2.6753019265,-1.8687005805	H,0,3.6727777167,2.6711365716,-1.5217679403
C,0,3.4472211202,0.7253497826,-0.9701620384	C,0,3.2677508186,0.6765248446,-0.7762562449
C,0,1.9663946215,-0.8752938024,-0.6170597368	C,0,1.7441721115,-0.9141361914,-0.6617815535
N,0,3.046578826,-1.344499717,-0.039475659	N,0,2.7562781821,-1.4390115165,-0.0186477565
N,0,2.1253243526,0.354554369,-1.1972444284	N,0,1.9694788587,0.3443487647,-1.151039596
H,0,1.3999054259,0.8639614016,-1.677104526	H,0,1.2792603703,0.9085811294,-1.621749075
N,0,0.7686371839,-1.5391699837,-0.6595736987	N,0,0.541385809,-1.5497446437,-0.8467249376
N,0,-0.3078997769,-0.9594843979,-1.2383678117	N,0,-0.4396061231,-0.9530846165,-1.5441975482
C,0,-1.4130732664,-1.6013326306,-1.2347409009	C,0,-1.5851735306,-1.5403657674,-1.6156823478
H,0,-1.5077454391,-2.5935048579,-0.7869995153	H,0,-1.7562953738,-2.4985154622,-1.1124745083
H,0,0.7042531816,-2.4253965795,-0.1686076755	H,0,0.4141953951,-2.4426527595,-0.378973377
H,0,6.1238409533,2.7497205112,-1.1564295623	H,0,5.9777202739,2.6536758996,-0.5886463137
C,0,-2.6428089406,-1.0285151183,-1.8284301335	C,0,-2.6929707176,-0.9811610617,-2.3573659252
C,0,-3.4827816601,-1.9477916962,-2.5656815385	C,0,-3.9116899292,-1.6578203896,-2.402891016
C,0,-2.6193988966,0.3383192506,-2.280219119	C,0,-2.5722787542,0.2859002385,-3.023514875
C,0,-4.3595282661,-1.4947281851,-3.524540968	C,0,-4.9756348778,-1.1698965991,-3.1660666351
C,0,-3.496576365,0.7792088664,-3.2344561511	C,0,-3.6138299471,0.6912988886,-3.8942046262
C,0,-4.3856263924,-0.1355488638,-3.8608539958	C,0,-4.8195970865,-0.0058114584,-3.9188351097

H,0,7.1257373067,0.8853526324,0.1081235821	H,0,6.8320134863,0.6966553933,0.6414300445
H,0,-5.0228904686,-2.1850205855,-4.0360636163	H,0,-5.9196140832,-1.7050760215,-3.1910268101
H,0,-3.4472089345,-2.9993388588,-2.3106072354	H,0,-4.0331945284,-2.5872009327,-1.8577670223
O,0,-3.5062293713,2.0904703981,-3.6049407772	O,0,-3.4260436222,1.7959320765,-4.6542214785
H,0,-4.1619332676,2.2158440335,-4.303778233	H,0,-4.233341165,1.9654584744,-5.1588232324
O,0,-3.5513006523,-1.0567459144,-0.205321653	O,0,-2.6915922118,1.548659112,-1.5345829278
C,0,-4.7462656439,-0.3246494939,-0.1867432271	C,0,-3.9526078505,1.6551475079,-0.9535355833
H,0,-4.5947423736,0.7506390753,-0.3530695594	H,0,-4.7100120652,2.0890439013,-1.6234900768
H,0,-5.4853339239,-0.6942294744,-0.9138005327	H,0,-4.3270306476,0.6997737773,-0.5550854174
H,0,-5.1788539351,-0.4553889161,0.8140865522	H,0,-3.8369295549,2.339512211,-0.0996150331
H,0,-1.929291075,1.0358193009,-1.8256563655	H,0,-1.586800736,0.685260954,-3.2092710692
O,0,-5.2119227861,0.4082262736,-4.797028678	O,0,-5.7903273853,0.5235243005,-4.7395166648
H,0,-5.7697946365,-0.2647959944,-5.2043082706	H,0,-6.5445173133,-0.0705505739,-4.8036026764

TS C15(•OCH_3), optimization in solv. water UB3LYP/6-311++G**, E= -1025.51267589 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231158 a.u. 1 imaginary frequency = 386.5566 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.0935918 a.u.	**TS C15(•OCH_3),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.49823780 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.232119 a.u. 1 imaginary frequency = 406.5271 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1025.0786002 a.u.
0, 2	0, 2
C,0,5.8476917689,0.6535978712,0.230553413	C,0,5.8380785264,0.6655322279,0.2209324803
C,0,5.0157737666,-0.4264802987,0.5248663531	C,0,5.0428815444,-0.4560271878,0.4478157697
C,0,5.4105579782,1.7170483925,-0.5766769802	C,0,5.3569463286,1.7725886503,-0.4969887386
H,0,5.3568697214,-1.2453367583,1.1479636292	H,0,5.4149349767,-1.3096531579,1.0020535761
C,0,3.7237454246,-0.4264962248,-0.0073710286	C,0,3.7421576563,-0.4543961712,-0.0609051802
C,0,4.122972882,1.735086613,-1.1172918891	C,0,4.0609993625,1.7930158485,-1.0143589445
H,0,3.783713079,2.5541208129,-1.7404194615	H,0,3.6893308757,2.6469523674,-1.5686283193
C,0,3.3009866455,0.654934621,-0.8182558302	C,0,3.2750783721,0.6705470241,-0.7831771317
C,0,1.7091344588,-0.8581179457,-0.5825303956	C,0,1.7347930626,-0.9023002964,-0.6300008905
N,0,2.7016978167,-1.361318284,0.1219511629	N,0,2.7499663674,-1.4257380523,0.0165031492
N,0,1.9940802268,0.3422246568,-1.1721211608	N,0,1.9715461471,0.344602621,-1.1408749006
H,0,1.3532553645,0.8741350105,-1.7416606304	H,0,1.2901865052,0.9060020053,-1.6283348004
N,0,0.4909947201,-1.458893274,-0.7322890409	N,0,0.5262961332,-1.5265053733,-0.7970504349
N,0,-0.467732379,-0.8633045778,-1.4741261133	N,0,-0.4493155654,-0.9284822127,-1.5062809152
C,0,-1.6049051739,-1.4644449534,-1.5787483492	C,0,-1.5938029786,-1.5175358087,-1.5849239485
H,0,-1.7797830256,-2.4246499839,-1.0855612525	H,0,-1.7683557319,-2.4750142447,-1.0835975533
H,0,0.3331918937,-2.3428129191,-0.2565575304	H,0,0.3929374922,-2.4219128888,-0.3357797479
H,0,6.0843567377,2.5400537775,-0.7850917075	H,0,6.0033991481,2.6284349919,-0.6532452562
C,0,-2.6946379882,-0.9180894049,-2.3572519871	C,0,-2.6941169885,-0.9609880543,-2.3406594739
C,0,-3.8861196711,-1.631478691,-2.4720617419	C,0,-3.9052822503,-1.6478088511,-2.4119352564
C,0,-2.5880449595,0.3675982121,-2.9927033511	C,0,-2.5726636089,0.3100327032,-3.0005025054
C,0,-4.9330882879,-1.1632461595,-3.2726394193	C,0,-4.9591651089,-1.1682409915,-3.1955812546
C,0,-3.6062000443,0.7561137853,-3.9006223765	C,0,-3.600175383,0.7061401668,-3.892654258
C,0,-4.7882077022,0.0227321733,-3.9944592099	C,0,-4.7996801303,-0.0015505755,-3.9443002825
H,0,6.8543773022,0.6743933396,0.6325548093	H,0,6.8510806325,0.6863655789,0.6066655493
H,0,-5.853538686,-1.7308540164,-3.3532728715	H,0,-5.89673462,-1.7126336536,-3.2409453495
H,0,-4.0005990628,-2.5762200366,-1.9532635864	H,0,-4.0288657541,-2.5800882085,-1.8725124905
O,0,-3.4217498339,1.8851581444,-4.6283895663	O,0,-3.406193406,1.8140621131,-4.647504368
H,0,-4.2099370475,2.0427618603,-5.1687768903	H,0,-4.2044686755,1.979942448,-5.1686794382
O,0,-2.846916597,1.6527119675,-1.5330676255	O,0,-2.7453633684,1.5855078904,-1.5246097055
C,0,-4.0412245181,1.4856276169,-0.8239651945	C,0,-4.0055283907,1.6174842846,-0.9276187697
H,0,-4.9370180984,1.6261275944,-1.4457863452	H,0,-4.7964614933,1.9910663146,-1.5945229629
H,0,-4.1088838755,0.5137580893,-0.3151978051	H,0,-4.3118698782,0.6444124213,-0.5155885821

H,0,-4.0565489394,2.2661735419,-0.0489139853	H,0,-3.9280892158,2.3184397529,-0.0831084477
H,0,-1.6066962908,0.7967795016,-3.1323991711	H,0,-1.5865892705,0.7168712776,-3.1671124216
O,0,-5.7336027897,0.5371451909,-4.8413152535	O,0,-5.7548281092,0.5198698809,-4.7829852453
H,0,-6.4937903361,-0.0519218447,-4.9162536367	H,0,-6.5088887235,-0.0743774404,-4.8601549711

TS C16(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.48533416 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231419 a.u. 1 imaginary frequency = 445.8642 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.0678127 a.u.	**TS C16(•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.51015321 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.232227 a.u. 1 imaginary frequency = 411.4063 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.0938086 a.u.
0, 2	0, 2
C,0,5.8510158154,0.6732122561,0.1048848466	C,0,5.86392677,0.6704397816,0.0610010193
C,0,5.0486669587,-0.4411261757,0.3388423316	C,0,5.0639979534,-0.4427755722,0.3203581317
C,0,5.405807473,1.7443290174,-0.685662179	C,0,5.4042474383,1.7343194323,-0.7323915342
H,0,5.39129894,-1.2685195579,0.9485971778	H,0,5.4227856011,-1.2619632509,0.9330651097
C,0,3.7776033958,-0.469039486,-0.2372314598	C,0,3.7815471664,-0.4755212607,-0.2328585089
C,0,4.1389056832,1.7354038196,-1.2700941194	C,0,4.1252792665,1.7194750491,-1.2939855077
H,0,3.7961171697,2.5631161317,-1.8803470366	H,0,3.7683906769,2.539009428,-1.9065604268
C,0,3.3459264052,0.6200569666,-1.0312494896	C,0,3.3358833012,0.6066675944,-1.0297261835
C,0,1.8070274735,-0.9559543932,-0.8865541529	C,0,1.7909666859,-0.9625236949,-0.8481775585
N,0,2.7856118354,-1.4417865969,-0.1672468564	N,0,2.7885600745,-1.4461552446,-0.1377307846
N,0,2.0610390942,0.2708261774,-1.4395105008	N,0,2.0453500931,0.2577065565,-1.4105900977
H,0,1.4129216901,0.7927259752,-2.0072449197	H,0,1.3970343353,0.7785317878,-1.9817425834
N,0,0.6148798354,-1.6063591911,-1.0925241058	N,0,0.5964239694,-1.6011282508,-1.0305237204
N,0,-0.3702178184,-1.0229145377,-1.8021788872	N,0,-0.3796910692,-1.0102995953,-1.7576032887
C,0,-1.4971142614,-1.6311234608,-1.8991861404	C,0,-1.5058431386,-1.6183816169,-1.863531342
H,0,-1.659965665,-2.5931871153,-1.4008055103	H,0,-1.678931087,-2.5786222634,-1.3702243409
H,0,0.484289386,-2.4894595659,-0.6084128422	H,0,0.4540584562,-2.4915734119,-0.5630581887
H,0,6.0573840481,2.5953813428,-0.8462826716	H,0,6.0527464044,2.5837151129,-0.9134342234
C,0,-2.618840551,-1.0863066488,-2.6633703009	C,0,-2.6143986852,-1.0627464228,-2.6414605201
C,0,-3.8552310686,-1.7715817817,-2.628786874	C,0,-3.8496349531,-1.7569363334,-2.6406791802
C,0,-2.5055109294,0.0595591177,-3.4381572582	C,0,-2.4894024223,0.0922966782,-3.3979980655
C,0,-4.9544158415,-1.3200056246,-3.3655773547	C,0,-4.9371119251,-1.3049949121,-3.3915482389
C,0,-3.6384927537,0.6189001138,-4.0946754809	C,0,-3.6166282423,0.6517409362,-4.0674190112
C,0,-4.8492259372,-0.1754115321,-4.1298784966	C,0,-4.8234037791,-0.1474497934,-4.1361875309
H,0,6.8421532793,0.7165146868,0.5419485655	H,0,6.8627530682,0.7165780371,0.4802028089
H,0,-5.8836216887,-1.8814907115,-3.35559643	H,0,-5.8622528287,-1.8703747385,-3.4099664641
H,0,-3.9515243557,-2.6730562814,-2.0341421853	H,0,-3.9499782931,-2.6667721172,-2.0605556126
O,0,-3.3818706436,1.4783003702,-5.111452715	O,0,-3.3485225183,1.5194202309,-5.078167385
H,0,-4.185371219,1.9846946838,-5.2917829127	H,0,-4.1827550109,1.8809351753,-5.4092386635
O,0,-4.2119690691,1.945425351,-2.8713459139	O,0,-4.1966039895,1.9719889523,-2.8195076197
C,0,-4.6796545349,1.5801031814,-1.6092246207	C,0,-4.7143312811,1.5566697779,-1.5867464002
H,0,-5.6529211329,1.0658836143,-1.6348018837	H,0,-5.6929747479,1.0627707177,-1.6736061057
H,0,-3.9631672609,0.9521960443,-1.0585949728	H,0,-4.0298057291,0.8844335141,-1.0482507327
H,0,-4.8015848764,2.5078827293,-1.0326666818	H,0,-4.8396940227,2.4525714129,-0.9625321848
O,0,-5.8317814178,0.3217271705,-4.9192989898	O,0,-5.7837816034,0.361299051,-4.9385696507
H,0,-6.6354766252,-0.2028382396,-4.8325713618	H,0,-6.5838436077,-0.1798942149,-4.9153295681
H,0,-1.5703098926,0.5958113603,-3.5192304868	H,0,-1.5519813865,0.6294326775,-3.4561387165

TS C16(•OCH_3), optimization in solv. benzene	**TS C17(•OCH_3),** optimization in gas phase

UB3LYP/6-311++G**, E= -1025.49561254 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234449 a.u. 1 imaginary frequency = 434.6316 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1025.0785973 a.u.	UB3LYP/6-311++G**, E= -1025.49824845 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.232611 a.u. 1 imaginary frequency = 348.7241 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.0775992 a.u.
0, 2 C,0,5.8869855646,0.6437542015,0.0384216506 C,0,5.0723253583,-0.4530864475,0.3141508087 C,0,5.4384403984,1.707922267,-0.760107017 H,0,5.4198155541,-1.274026348,0.9302805673 C,0,3.7855840136,-0.4699251996,-0.2277096011 C,0,4.1556230616,1.7096701058,-1.3103727169 H,0,3.8088839,2.5307183879,-1.9271049857 C,0,3.350842941,0.6124212176,-1.0296744247 C,0,1.7878571732,-0.933463661,-0.8206204306 N,0,2.7794712816,-1.4246945888,-0.1162677451 N,0,2.0509054055,0.2793411309,-1.3975394515 H,0,1.4026099466,0.8017399259,-1.9657375989 N,0,0.5797241373,-1.5597668437,-0.9844721058 N,0,-0.3892788692,-0.9854261337,-1.7271532994 C,0,-1.5127949591,-1.5968568207,-1.8411638208 H,0,-1.6852565022,-2.5552386928,-1.3410715302 H,0,0.4494584199,-2.4554575784,-0.5239795223 H,0,6.0995017658,2.544653526,-0.9541098675 C,0,-2.6177206373,-1.0561055851,-2.6333410427 C,0,-3.8412642681,-1.7666640252,-2.6568435697 C,0,-2.498786129,0.1065108113,-3.3809844619 C,0,-4.9217559928,-1.3247972402,-3.4256640421 C,0,-3.6200301733,0.6551801618,-4.0665547496 C,0,-4.812209847,-0.1623052179,-4.1626713076 H,0,6.8900539318,0.6776851767,0.4484311817 H,0,-5.8375108355,-1.90586552,-3.4638280882 H,0,-3.939624928,-2.6813492527,-2.0833985654 O,0,-3.3461161601,1.5394141614,-5.0588180827 H,0,-4.1675072059,1.9825263661,-5.3121234395 O,0,-4.259390934,1.9468531881,-2.8300538473 C,0,-4.7652640285,1.5325343927,-1.5961668896 H,0,-5.7281053216,1.0054036521,-1.674850956 H,0,-4.0590388345,0.8948840711,-1.0436360614 H,0,-4.9215984709,2.4363314622,-0.9905656475 O,0,-5.7710434456,0.3335876384,-4.9787577985 H,0,-6.5698010006,-0.2059155972,-4.9406286525 H,0,-1.57160337,0.6617021182,-3.4167257588	0, 2 C,0,5.917357724,0.6604769789,0.0634416706 C,0,5.0567393375,-0.3871416923,0.3784613709 C,0,5.5290525003,1.6930681748,-0.8059460684 H,0,5.3543098671,-1.1844709176,1.0487161327 C,0,3.7842541385,-0.3872704717,-0.1967745512 C,0,4.2631658209,1.7113568676,-1.3907412985 H,0,3.9655852387,2.5090370985,-2.0614923161 C,0,3.4105013827,0.6618248739,-1.0709259009 C,0,1.7898440705,-0.8122013105,-0.8124279396 N,0,2.7421192722,-1.2959422481,-0.056757736 N,0,2.1075887762,0.3547429438,-1.4535586139 H,0,1.4929506653,0.8605894262,-2.0709654307 N,0,0.562725949,-1.410224834,-0.9640351275 N,0,-0.375828973,-0.8669892596,-1.7522359301 C,0,-1.5173547757,-1.4703703872,-1.8401538793 H,0,-1.7017165647,-2.391931304,-1.2782825122 H,0,0.4065657416,-2.2701155095,-0.4449685026 H,0,6.2264057409,2.4924144601,-1.0278897272 C,0,-2.5964769585,-0.9767780231,-2.6632311181 C,0,-3.8193706133,-1.700743795,-2.6790321324 C,0,-2.4668055817,0.1769982856,-3.4610989396 C,0,-4.8779973302,-1.28206856,-3.446974979 C,0,-3.526108585,0.6071586451,-4.2304390304 C,0,-4.7977555997,-0.0590798564,-4.1619522702 H,0,6.9104656508,0.6825289841,0.4973084128 H,0,-5.8063737862,-1.8379157959,-3.4886856743 H,0,-3.9032993031,-2.6108683618,-2.0952020619 O,0,-3.4024289964,1.6795019726,-5.033497528 H,0,-4.2471815398,1.7892125418,-5.4984001099 O,0,-5.8083775227,1.1652506788,-2.9431184821 C,0,-5.358725238,1.3591977843,-1.6430530957 H,0,-6.1521358226,1.8845462354,-1.0898085223 H,0,-5.1815658941,0.4081403517,-1.116137132 H,0,-4.4465333925,1.9716109383,-1.5921207447 O,0,-5.6747911894,0.2397309205,-5.1783292567 H,0,-6.4691286124,0.5975168928,-4.7499392284 H,0,-1.5308665872,0.7181388219,-3.4954866472

TS C17(•OCH$_3$), optimization in solv. water UB3LYP/6-311++G**, E= -1025.51707983 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.231709 a.u. 1 imaginary frequency = 325.6437 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.0975476 a.u.	**TS C17(•OCH$_3$),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.50618598 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.232390 a.u. 1 imaginary frequency = 340.8228 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1025.086037 a.u.
0, 2 C,0,5.9167654584,0.5729397984,0.0155506742 C,0,5.0299963075,-0.4293727678,0.4053663767 C,0,5.5469269066,1.5582445033,-0.9160904797 H,0,5.3182449378,-1.1879218449,1.1239884691	0, 2 C,0,5.9121712586,0.6657151448,0.0513805783 C,0,5.0547758618,-0.3828062908,0.3753752096 C,0,5.5176540508,1.6933739905,-0.8216937815 H,0,5.3592217776,-1.1753176544,1.0486240384

C,0,3.7510651826,-0.4310004448,-0.158433861	C,0,3.779402666,-0.3884567824,-0.1945788594
C,0,4.2745697068,1.5733773839,-1.4900072948	C,0,4.2487293665,1.7056885709,-1.4011817155
H,0,3.9873819168,2.3319186372,-2.2084573701	H,0,3.9448195981,2.4983799454,-2.0748103255
C,0,3.3966565737,0.5702653509,-1.095213019	C,0,3.3996881912,0.6555585076,-1.0723914263
C,0,1.732964995,-0.8340149191,-0.735707659	C,0,1.780431765,-0.8183936797,-0.8026516062
N,0,2.683781722,-1.2985987837,0.0464859708	N,0,2.7386882757,-1.2981341853,-0.0465716007
N,0,2.0846563371,0.2783333936,-1.4469121375	N,0,2.0969541103,0.3450928374,-1.4483840191
H,0,1.4856639493,0.7681327215,-2.0945583614	H,0,1.4823975697,0.8502781629,-2.0674676898
N,0,0.4904690622,-1.3980957835,-0.8457449751	N,0,0.5542564529,-1.4157890731,-0.948835391
N,0,-0.4239387058,-0.8636200939,-1.6715285974	N,0,-0.3818577491,-0.8709393305,-1.7404222344
C,0,-1.5823785961,-1.4375471288,-1.7400412973	C,0,-1.5235358604,-1.4742882159,-1.829703114
H,0,-1.8034228435,-2.3247750598,-1.1418730493	H,0,-1.7111443324,-2.3949138219,-1.2693947545
H,0,0.2967027117,-2.2279177598,-0.2909201751	H,0,0.3928850125,-2.276201917,-0.4318531709
H,0,6.2631551656,2.3222338543,-1.1954048183	H,0,6.2122285989,2.4932393216,-1.0505929246
C,0,-2.6302995197,-0.9392505169,-2.6004535585	C,0,-2.5976637253,-0.9756194098,-2.656623818
C,0,-3.8768500369,-1.6229926265,-2.6105652609	C,0,-3.8227387563,-1.6962629005,-2.6785567006
C,0,-2.448862505,0.1812813722,-3.4380144503	C,0,-2.4612104788,0.1797078248,-3.4521620901
C,0,-4.9065135192,-1.2012034169,-3.4148035051	C,0,-4.876237333,-1.2738589326,-3.4513221299
C,0,-3.4790250816,0.6149178316,-4.2418870529	C,0,-3.5156292079,0.613676707,-4.2253295658
C,0,-4.7701491773,-0.0117124508,-4.1782590038	C,0,-4.7885181634,-0.0505470298,-4.1655310382
H,0,6.9144751628,0.5946753989,0.4391149249	H,0,6.90707151,0.6917405069,0.4810613766
H,0,-5.8501684355,-1.7316644362,-3.4508634586	H,0,-5.8053767121,-1.8282423867,-3.4977163759
H,0,-4.0015708178,-2.5047775866,-1.9926297686	H,0,-3.9119823033,-2.6061576879,-2.0955318076
O,0,-3.308182739,1.6620270102,-5.0778510745	O,0,-3.3854021645,1.6903144138,-5.0249088387
H,0,-4.139209838,1.7932335016,-5.5622097713	H,0,-4.2268365662,1.8078340902,-5.4943428628
O,0,-5.7489751523,1.2988372087,-2.9954975107	O,0,-5.7993177723,1.1786222605,-2.9428335926
C,0,-5.2744714866,1.4913670553,-1.7003015073	C,0,-5.3424099095,1.3551817897,-1.6412875151
H,0,-4.3461060798,2.0806864692,-1.6661792342	H,0,-6.1292118071,1.8777710428,-1.0761202836
H,0,-6.0430485099,2.0381236971,-1.1325868957	H,0,-5.1664568475,0.3973464853,-1.1267999912
H,0,-5.1085099922,0.5407853715,-1.1696115	H,0,-4.4266712061,1.9620219449,-1.5874485699
O,0,-5.6002898004,0.275244818,-5.2315745316	O,0,-5.6555705195,0.2497703744,-5.1896616191
H,0,-6.4763738211,0.4826137864,-4.8737558023	H,0,-6.4709368848,0.5744257692,-4.7758521474
H,0,-1.4963204282,0.694158006,-3.4683043343	H,0,-1.5238587564,0.7191211576,-3.479614543

TS C19(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.49169875 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.232364 a.u. 1 imaginary frequency = 400.0483 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1025.0707614 a.u.	**TS C19(•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.51449991 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.232219 a.u. 1 imaginary frequency = 364.0472 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1025.0945319 a.u.
0, 2	0, 2
C,0,6.0841264683,0.7600787977,0.248243405	C,0,6.0818224136,0.7745016546,0.209214145
C,0,5.2333641988,-0.2969025097,0.5611094329	C,0,5.2600877905,-0.3139683301,0.4998475123
C,0,5.6650017784,1.8217520324,-0.5695517219	C,0,5.6194757148,1.8586690135,-0.555654823
H,0,5.5552289527,-1.1166853582,1.191985892	H,0,5.6203370415,-1.1489034633,1.0898807111
C,0,3.9393441122,-0.2767057515,0.0371511133	C,0,3.9522551412,-0.3009384875,0.0076858524
C,0,4.37657462,1.8606378765,-1.1028858105	C,0,4.3162013873,1.8898927628,-1.055909252
H,0,4.0546370175,2.6809223728,-1.7341430966	H,0,3.9577991536,2.7248362774,-1.6462697758
C,0,3.5344544654,0.8021507624,-0.7854916244	C,0,3.5041844278,0.8009413774,-0.760866486
C,0,1.9204761082,-0.6789533665,-0.5134085721	C,0,1.9219442382,-0.7198552447,-0.5171967423
N,0,2.9015360887,-1.1889523009,0.1869426281	N,0,2.9352917533,-1.2402328164,0.1429758492
N,0,2.2168801223,0.5094638973,-1.1264587944	N,0,2.1871057308,0.4962275105,-1.0824597082
H,0,1.5774705866,1.0370792563,-1.6985330205	H,0,1.5311590035,1.0403305611,-1.6225301468
N,0,0.6874520018,-1.2668226563,-0.641684343	N,0,0.6997384118,-1.3200069137,-0.6435309915

N,0,-0.2800366011,-0.683215565,-1.370442381	N,0,-0.2808502141,-0.7149469441,-1.3423034446
C,0,-1.4193009927,-1.2875706258,-1.4537972579	C,0,-1.4162209075,-1.3260864711,-1.4377147051
H,0,-1.5877029355,-2.2379108838,-0.9394636436	H,0,-1.5728557547,-2.2965760567,-0.9612330956
H,0,0.5389130374,-2.1391198368,-0.1423515036	H,0,0.5655306921,-2.2238846326,-0.1985272055
H,0,6.3549381172,2.6274745556,-0.7918814281	H,0,6.2862961504,2.6877392153,-0.7623982431
C,0,-2.5304817582,-0.7465588613,-2.2025911409	C,0,-2.5270833032,-0.7639859073,-2.1719053877
C,0,-3.7569811071,-1.4888629552,-2.2131534	C,0,-3.766464248,-1.4894762035,-2.1790745432
C,0,-2.4729292894,0.4926857469,-2.8509267922	C,0,-2.4534457674,0.4713355796,-2.8260860004
C,0,-4.8211793933,-1.0461669099,-3.0474996618	C,0,-4.8221421265,-1.0461811983,-3.0250752206
C,0,-3.5580389401,0.9580830708,-3.5730840634	C,0,-3.5329703763,0.9415152549,-3.5541837091
C,0,-4.7395677598,0.169958253,-3.6724251792	C,0,-4.7254970199,0.1630595663,-3.6615151296
H,0,7.0934845161,0.7659570968,0.6436168344	H,0,7.1003683844,0.786000747,0.5804618623
H,0,-5.7165382617,-1.6522868284,-3.1326783822	H,0,-5.7195536177,-1.6461479364,-3.1208277647
H,0,-3.7255768735,-2.5359380854,-1.9476564569	H,0,-3.7449249043,-2.535118267,-1.9063228183
O,0,-3.492579955,2.1588844842,-4.1974766452	O,0,-3.4521929001,2.1365642781,-4.1862250153
H,0,-4.3315126877,2.3198919584,-4.6509198457	H,0,-4.2836624909,2.3043132085,-4.6543991405
O,0,-4.4204302609,-1.2171244536,-0.3766901276	O,0,-4.4263417098,-1.159550479,-0.3395412594
C,0,-4.6724872134,0.115991548,-0.0633073423	C,0,-4.6817717858,0.1903887852,-0.0874148126
H,0,-3.7620284296,0.7315389474,-0.0050249977	H,0,-3.7685588036,0.8020909607,-0.0371317194
H,0,-5.3816306917,0.5958417775,-0.7563738984	H,0,-5.3661728843,0.6406910811,-0.8224179525
H,0,-5.1425669137,0.1223381622,0.9317631835	H,0,-5.1783040405,0.2523139245,0.8927558193
O,0,-5.7225594677,0.7291990467,-4.4503475837	O,0,-5.6843375996,0.7232687642,-4.4538687261
H,0,-6.5181768318,0.1870608096,-4.4363629781	H,0,-6.4832189436,0.1820170442,-4.474667876
H,0,-1.5758998879,1.0959748456,-2.8058874162	H,0,-1.5473520971,1.062350135,-2.7872566768

TS C19(•OCH_3), optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.50143343 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.232471 a.u. 1 imaginary frequency = 386.1168 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1025.0809057 a.u.	
0, 2 C,0,6.0896826754,0.7613190219,0.2202107657 C,0,5.2473902544,-0.3029269985,0.5349782419 C,0,5.6547010633,1.828567071,-0.5825227249 H,0,5.5836978752,-1.1259744087,1.1543756003 C,0,3.9459653046,-0.2838618689,0.0283308035 C,0,4.3584683594,1.8661037041,-1.0981041486 H,0,4.0227623619,2.6895791393,-1.7176892648 C,0,3.5253323793,0.8007079075,-0.7789099102 C,0,1.9185915241,-0.6879388206,-0.5020757103 N,0,2.9131021944,-1.2017763238,0.1824410143 N,0,2.2056427117,0.5065117748,-1.105457322 H,0,1.5600576007,1.0402295154,-1.6660047 N,0,0.6868060436,-1.2757593453,-0.6217226945 N,0,-0.2833201828,-0.6859467523,-1.3447015496 C,0,-1.4208562556,-1.293220013,-1.4337098649 H,0,-1.5855839152,-2.2501346906,-0.9318142569 H,0,0.5416697219,-2.1593161863,-0.1412157547 H,0,6.3379531597,2.6394462553,-0.8069453854 C,0,-2.5298114898,-0.7466953974,-2.1821097151 C,0,-3.7568759036,-1.4893775513,-2.2049565871 C,0,-2.4679121824,0.4944872043,-2.8263482666 C,0,-4.8134804424,-1.0481989829,-3.0503879923	

C,0,-3.5474795667,0.9591392989,-3.5573457173 C,0,-4.72800814,0.1687119375,-3.6734704317 H,0,7.1042093499,0.7678743721,0.6022897452 H,0,-5.7053989073,-1.6565523287,-3.1497765485 H,0,-3.7255099622,-2.5370700761,-1.9417073972 O,0,-3.4776876243,2.1615642791,-4.1779576153 H,0,-4.3107968855,2.3231984262,-4.6433168103 O,0,-4.4400063622,-1.2094363794,-0.3716030573 C,0,-4.6918975027,0.1291059982,-0.0740089115 H,0,-3.7788290925,0.7390119059,-0.0021236047 H,0,-5.3805066007,0.6062570641,-0.7887837374 H,0,-5.1851134096,0.1510182076,0.9095609923 O,0,-5.698165034,0.7267241684,-4.4622370346 H,0,-6.4917337673,0.1797024457,-4.4737814737 H,0,-1.5713834128,1.0981147761,-2.7730855959	

TS C1(•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.34004565 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208297 a.u. 1 imaginary frequency = 494.5671 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9136051 a.u.	**TS C1(•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.36547757 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.207878 a.u. 1 imaginary frequency = 448.0346 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9402128 a.u.
0, 2 C,0,5.9722483963,0.9581377126,-0.0659542835 C,0,5.1193821088,-0.0813644089,0.3614573262 C,0,5.5826574463,1.8819421686,-1.016957509 H,0,5.4366457206,-0.8026528679,1.1041477611 C,0,3.8454523161,-0.1653566437,-0.2157247903 C,0,4.2366348998,1.9092678218,-1.5479725396 H,0,4.0912013591,2.3479241814,-2.5314821523 C,0,3.449763697,0.7767396254,-1.1745989923 C,0,1.8607004658,-0.6929462672,-0.7791358687 N,0,2.8292126939,-1.0868224008,0.0086266351 N,0,2.1642956101,0.417965527,-1.5265585897 H,0,1.5134836124,0.9149555839,-2.1148679264 N,0,0.650247664,-1.3269594596,-0.8916451627 N,0,-0.325202466,-0.8051058775,-1.6690578525 C,0,-1.472513345,-1.3814934568,-1.6656721599 H,0,-1.6526111226,-2.2630882983,-1.0400020919 H,0,0.4774343493,-2.1020110885,-0.2588247379 H,0,6.2707578199,2.6521105455,-1.3439953169 C,0,-2.5947145999,-0.9176785326,-2.4759328933 C,0,-3.8148411977,-1.6007912298,-2.3945856374 C,0,-2.4886238441,0.1910656645,-3.3326246661 C,0,-4.9101445857,-1.1878908724,-3.1512866437 C,0,-3.5735926767,0.6037578134,-4.0854931401 C,0,-4.7931584294,-0.0914074865,-3.9929244182 H,0,6.9749483281,1.0139891931,0.3436009193 H,0,-5.8538505926,-1.7204927481,-3.0846245874 H,0,-3.9131858485,-2.4585654615,-1.738991703 O,0,-3.4546340818,1.6796378352,-4.9113067696 H,0,-4.3027147348,1.8287207903,-5.3491899683 O,0,3.4319995618,3.3465265741,-0.8203663043 H,0,-1.5578693498,0.7369611481,-3.4129259496 O,0,-5.8052654582,0.400595057,-4.7819545472 H,0,-6.6132765692,-0.1071092482,-4.6573359795 O,0,3.2191982036,3.1660510577,0.5626286338 H,0,4.0325145891,3.514583729,0.9577370455	0, 2 C,0,5.9785016217,0.8824756838,-0.1402702211 C,0,5.1144889779,-0.1332817075,0.3303876673 C,0,5.5733454489,1.8127380462,-1.0755817508 H,0,5.4518219804,-0.8588061657,1.0606028834 C,0,3.8164377879,-0.1883317208,-0.1930787192 C,0,4.2041291274,1.874377262,-1.5449281034 H,0,4.0202109639,2.3191042814,-2.5186431378 C,0,3.4038263939,0.7610206532,-1.1392703422 C,0,1.8022674611,-0.6906333025,-0.7072321282 N,0,2.791575233,-1.0954103794,0.0609232258 N,0,2.1046292517,0.4232866952,-1.4510442938 H,0,1.4715197974,0.8825458886,-2.0896860577 N,0,0.5839711818,-1.2971430657,-0.7949689736 N,0,-0.3737710435,-0.7747374052,-1.6035682926 C,0,-1.5140646095,-1.3657825482,-1.6362593417 H,0,-1.7022255746,-2.2570349031,-1.0307200535 H,0,0.4117492621,-2.1146954028,-0.2177203873 H,0,6.2663980784,2.5635310994,-1.435054485 C,0,-2.6162766249,-0.8938516409,-2.4697375628 C,0,-3.8303984162,-1.5930348786,-2.442243113 C,0,-2.4985872905,0.2385504911,-3.2961737869 C,0,-4.9089239884,-1.1758935833,-3.2210514371 C,0,-3.567589085,0.6545556422,-4.0693037441 C,0,-4.782669314,-0.0563233839,-4.0329947483 H,0,6.9982496951,0.9112355687,0.226860136 H,0,-5.8469060976,-1.7201581299,-3.1983394255 H,0,-3.936814644,-2.4674196454,-1.810605884 O,0,-3.4396474069,1.7565739992,-4.8666508683 H,0,-4.2762277644,1.9049011199,-5.3292492687 O,0,3.4866376525,3.3369871818,-0.7617242023 H,0,-1.5717119791,0.7969567567,-3.3349701417 O,0,-5.7722559358,0.4414167566,-4.836256642 H,0,-6.5801101441,-0.0798125651,-4.756518456 O,0,3.440664256,3.201827856,0.6493442447 H,0,4.3141541074,3.5127601257,0.9340075214

TS C1(•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.35088176 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208435 a.u. 1 imaginary frequency = 475.9884 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9248724 a.u.	**TS C2(•OOH),** optimization in gas phase UB3LYP/6-311++G**, E= -1061.34014690 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.207680 a.u. 1 imaginary frequency = 478.8967 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9130651 a.u.
0, 2 C,0,5.9763342234,0.8892862145,-0.0772549585 C,0,5.1096085032,-0.1331276833,0.3675048547 C,0,5.592418325,1.8119073197,-1.0305478196	0, 2 C,0,5.8793220975,0.333447221,0.1960301503 C,0,5.0267249748,-0.7242363795,0.3729690474 C,0,5.4505272725,1.5731422746,-0.4241711894

H,0,5.425702526,-0.8535359567,1.1117502761	H,0,5.3371787459,-1.626104856,0.8866525065
C,0,3.8294536316,-0.202004684,-0.1971167289	C,0,3.7210237492,-0.6302988668,-0.154584428
C,0,4.2403880567,1.8578023882,-1.5466306258	C,0,4.1764972472,1.5994650943,-1.0971504098
H,0,4.0898032411,2.2919097439,-2.5311741602	H,0,3.8904749862,2.4658339097,-1.6812632276
C,0,3.4379910397,0.740796026,-1.1580172386	C,0,3.3365483257,0.5364652391,-0.8842549306
C,0,1.8351293634,-0.714288378,-0.7548355378	C,0,1.7251860559,-0.9772723955,-0.8110480696
N,0,2.8046072688,-1.1129778641,0.034466245	N,0,2.6972203404,-1.5468559548,-0.1272347325
N,0,2.1486500463,0.3932405231,-1.5031751624	N,0,2.0310166077,0.2632602981,-1.2989884738
H,0,1.5097508051,0.8775105044,-2.1157365828	H,0,1.4048910916,0.8390852931,-1.8382870873
N,0,0.6212029236,-1.3349466863,-0.8672946678	N,0,0.5106683478,-1.5600268021,-1.0238762181
N,0,-0.3433892487,-0.8035077212,-1.6565955753	N,0,-0.4499659069,-0.9156763553,-1.7247590824
C,0,-1.4919251931,-1.3778815441,-1.6689383524	C,0,-1.5811038092,-1.5067472036,-1.876436227
H,0,-1.6808290425,-2.2640617673,-1.0539653593	H,0,-1.7544947379,-2.4995550657,-1.4463053667
H,0,0.4361863206,-2.1164195082,-0.245848052	H,0,0.3611319191,-2.4781536458,-0.6158071542
H,0,6.2897439879,2.5676764979,-1.3712669433	H,0,6.2327114451,2.1986417767,-0.8436517012
C,0,-2.6046521817,-0.8994076163,-2.4840542592	C,0,-2.6908937724,-0.9125798338,-2.612926226
C,0,-3.822612575,-1.5899935653,-2.4362893255	C,0,-3.8954779865,-1.6213043546,-2.709653288
C,0,-2.4933410361,0.2327128791,-3.3098780726	C,0,-2.5878705053,0.3479435828,-3.2260781129
C,0,-4.9112113243,-1.1624333459,-3.1948481952	C,0,-4.9788347329,-1.0844125019,-3.402604824
C,0,-3.5721654796,0.6603871431,-4.0628371116	C,0,-3.6610036529,0.8839953867,-3.9148633642
C,0,-4.7909588822,-0.0408610172,-4.0034225511	C,0,-4.8654058629,0.1614745118,-4.0026830711
H,0,6.9837236162,0.9307341498,0.3220939399	H,0,6.8869589439,0.2935609135,0.5909483726
H,0,-5.8517807263,-1.7025088401,-3.1573683865	H,0,-5.9107651294,-1.6365229828,-3.4746563888
H,0,-3.9243877973,-2.4655751384,-1.8052930832	H,0,-3.990931536,-2.5948786181,-2.2424984844
O,0,-3.4496565119,1.7614488078,-4.8576414305	O,0,-3.5452214629,2.1057263593,-4.5033842987
H,0,-4.2966168617,1.9248572199,-5.293952169	H,0,-4.3810063459,2.3215955345,-4.9372387768
O,0,3.4781929971,3.3202772934,-0.8147844546	O,0,5.3122625937,2.7331262022,0.9586217113
H,0,-1.5647689084,0.7861106199,-3.3622619847	O,0,-5.866083889,0.783623853,-4.7079876979
O,0,-5.7949273343,0.469464055,-4.7867669293	H,0,-6.6605303418,0.2406288819,-4.7280001838
H,0,-6.6165633359,-0.0156401381,-4.6538736787	H,0,-1.6678164323,0.9142262293,-3.1674326971
O,0,3.3176819865,3.1732017811,0.5820947557	O,0,4.3710830956,2.2792324229,1.9092916658
H,0,4.1589794267,3.4976589578,0.9380345452	H,0,3.5447402343,2.6837486518,1.6065926579

TS C2(•OOH), optimization in solv. water UB3LYP/6-311++G**, E= -1061.36857189 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208444 a.u. 1 imaginary frequency = 402.5181 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9425009 a.u.	**TS C2(•OOH),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.35224038 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208916 a.u. 1 imaginary frequency = 449.4985 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9255452 a.u.
0, 2	0, 2
C,0,5.8781267086,0.3315673063,0.1932699702	C,0,5.8784787692,0.3321717633,0.1915064838
C,0,5.0320036113,-0.7325488326,0.3725430758	C,0,5.0280630172,-0.7270873266,0.374069356
C,0,5.4390222413,1.5711460727,-0.4254060604	C,0,5.4458946413,1.5697412324,-0.4316317457
H,0,5.358215297,-1.6360271303,0.8748523114	H,0,5.3449513071,-1.627836461,0.8862440302
C,0,3.7206811806,-0.6441843019,-0.1470038021	C,0,3.7194755141,-0.6364071432,-0.1485878521
C,0,4.1571333957,1.5919985269,-1.0873291522	C,0,4.1667913083,1.5936481986,-1.0961300034
H,0,3.8597409814,2.4540475864,-1.6712474574	H,0,3.8755330659,2.456690593,-1.6823492441
C,0,3.3257241526,0.5247755324,-0.8736860937	C,0,3.3300658649,0.5297985317,-0.8787967781
C,0,1.7163102025,-0.9917326814,-0.7985933332	C,0,1.7191341367,-0.9846882662,-0.8002915431
N,0,2.7041427025,-1.5628037368,-0.1158421783	N,0,2.6983455566,-1.5536961346,-0.1169222158
N,0,2.0236563618,0.2471036698,-1.2830077986	N,0,2.0250821377,0.2546640066,-1.2884568835
H,0,1.3946177413,0.8345314169,-1.8094979995	H,0,1.3985288199,0.8325572172,-1.8263634726
N,0,0.5102519547,-1.5710472455,-1.0041688714	N,0,0.5077737189,-1.5656259961,-1.0091878757
N,0,-0.4480673455,-0.9142402714,-1.7108804275	N,0,-0.4510991464,-0.9155735251,-1.7140501852

C,0,-1.576745991,-1.5101547403,-1.8668358808	C,0,-1.5802588284,-1.5092803589,-1.8709866044
H,0,-1.7509993551,-2.5038508588,-1.4445296801	H,0,-1.7539175737,-2.5036246121,-1.446713164
H,0,0.3499186594,-2.4936909741,-0.6090926181	H,0,0.3538368772,-2.4865933765,-0.6087157838
H,0,6.2175735283,2.1899475193,-0.8623778217	H,0,6.2262171947,2.1906137418,-0.8617325574
C,0,-2.6819120403,-0.9091803849,-2.6044685956	C,0,-2.6874692169,-0.9122149526,-2.6090076451
C,0,-3.883146371,-1.6223123624,-2.7178981375	C,0,-3.8883913618,-1.6255010992,-2.7191839609
C,0,-2.5790925037,0.359979299,-3.2034475223	C,0,-2.5860005596,0.3544094864,-3.2110396495
C,0,-4.9645045139,-1.0850044578,-3.4137278453	C,0,-4.9699311727,-1.08897755,-3.4153141255
C,0,-3.650763546,0.895015285,-3.8945401698	C,0,-3.65750677,0.889759934,-3.902419778
C,0,-4.8531766093,0.168537202,-4.002080199	C,0,-4.8586993293,0.1624971919,-4.005835944
H,0,6.8940302186,0.2875600693,0.5671341018	H,0,6.8897719919,0.2911697462,0.5771748883
H,0,-5.892917514,-1.6391535867,-3.4990326537	H,0,-5.8985656349,-1.6442916429,-3.4980962331
H,0,-3.9768255566,-2.6007467203,-2.2612511573	H,0,-3.9820673562,-2.6029870252,-2.2601603626
O,0,-3.5385305634,2.1274105826,-4.4717896753	O,0,-3.5444204609,2.1186809897,-4.4806874125
H,0,-4.3720692059,2.3420590827,-4.9134887555	H,0,-4.3789718692,2.3348236123,-4.9180829051
O,0,5.3200050125,2.7479426144,0.9479524031	O,0,5.3217916503,2.7442136948,0.9451513721
O,0,-5.8455331119,0.7906562264,-4.7069065971	O,0,-5.8546832943,0.7842795614,-4.7125931758
H,0,-6.6366201306,0.2405869856,-4.7575394609	H,0,-6.6471914585,0.2374819176,-4.7497624887
H,0,-1.6611785916,0.9295703607,-3.1307073941	H,0,-1.6687996073,0.9244806091,-3.1411454125
O,0,4.3115181781,2.357443768,1.8755581373	O,0,4.3625879958,2.316901816,1.8970220903
H,0,3.4997320415,2.7142402189,1.4838816786	H,0,3.5374309125,2.6998884961,1.5637196611

TS C4(•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.34004209 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208405 a.u. 1 imaginary frequency = 499.7302 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9133966 a.u.	**TS C4(•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.36823106 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208104 a.u. 1 imaginary frequency = 430.1120 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.942175 a.u.
0, 2	0, 2
C,0,5.9394679492,0.6174720291,0.2438927155	C,0,5.9280784831,0.6183463118,0.1958455782
C,0,5.0269198964,-0.4254028008,0.6493918943	C,0,5.0255209084,-0.4268149785,0.6202615368
C,0,5.5208749516,1.6983744218,-0.5054326091	C,0,5.4936526195,1.6947868198,-0.5478412547
H,0,5.4326427969,-1.3894449817,0.9370990406	H,0,5.4429145014,-1.3970721425,0.8709904794
C,0,3.7517072496,-0.4079355037,-0.0081769143	C,0,3.7245399249,-0.3948683868,0.0120584646
C,0,4.2085389481,1.782423954,-1.0284598733	C,0,4.1664552851,1.7817833363,-1.0411556566
H,0,3.8980775747,2.6331975116,-1.6228526811	H,0,3.8447835008,2.6274079899,-1.6360260246
C,0,3.3635249867,0.7109539396,-0.7691210787	C,0,3.3224872703,0.7202780313,-0.7510083274
C,0,1.7638662756,-0.8014672249,-0.6469981166	C,0,1.7107485898,-0.7784766445,-0.5811091218
N,0,2.7445909256,-1.338062981,0.0511080858	N,0,2.7131798319,-1.3156890407,0.1076935505
N,0,2.0592125338,0.4241085601,-1.1699752929	N,0,2.0079284279,0.4387684638,-1.1151432748
H,0,1.427948864,0.9824375339,-1.7218410966	H,0,1.3811275453,0.992856479,-1.679453557
N,0,0.5571334372,-1.4110778299,-0.8492623357	N,0,0.502551957,-1.374530733,-0.7508566008
N,0,-0.4139415227,-0.7927384987,-1.5569357684	N,0,-0.4567372118,-0.7598821418,-1.4910261123
C,0,-1.5568374253,-1.3729233618,-1.6468062062	C,0,-1.5883550513,-1.3582740791,-1.6087725634
H,0,-1.7359255329,-2.3337981888,-1.1515068682	H,0,-1.767363567,-2.3226629804,-1.1248706796
H,0,0.3983262286,-2.2884853781,-0.3629005449	H,0,0.3473210858,-2.2769628106,-0.3106692911
H,0,6.2221110782,2.4941508275,-0.7310975661	H,0,6.190473751,2.4878796966,-0.7942414719
C,0,-2.6737698517,-0.806475669,-2.395392665	C,0,-2.6906508989,-0.7991530756,-2.3840440695
C,0,-3.8996087295,-1.4845220577,-2.3988503617	C,0,-3.901030523,-1.503414222,-2.4402583335
C,0,-2.5573207975,0.3981927338,-3.1097114439	C,0,-2.5758673951,0.4211657057,-3.0750241826
C,0,-4.9908696141,-0.9713857227,-3.0976430058	C,0,-4.9796651147,-1.0048824516,-3.1688517984
C,0,-3.6382851144,0.9105793694,-3.8044130392	C,0,-3.6446233035,0.9174338317,-3.7990411694
C,0,-4.864117624,0.2201035631,-3.7969613851	C,0,-4.8565272875,0.2009107771,-3.8473704194
H,0,6.9580642314,0.575132918,0.6108545777	H,0,6.956869802,0.5725684145,0.5325499148

H,0,-5.9392542036,-1.4997420493,-3.0968113322	H,0,-5.9151661246,-1.5521388644,-3.209345772
H,0,-4.0057294363,-2.415276666,-1.8532926506	H,0,-4.0042760419,-2.4445338434,-1.9126593705
O,0,-3.5091814424,2.0788589808,-4.4917636858	O,0,-3.5199457877,2.1025118042,-4.4664941776
H,0,-4.3538552904,2.2852328848,-4.9127378069	H,0,-4.3533164433,2.2946595537,-4.9187369604
O,0,4.6826183522,-0.0616645392,2.3980493141	O,0,4.7551581756,-0.1222941647,2.4075021385
H,0,-1.6204351577,0.9391454654,-3.1252208086	H,0,-1.6506307679,0.9828700697,-3.0483772653
O,0,-5.8711011169,0.8146392506,-4.5183299385	O,0,-5.8451507583,0.7824726102,-4.5919052152
H,0,-6.6819766492,0.2991540867,-4.4632227881	H,0,-6.6461912102,0.2447117984,-4.5902544102
O,0,3.9776191002,1.1489994738,2.537975152	O,0,4.1415069194,1.1363782257,2.638017125
H,0,4.6838809689,1.8083167694,2.6142555334	H,0,4.8895045779,1.7536111102,2.6471480622

TS C4(•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.35190585 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209070 a.u. 1 imaginary frequency = 474.1690 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.925476 a.u.	**TS C6(•OOH),** optimization in gas phase UB3LYP/6-311++G**, E= -1061.34275568 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209936 a.u. 1 imaginary frequency = 510.4346 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9154501 a.u.
0, 2	0, 2
C,0,5.9377850627,0.6155007905,0.2188537056	C,0,6.1068072951,0.6026725575,0.0054358541
C,0,5.0297204078,-0.4294597487,0.6295210499	C,0,5.2850705498,-0.4815218957,0.257166087
C,0,5.5113673457,1.6993628513,-0.5206919361	C,0,5.628577213,1.7441016875,-0.675496866
H,0,5.4400287225,-1.3979048935,0.8960191023	H,0,5.6398588418,-1.3592379048,0.7833287816
C,0,3.7409730691,-0.4003169058,-0.0013919191	C,0,3.9507929892,-0.4225365972,-0.1928601124
C,0,4.1908786202,1.7891963746,-1.0255904709	C,0,4.3145580477,1.8332922857,-1.1324335956
H,0,3.8745224097,2.641434545,-1.6144733695	H,0,3.960185802,2.7147187137,-1.653148683
C,0,3.3455646135,0.7219764532,-0.7555124177	C,0,3.4896812183,0.7411691276,-0.8928846016
C,0,1.7388893912,-0.7828431077,-0.6143069749	C,0,1.8525290056,-0.7344886822,-0.6029424407
N,0,2.7310714491,-1.325233225,0.072116873	N,0,2.9638674661,-1.337015441,-0.0676143607
N,0,2.0349027751,0.4414291516,-1.1371210215	N,0,2.1830452351,0.4714088174,-1.2171326566
H,0,1.403382864,1.0031664956,-1.6865097201	H,0,1.489084153,1.1046410659,-1.5813459877
N,0,0.5292045825,-1.383025442,-0.7989462222	N,0,0.8481110498,-1.5263694271,-1.1387760395
N,0,-0.4346001971,-0.7687832048,-1.5259952478	N,0,-0.1967239904,-0.8484082077,-1.7109579309
C,0,-1.5748980586,-1.3536015292,-1.6217314573	C,0,-1.3214358744,-1.4540833899,-1.7844423563
H,0,-1.7574567871,-2.3096831398,-1.1202793174	H,0,-1.4506134106,-2.45369779,-1.3541839716
H,0,0.3713116977,-2.2715001183,-0.3326320114	H,0,0.6172887892,-2.3114107663,-0.5302308701
H,0,6.211201453,2.4941612063,-0.7536856793	H,0,6.3036696819,2.5742914356,-0.8484198372
C,0,-2.6840608611,-0.7962947351,-2.3884507448	C,0,-2.4943260176,-0.8674470641,-2.431178902
C,0,-3.9071725788,-1.479566722,-2.4007017703	C,0,-3.7072233055,-1.5655756855,-2.3966600104
C,0,-2.5633986813,0.4025790305,-3.1128934207	C,0,-2.4395097133,0.3768616197,-3.08026429
C,0,-4.99238823,-0.9784330157,-3.1174470752	C,0,-4.8484308639,-1.0324306749,-2.9938882941
C,0,-3.6383197117,0.9022310694,-3.8256468804	C,0,-3.5697378497,0.9097502144,-3.6741840143
C,0,-4.8624936953,0.2073081356,-3.8272869359	C,0,-4.7826307263,0.1993426042,-3.6286329748
H,0,6.9621868563,0.5679933916,0.5686987503	H,0,7.1380200421,0.5842505457,0.337971843
H,0,-5.9383252115,-1.5101788066,-3.1232312342	H,0,-5.7878851344,-1.5758663381,-2.9638159886
H,0,-4.0156418132,-2.4055465531,-1.8477082247	H,0,-3.764570044,-2.527254413,-1.8996261387
O,0,-3.5061083127,2.0654935613,-4.524460584	O,0,-3.5012157088,2.1178849078,-4.3006499013
H,0,-4.3461687724,2.2632686394,-4.9599540906	H,0,-4.3750092854,2.3331377229,-4.6516749115
O,0,4.7207116653,-0.1004207888,2.3997294443	O,0,1.0769419386,-0.0670548191,0.965052994
H,0,-1.6282925477,0.9472254814,-3.1220718772	H,0,-1.5113954275,0.9313055387,-3.1228587675
O,0,-5.8605649733,0.7900267532,-4.5651087758	O,0,-5.8432853122,0.8161985389,-4.249299636
H,0,-6.6709985033,0.2707763969,-4.5219184399	H,0,-6.6406923219,0.2831869909,-4.1707954205
O,0,4.0499029154,1.1282261287,2.5863487046	O,0,0.4752679338,-1.1521514217,1.6276992644
H,0,4.7732137745,1.7715861399,2.6378212187	H,0,1.1459984438,-1.4072230456,2.2794444953

TS C6(•OOH), optimization in solv. water UB3LYP/6-311++G**, E= -1061.36593020 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208571 a.u. 1 imaginary frequency = 460.7358 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9390835 a.u.	**TS C6(•OOH),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.35248114 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209728 a.u. 1 imaginary frequency = 495.3622 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9253862 a.u.
0, 2 C,0,6.1452601973,0.5368278864,-0.0316727359 C,0,5.2953804923,-0.5102391345,0.2701356805 C,0,5.6939755656,1.6688228308,-0.7536116969 H,0,5.6322791827,-1.3766696524,0.8262299512 C,0,3.9561388747,-0.4245597581,-0.1700518071 C,0,4.3792719871,1.785935116,-1.1988516251 H,0,4.0449001322,2.6559926564,-1.7498961765 C,0,3.522685682,0.7295997838,-0.9074266609 C,0,1.8425038109,-0.6838483453,-0.5569823315 N,0,2.944027671,-1.3020943044,-0.0071960175 N,0,2.2053854036,0.4946575508,-1.2031080067 H,0,1.5471474919,1.1252872102,-1.6349736227 N,0,0.8273227949,-1.4670793646,-1.0663532958 N,0,-0.220169278,-0.7974300775,-1.6496633609 C,0,-1.3209910872,-1.4412187944,-1.7821127171 H,0,-1.4228340578,-2.4648519833,-1.4086514137 H,0,0.6125418401,-2.2797189022,-0.4906405013 H,0,6.3947590063,2.4676101866,-0.9661238375 C,0,-2.4968268743,-0.864514754,-2.4305844356 C,0,-3.6638708985,-1.6344279673,-2.5172872803 C,0,-2.4935656956,0.4364277321,-2.9652538415 C,0,-4.8095330353,-1.122403926,-3.1245323695 C,0,-3.6288225214,0.9468859837,-3.5686838412 C,0,-4.7967306997,0.1635733346,-3.6492521402 H,0,7.1792078578,0.499821526,0.2899179981 H,0,-5.7112263653,-1.7214773707,-3.1896640172 H,0,-3.6808448944,-2.6386418828,-2.1098654258 O,0,-3.6123046325,2.2115597752,-4.0847933428 H,0,-4.4800284923,2.4035619305,-4.4670374979 O,0,1.0893333163,0.076557391,1.0063952708 H,0,-1.6034883011,1.0504893905,-2.9104410468 O,0,-5.8590623067,0.767173779,-4.2642834055 H,0,-6.6245037181,0.1806601826,-4.2976381453 O,0,0.4286422311,-0.9581156381,1.7093163301 H,0,1.0915471603,-1.2536500406,2.3525778359	0, 2 C,0,6.1170418554,0.5877894182,-0.0104694507 C,0,5.2897021618,-0.4881991578,0.2546180483 C,0,5.6420776804,1.7299012368,-0.6957161258 H,0,5.6432159115,-1.3646070109,0.7839358729 C,0,3.9514935203,-0.4208409705,-0.1862481528 C,0,4.3257313337,1.8280132214,-1.1426495693 H,0,3.9730460997,2.7084198609,-1.6658190345 C,0,3.4940382273,0.7433944684,-0.8894488654 C,0,1.8465378672,-0.7172961885,-0.5828261727 N,0,2.9586019298,-1.3263602018,-0.0506561956 N,0,2.1831289198,0.4843545006,-1.2001310363 H,0,1.4993094936,1.1180914942,-1.5834172217 N,0,0.8384455964,-1.5050620812,-1.1118405567 N,0,-0.2052023405,-0.8276229118,-1.6910568463 C,0,-1.3259910373,-1.4408969073,-1.775711988 H,0,-1.4516993585,-2.4433302858,-1.3526129961 H,0,0.6083023678,-2.2965359475,-0.5117254362 H,0,6.3230265437,2.5529713591,-0.8789608235 C,0,-2.497346552,-0.859358892,-2.4291232096 C,0,-3.7025707917,-1.5719539021,-2.4149923806 C,0,-2.4499093854,0.3922107721,-3.0661176258 C,0,-4.8436830814,-1.0479086875,-3.0206222092 C,0,-3.5798685593,0.9150784853,-3.6689570123 C,0,-4.7858526099,0.1903361804,-3.645166605 H,0,7.1506062854,0.5638088746,0.3140944816 H,0,-5.7763721691,-1.6025906693,-3.0055633168 H,0,-3.7538409019,-2.5389256407,-1.9276916304 O,0,-3.5189673946,2.1306609729,-4.2851815149 H,0,-4.3907746432,2.338398257,-4.6472548319 O,0,1.0818353963,-0.0333638872,0.9933840464 H,0,-1.5284943044,0.9591597532,-3.0921539979 O,0,-5.8430194598,0.7999125027,-4.2725172713 H,0,-6.6356529421,0.2545694869,-4.2228685477 O,0,0.4672293946,-1.1099268957,1.6644429834 H,0,1.1387167762,-1.3796934771,2.3098120423

TS C9(•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.33643221 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209310 a.u. 1 imaginary frequency = 409.5558 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9124823 a.u.	**TS C9(•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.36287054 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209396 a.u. 1 imaginary frequency = 324.0468 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9407079 a.u.
0, 2 C,0,5.7773304013,0.1942679977,-0.3046812491 C,0,4.7450313928,-0.7359638637,-0.2400722448 C,0,5.5598462557,1.5156906843,-0.7982693292	0, 2 C,0,5.760353917,0.1871117971,-0.3480599397 C,0,4.7275693825,-0.7392428766,-0.2306031326 C,0,5.5248370211,1.5066024694,-0.8457190692

H,0,4.9300303988,-1.7696496688,0.02541414	H,0,4.9268751515,-1.7726551992,0.028449646
C,0,3.4676809186,-0.3270669671,-0.6044940742	C,0,3.4359244937,-0.3306406281,-0.5496819821
C,0,4.3144896456,1.9550321622,-1.1614906917	C,0,4.2679200899,1.9503696741,-1.1549034364
H,0,4.1470268907,2.9459463389,-1.5667370546	H,0,4.0863289537,2.9385812166,-1.5600774198
C,0,3.1908615967,1.0950934282,-0.8623390783	C,0,3.1485379724,1.0966577621,-0.8023616789
C,0,1.491750034,-0.2323294748,-1.3832878374	C,0,1.4394632922,-0.2411892653,-1.30350023
N,0,2.3483117309,-1.080059347,-0.8530884846	N,0,2.3138227712,-1.0861040275,-0.771960391
N,0,1.9694478741,1.0410541243,-1.5832658993	N,0,1.9162509478,1.0301711489,-1.496774514
H,0,1.3426872528,1.8279348182,-1.671786794	H,0,1.3130821819,1.8189412277,-1.6817724301
N,0,0.2365560087,-0.5923363204,-1.756111736	N,0,0.1923560259,-0.5981478464,-1.6727777712
N,0,-0.6260691173,0.3177051634,-2.2666494392	N,0,-0.6549527549,0.3252550076,-2.2059729838
C,0,-1.8091873346,-0.0849305857,-2.5633482498	C,0,-1.8227902207,-0.0873181236,-2.5509595931
H,0,-2.1029389987,-1.1280876416,-2.4000901754	H,0,-2.1092425465,-1.1345870019,-2.4200724489
H,0,-0.0378112315,-1.5539895685,-1.574997562	H,0,-0.0886981014,-1.5656245355,-1.5351469213
H,0,6.4151687458,2.1712249824,-0.9220443404	H,0,6.3766248992,2.156595532,-1.0129389858
C,0,-2.8237193321,0.7974870327,-3.1285469171	C,0,-2.825397991,0.797651218,-3.1311551404
C,0,-4.0955304724,0.2784800142,-3.4030220499	C,0,-4.0691362135,0.2604374896,-3.490000326
C,0,-2.5598711292,2.1492146772,-3.4088085614	C,0,-2.5824061491,2.167265866,-3.3437582486
C,0,-5.0890117627,1.0912090502,-3.9455945147	C,0,-5.0556333505,1.0687262906,-4.0513057938
C,0,-3.5436010652,2.9587998489,-3.9475911096	C,0,-3.5601732916,2.9713919527,-3.9001791163
C,0,-4.8171411142,2.4244156805,-4.2174993319	C,0,-4.8066591614,2.4198371081,-4.2576792676
H,0,6.7837742183,-0.1024445617,-0.0338033096	H,0,6.7770652175,-0.11184148,-0.1221547514
H,0,-6.0738594922,0.6861154094,-4.1565750056	H,0,-6.0166640351,0.6502918446,-4.3292359312
H,0,-4.3135795827,-0.7624024725,-3.1926909311	H,0,-4.2693674386,-0.7929475997,-3.3322539365
O,0,-3.2737532065,4.2657211141,-4.2151424946	O,0,-3.3130154825,4.2989532373,-4.1014338907
H,0,-4.0656619585,4.6762464137,-4.586099151	H,0,-4.0982927736,4.7071671035,-4.4921474842
O,0,2.5199646435,1.7225128388,0.6167650123	O,0,2.5266865836,1.7243857071,0.6732076436
O,0,-5.7186234031,3.3123175594,-4.7516594146	O,0,-5.6975757993,3.3033679835,-4.7989335241
H,0,-6.5644660354,2.8840630097,-4.9174132634	H,0,-6.5318939849,2.8706042305,-5.0175434303
H,0,-1.5840542397,2.5712619962,-3.207832515	H,0,-1.6296116989,2.6052962259,-3.0743253286
O,0,3.4357221056,1.6871747664,1.6972499376	O,0,3.5029713287,1.790351241,1.7143120302
H,0,3.883867352,2.5432670808,1.6290040694	H,0,3.9504774939,2.6333807002,1.5437215779

TS C9(•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.34755915 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209656 a.u. 1 imaginary frequency = 377.9069 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9242744 a.u.	**TS C13(•OOH),** optimization in gas phase UB3LYP/6-311++G**, E= -1061.35460736 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209346 a.u. 1 imaginary frequency = 418.6826 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9257125 a.u.
0, 2	0, 2
C,0,5.7698705206,0.1959372258,-0.313252544	C,0,6.0337830576,0.6858178104,0.1301111668
C,0,4.7384746501,-0.7343407424,-0.2318417539	C,0,5.1566279085,-0.3257117936,0.5048450983
C,0,5.5453022842,1.5160949246,-0.8099754833	C,0,5.6559370267,1.6838933571,-0.7855112084
H,0,4.9294541208,-1.767196123,0.0335987175	H,0,5.4438490381,-1.0955466944,1.2106705933
C,0,3.455845552,-0.327868317,-0.5839823479	C,0,3.8764366726,-0.3261671142,-0.0569400407
C,0,4.2956120207,1.9547921085,-1.1572165869	C,0,4.3856171529,1.7020321201,-1.3582548393
H,0,4.1224859768,2.9440790749,-1.5639058438	H,0,4.0977711145,2.4727293114,-2.0637165309
C,0,3.1739852626,1.0953079702,-0.8416944745	C,0,3.5135721741,0.6877159825,-0.9791611039
C,0,1.4738673148,-0.2382431594,-1.3590914428	C,0,1.8673126064,-0.7347682902,-0.6288912098
N,0,2.3377896486,-1.0836822027,-0.8264053198	N,0,2.8213227982,-1.2030535131,0.1388903444
N,0,1.950388045,1.0348721797,-1.5550321639	N,0,2.2041693603,0.3894003686,-1.333908586
H,0,1.3309854169,1.8223403291,-1.6822754594	H,0,1.580150029,0.8889527194,-1.9479155477
N,0,0.2232817529,-0.5976406158,-1.7335608277	N,0,0.630144741,-1.3125986664,-0.7491911033
N,0,-0.6328807041,0.3190616939,-2.2527673341	N,0,-0.3115023963,-0.7477840504,-1.5073913342

C,0,-1.8127776442,-0.0850776983,-2.5615229135	C,0,-1.4686418023,-1.4048954854,-1.5330517653
H,0,-2.1066307219,-1.1282143478,-2.4051619603	H,0,-1.4842332591,-2.4736575105,-1.3272941118
H,0,-0.0564548376,-1.560308418,-1.5654114093	H,0,0.4096606913,-2.0723294816,-0.108070696
H,0,6.3990046871,2.1708455288,-0.9476563059	H,0,6.3676880384,2.4564258319,-1.0523186719
C,0,-2.8231654398,0.7983919694,-3.1316914207	C,0,-2.5723976446,-0.8842609148,-2.3407567037
C,0,-4.0872731125,0.2732831326,-3.4303280392	C,0,-3.627872029,-1.7378347524,-2.6813838646
C,0,-2.5654108388,2.1558097618,-3.3923766566	C,0,-2.6102912221,0.4564578964,-2.7561177729
C,0,-5.0793696669,1.0839975727,-3.9782695339	C,0,-4.6984802857,-1.2668999782,-3.4405087737
C,0,-3.5481369845,2.9630377911,-3.9359251266	C,0,-3.6685411995,0.9259463544,-3.5144958881
C,0,-4.8145698298,2.423104928,-4.2311898454	C,0,-4.7192452614,0.056425579,-3.8574712792
H,0,6.7799289185,-0.099707785,-0.055088097	H,0,7.0320677783,0.7091285444,0.5517045857
H,0,-6.0574331893,0.6744726744,-4.2087197169	H,0,-5.5142352491,-1.9313173028,-3.7084851337
H,0,-4.2999954221,-0.7714989333,-3.2348826577	H,0,-3.6143757023,-2.7711103441,-2.3565738505
O,0,-3.2850549034,4.2770276918,-4.1840458682	O,0,-3.6889480165,2.2270377467,-3.9185660489
H,0,-4.0764740716,4.6878564509,-4.557258539	H,0,-4.4956101721,2.3793469182,-4.4277188287
O,0,2.5164137986,1.7237012692,0.6373489504	O,0,-1.9897658051,-1.146119199,0.38051215
O,0,-5.7129781983,3.3086628276,-4.7666782615	O,0,-5.7215119936,0.6223843808,-4.6084054525
H,0,-6.5595902745,2.8819627863,-4.9387822973	H,0,-6.4033986732,-0.0257376072,-4.811552946
H,0,-1.5962849911,2.5835326907,-3.1708932191	H,0,-1.8132017275,1.1368993884,-2.4873726463
O,0,3.4530756194,1.7285363899,1.7065223906	O,0,-3.1974401454,-1.7936720852,0.631587734
H,0,3.9026427012,2.5801633007,1.5989298318	H,0,-3.8522938729,-1.0810234566,0.5679339653

TS C13(•OOH), optimization in solv. water UB3LYP/6-311++G**, E= -1061.37835707 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208872 a.u. 1 imaginary frequency = 390.6870 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9498224 a.u.	**TS C13(•OOH),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.36468603 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209302 a.u. 1 imaginary frequency = 412.6628 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9360588 a.u.
0, 2	0, 2
C,0,6.0784630339,0.6344107981,0.0569296469	C,0,6.0401237398,0.6549596341,0.1793477936
C,0,5.2547087432,-0.4569493026,0.3145456607	C,0,5.1994425375,-0.4148904001,0.4675029154
C,0,5.6134485998,1.7531996181,-0.6597835667	C,0,5.6082719158,1.7372641565,-0.6087161464
H,0,5.6137526203,-1.3180172917,0.8659531207	H,0,5.5303145744,-1.248827456,1.0748061289
C,0,3.9396148036,-0.412534194,-0.1615490229	C,0,3.9008698671,-0.387218501,-0.0509185774
C,0,4.3073278492,1.8174348264,-1.1425636613	C,0,4.3187627776,1.7847283728,-1.1354387703
H,0,3.9497108988,2.6782197484,-1.6944684348	H,0,3.9877651244,2.6192162118,-1.7422622824
C,0,3.4890526784,0.7229608515,-0.8808458051	C,0,3.4835018873,0.7118514559,-0.8431010704
C,0,1.904101184,-0.7921498688,-0.6777724837	C,0,1.8812795161,-0.7812676569,-0.6049454484
N,0,2.9206875731,-1.3472753104,-0.0514102564	N,0,2.8721093181,-1.3078138121,0.0778870823
N,0,2.1683612163,0.4420667247,-1.1979659755	N,0,2.1703832241,0.4217558459,-1.1871769805
H,0,1.5088886762,1.0138781272,-1.7050563551	H,0,1.5214819913,0.9708436217,-1.7298953233
N,0,0.677340038,-1.3862752797,-0.810695476	N,0,0.6540578037,-1.3734739913,-0.7486043405
N,0,-0.3055040609,-0.7735010493,-1.4683666553	N,0,-0.3131342405,-0.771127765,-1.4406574119
C,0,-1.4606169245,-1.4365486567,-1.508928045	C,0,-1.464548052,-1.4377122453,-1.4933476574
H,0,-1.4723124321,-2.5082602978,-1.3194657196	H,0,-1.4699438494,-2.5146955179,-1.334961686
H,0,0.5524721691,-2.3011236411,-0.3802160414	H,0,0.4852738116,-2.2276045441,-0.2205460748
H,0,6.2855867033,2.5838669731,-0.8407694795	H,0,6.2928209974,2.5527359463,-0.8112555479
C,0,-2.5596057139,-0.9038640331,-2.3137353704	C,0,-2.5707420461,-0.8902633953,-2.2799004608
C,0,-3.5949191654,-1.7618091009,-2.7033955172	C,0,-3.6078603884,-1.7398101956,-2.6815368468
C,0,-2.6117367759,0.4508830153,-2.6857181115	C,0,-2.6275183314,0.4720236229,-2.617736845
C,0,-4.6617422578,-1.2844093251,-3.4636830779	C,0,-4.6794854545,-1.2443246789,-3.4237511643
C,0,-3.6688771285,0.9269758146,-3.440389977	C,0,-3.6875456572,0.9662765501,-3.3570422811
C,0,-4.7020071499,0.0540463817,-3.8327609289	C,0,-4.720890286,0.1014265007,-3.7622503558
H,0,7.1017068418,0.6256987331,0.4143849105	H,0,7.0514136393,0.6581343331,0.5694420925

H,0,-5.4600686546,-1.951305636,-3.7704415158	H,0,-5.4803402647,-1.905553205,-3.7387173099
H,0,-3.5663561321,-2.8076583144,-2.4224597493	H,0,-3.5789155291,-2.7907554951,-2.4205150097
O,0,-3.7073440888,2.2444627944,-3.7994695097	O,0,-3.7275405542,2.2899477866,-3.684489152
H,0,-4.5101858766,2.4033551448,-4.3152427774	H,0,-4.5324445959,2.459438798,-4.1921574771
O,0,-2.0227349418,-1.1375868073,0.4030381051	O,0,-2.0018891524,-1.2353290252,0.4258162508
O,0,-5.6961015114,0.6281314137,-4.5755170454	O,0,-5.7230472456,0.6935280286,-4.4873949895
H,0,-6.372902253,-0.0176772627,-4.8117102087	H,0,-6.3983224231,0.0514920301,-4.7322568414
H,0,-1.8261839825,1.1338855585,-2.3884093653	H,0,-1.8437742141,1.1487806898,-2.3035573673
O,0,-3.298750803,-1.6717694043,0.6184556956	O,0,-3.239513837,-1.8432143956,0.6402963102
H,0,-3.8957446065,-0.921434708,0.4678954132	H,0,-3.8705337838,-1.1094323944,0.5714784247

TS C14(•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.33192320 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208460 a.u. 1 imaginary frequency = 421.6750 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9095323 a.u.	**TS C14(•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.35882449 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209006 a.u. 1 imaginary frequency = 352.3597 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.937826 a.u.
0, 2	0, 2
C,0,6.1109463848,0.7958465249,-0.2458759712	C,0,6.1005241694,0.7941157283,-0.2457096169
C,0,5.3661263361,-0.3317102425,0.091877062	C,0,5.3827145497,-0.3737067121,0.0121603314
C,0,5.5334803156,1.8788582552,-0.9270828585	C,0,5.4857347676,1.9215877245,-0.8150432044
H,0,5.8103450528,-1.1680366352,0.6181669358	H,0,5.8605340612,-1.2417323551,0.4518847159
C,0,4.0175285535,-0.3606468772,-0.2663583941	C,0,4.024123444,-0.3961948898,-0.3123770801
C,0,4.1874156548,1.8691497941,-1.2938401246	C,0,4.1290273184,1.9178897352,-1.1463115428
H,0,3.7427513436,2.706265961,-1.8197550758	H,0,3.6528987577,2.7862411601,-1.5860238246
C,0,3.4526110615,0.7405299934,-0.9527648574	C,0,3.4222880095,0.7498187501,-0.8854760613
C,0,1.9707293105,-0.8553544024,-0.5920511067	C,0,1.9688394255,-0.8933015756,-0.631998093
N,0,3.0577789609,-1.3457032769,-0.0562447926	N,0,3.0839290406,-1.4123220295,-0.1655571636
N,0,2.120108255,0.3865756481,-1.1497696403	N,0,2.0928732942,0.3923794597,-1.0790223266
H,0,1.3869166458,0.9059444262,-1.6051372563	H,0,1.3451677706,0.9468266203,-1.4681937081
N,0,0.7640706529,-1.5126075116,-0.6123548204	N,0,0.7730525363,-1.5584746235,-0.6767826769
N,0,-0.3191717298,-0.932806477,-1.1620031199	N,0,-0.3201051707,-0.9428278766,-1.1735729769
C,0,-1.4192756721,-1.5850483237,-1.1814348615	C,0,-1.4160372365,-1.6015443088,-1.2280980315
H,0,-1.5029555477,-2.5933099182,-0.7662241218	H,0,-1.4869223954,-2.6371930492,-0.8890140945
H,0,0.7263636744,-2.4261834162,-0.1710124063	H,0,0.7454564955,-2.5161140959,-0.3388567066
H,0,6.1435717217,2.7401065606,-1.1735260778	H,0,6.0742298242,2.8124281635,-1.0017485431
C,0,-2.661350097,-1.002093588,-1.7535979089	C,0,-2.6642561294,-0.9819947978,-1.7507418412
C,0,-3.4762967448,-1.9367611677,-2.5210217114	C,0,-3.5412902158,-1.9166776038,-2.4521839202
C,0,-2.6116411311,0.3621678874,-2.2468145734	C,0,-2.5824841835,0.3600858701,-2.3072130335
C,0,-4.325861584,-1.4942855358,-3.5022467724	C,0,-4.396761559,-1.4911446323,-3.4351355755
C,0,-3.476028613,0.7895908332,-3.2137140246	C,0,-3.4526718515,0.7709775755,-3.274087485
C,0,-4.3552297249,-0.135728323,-3.8439137648	C,0,-4.3851361325,-0.1482907985,-3.8436224725
H,0,7.1602774457,0.8405763476,0.0226990576	H,0,7.1561186735,0.8341732757,-0.0016986291
H,0,-4.9741721391,-2.1916009355,-4.0245018093	H,0,-5.0765564485,-2.1868479907,-3.9158062607
H,0,-3.4509916345,-2.9843594255,-2.2483030838	H,0,-3.5373434153,-2.9543340398,-2.1420048121
O,0,-3.4846333255,2.0960216875,-3.6026189216	O,0,-3.4187080675,2.0554040211,-3.7308991777
H,0,-4.1291912204,2.206679195,-4.3132213825	H,0,-4.0724048165,2.158868285,-4.4363956813
O,0,-3.5000958222,-0.9246271312,-0.2143271011	O,0,-3.40220636,-0.7920096871,-0.1779878191
H,0,-1.9235414219,1.0619974078,-1.7930669987	H,0,-1.854163327,1.0530769297,-1.9080405996
O,0,-5.1722540588,0.3984339967,-4.7983577065	O,0,-5.1939101418,0.3708171024,-4.7989902727
H,0,-5.7498706771,-0.2747605651,-5.1740805463	H,0,-5.7896573124,-0.2965640532,-5.1634310476
O,0,-4.8348159676,-0.4737296649,-0.3773698875	O,0,-4.7391736874,-0.300592962,-0.2821424503
H,0,-4.746119118,0.485899349,-0.2762077471	H,0,-4.6141950872,0.6592720498,-0.3419364783

TS C14(•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.34340850 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208990 a.u. 1 imaginary frequency = 399.8116 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9215493 a.u.	**TS C15(•OOH),** optimization in gas phase UB3LYP/6-311++G**, E= -1061.34136372 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208576 a.u. 1 imaginary frequency = 509.8898 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9138515 a.u.
0, 2	0, 2
C,0,6.1051852736,0.7988066104,-0.24248	C,0,5.8279632847,0.6628637242,0.2467084473
C,0,5.3712634148,-0.3455146936,0.0645427531	C,0,5.033836221,-0.4631116868,0.4472760166
C,0,5.5135614111,1.8987387666,-0.8839717583	C,0,5.3499979578,1.7821825107,-0.4538568169
H,0,5.828094411,-1.1938215055,0.5604560726	H,0,5.4009153616,-1.3272778168,0.987814184
C,0,4.0197088445,-0.3735594852,-0.2844213116	C,0,3.7369417828,-0.4538805788,-0.0701946313
C,0,4.1641929875,1.8896248205,-1.2407188604	C,0,4.0583906563,1.8108485144,-0.9797203684
H,0,3.7077825728,2.7390649759,-1.7355229511	H,0,3.6907865302,2.6754461447,-1.5202679789
C,0,3.4407794773,0.7444782635,-0.9310510917	C,0,3.2726634924,0.6833374663,-0.774910359
C,0,1.970579536,-0.8716407257,-0.6123982521	C,0,1.7379202838,-0.8966079346,-0.6581555009
N,0,3.0681917434,-1.3718002538,-0.0992456421	N,0,2.7475694838,-1.4283758893,-0.0164361506
N,0,2.1105371916,0.3874610364,-1.1301656827	N,0,1.9717711099,0.3601114412,-1.1482427671
H,0,1.3721204935,0.920752665,-1.5618483994	H,0,1.2851488102,0.9298277584,-1.6171013666
N,0,0.7695345558,-1.5337938607,-0.6445934992	N,0,0.531420923,-1.5247129083,-0.8408637638
N,0,-0.3185064976,-0.9406380395,-1.174231249	N,0,-0.4475263147,-0.9271717071,-1.5400129763
C,0,-1.4164763219,-1.5967609127,-1.2028180876	C,0,-1.5931457872,-1.5207173561,-1.6129234025
H,0,-1.4926349278,-2.6152925809,-0.813684623	H,0,-1.7587083137,-2.4795753819,-1.1098369306
H,0,0.7326590839,-2.4601619548,-0.2301980594	H,0,0.4004526608,-2.4162111942,-0.3712371136
H,0,6.1146732925,2.7726378415,-1.1069750915	H,0,5.9962709207,2.641618292,-0.5894230732
C,0,-2.6622750934,-1.0031192217,-1.7566953358	C,0,-2.6998838105,-0.9672461282,-2.3491378348
C,0,-3.4984412475,-1.9390071627,-2.500843064	C,0,-3.9179770055,-1.6428386924,-2.39539204
C,0,-2.6037888085,0.354352562,-2.270504031	C,0,-2.5838295437,0.3202119212,-2.9999207399
C,0,-4.3503947024,-1.5032501412,-3.4828615908	C,0,-4.9827650222,-1.1547209257,-3.1534160771
C,0,-3.4696281436,0.774824885,-3.238300643	C,0,-3.6269498459,0.7044741477,-3.8961672609
C,0,-4.3657144696,-0.1499412,-3.8489168549	C,0,-4.824827753,0.0093935522,-3.9161053691
H,0,7.156255507,0.8429276889,0.0195333059	H,0,6.8382381445,0.678681683,0.639533569
H,0,-5.0109300507,-2.2001297508,-3.9891543198	H,0,-5.9291988362,-1.6853532753,-3.1721189757
H,0,-3.4805725207,-2.9832551282,-2.2147089483	H,0,-4.038562935,-2.5715023959,-1.849037222
O,0,-3.4646628073,2.0746745349,-3.6505851414	O,0,-3.4339051557,1.8094951144,-4.6616736096
H,0,-4.1114109379,2.1822910556,-4.3606270444	H,0,-4.2235236883,1.9493178191,-5.2022781325
O,0,-3.4668238004,-0.8872351554,-0.2015533717	O,0,-2.6591298814,1.5398406421,-1.6216086246
H,0,-1.9037462023,1.0533829425,-1.8338492822	H,0,-1.5888885533,0.6757166436,-3.238864178
O,0,-5.178577677,0.3774689297,-4.8045666609	O,0,-5.8014996293,0.5284671803,-4.7396583602
H,0,-5.7567081626,-0.2956511671,-5.1826386065	H,0,-6.5216350275,-0.1000027554,-4.850466578
O,0,-4.804369203,-0.4262343365,-0.3438351857	O,0,-3.8930718869,1.5080029615,-0.9552391885
H,0,-4.7037958221,0.5368208375,-0.2992562218	H,0,-4.3953576332,2.2152175396,-1.3881889664

TS C15(•OOH), optimization in solv. water UB3LYP/6-311++G**, E= -1061.36832162 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208545 a.u. 1 imaginary frequency = 461.7560 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.942007 a.u.	**TS C15(•OOH),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.35265495 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208981 a.u. 1 imaginary frequency = 493.6570 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9255858 a.u.
0, 2	0, 2
C,0,5.8564019283,0.6426789686,0.2070997147	C,0,5.8489126081,0.6479153429,0.210614563
C,0,5.025577982,-0.4382674005,0.5004426081	C,0,5.0424743849,-0.4635676625,0.4460615652
C,0,5.4122627986,1.7152146521,-0.58439035	C,0,5.3772178576,1.7567087767,-0.5111392488

H,0,5.3719213334,-1.2641839541,1.1111671418	H,0,5.4069619956,-1.318454196,1.0033250306
C,0,3.7273105709,-0.4298542762,-0.0165809132	C,0,3.7398620385,-0.4499906637,-0.0579404406
C,0,4.1185443416,1.7419264203,-1.1094111467	C,0,4.0796639038,1.7891783971,-1.0235786107
H,0,3.7740450668,2.5678970914,-1.7203503593	H,0,3.7154601607,2.6445536095,-1.5805705334
C,0,3.2974679549,0.660684546,-0.8114846871	C,0,3.2823003302,0.6765560576,-0.7839170219
C,0,1.7056444303,-0.8514300024,-0.5729953358	C,0,1.7257947569,-0.878924317,-0.6174943575
N,0,2.7050509397,-1.3637974453,0.1149387753	N,0,2.7379381178,-1.4100309882,0.0276706418
N,0,1.9859084913,0.3544430648,-1.153192594	N,0,1.9740106196,0.3629725196,-1.1352157129
H,0,1.3404546899,0.8928319308,-1.7113248544	H,0,1.2975443232,0.9294895983,-1.6231837201
N,0,0.4848865406,-1.4491425904,-0.7146666174	N,0,0.5114550952,-1.4927527099,-0.7774586776
N,0,-0.4784121393,-0.8512304342,-1.4464762393	N,0,-0.4613655837,-0.8952944156,-1.489795318
C,0,-1.6113291932,-1.4641123275,-1.5598499696	C,0,-1.603819561,-1.4938076035,-1.5747101366
H,0,-1.7738158191,-2.4345341621,-1.0829282912	H,0,-1.7706680077,-2.4546298904,-1.077725997
H,0,0.3360129188,-2.3432298059,-0.255059043	H,0,0.375115052,-2.3875789447,-0.3156631178
H,0,6.0856854846,2.5385637883,-0.7926171032	H,0,6.0325727347,2.6044891341,-0.6740554658
C,0,-2.7030276242,-0.9186046498,-2.3270383195	C,0,-2.703015335,-0.9450973848,-2.3270839092
C,0,-3.885628923,-1.6403253524,-2.4660087433	C,0,-3.9066093858,-1.6414353845,-2.4147503173
C,0,-2.607338407,0.3950071164,-2.9320038357	C,0,-2.5933561218,0.3518134582,-2.961437089
C,0,-4.9264383946,-1.1736115772,-3.2738939541	C,0,-4.9583728944,-1.166198802,-3.2004714696
C,0,-3.6139334641,0.7631394747,-3.8775607326	C,0,-3.6165004803,0.7240336958,-3.8861820518
C,0,-4.7801165656,0.0203862701,-3.9925376986	C,0,-4.8007297233,0.0068018619,-3.9501533995
H,0,6.8678410277,0.6572122215,0.5972283395	H,0,6.8634932276,0.6596530732,0.5925004158
H,0,-5.8405283524,-1.7484441126,-3.3721458379	H,0,-5.8922981513,-1.7156083276,-3.2537920487
H,0,-3.9952103894,-2.5949521667,-1.9643829611	H,0,-4.0251576082,-2.5787558152,-1.8831333365
O,0,-3.4222242927,1.9017846475,-4.5920021671	O,0,-3.4185582295,1.8380210699,-4.637380312
H,0,-4.1947838203,2.0517367278,-5.1566175856	H,0,-4.195319339,1.9748954424,-5.1981529321
O,0,-2.829674023,1.5873004972,-1.5427393815	O,0,-2.7374857341,1.5645944954,-1.5805131165
H,0,-1.6155952304,0.797952706,-3.102191044	H,0,-1.5984899098,0.727982401,-3.1676737682
O,0,-5.7199527993,0.5214664651,-4.854779998	O,0,-5.7581219068,0.5130751608,-4.7986312422
H,0,-6.4552013885,-0.0928062517,-4.9662147324	H,0,-6.4656886189,-0.1252578232,-4.9389792319
O,0,-4.0863584838,1.4511898674,-0.9138998221	O,0,-3.9795316073,1.4820226081,-0.9263947375
H,0,-4.6534250698,2.0708757631,-1.3991076419	H,0,-4.5143272784,2.1539866961,-1.3766135559

TS C16(•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.33586019 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208540 a.u. 1 imaginary frequency = 480.6414 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9117971 a.u.	**TS C16(•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.36474281 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208338 a.u. 1 imaginary frequency = 418.6930 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.94198 a.u.
0, 2	0, 2
C,0,5.8336193581,0.6763570321,0.1086583647	C,0,5.849084195,0.6763183766,0.0723744161
C,0,5.0447698893,-0.453613028,0.3114055095	C,0,5.0566338732,-0.4463288754,0.313022075
C,0,5.371834895,1.7674443802,-0.6442331742	C,0,5.382473986,1.7500242683,-0.703628341
H,0,5.4000318518,-1.2963099022,0.8923033049	H,0,5.4206573704,-1.2730478574,0.91236392
C,0,3.770420065,-0.4768690721,-0.2576118335	C,0,3.7746352846,-0.4785375276,-0.2413163198
C,0,4.1016062383,1.7633066914,-1.2213704225	C,0,4.1038502878,1.7359670128,-1.2658622561
H,0,3.7458497822,2.6065351527,-1.8022240137	H,0,3.7416423167,2.5631912181,-1.8647921422
C,0,3.3221066033,0.6322838579,-1.0138159577	C,0,3.3218866675,0.613617553,-1.0203429654
C,0,1.8010349714,-0.9636143586,-0.9100605178	C,0,1.7875781928,-0.9684045795,-0.8650628023
N,0,2.7893210158,-1.462018553,-0.2129533235	N,0,2.7880497511,-1.4571733342,-0.1625418764
N,0,2.0390880575,0.281953453,-1.4264406682	N,0,2.0338426223,0.2624065447,-1.4073599626
H,0,1.3765078358,0.8201134368,-1.961519283	H,0,1.3816593271,0.7889516752,-1.9687997876
N,0,0.6137110223,-1.6193650146,-1.1284242348	N,0,0.5973635022,-1.6125926687,-1.0588148276
N,0,-0.3771326028,-1.0269177216,-1.8212791056	N,0,-0.3841261344,-1.0140057234,-1.7707179432

C,0,-1.5068965447,-1.6299825038,-1.9114276171	C,0,-1.5102027592,-1.6217990502,-1.8784102215
H,0,-1.67055687,-2.5926162558,-1.4146117788	H,0,-1.6808755435,-2.5873963697,-1.3949733059
H,0,0.4859558655,-2.5071941492,-0.6521044055	H,0,0.4590189282,-2.5085415677,-0.6005824464
H,0,6.012947319,2.6305803361,-0.7807319899	H,0,6.025286748,2.6066476214,-0.8703032053
C,0,-2.6314764113,-1.0745480404,-2.6645779381	C,0,-2.6227252024,-1.0556133355,-2.644233646
C,0,-3.8813565442,-1.7379894605,-2.5922787904	C,0,-3.8664107102,-1.7413985244,-2.6208590915
C,0,-2.5091672474,0.0501259484,-3.4580935015	C,0,-2.4960942475,0.0905861172,-3.4040841363
C,0,-4.9872655482,-1.2859747411,-3.3271184834	C,0,-4.9604439131,-1.2908150459,-3.3689770706
C,0,-3.6612169196,0.648386411,-4.0742507165	C,0,-3.6419579404,0.6797832359,-4.0428868609
C,0,-4.8762345093,-0.1577157615,-4.1047832137	C,0,-4.848138443,-0.1409458083,-4.1179300741
H,0,6.8269064599,0.7165432255,0.5411428827	H,0,6.8474180554,0.7223287062,0.4927439051
H,0,-5.9187825814,-1.8437836143,-3.3048956332	H,0,-5.8837962441,-1.8593592443,-3.3838889983
H,0,-3.9823647931,-2.6247704951,-1.9771563522	H,0,-3.9652630878,-2.6465038051,-2.0334211973
O,0,-3.40349699,1.4568359176,-5.1404920873	O,0,-3.3700071062,1.5049892999,-5.0960714402
H,0,-4.237892608,1.8205017791,-5.4654112433	H,0,-4.203277446,1.7735401848,-5.509388999
O,0,-4.1170027426,1.9561170763,-2.9434466958	O,0,-4.1517938879,1.9852349156,-2.9201308641
O,0,-5.8555837279,0.3447444701,-4.9038510791	O,0,-5.8028129722,0.3680540171,-4.9282379535
H,0,-6.635748747,-0.2205247165,-4.8853058199	H,0,-6.593387842,-0.1875440888,-4.9359353306
H,0,-1.5649710266,0.5647978192,-3.5702036799	H,0,-1.5547022474,0.61861112,-3.4807254864
O,0,-4.3937758242,1.5248682473,-1.6297454664	O,0,-4.4893181734,1.5462627566,-1.6144472144
H,0,-5.3576639117,1.4253440735,-1.6281062356	H,0,-5.4383272975,1.3553993227,-1.6763146397

TS C16(•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.34783607 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208283 a.u. 1 imaginary frequency = 458.6317 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9243214 a.u.	**TS C17(•OOH),** optimization in gas phase UB3LYP/6-311++G**, E= -1061.34988505 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.210236 a.u. 1 imaginary frequency = 458.9467 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9225336 a.u.
0, 2	0, 2
C,0,5.846575604,0.6753429747,0.0640109469	C,0,5.9218378464,0.6432798594,0.0666362866
C,0,5.0634458198,-0.457036478,0.2811603929	C,0,5.0458578793,-0.3877395879,0.3935606568
C,0,5.3672996464,1.7670372797,-0.6775444336	C,0,5.5512381365,1.6678154255,-0.8199410046
H,0,5.4344150007,-1.2989535885,0.8537599908	H,0,5.3297466353,-1.1787363003,1.0771099478
C,0,3.7772335081,-0.4818204698,-0.2617221009	C,0,3.7758200409,-0.3795208958,-0.1872856085
C,0,4.0848914359,1.761000392,-1.2286187556	C,0,4.2882154829,1.6943529199,-1.4105780617
H,0,3.7142953823,2.6033866503,-1.8010591601	H,0,4.0043580982,2.4857642251,-2.0945838378
C,0,3.3118041117,0.6280486901,-1.0068611823	C,0,3.4200367993,0.661340656,-1.0789048077
C,0,1.7925817577,-0.9688660328,-0.8785766543	C,0,1.7783198523,-0.7866264328,-0.8053518984
N,0,2.7980228322,-1.4685980525,-0.2003621496	N,0,2.7211809307,-1.2716620675,-0.0380872767
N,0,2.0221969824,0.2778652349,-1.3937524971	N,0,2.1147295718,0.3664124592,-1.4622549865
H,0,1.3535330827,0.8166092833,-1.9217783993	H,0,1.510328839,0.8687862801,-2.0924351
N,0,0.601496376,-1.6187158995,-1.075881648	N,0,0.5445085395,-1.3695802775,-0.9545860318
N,0,-0.3841367052,-1.0274509748,-1.7811426959	N,0,-0.3846455323,-0.8221674949,-1.7518056845
C,0,-1.5121568301,-1.6321635725,-1.8818642401	C,0,-1.5344007652,-1.4201368099,-1.8351048329
H,0,-1.6823458244,-2.5944585407,-1.3887896377	H,0,-1.723665884,-2.3337562402,-1.2622814255
H,0,0.4780686853,-2.5193707564,-0.6230986203	H,0,0.3746362256,-2.2207141602,-0.4253268127
H,0,6.0037432401,2.6317542541,-0.8257934962	H,0,6.2603265863,2.4542262792,-1.0507468244
C,0,-2.6262459571,-1.0712610771,-2.6480225407	C,0,-2.6044409079,-0.9314753532,-2.6590499901
C,0,-3.8783701707,-1.7352168378,-2.5983857573	C,0,-3.8335589078,-1.6517906985,-2.6758889091
C,0,-2.4902401037,0.0569879066,-3.4334287987	C,0,-2.4696584966,0.2190435715,-3.4713291985
C,0,-4.9733426591,-1.279622738,-3.3459700295	C,0,-4.8896745032,-1.2331187844,-3.4353859497
C,0,-3.6324703837,0.6568269193,-4.0658136272	C,0,-3.5225524889,0.6498503552,-4.2378379139
C,0,-4.849542691,-0.1465806929,-4.1165438929	C,0,-4.8187191378,0.0131103578,-4.1332828362
H,0,6.8484668602,0.7162068248,0.476278489	H,0,6.9132911146,0.6585879828,0.5045520254

H,0,-5.9053092192,-1.8363444425,-3.340692348	H,0,-5.8216582003,-1.7844168085,-3.4641692492
H,0,-3.9875632335,-2.6262771516,-1.9911403622	H,0,-3.9192531703,-2.5594771767,-2.0885882377
O,0,-3.3594482088,1.4671899031,-5.127906648	O,0,-3.3949788456,1.7138809258,-5.0570568902
H,0,-4.1919717276,1.7961811954,-5.4940117587	H,0,-4.2415152072,1.8380708688,-5.5128097969
O,0,-4.1040917036,1.9707109818,-2.9412327279	O,0,-5.7410761329,1.2040216687,-3.0068733792
O,0,-5.8097976556,0.36212035,-4.9290182073	O,0,-5.6523783861,0.2915547534,-5.1938291609
H,0,-6.5958704246,-0.1967951131,-4.9315420567	H,0,-6.5570078969,0.3608181011,-4.8572246779
H,0,-1.5429681793,0.5697177463,-3.5293139779	H,0,-1.5265775802,0.7468915319,-3.5192910143
O,0,-4.4010801827,1.5416014631,-1.6280769701	O,0,-5.3943918091,1.1153185106,-1.654904795
H,0,-5.3616577756,1.4128431791,-1.6464626655	H,0,-4.7206661863,1.8055413861,-1.5547810038

TS C17(•OOH), optimization in solv. water UB3LYP/6-311++G**, E= -1061.37322911 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209468 a.u. 1 imaginary frequency = 415.1296 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9468371 a.u.	**TS C17(•OOH),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.35966062 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209979 a.u. 1 imaginary frequency = 446.6193 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9326892 a.u.
0, 2	0, 2
C,0,5.9107542286,0.5579782293,0.0162166881	C,0,5.9212276939,0.6396726186,0.0515693955
C,0,5.01739784,-0.4395331939,0.4029738925	C,0,5.0431524514,-0.3853820176,0.3944821075
C,0,5.5479727503,1.5477804201,-0.9135532806	C,0,5.5494669158,1.655322559,-0.8452960213
H,0,5.3001790417,-1.2014797359,1.1201642956	H,0,5.3300238775,-1.1685438259,1.0861300327
C,0,3.7388942931,-0.431845979,-0.1620137624	C,0,3.7701120041,-0.3798592885,-0.1809060401
C,0,4.2763172631,1.5723566464,-1.4885807661	C,0,4.2832319818,1.6787836749,-1.4303196123
H,0,3.9946299282,2.3344259931,-2.2054709397	H,0,3.9969374042,2.4621595777,-2.1223390832
C,0,3.3916759289,0.5739019238,-1.0968965252	C,0,3.4133655518,0.6520194021,-1.0826517729
C,0,1.7186527431,-0.8203102762,-0.741806979	C,0,1.7660827678,-0.7861114205,-0.7890476428
N,0,2.6661095098,-1.292893288,0.0401852659	N,0,2.7125639316,-1.2668513357,-0.0182266796
N,0,2.0781949894,0.2914585255,-1.450116596	N,0,2.1066948204,0.3577517299,-1.4575228703
H,0,1.4828919111,0.7857340197,-2.0977732652	H,0,1.5049423946,0.8583376136,-2.0926709841
N,0,0.4728856927,-1.3755316779,-0.8548150735	N,0,0.5310402978,-1.3644475456,-0.9301915574
N,0,-0.4380505558,-0.830910255,-1.6778386238	N,0,-0.3938667594,-0.8165563383,-1.7337204926
C,0,-1.6039665565,-1.4014171911,-1.7426876638	C,0,-1.5423355539,-1.4169171882,-1.822520016
H,0,-1.8241215275,-2.2875708296,-1.1426187319	H,0,-1.7335201328,-2.3317660604,-1.2542365378
H,0,0.2726520497,-2.204198369,-0.3003978937	H,0,0.3543514906,-2.2148275341,-0.401610761
H,0,6.2693062453,2.3078358846,-1.1904480017	H,0,6.2599125233,2.4367886556,-1.088586803
C,0,-2.6474565384,-0.9018525737,-2.5930613567	C,0,-2.6071217461,-0.9244657432,-2.6510127535
C,0,-3.9018393402,-1.5785171468,-2.6012577946	C,0,-3.8323353642,-1.651024445,-2.6865682084
C,0,-2.4632961383,0.2199458781,-3.4405776184	C,0,-2.4715991175,0.2368779265,-3.4493842946
C,0,-4.9343685745,-1.1475364737,-3.3862505112	C,0,-4.8829937701,-1.2303715907,-3.4525581649
C,0,-3.486932447,0.6596695803,-4.2361296565	C,0,-3.518557377,0.6704824185,-4.220915035
C,0,-4.8065174913,0.0679895543,-4.1338258207	C,0,-4.810903245,0.0225116016,-4.1396959687
H,0,6.9081958448,0.5725285777,0.4407077716	H,0,6.9147283564,0.6565832582,0.4849264576
H,0,-5.883978754,-1.6694992968,-3.4085645789	H,0,-5.8110506869,-1.7875354317,-3.4967854603
H,0,-4.025709888,-2.4638205245,-1.9878788208	H,0,-3.9187337212,-2.5649211732,-2.1093568197
O,0,-3.3066717503,1.6949512027,-5.0893817911	O,0,-3.3880332907,1.7485376843,-5.024756001
H,0,-4.133948784,1.8536332827,-5.5682240283	H,0,-4.2311575143,1.8880648212,-5.4821862945
O,0,-5.6587834391,1.3458134926,-3.0201697496	O,0,-5.7424835495,1.1988663261,-2.9927754806
O,0,-5.597891526,0.3409193431,-5.2110360367	O,0,-5.6272147471,0.308436481,-5.2055108088
H,0,-6.5024491283,0.0384472817,-5.0565679068	H,0,-6.5506916131,0.2214912106,-4.9323830798
H,0,-1.5024806551,0.7161010228,-3.4866985222	H,0,-1.5321209203,0.7727638836,-3.478725147
O,0,-5.1915355949,1.3666906613,-1.6905437792	O,0,-5.3624998535,1.1219760972,-1.6449877463
H,0,-4.4502374704,1.9920715213,-1.7175139991	H,0,-4.6813101602,1.8077540085,-1.5648712458

TS C19(•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.34539648 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209490 a.u. 1 imaginary frequency = 489.2165 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1060.9178658 a.u.	**TS C19(•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.37059766 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208818 a.u. 1 imaginary frequency = 436.8758 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1060.9438113 a.u.
0, 2 C,0,6.1156681026,0.7459111088,0.2341557773 C,0,5.269610659,-0.318855861,0.5324974125 C,0,5.6869352827,1.8244148095,-0.5563268158 H,0,5.5988389746,-1.1516591614,1.1421353313 C,0,3.9703637495,-0.2891552499,0.0219206794 C,0,4.3931439851,1.8732742573,-1.075441291 H,0,4.0639173367,2.7065918805,-1.6854815806 C,0,3.5556432748,0.8068262877,-0.7726917828 C,0,1.9466401982,-0.6823331784,-0.5169633018 N,0,2.9353656849,-1.2059913283,0.162295466 N,0,2.2346921264,0.5201232081,-1.1059730024 H,0,1.5908748255,1.0563819898,-1.6649429528 N,0,0.7137900055,-1.2703405234,-0.6461364623 N,0,-0.2636904423,-0.6729194876,-1.3497181687 C,0,-1.401519982,-1.2855338028,-1.4392306231 H,0,-1.5503616922,-2.2524858852,-0.9489328574 H,0,0.5779164244,-2.1605629936,-0.1754586264 H,0,6.3736879915,2.6356243117,-0.7682348523 C,0,-2.5209866881,-0.7433747695,-2.1663454732 C,0,-3.7621191783,-1.4849603906,-2.1481872291 C,0,-2.4753386672,0.4945224013,-2.8175360528 C,0,-4.810519452,-1.0765222483,-3.0355961239 C,0,-3.5656662402,0.9465504278,-3.539436619 C,0,-4.7368045972,0.1356949246,-3.6549673615 H,0,7.1289569306,0.7447809975,0.6193201451 H,0,-5.6974271459,-1.6934175842,-3.1260133519 H,0,-3.7038386909,-2.5416300566,-1.9096359022 O,0,-3.518190654,2.1476557445,-4.1612853086 H,0,-4.3644028805,2.2999357585,-4.6050360653 O,0,-4.4382636346,-1.1818923737,-0.451335763 O,0,-5.7120591196,0.683197455,-4.4484585101 H,0,-6.5319597518,0.1839359857,-4.3728527077 H,0,-1.5804458259,1.1020161688,-2.7839124739 O,0,-4.8663345289,0.1504513277,-0.314424275 H,0,-4.0890809505,0.5969754196,0.0549155029	0, 2 C,0,6.1054200344,0.7598996901,0.1941079807 C,0,5.280331091,-0.3253075101,0.4868765374 C,0,5.6436168215,1.8483809095,-0.5651114364 H,0,5.6400476749,-1.1635803574,1.0724639893 C,0,3.9695490878,-0.3045551441,0.0026912448 C,0,4.3375024234,1.8874789819,-1.057115718 H,0,3.9795992134,2.7257172845,-1.6430716657 C,0,3.521980416,0.8016729658,-0.7599734979 C,0,1.9342344359,-0.7121970163,-0.5109567783 N,0,2.9491093136,-1.2392842706,0.1416136891 N,0,2.2015388898,0.5042508045,-1.0742608036 H,0,1.5449840597,1.0530706007,-1.6088202064 N,0,0.7090265065,-1.3072255611,-0.6322958159 N,0,-0.2738991648,-0.6966548359,-1.3217388779 C,0,-1.4109084536,-1.3103676891,-1.4159519226 H,0,-1.5591271684,-2.2856454435,-0.9461645582 H,0,0.5758018856,-2.2134692389,-0.1915608488 H,0,6.3132881059,2.6746371161,-0.7738629306 C,0,-2.5248355011,-0.7491431327,-2.1387821262 C,0,-3.7728641978,-1.4824241925,-2.1350786014 C,0,-2.4644204875,0.4902518453,-2.785002132 C,0,-4.8147446616,-1.0620766636,-3.0250296739 C,0,-3.5450005082,0.948984536,-3.5184483122 C,0,-4.7243540629,0.1466382272,-3.6519190864 H,0,7.1262765423,0.7655319278,0.559066177 H,0,-5.6996722206,-1.6771996563,-3.1373458291 H,0,-3.7213396087,-2.5413313489,-1.9056258677 O,0,-3.4783048082,2.1480234302,-4.1422574314 H,0,-4.3073913757,2.3038022427,-4.6190723703 O,0,-4.4391195369,-1.1906044502,-0.4201619136 O,0,-5.6729316846,0.6965804763,-4.463309694 H,0,-6.4671285416,0.1490435003,-4.4963463299 H,0,-1.5640503493,1.0899062915,-2.7437253633 O,0,-4.810729746,0.1622369856,-0.2354613799 H,0,-3.9954156541,0.5805607053,0.0827788031

TS C19(•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.35624856 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209209 a.u. 1 imaginary frequency = 469.4922 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1060.9290135 a.u.	
0, 2 C,0,6.1239995456,0.7423112057,0.1951718336 C,0,5.2822912606,-0.3232662684,0.5063663878 C,0,5.6822272388,1.8220435571,-0.5870698418	

H,0,5.6237641379,-1.1559852255,1.109773722 C,0,3.9743632192,-0.2926543487,0.0171377561 C,0,4.3794406162,1.8715062159,-1.084534851 H,0,4.0386585518,2.704561116,-1.6883126039 C,0,3.5468102276,0.8045378546,-0.7691177601 C,0,1.9391143753,-0.6828491935,-0.4926492979 N,0,2.9405873298,-1.2093142652,0.1718417458 N,0,2.2216454893,0.5196784583,-1.0817555344 H,0,1.5729488702,1.0600492691,-1.6322629784 N,0,0.7045535775,-1.2664161204,-0.6052372529 N,0,-0.2729582212,-0.6664503443,-1.3090380982 C,0,-1.4086943134,-1.282237716,-1.4053225933 H,0,-1.5563506423,-2.2535606834,-0.9251063307 H,0,0.5705909492,-2.1655162839,-0.1508073633 H,0,6.3655224064,2.6333867686,-0.8096002718 C,0,-2.5236123087,-0.735873455,-2.1369375024 C,0,-3.7599755164,-1.486819561,-2.1478037499 C,0,-2.4762588547,0.5088662067,-2.774667869 C,0,-4.7971212076,-1.0772335957,-3.048115412 C,0,-3.5570936972,0.9584403334,-3.5124394461 C,0,-4.7208259644,0.1394908754,-3.6594820304 H,0,7.1435304052,0.7401729497,0.5636791192 H,0,-5.6754657543,-1.7015647566,-3.1643632224 H,0,-3.6965026723,-2.5457995978,-1.9213324832 O,0,-3.5064001915,2.165225081,-4.1229751671 H,0,-4.3427881124,2.31616098,-4.5868081229 O,0,-4.4607354328,-1.2105114578,-0.4512827819 O,0,-5.6786568146,0.6844398258,-4.4701461868 H,0,-6.4881879773,0.1616109339,-4.4482986897 H,0,-1.5864249934,1.1224410905,-2.7199832365 O,0,-4.894521422,0.1213032833,-0.2933238582 H,0,-4.1156492041,0.5696038083,0.0709851118	

TS C1(•OOCH$_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.65474526 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234144 a.u. 1 imaginary frequency = 509.8826 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2066818 a.u.	**TS C1(•OOCH$_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.67867657 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234030 a.u. 1 imaginary frequency = 469.7309 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2320136 a.u.
0, 2 C,0,6.0492466695,0.8217361215,-0.1301917517 C,0,5.2013255229,-0.2307737039,0.2652744432 C,0,5.6473407552,1.7896989003,-1.0330026518 H,0,5.5272209432,-0.9854553153,0.970075901 C,0,3.9160154039,-0.2845505951,-0.2953051428 C,0,4.2964492358,1.8402144238,-1.5553468398 H,0,4.1639708449,2.2803985558,-2.5409158134 C,0,3.5107037769,0.6955229916,-1.2078346401 C,0,1.9218436303,-0.7839310419,-0.8523953531 N,0,2.9000078542,-1.2118282371,-0.0942755013 N,0,2.219491059,0.3537371692,-1.5590702084 H,0,1.5617602844,0.8812558403,-2.1119983465 N,0,0.7071006559,-1.4105200284,-0.9710535039 N,0,-0.2798162847,-0.8551991125,-1.7088390638 C,0,-1.4306810342,-1.4246198289,-1.7042437227 H,0,-1.6048382791,-2.3268493116,-1.1069078818 H,0,0.5407210891,-2.2058553911,-0.3620979709 H,0,6.3356671166,2.5674424377,-1.3407727674 C,0,-2.5646386011,-0.9254028473,-2.4763254721 C,0,-3.7895034666,-1.599653979,-2.3918285197 C,0,-2.4650818396,0.2087755411,-3.2998540783 C,0,-4.8957838491,-1.1529929922,-3.11263559 C,0,-3.5610003097,0.655021122,-4.0169243636 C,0,-4.7851229476,-0.0315128945,-3.9214955828 H,0,7.0577757475,0.8592548775,0.2670001028 H,0,-5.8430832597,-1.6789164364,-3.0436257882 H,0,-3.8829554713,-2.4768564734,-1.7616943293 O,0,-3.4481766744,1.7553417877,-4.8110412649 H,0,-4.3033335858,1.9253822929,-5.2269399748 O,0,3.4570791907,3.2595319862,-0.868162164 H,0,-1.5305962713,0.7479560822,-3.3822761703 O,0,-5.8081533795,0.494210142,-4.6742926739 H,0,-6.6183093264,-0.0098436023,-4.5489089745 O,0,3.2265280565,3.1179469625,0.5143213414 C,0,4.1272574402,3.9667861996,1.2183676807 H,0,3.8552798847,3.8570783483,2.2707992562 H,0,5.1629934918,3.6509981926,1.0661664197 H,0,4.0009157266,5.007399566,0.9056821609	0, 2 C,0,6.0185385738,0.7990113924,-0.1797344877 C,0,5.1695921231,-0.2420369605,0.2539601035 C,0,5.5940052224,1.771431649,-1.0642600612 H,0,5.520818325,-0.9994217614,0.9442031521 C,0,3.8635415514,-0.281856218,-0.2570818429 C,0,4.219544989,1.8437952891,-1.5231410651 H,0,4.0424021596,2.2950511433,-2.4960387849 C,0,3.4335074289,0.704319253,-1.1532308112 C,0,1.848733775,-0.7800987523,-0.7739040276 N,0,2.8498066535,-1.2096252737,-0.0344696104 N,0,2.1337376328,0.3678680117,-1.4693047699 H,0,1.4897095977,0.8516620989,-2.0780652044 N,0,0.6351231909,-1.3955907792,-0.8764658459 N,0,-0.3379490881,-0.8461067423,-1.6472938021 C,0,-1.4765017133,-1.4403242236,-1.684633867 H,0,-1.6519586959,-2.3546023066,-1.1103163266 H,0,0.4733581223,-2.2319788773,-0.3237445777 H,0,6.2800840854,2.5385638904,-1.4015190509 C,0,-2.5935445081,-0.942149062,-2.482465296 C,0,-3.8058953798,-1.6445551209,-2.4586790834 C,0,-2.4919911267,0.2184225651,-3.2710641846 C,0,-4.898406952,-1.2030264454,-3.2038745502 C,0,-3.5748916667,0.6586343359,-4.0108135198 C,0,-4.7881122616,-0.0555033245,-3.9782053478 H,0,7.0428580169,0.8196220686,0.1752035987 H,0,-5.834962085,-1.7497810533,-3.1835578939 H,0,-3.8999444777,-2.5405990931,-1.856079837 O,0,-3.4622915855,1.7877894275,-4.7718072017 H,0,-4.3070261624,1.9502952096,-5.2144069447 O,0,3.4508496095,3.2696663814,-0.7626396302 H,0,-1.56674576,0.7797461565,-3.3065570709 O,0,-5.7923579008,0.4677679929,-4.7465051154 H,0,-6.5981237025,-0.0571983144,-4.6702393279 O,0,3.4017048806,3.1646853871,0.6488156715 C,0,4.3733384929,4.0471156183,1.2122764629 H,0,4.2501675962,3.9518219151,2.2932641887 H,0,5.3838634907,3.7491363371,0.9238889366 H,0,4.1810373488,5.0789759357,0.9059182247

TS C1(•OOCH$_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.66484695 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234470 a.u. 1 imaginary frequency = 494.5578 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2173231 a.u.	**TS C2(•OOCH$_3$),** optimization in gas phase UB3LYP/6-311++G**, E= -1100.65465258 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.233540 a.u. 1 imaginary frequency = 488.3830 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.206182 a.u.
0, 2	0, 2

C,0,6.0345247518,0.8189763035,-0.1243263896	C,0,5.8560311468,0.285687128,0.1651290541
C,0,5.1839699771,-0.22682868,0.2872356487	C,0,5.0011974667,-0.7678469477,0.3470128294
C,0,5.632245445,1.7765730106,-1.0368133226	C,0,5.4368685069,1.5199396501,-0.4788760547
H,0,5.5131477872,-0.9732597925,0.9994916253	H,0,5.3060424507,-1.663285262,0.8752935602
C,0,3.8974979482,-0.2856853965,-0.2698448512	C,0,3.6991230273,-0.679217553,-0.1932547898
C,0,4.2780570749,1.8254977659,-1.5526668643	C,0,4.1675271062,1.5356021113,-1.1627267701
H,0,4.1404734344,2.2559535,-2.5416129084	H,0,3.8890443152,2.3915087004,-1.7651869949
C,0,3.4901185047,0.6857660477,-1.1915136988	C,0,3.3251211553,0.4752030433,-0.9433140628
C,0,1.9038738877,-0.7980101147,-0.8312069138	C,0,1.7052187779,-1.0280299623,-0.8538942112
N,0,2.8835031309,-1.2150059215,-0.0636908537	N,0,2.6711010931,-1.591406846,-0.1565965184
N,0,2.2015476424,0.3367870379,-1.5421601425	N,0,2.020181528,0.2024555117,-1.360267234
H,0,1.5521550019,0.8409951845,-2.1268542224	H,0,1.3980746083,0.7751075591,-1.9074529927
N,0,0.6943750258,-1.427683983,-0.9552931345	N,0,0.4886548509,-1.6091570957,-1.0650734046
N,0,-0.2874672229,-0.8698680841,-1.703760137	N,0,-0.4697903421,-0.9657228017,-1.7686171675
C,0,-1.4373184837,-1.4417276791,-1.7077926385	C,0,-1.6058745842,-1.5497456326,-1.9110539329
H,0,-1.6149275287,-2.3451223296,-1.1147938641	H,0,-1.7854709615,-2.537021716,-1.4708369162
H,0,0.5183351176,-2.2215527858,-0.3470046199	H,0,0.3312796097,-2.5179915232,-0.6395890411
H,0,6.3214575735,2.548501784,-1.3567985803	H,0,6.2267932011,2.120598974,-0.9207862723
C,0,-2.5667474486,-0.9375143966,-2.4836556643	C,0,-2.7136675586,-0.9534787718,-2.649052377
C,0,-3.7886513573,-1.6197124825,-2.4191752824	C,0,-3.9244378169,-1.6530457542,-2.7349851457
C,0,-2.4677102679,0.211176437,-3.2878634278	C,0,-2.6033290335,0.3011832601,-3.2729065597
C,0,-4.8932294617,-1.1672176782,-3.1392502147	C,0,-5.0064864347,-1.1129470844,-3.4275816014
C,0,-3.5622410721,0.6632333317,-4.0030674165	C,0,-3.6752300079,0.8404507326,-3.9611651473
C,0,-4.784801205,-0.0297065933,-3.9269101792	C,0,-4.8857767967,0.1272032813,-4.0379461124
H,0,7.0443505413,0.8575920723,0.269187392	H,0,6.8597659013,0.2501338882,0.5703472961
H,0,-5.837309431,-1.6999220433,-3.0873565059	H,0,-5.9431253466,-1.6581145565,-3.4912514493
H,0,-3.881081717,-2.5081116452,-1.8048638365	H,0,-4.0257564777,-2.6220102731,-2.2595338761
O,0,-3.4511652005,1.7799016372,-4.777731939	O,0,-3.5523902991,2.0567870636,-4.5597331668
H,0,-4.3069190405,1.9570645887,-5.1908712434	H,0,-4.3885747929,2.2758483883,-4.9911798085
O,0,3.4569584845,3.2593113597,-0.8684795824	O,0,5.3473907432,2.713037108,0.8649505695
H,0,-1.5359314105,0.7577600756,-3.3533864984	O,0,-5.8848459936,0.7519835886,-4.7437684941
O,0,-5.8045539123,0.5049132752,-4.6730700579	H,0,-6.6843927273,0.2162837696,-4.7535341431
H,0,-6.6231884808,0.0148245974,-4.5398458053	H,0,-1.6785780628,0.8605623088,-3.2224415245
O,0,3.2652697965,3.1483972954,0.5255512018	O,0,4.3997568064,2.3208725513,1.8344931592
C,0,4.1881480003,4.0100286429,1.1875529895	C,0,3.2808644389,3.1931814818,1.7504660052
H,0,3.9503393442,3.9170411054,2.2496346345	H,0,2.7745470479,3.0945351961,0.7851726248
H,0,5.2181508031,3.6920795759,1.0070183908	H,0,2.6117207519,2.8786936699,2.5553732544
H,0,4.0503637677,5.0454827271,0.8634201124	H,0,3.5862625525,4.2326309642,1.9046674862

TS C2(•OOCH$_3$), optimization in solv. water UB3LYP/6-311++G**, E= -1100.68133840 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234192 a.u. 1 imaginary frequency = 418.3103 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.234085 a.u.	**TS C2(•OOCH$_3$),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.66588625 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234167 a.u. 1 imaginary frequency = 461.6088 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2179875 a.u.
0, 2	0, 2
C,0,5.8567756602,0.2731333705,0.1426467393	C,0,5.8594043268,0.2875396659,0.1485777982
C,0,5.0100878595,-0.7884678502,0.3266516873	C,0,5.0099286592,-0.7709144744,0.3310594904
C,0,5.4194915052,1.5150546271,-0.4797858996	C,0,5.4293763236,1.5251217083,-0.4834085422
H,0,5.3370002985,-1.6912415506,0.8299773299	H,0,5.3254777337,-1.6690054105,0.8489080533
C,0,3.6960486143,-0.6993714354,-0.1880810061	C,0,3.7022059009,-0.6835739228,-0.1970389148
C,0,4.134217978,1.5314779895,-1.1379154542	C,0,4.1536675386,1.5393355298,-1.1570304104
H,0,3.8375969996,2.3887223785,-1.7288966119	H,0,3.8655883819,2.3962551816,-1.7532959864
C,0,3.3028365917,0.4649056131,-0.9185681202	C,0,3.3179852724,0.4743820874,-0.9384432633

C,0,1.6881589347,-1.0455521833,-0.8299761823	C,0,1.7018475414,-1.0336024851,-0.847470015
N,0,2.6764468355,-1.6160851133,-0.148602118	N,0,2.6785079839,-1.5989219479,-0.1581153386
N,0,1.9973189826,0.190245871,-1.3206364383	N,0,2.0125364449,0.199527585,-1.3475766704
H,0,1.3688192381,0.776116689,-1.8493866209	H,0,1.38729967,0.7755070502,-1.888939054
N,0,0.4784789461,-1.6220924557,-1.0298213659	N,0,0.4876335666,-1.6126252776,-1.0520728137
N,0,-0.4772702393,-0.9666056929,-1.7403279445	N,0,-0.4694664495,-0.9640753389,-1.7595058605
C,0,-1.607830243,-1.5590798634,-1.8955368087	C,0,-1.6061972127,-1.5474816054,-1.8999704686
H,0,-1.7864424197,-2.5504147311,-1.4694930253	H,0,-1.7889479823,-2.5322366757,-1.4575279313
H,0,0.3168946898,-2.5438864321,-0.6335098388	H,0,0.3273847968,-2.5257152548,-0.6364754374
H,0,6.2000871007,2.1118454589,-0.944318833	H,0,6.2136861221,2.1291415564,-0.9311110739
C,0,-2.7095077119,-0.9568209301,-2.6378025241	C,0,-2.7110504841,-0.9496844409,-2.6412580305
C,0,-3.913019321,-1.6659702696,-2.7518375324	C,0,-3.9255175122,-1.6439123252,-2.720503999
C,0,-2.6011261147,0.3100523409,-3.2406159216	C,0,-2.5947090672,0.299874773,-3.2754247793
C,0,-4.9908792832,-1.127151358,-3.4520746388	C,0,-5.0060478259,-1.1047638223,-3.4162633473
C,0,-3.6693812554,0.8466622878,-3.935878194	C,0,-3.6651057979,0.8375720055,-3.9668377425
C,0,-4.8739795535,0.1241049113,-4.0440786479	C,0,-4.8802603357,0.130115909,-4.0378371298
H,0,6.8737778698,0.2283313963,0.5135699722	H,0,6.8687015373,0.2498104781,0.5398659503
H,0,-5.9209468003,-1.6784544293,-3.537948827	H,0,-5.9453479634,-1.6450394186,-3.4744776959
H,0,-4.0112786848,-2.642631488,-2.2923344393	H,0,-4.0307225097,-2.6083054847,-2.2369090104
O,0,-3.5515055852,2.0769780094,-4.5166756616	O,0,-3.5372732784,2.0498029537,-4.5768114124
H,0,-4.383692724,2.2935461693,-4.9599769738	H,0,-4.3724156284,2.2688460244,-5.0116071023
O,0,5.3711919298,2.7051344043,0.865938051	O,0,5.3494892418,2.7108942935,0.868522991
O,0,-5.8626407441,0.7474002391,-4.7534619709	O,0,-5.8742370431,0.7527739155,-4.7472037318
H,0,-6.6566507939,0.2013091275,-4.8010291554	H,0,-6.6758444216,0.2183664678,-4.7631192691
H,0,-1.6814869837,0.8768076612,-3.1674496748	H,0,-1.6665755234,0.8545850008,-3.2307776165
O,0,4.3928368836,2.3577744628,1.8391482177	O,0,4.3956648759,2.3203203597,1.8393233093
C,0,3.2881170189,3.2511641758,1.7169881187	C,0,3.272673965,3.189547609,1.7478568629
H,0,2.7996507197,3.1426116196,0.7455060061	H,0,2.7739452183,3.0887515109,0.7796269065
H,0,2.5981113231,2.9637783044,2.5139742138	H,0,2.599159181,2.8722616282,2.5477802725
H,0,3.6085323284,4.2871368258,1.8619201633	H,0,3.5723946031,4.229992741,1.9057910829

TS C4(•OOCH$_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.65426226 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234001 a.u. 1 imaginary frequency = 518.7530 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2059642 a.u.	**TS C4(•OOCH$_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.68110710 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234434 a.u. 1 imaginary frequency = 455.0144 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2337661 a.u.
0, 2	0, 2
C,0,5.9769365424,0.6081272314,0.0926124182	C,0,5.9392915736,0.6467753868,0.0553983918
C,0,5.0525397966,-0.3986257079,0.5622829614	C,0,5.0285371965,-0.3637340138,0.5485165725
C,0,5.5727617294,1.6494637904,-0.7201167154	C,0,5.5155240728,1.6780510259,-0.7569041659
H,0,5.4524253616,-1.3617964408,0.8630326008	H,0,5.4438328613,-1.3313349622,0.8155794714
C,0,3.7695213161,-0.3899239563,-0.0864592991	C,0,3.7230075403,-0.3491591189,-0.0584850031
C,0,4.2601175265,1.7286608815,-1.2354315268	C,0,4.1886624955,1.7523934181,-1.2467558176
H,0,3.9600652869,2.5476786304,-1.8778676066	H,0,3.8737328219,2.5614924867,-1.8938586296
C,0,3.3960891981,0.6894805875,-0.9051732387	C,0,3.3316390948,0.7208574008,-0.8843708983
C,0,1.7708171283,-0.7849667963,-0.690312724	C,0,1.7025670336,-0.7455024106,-0.6213772825
N,0,2.7469628047,-1.298898491,0.0298572328	N,0,2.7011335796,-1.2524102094,0.093932715
N,0,2.083890642,0.4043950004,-1.2818856956	N,0,2.0121808442,0.4344811831,-1.2271172925
H,0,1.4586807311,0.9434182844,-1.8592329203	H,0,1.3903832675,0.9617239593,-1.8218067642
N,0,0.5513476438,-1.3841476387,-0.8512453554	N,0,0.4853333951,-1.3358500495,-0.7524197003
N,0,-0.4193376255,-0.7821314845,-1.572324057	N,0,-0.4733669953,-0.746382186,-1.5125981444
C,0,-1.5741569156,-1.3438858526,-1.6171988461	C,0,-1.6163182808,-1.3302925077,-1.5848217083
H,0,-1.7626712396,-2.2767930241,-1.0742029612	H,0,-1.8051952047,-2.2643025396,-1.0479314471

H,0,0.3810290944,-2.2285096449,-0.3130451712	H,0,0.3190260406,-2.2065550444,-0.2561438389
H,0,6.286905692,2.4176030194,-0.9954963128	H,0,6.2222302079,2.443729385,-1.0563631325
C,0,-2.6927575076,-0.7919626658,-2.374194704	C,0,-2.7194256012,-0.7928492957,-2.3745296643
C,0,-3.9290376587,-1.4494993806,-2.3315996978	C,0,-3.942382498,-1.4773639605,-2.3788064001
C,0,-2.5684783826,0.3791939876,-3.1409963261	C,0,-2.5940948535,0.3886517491,-3.1282438575
C,0,-5.022420289,-0.9491371141,-3.0363712105	C,0,-5.0229129464,-0.997096282,-3.1169443486
C,0,-3.6515316132,0.8787656011,-3.8418497237	C,0,-3.6648054355,0.8668432622,-3.8615790465
C,0,-4.8876247421,0.2091855005,-3.7878483451	C,0,-4.8894085585,0.1708381759,-3.8567794934
H,0,6.9991568388,0.5656634737,0.4489754261	H,0,6.9706532411,0.6063176643,0.3843539891
H,0,-5.9787467434,-1.4617037049,-2.9995306562	H,0,-5.9680305262,-1.5291381457,-3.1174300177
H,0,-4.0416297391,-2.3544453546,-1.7454179655	H,0,-4.0540800234,-2.3888567833,-1.8030788293
O,0,-3.5146743562,2.0148887134,-4.5800630041	O,0,-3.5298248307,2.0148881409,-4.5893050001
H,0,-4.362451525,2.2168015514,-4.9969160982	H,0,-4.3678997584,2.2015425832,-5.0351025648
O,0,4.731347092,-0.0288432975,2.2991284902	O,0,4.7681999537,-0.0464469375,2.3134457488
H,0,-1.623838239,0.9042406212,-3.1924319246	H,0,-1.6595123906,0.9351472498,-3.1421791206
O,0,-5.896016723,0.7887214247,-4.5198944377	O,0,-5.879152756,0.7321725416,-4.6156318839
H,0,-6.7138229008,0.2892038549,-4.4309632535	H,0,-6.6921631962,0.2150183488,-4.567282089
O,0,4.0778897545,1.2055779411,2.458421742	O,0,4.2036620297,1.2297861637,2.5569614074
C,0,4.9902964077,2.1330457169,3.0361117055	C,0,5.2101467257,2.0842062392,3.1005172022
H,0,5.358807685,1.7631550606,3.9975387388	H,0,5.6109896335,1.66655179,4.028452768
H,0,5.8298275827,2.3282339915,2.3631539371	H,0,6.0159613428,2.2455234924,2.3808910125
H,0,4.4112679258,3.0476089807,3.1859209542	H,0,4.7013664838,3.0281260901,3.3087632923

TS C4(•OOCH$_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.66540717 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234225 a.u. 1 imaginary frequency = 495.9406 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.217469 a.u.	**TS C6(•OOCH$_3$),** optimization in gas phase UB3LYP/6-311++G**, E= -1100.65908086 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235121 a.u. 1 imaginary frequency = 518.4392 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.210566 a.u.
0, 2	0, 2
C,0,5.9621415802,0.622139975,0.0786407498	C,0,6.1570712196,0.5963153303,-0.0820940502
C,0,5.0428022001,-0.3859435499,0.5572300859	C,0,5.3360876713,-0.4886588553,0.1736532488
C,0,5.5508051383,1.6598773996,-0.7338588432	C,0,5.6680112541,1.7475610553,-0.7361362985
H,0,5.4487071908,-1.3510897951,0.8443951883	H,0,5.6999599288,-1.3745922594,0.679591817
C,0,3.7505412183,-0.3738500591,-0.0742363597	C,0,3.9924062065,-0.4186631351,-0.2435494357
C,0,4.2325060891,1.7377139086,-1.2390279643	C,0,4.3433313716,1.8464420411,-1.1618001441
H,0,3.9267781597,2.553166457,-1.8830865839	H,0,3.9807386015,2.7352449821,-1.6640966977
C,0,3.3704940757,0.7023029785,-0.8957405183	C,0,3.5199360872,0.7549670521,-0.9171622659
C,0,1.742887985,-0.7681823999,-0.6618399964	C,0,1.8788228982,-0.7181279848,-0.608322253
N,0,2.7281416882,-1.2802913394,0.0557578244	N,0,3.0057448677,-1.3338725544,-0.1106072584
N,0,2.0552684087,0.4173897694,-1.2588632521	N,0,2.2056443032,0.4933307816,-1.2196793516
H,0,1.4312884196,0.9531484907,-1.8417510709	H,0,1.5066592855,1.1388194678,-1.5509710244
N,0,0.5240438534,-1.3629285747,-0.8109878118	N,0,0.8833678699,-1.5126948357,-1.1649688638
N,0,-0.4403898718,-0.7664503402,-1.5508441831	N,0,-0.1735320863,-0.8369516093,-1.7152900679
C,0,-1.5918861538,-1.3345907537,-1.604049283	C,0,-1.287528903,-1.4593245482,-1.8079330547
H,0,-1.7828694354,-2.264521575,-1.0584572281	H,0,-1.3993114005,-2.4742871634,-1.4095638799
H,0,0.3520319477,-2.2145851761,-0.284856389	H,0,0.6662364891,-2.3179195101,-0.5786378635
H,0,6.2624843059,2.4267531034,-1.0187824329	H,0,6.3416672513,2.5778773447,-0.9141062326
C,0,-2.7036784731,-0.7903450604,-2.3766316136	C,0,-2.4703936675,-0.8738457944,-2.4377696075
C,0,-3.9350101113,-1.4583697958,-2.351376596	C,0,-3.6680543201,-1.5986169915,-2.4361015994
C,0,-2.5785070653,0.3827640483,-3.1413565475	C,0,-2.4397378705,0.3948535853,-3.0395712216
C,0,-5.0234900399,-0.9674741033,-3.0704152854	C,0,-4.8176559555,-1.0685743493,-3.0199866878
C,0,-3.656801761,0.8725176651,-3.8559404513	C,0,-3.5783427241,0.9246964042,-3.620153375
C,0,-4.8891481591,0.1934157531,-3.8193205066	C,0,-4.7755444342,0.1869757143,-3.6084059087

H,0,6.9881529658,0.5796031947,0.4239925766	H,0,7.1954971168,0.569154359,0.2266406405
H,0,-5.9753707376,-1.4881134263,-3.0477353113	H,0,-5.7451200818,-1.6330648329,-3.0157552384
H,0,-4.0473580336,-2.3647742318,-1.7675608542	H,0,-3.7067822682,-2.5794003533,-1.9759363724
O,0,-3.5202939164,2.0118004923,-4.5926993087	O,0,-3.533261271,2.1567340432,-4.2007944446
H,0,-4.3649791339,2.2082264342,-5.0197549474	H,0,-4.4098617959,2.3656922855,-4.548563329
O,0,4.7444530932,-0.040437633,2.3074299592	O,0,1.1096093379,-0.0751645486,0.9338428616
H,0,-1.6376550651,0.9161777629,-3.1791035435	H,0,-1.5237632521,0.9704997878,-3.0556703689
O,0,-5.8903306305,0.7652059074,-4.5619616011	O,0,-5.8465430446,0.8033871762,-4.2121100639
H,0,-6.709789608,0.26508988,-4.4809481082	H,0,-6.631861851,0.2497037629,-4.1592792612
O,0,4.1277734354,1.2119312637,2.5046667933	O,0,0.4946391232,-1.1442619384,1.5949059756
C,0,5.081539156,2.110319718,3.0652335786	C,0,1.2921473314,-1.5170028784,2.7196788206
H,0,5.4694678241,1.7204879675,4.0108368174	H,0,1.4198532812,-0.6636718389,3.3906756534
H,0,5.9039496948,2.2927532564,2.3687700104	H,0,0.7316732222,-2.3100444058,3.2199922279
H,0,4.5307873458,3.0370056783,3.2431994375	H,0,2.2649337381,-1.8854124062,2.383947195

TS C6(•OOCH$_3$), optimization in solv. water UB3LYP/6-311++G**, E= -1100.68070929 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234529 a.u. 1 imaginary frequency = 477.0433 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2329851 a.u.	**TS C6(•OOCH$_3$),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.66799883 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234773 a.u. 1 imaginary frequency = 505.9014 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2197838 a.u.
0, 2	0, 2
C,0,6.1938866907,0.5302560639,-0.1124424346	C,0,6.1705117233,0.5753475799,-0.0986530095
C,0,5.3503139762,-0.5273804202,0.1748854338	C,0,5.343207988,-0.501810506,0.1669774044
C,0,5.726896166,1.6810602718,-0.7908320572	C,0,5.6859342276,1.7293330814,-0.7542745709
H,0,5.699396838,-1.4089922051,0.6987971659	H,0,5.7045974873,-1.3881147893,0.6741675733
C,0,4.0028072906,-0.4310826468,-0.2345026606	C,0,3.996326914,-0.4215651841,-0.2418400115
C,0,4.4023661836,1.8072903995,-1.2067591856	C,0,4.3594753179,1.8390353141,-1.1704901973
H,0,4.0561055597,2.692033755,-1.7263167458	H,0,3.9996425544,2.7285678992,-1.6730817892
C,0,3.5531491875,0.7420396489,-0.9290173926	C,0,3.528627716,0.7548038256,-0.91564703
C,0,1.876004065,-0.6828556361,-0.5827707236	C,0,1.8765229332,-0.703762275,-0.5951511533
N,0,2.9960564436,-1.3176178428,-0.0792739521	N,0,3.0035678888,-1.3281052561,-0.1022015147
N,0,2.2309954717,0.5116913753,-1.211224576	N,0,2.2105347306,0.5050412361,-1.2067493152
H,0,1.5626917392,1.1624765667,-1.5947068189	H,0,1.5216171893,1.1535085085,-1.5542566666
N,0,0.8753974758,-1.4695563396,-1.1266660654	N,0,0.8782766968,-1.4935141578,-1.1487013993
N,0,-0.1887540287,-0.7982344824,-1.6768709138	N,0,-0.1794775563,-0.8170291114,-1.7012775868
C,0,-1.2785285327,-1.4563886054,-1.8271285194	C,0,-1.2877123978,-1.4490886343,-1.808257618
H,0,-1.3598214813,-2.4950238234,-1.4916958782	H,0,-1.3921563556,-2.4695422414,-1.4238869527
H,0,0.6760589263,-2.3051824821,-0.579044716	H,0,0.6634059741,-2.3075212688,-0.5740551083
H,0,6.4213832136,2.4878411113,-0.993825213	H,0,6.3658339286,2.5527390563,-0.9400719747
C,0,-2.4686461175,-0.8774802358,-2.4477889847	C,0,-2.4720233009,-0.8682767455,-2.4390660866
C,0,-3.6209428885,-1.6658686293,-2.5612846984	C,0,-3.657120845,-1.6134869957,-2.466269318
C,0,-2.4930927951,0.4435956347,-2.9297507367	C,0,-2.4567904526,0.4134743361,-3.0147442956
C,0,-4.7788571488,-1.1524038892,-3.1437718696	C,0,-4.8094378332,-1.0930292531,-3.0535753864
C,0,-3.6405020962,0.9554694423,-3.5086652465	C,0,-3.5980019711,0.9329108791,-3.5992667391
C,0,-4.7930966223,0.1532991511,-3.6168374899	C,0,-4.7832566204,0.174738271,-3.6180075891
H,0,7.2339287539,0.4852386044,0.1879110922	H,0,7.2107968148,0.541191291,0.2028440654
H,0,-5.6695530775,-1.7652216115,-3.2297073199	H,0,-5.7262159949,-1.6735526857,-3.0711181362
H,0,-3.6167406533,-2.6856540826,-2.1941429587	H,0,-3.683717069,-2.6039209777,-2.0264177418
O,0,-3.6508008145,2.2400074994,-3.9736491204	O,0,-3.5683644398,2.1781346667,-4.1560433944
H,0,-4.5252335296,2.4315147699,-4.340509301	H,0,-4.4445253218,2.3792350688,-4.5112341176
O,0,1.1236693043,0.0237860891,0.957320786	O,0,1.1177765198,-0.0490464398,0.9542349275
H,0,-1.6150169626,1.0723832805,-2.852585011	H,0,-1.5517344289,1.0067380635,-3.007080194
O,0,-5.8699167993,0.7593072592,-4.2041308156	O,0,-5.8543058672,0.7840848124,-4.2222688222

H,0,-6.6253716528,0.1609201006,-4.2505521375	H,0,-6.6329152794,0.217185153,-4.1987601918
O,0,0.4481256572,-1.0052477424,1.6391300583	O,0,0.485316804,-1.1097373324,1.6184339094
C,0,1.2309684678,-1.4297471959,2.7576897156	C,0,1.281037986,-1.505201773,2.7376504539
H,0,1.4079834683,-0.5932525327,3.4390237725	H,0,1.4249173468,-0.6612732602,3.4171669085
H,0,0.6328098172,-2.1968483919,3.2534527909	H,0,0.7100214976,-2.2937986175,3.2325416847
H,0,2.1806240346,-1.8480698484,2.4161549475	H,0,2.2465490252,-1.8865891578,2.3963432039

TS C9(•OOCH$_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.65062248 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234930 a.u. 1 imaginary frequency = 417.7784 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2052453 a.u.	**TS C9(•OOCH$_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.67555895 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234745 a.u. 1 imaginary frequency = 344.6139 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2320522 a.u.
0, 2	0, 2
C,0,5.8316628099,0.1029201173,-0.4317570016	C,0,5.8251365294,0.0834459224,-0.4875203125
C,0,4.7779743088,-0.7978499157,-0.3042545232	C,0,4.7753848206,-0.8172881632,-0.3181726119
C,0,5.6337741435,1.4074982812,-0.9717449167	C,0,5.6041032905,1.3921113886,-1.014986225
H,0,4.9443374315,-1.8258792361,-0.0062136505	H,0,4.9595713157,-1.8483872442,-0.039204567
C,0,3.5035440829,-0.3707203983,-0.6525102964	C,0,3.4862064988,-0.3890616806,-0.6146292673
C,0,4.3907036956,1.8669004582,-1.316220356	C,0,4.348828848,1.856834191,-1.2987571053
H,0,4.2377932955,2.8453900634,-1.7552157029	H,0,4.1778981587,2.837316493,-1.726006717
C,0,3.2518709948,1.0506633937,-0.9554789936	C,0,3.219166566,1.0400349078,-0.8936790896
C,0,1.515675756,-0.2589253485,-1.3976482209	C,0,1.476196637,-0.2788689365,-1.3284748207
N,0,2.3612696604,-1.1052117371,-0.8495183219	N,0,2.3433937317,-1.1267260778,-0.7919770622
N,0,2.0198154901,0.9932256166,-1.6609378306	N,0,1.9755030622,0.9759176707,-1.5723690192
H,0,1.4081350442,1.7899628154,-1.7653977723	H,0,1.3792065139,1.7717106001,-1.7500581578
N,0,0.2448046392,-0.6030379331,-1.7324256526	N,0,0.2132176599,-0.6188989027,-1.6601195386
N,0,-0.6064483656,0.3056246747,-2.2627483533	N,0,-0.6241068568,0.3057210118,-2.2060771564
C,0,-1.8056044148,-0.0786412373,-2.5167677526	C,0,-1.8117003652,-0.0866878734,-2.5037516678
H,0,-2.1219101237,-1.1057382729,-2.3018677519	H,0,-2.1245582646,-1.1185792722,-2.321346114
H,0,-0.0487292818,-1.549214927,-1.5055964307	H,0,-0.0874663726,-1.5737641828,-1.4819559424
H,0,6.5013819053,2.0359915817,-1.1413392158	H,0,6.464650447,2.0184593331,-1.2230330241
C,0,-2.8101411762,0.8052363939,-3.0975395	C,0,-2.80357789,0.8032258895,-3.095211711
C,0,-4.1030865431,0.3114454427,-3.3137717956	C,0,-4.0767556149,0.294266381,-3.3852509818
C,0,-2.5166313051,2.1342405047,-3.4482426157	C,0,-2.5207548834,2.1507868724,-3.38546436
C,0,-5.0882399751,1.1267817379,-3.8675486049	C,0,-5.053952513,1.1092430069,-3.9533948244
C,0,-3.4921152539,2.9463364229,-3.9982027788	C,0,-3.4889656452,2.961363741,-3.9491003754
C,0,-4.7870826924,2.4375597752,-4.2086823284	C,0,-4.7657284784,2.4386266556,-4.2356754426
H,0,6.8373295905,-0.2094163703,-0.1757222532	H,0,6.8409482321,-0.2324867629,-0.2811115294
H,0,-6.0894007968,0.7411104891,-4.0334079225	H,0,-6.0380528011,0.7125337919,-4.1775873846
H,0,-4.3442562927,-0.7116691442,-3.0486256786	H,0,-4.307729111,-0.7420093082,-3.1674837816
O,0,-3.193633868,4.2312732765,-4.3339714967	O,0,-3.2029655662,4.2672239517,-4.2267871068
H,0,-3.9832781929,4.6459470963,-4.705109039	H,0,-3.9860599035,4.6828424527,-4.6140326313
O,0,2.6015097483,1.7269935472,0.5007194609	O,0,2.6185226768,1.6939014965,0.5699322394
O,0,-5.6781868877,3.3257264965,-4.7602037658	O,0,-5.6442504142,3.3261992147,-4.7907246565
H,0,-6.5401787203,2.9151915044,-4.8815344727	H,0,-6.5006075699,2.9137953566,-4.9568041882
H,0,-1.5241693406,2.5363823944,-3.2931760486	H,0,-1.5441258888,2.5660925852,-3.1710827258
O,0,3.5480095404,1.7662729504,1.5569142984	O,0,3.6160452386,1.8049283609,1.5876420081
C,0,3.8322948036,3.1282966906,1.8456809675	C,0,3.8705958071,3.1895861803,1.8145480061
H,0,4.5255882344,3.1000816725,2.6899095193	H,0,4.6029819743,3.2139412599,2.6247681741
H,0,4.3051656144,3.6250170651,0.9930433984	H,0,4.2865141396,3.6656614756,0.9231997282
H,0,2.9213592411,3.6633109581,2.1321496598	H,0,2.9581927911,3.7060651139,2.1267762024

TS C9(•$OOCH_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.66100323 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235159 a.u. 1 imaginary frequency = 390.0807 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2163617 a.u.	**TS C13(•$OOCH_3$),** optimization in gas phase UB3LYP/6-311++G**, E= -1100.67028212 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235096 a.u. 1 imaginary frequency = 469.7758 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2208945 a.u.
0, 2 C,0,5.8299320378,0.1020907502,-0.4450624427 C,0,4.7794618416,-0.801238836,-0.3051770542 C,0,5.6219365305,1.4070158841,-0.9829505769 H,0,4.9541140927,-1.8292253136,-0.0108643266 C,0,3.4993981964,-0.3779970022,-0.640564047 C,0,4.3739158427,1.8643337615,-1.3106490957 H,0,4.2130247532,2.8425595064,-1.7472489912 C,0,3.2391993379,1.0448541759,-0.9377058449 C,0,1.505357692,-0.2731932278,-1.3818280463 N,0,2.359990592,-1.1172110714,-0.8342611732 N,0,2.0058713276,0.9808015982,-1.637756977 H,0,1.3973483751,1.7755811598,-1.7723177188 N,0,0.2391934562,-0.617557247,-1.7187204708 N,0,-0.6065000811,0.2985677765,-2.2545008983 C,0,-1.8048299428,-0.0847431503,-2.5152087075 H,0,-2.1240303636,-1.1106367022,-2.3039504304 H,0,-0.0600173825,-1.5650915747,-1.5045415956 H,0,6.4861046701,2.0370638754,-1.1637328381 C,0,-2.8041397948,0.8029608043,-3.0987246652 C,0,-4.0952928942,0.3094848809,-3.3274613152 C,0,-2.5089837942,2.134994848,-3.4387535646 C,0,-5.0778201276,1.1270347976,-3.8827180056 C,0,-3.4820070121,2.9488190488,-3.989784098 C,0,-4.7762478121,2.4413577142,-4.2126095885 H,0,6.8393923371,-0.2082710214,-0.2019970703 H,0,-6.0770308157,0.7421273246,-4.058926507 H,0,-4.3369728279,-0.7155986885,-3.0708558032 O,0,-3.1827611578,4.2380743441,-4.3153365389 H,0,-3.9716717756,4.6564018906,-4.6855053098 O,0,2.5989827001,1.7132914889,0.5197800066 O,0,-5.6624323711,3.3312144062,-4.7617447513 H,0,-6.5296233001,2.9281045192,-4.8791818341 H,0,-1.5181389136,2.537441714,-3.2730867061 O,0,3.5589415781,1.7788348367,1.5678944571 C,0,3.8323369055,3.1494724506,1.8348967796 H,0,4.5353579338,3.1406136224,2.6712718895 H,0,4.2901608407,3.6380496082,0.9700821334 H,0,2.9193861259,3.6786939479,2.1248379864	0, 2 C,0,6.0085876753,0.6866550856,0.1498423803 C,0,5.1324414354,-0.3317906227,0.5082464811 C,0,5.6339336026,1.6918867831,-0.7591354271 H,0,5.4174443202,-1.1071907883,1.2088887219 C,0,3.8565687632,-0.3321012486,-0.0632752329 C,0,4.3679177631,1.7102995032,-1.3414783776 H,0,4.0823913867,2.4864073845,-2.041965891 C,0,3.4969540786,0.6890411064,-0.9788644709 C,0,1.8535689527,-0.7433676195,-0.65519171 N,0,2.8035984894,-1.2151011766,0.1159197297 N,0,2.1917119954,0.3890651001,-1.3464805223 H,0,1.5698900742,0.8912428286,-1.9605987771 N,0,0.6197502736,-1.3235528184,-0.7929468745 N,0,-0.3174583326,-0.7499558382,-1.5526397924 C,0,-1.4773355678,-1.4131930488,-1.5785742324 H,0,-1.477723646,-2.4896107678,-1.4155893697 H,0,0.3926891206,-2.0862514613,-0.1577604147 H,0,6.3446283217,2.4696791399,-1.0132346765 C,0,-2.5714437536,-0.8940959182,-2.404553605 C,0,-3.6175896167,-1.7508142955,-2.7620969465 C,0,-2.6049951079,0.4457476993,-2.8215344783 C,0,-4.6807521694,-1.2814753782,-3.5323932785 C,0,-3.6552317231,0.9139497085,-3.5918053762 C,0,-4.7006068642,0.042812521,-3.9465863978 H,0,7.003540219,0.7097067644,0.5793079303 H,0,-5.4917019099,-1.9474483636,-3.8109971603 H,0,-3.6063841955,-2.7837987478,-2.4363382929 O,0,-3.6731413677,2.2153307881,-3.996422819 H,0,-4.4731564506,2.3652668053,-4.5166258151 O,0,-1.9610328099,-1.1913916208,0.3038075742 O,0,-5.6961001919,0.6073897131,-4.7080810696 H,0,-6.3729501503,-0.0429640728,-4.9206421586 H,0,-1.8120592037,1.1270066145,-2.5426893147 O,0,-3.2105680269,-1.7365415786,0.5676583831 C,0,-4.1378049369,-0.6786067915,0.8238876871 H,0,-5.0870635571,-1.1742597902,1.037135766 H,0,-3.8126402025,-0.0958330882,1.6895840225 H,0,-4.2358277574,-0.0312562999,-0.0503105742

TS C13(•$OOCH_3$), optimization in solv. water UB3LYP/6-311++G**, E= -1100.69256294 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235101 a.u. 1 imaginary frequency = 443.1964 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2439202 a.u.	**TS C13(•$OOCH_3$),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.67964999 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235201 a.u. 1 imaginary frequency = 464.8213 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2306742 a.u.
0, 2	0, 2

C,0,6.0441172686,0.6516927359,0.0710161722	C,0,6.0245060171,0.6693280489,0.1121790225
C,0,5.2178051514,-0.435874621,0.3369536104	C,0,5.1762326679,-0.3886514687,0.4216613691
C,0,5.5857335758,1.7601040412,-0.6656451583	C,0,5.604875926,1.7315598701,-0.7089528495
H,0,5.5719572774,-1.288995809,0.9036970072	H,0,5.4978744712,-1.2071046429,1.0544855955
C,0,3.9069969659,-0.3984087939,-0.1513344369	C,0,3.882553118,-0.3697497349,-0.1091972082
C,0,4.2838539083,1.8172956252,-1.1608382955	C,0,4.3204492129,1.7698153025,-1.2489003576
H,0,3.9311956963,2.6700934259,-1.7281667931	H,0,3.9987299083,2.5888391928,-1.8812876552
C,0,3.4630930564,0.7267229353,-0.8907929086	C,0,3.4776574615,0.7089030123,-0.9352992919
C,0,1.8759835078,-0.7856250622,-0.6805510056	C,0,1.8660244263,-0.7699945692,-0.6708324179
N,0,2.8871017141,-1.3317104358,-0.0371319067	N,0,2.8483958421,-1.2819026831,0.0355403173
N,0,2.1452859937,0.4413456042,-1.2156070112	N,0,2.166469488,0.4152967963,-1.2832547974
H,0,1.4900202083,1.0056181729,-1.7363754019	H,0,1.5244001819,0.9519284776,-1.8461847896
N,0,0.650454369,-1.380393036,-0.8177954644	N,0,0.6370754968,-1.3585893955,-0.8099481752
N,0,-0.3248835008,-0.7766550885,-1.4975669254	N,0,-0.3195173484,-0.7707228139,-1.5314181684
C,0,-1.4827871577,-1.4484767221,-1.5259186765	C,0,-1.4801061343,-1.4347455453,-1.5535361828
H,0,-1.4766169203,-2.5234416162,-1.3554267714	H,0,-1.4794274738,-2.5104865277,-1.3857241617
H,0,0.518691986,-2.287023919,-0.3726144395	H,0,0.4554991883,-2.1927013344,-0.2550225694
H,0,6.2595600318,2.5880837305,-0.8526182016	H,0,6.294857314,2.5383772804,-0.9271641327
C,0,-2.5684170338,-0.940799868,-2.3691228695	C,0,-2.5706912485,-0.9208470232,-2.3878692256
C,0,-3.605298058,-1.8066072648,-2.733290164	C,0,-3.6131585359,-1.7810165361,-2.7478939985
C,0,-2.6032882744,0.3957707895,-2.8018283351	C,0,-2.6044955217,0.4173154033,-2.8121651676
C,0,-4.6644199801,-1.3522469111,-3.518267644	C,0,-4.6743247091,-1.3179914548,-3.5250879507
C,0,-3.6511481025,0.848824919,-3.5831739319	C,0,-3.6531541302,0.8790735677,-3.5878964811
C,0,-4.6914428366,-0.0298601431,-3.9423547174	C,0,-4.6965979595,0.0051072159,-3.9446059947
H,0,7.0641764601,0.6479443595,0.4375854706	H,0,7.0322125173,0.6786999443,0.5113996849
H,0,-5.4663246549,-2.0249672341,-3.8020444145	H,0,-5.4820249323,-1.9867076134,-3.8044624891
H,0,-3.5877533951,-2.8398879428,-2.4084582702	H,0,-3.6002347426,-2.8139523035,-2.421935629
O,0,-3.6735518437,2.1493971202,-4.0013403437	O,0,-3.6722969534,2.180234191,-3.9985805669
H,0,-4.4709933053,2.292578033,-4.5299567786	H,0,-4.4706974034,2.3274771354,-4.5231421775
O,0,-2.0081041124,-1.1621481615,0.3408955379	O,0,-1.9799058615,-1.1776484573,0.318809022
O,0,-5.6767148252,0.5216134577,-4.7138613732	O,0,-5.687305516,0.5642233225,-4.7111502273
H,0,-6.3567113602,-0.128225573,-4.9289536497	H,0,-6.3658846315,-0.0853003217,-4.9255133668
H,0,-1.8136347574,1.0838013044,-2.5279860617	H,0,-1.8136040027,1.1016552118,-2.5344207868
O,0,-3.3154766279,-1.59104822,0.5782924375	O,0,-3.260567449,-1.6592302945,0.5711420313
C,0,-4.1699511375,-0.4551776562,0.754931863	C,0,-4.1467572489,-0.5568118738,0.7889069831
H,0,-5.1608738076,-0.8688065934,0.950499632	H,0,-5.1204698085,-1.0068994159,0.9916825426
H,0,-3.8360032691,0.1394741706,1.6091796993	H,0,-3.8146543407,0.0281564617,1.6503828456
H,0,-4.1895832801,0.1569064568,-0.1485638596	H,0,-4.1998883555,0.0759497849,-0.0992769748

TS C14(•OOCH$_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.64632498 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.233958 a.u. 1 imaginary frequency = 437.8670 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2026951 a.u.	**TS C14(•OOCH$_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.67140071 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234156 a.u. 1 imaginary frequency = 373.2810 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2292264 a.u.
0, 2	0, 2
C,0,6.1408482003,0.770870358,-0.2830627294	C,0,6.109753951,0.7930799165,-0.2614368161
C,0,5.3756015411,-0.3267115486,0.1044498182	C,0,5.3836793478,-0.3637787829,0.021815458
C,0,5.5859037937,1.8269952904,-1.0225936254	C,0,5.5059548628,1.9072085922,-0.8674663504
H,0,5.8026251893,-1.142427089,0.6754415449	H,0,5.8530094434,-1.2214813571,0.4900407198
C,0,4.0295074686,-0.3529596064,-0.2631823819	C,0,4.0280620187,-0.3888202334,-0.3146508903
C,0,4.242532993,1.8196622222,-1.3994135105	C,0,4.1523944343,1.9006079224,-1.2115408945
H,0,3.8151442395,2.6361535723,-1.9701873043	H,0,3.6847573031,2.7587551687,-1.6794890156
C,0,3.487304832,0.7211326705,-1.0084502263	C,0,3.4374159604,0.7435908341,-0.9252592619

C,0,1.9776315294,-0.831933456,-0.5813013301	C,0,1.9728974363,-0.8843875157,-0.6383649432
N,0,3.0528210957,-1.3114850697,-0.0123677348	N,0,3.0812739936,-1.3956680576,-0.1476372021
N,0,2.150955811,0.3783530032,-1.1986567977	N,0,2.1079509306,0.3873265191,-1.1209783313
H,0,1.429340515,0.8848685645,-1.6859885802	H,0,1.3659815724,0.9350171952,-1.53016013
N,0,0.7610526782,-1.4702462117,-0.5802344037	N,0,0.773871967,-1.5436572093,-0.6738719783
N,0,-0.3090599469,-0.8978563799,-1.1645543646	N,0,-0.312075557,-0.9360138884,-1.1977445493
C,0,-1.4201463169,-1.5306959196,-1.1596801494	C,0,-1.4141683377,-1.5851756836,-1.2292246439
H,0,-1.5246910276,-2.5168442207,-0.6986104547	H,0,-1.4964444968,-2.6058093281,-0.8495510785
H,0,0.7041656463,-2.3602726777,-0.0951569388	H,0,0.7353350459,-2.4871589104,-0.2993874309
H,0,6.2114084414,2.6652186521,-1.3069115668	H,0,6.1004838072,2.7898956715,-1.0728809977
C,0,-2.6486243011,-0.9553210974,-1.7717949558	C,0,-2.6555798689,-0.9770988861,-1.7853923936
C,0,-3.4433743198,-1.9071217211,-2.5430131712	C,0,-3.516321115,-1.9330029038,-2.4820457811
C,0,-2.5735796912,0.3928768249,-2.3029236463	C,0,-2.5569354336,0.3446151129,-2.3846761277
C,0,-4.2523070046,-1.4877187885,-3.5664711561	C,0,-4.3450286206,-1.5374735573,-3.4988757754
C,0,-3.4017470166,0.7977173218,-3.3112375914	C,0,-3.403881904,0.7261919509,-3.3842291008
C,0,-4.2625405766,-0.1377942513,-3.945366507	C,0,-4.3231985343,-0.2065644827,-3.9464552405
H,0,7.1887051453,0.8127318426,-0.0082814208	H,0,7.1631973507,0.8348814434,-0.008558978
H,0,-4.8841072311,-2.1962620034,-4.0940573146	H,0,-5.0116215389,-2.2480655727,-3.9764164482
H,0,-3.4353584003,-2.9465704546,-2.23975987	H,0,-3.5218390717,-2.9606039464,-2.1398988876
O,0,-3.3920979134,2.0960653309,-3.7292384087	O,0,-3.3599628792,2.0000670648,-3.8729337393
H,0,-4.0143926212,2.1929058009,-4.4612925917	H,0,-3.9952498744,2.0835083129,-4.5975397381
O,0,-3.5154218509,-0.8590773792,-0.2538674335	O,0,-3.4156305538,-0.7707136987,-0.2298691993
H,0,-1.8967356835,1.10138159,-1.8461466177	H,0,-1.8365864977,1.0489252266,-1.9913366964
O,0,-5.0446950238,0.372543431,-4.9426059864	O,0,-5.1108206988,0.2831620402,-4.9363232086
H,0,-5.6102898085,-0.3100516681,-5.3193482494	H,0,-5.698489456,-0.395575085,-5.2925088882
O,0,-4.8487671222,-0.4150905885,-0.4497190514	O,0,-4.7536908455,-0.2857903824,-0.3609977296
C,0,-4.9623674762,0.8970839418,0.0927397643	C,0,-4.7889908695,1.0651456947,0.0974883767
H,0,-4.7047087353,0.8994418216,1.155588569	H,0,-4.4685961028,1.1295514088,1.1412173057
H,0,-4.3299956473,1.6059942095,-0.448750088	H,0,-4.1681964459,1.71086796,-0.5279004161
H,0,-6.0146529246,1.163151273,-0.0344692676	H,0,-5.836822243,1.3631490367,0.0145652722

TS C14(•OOCH$_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.65695526 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234147 a.u. 1 imaginary frequency = 414.3499 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2139171 a.u.	**TS C15(•OOCH$_3$),** optimization in gas phase UB3LYP/6-311++G**, E= -1100.65644657 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234391 a.u. 1 imaginary frequency = 532.6497 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2081936 a.u.
0, 2	0, 2
C,0,6.1321819614,0.7773167371,-0.2686033862	C,0,5.7947027691,0.6846163423,0.2671229639
C,0,5.3790625012,-0.3419532052,0.0815741863	C,0,4.9906971077,-0.4291242586,0.4956765553
C,0,5.5625000804,1.8553781725,-0.9646110983	C,0,5.3348070383,1.7799370144,-0.4815897823
H,0,5.8190872205,-1.1735168539,0.619293343	H,0,5.3440978738,-1.2749218959,1.0731656348
C,0,4.0306559882,-0.3670413225,-0.2794696851	C,0,3.7023319435,-0.4321118234,-0.0426120181
C,0,4.2164959679,1.8488849344,-1.3342069089	C,0,4.0518221975,1.796001924,-1.0290193714
H,0,3.7773266694,2.6816868232,-1.8711011323	H,0,3.6980185983,2.642023793,-1.6069264002
C,0,3.4737968311,0.7289423244,-0.9810686304	C,0,3.2561614936,0.6810930131,-0.7958469669
C,0,1.9777047949,-0.8510938379,-0.6055417217	C,0,1.7101007494,-0.8852737956,-0.6459297335
N,0,3.0634364325,-1.342881909,-0.0596386861	N,0,2.7064596479,-1.3987075542,0.0308721795
N,0,2.1404748433,0.3817725701,-1.1772052818	N,0,1.9594709916,0.3514195231,-1.1779223556
H,0,1.4133393472,0.90516494,-1.6391780537	H,0,1.2823266462,0.9073750141,-1.6763214004
N,0,0.7679818292,-1.4971131933,-0.6210790934	N,0,0.5025826769,-1.5115036107,-0.8256057419
N,0,-0.3078477135,-0.9096344918,-1.1835247422	N,0,-0.4620978291,-0.9283301478,-1.5581022161
C,0,-1.4156671018,-1.5487554772,-1.1889568647	C,0,-1.6138505816,-1.5102646932,-1.6208884553
H,0,-1.5102166115,-2.5479782043,-0.7561397486	H,0,-1.7961138427,-2.4478997647,-1.084400616

H,0,0.7125235846,-2.4024592976,-0.1645573156	H,0,0.3542863239,-2.3811123682,-0.3215538598
H,0,6.1780721414,2.7100108563,-1.2204617308	H,0,5.9882959385,2.6303082724,-0.6382123456
C,0,-2.6500987355,-0.9626646167,-1.7797893717	C,0,-2.7071466317,-0.9711727552,-2.387194921
C,0,-3.4668131208,-1.9155318568,-2.5279700501	C,0,-3.9313784456,-1.6328233056,-2.4212361856
C,0,-2.5688216068,0.3786827289,-2.3304081444	C,0,-2.5685024708,0.2942440155,-3.0811867101
C,0,-4.2843728932,-1.5024435038,-3.5470927171	C,0,-4.9859448767,-1.1607612133,-3.2063694757
C,0,-3.4043003807,0.7769248133,-3.3343373018	C,0,-3.5984032588,0.6497326112,-4.0088301182
C,0,-4.2855810892,-0.1573389282,-3.945597476	C,0,-4.8051468576,-0.0323975134,-4.0136114957
H,0,7.1812342035,0.8185501375,0.0018874926	H,0,6.7986602961,0.7092813644,0.6754457371
H,0,-4.9287869369,-2.2108826548,-4.0583509985	H,0,-5.9383480047,-1.6808415903,-3.2131664401
H,0,-3.4619409565,-2.9521125563,-2.2146815163	H,0,-4.0671664317,-2.5406065434,-1.8439976715
O,0,-3.3843710194,2.0689428958,-3.7734787988	O,0,-3.3736007881,1.7031528372,-4.8348257813
H,0,-4.0135429443,2.1631684012,-4.5008964789	H,0,-4.1558865156,1.8307672881,-5.3888082401
O,0,-3.4805294331,-0.8328770524,-0.245576736	O,0,-2.5950386268,1.5621582883,-1.7729959007
H,0,-1.8786120257,1.0862618467,-1.8923254817	H,0,-1.5657907353,0.6108057118,-3.3437291214
O,0,-5.0717917432,0.3476812589,-4.9367184474	O,0,-5.7656133707,0.464420027,-4.8701192864
H,0,-5.6484113426,-0.3319373598,-5.3049666462	H,0,-6.4880803724,-0.1632987469,-4.9698519438
O,0,-4.8182002687,-0.3799764804,-0.4177191846	O,0,-3.755760203,1.5105578619,-0.9945805069
C,0,-4.9085842984,0.9472459383,0.0948237564	C,0,-4.5932130808,2.6153216522,-1.3323125209
H,0,-4.6299399805,0.9738133957,1.1519652809	H,0,-4.9616112658,2.5325351705,-2.3583425504
H,0,-4.2810864219,1.6356140572,-0.4770091462	H,0,-5.428088529,2.5621213809,-0.630165973
H,0,-5.9604692927,1.2208575603,-0.0177572139	H,0,-4.0538789838,3.557247925,-1.2039715846

TS C15(•$OOCH_3$), optimization in solv. water UB3LYP/6-311++G**, E= -1100.68179553 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234676 a.u. 1 imaginary frequency = 489.3497 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2348035 a.u.	**TS C15(•$OOCH_3$),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.66697616 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234772 a.u. 1 imaginary frequency = 517.9952 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2192455 a.u.
0, 2	0, 2
C,0,5.8642072145,0.6272116802,0.2078273779	C,0,5.8330536376,0.6528725113,0.2315282552
C,0,5.0202207357,-0.4365048353,0.5261096442	C,0,5.0129690526,-0.4425171627,0.4944815632
C,0,5.4357513092,1.6823506675,-0.6149067206	C,0,5.3826778523,1.7384509753,-0.5373817797
H,0,5.3546271262,-1.2489555532,1.1610950386	H,0,5.3612231764,-1.2795916964,1.0880320855
C,0,3.7247947802,-0.4286392411,0.0020991572	C,0,3.7184150088,-0.4364552964,-0.0298813167
C,0,4.1450445192,1.7081338584,-1.1476163079	C,0,4.0932850291,1.7630713582,-1.0708035333
H,0,3.8123635625,2.5206937152,-1.7826628114	H,0,3.7453098512,2.6005500567,-1.6642398503
C,0,3.3109831566,0.6441933464,-0.8248142772	C,0,3.2822666943,0.6668630509,-0.8032866466
C,0,1.7012496822,-0.8437291295,-0.5534778102	C,0,1.7089429798,-0.8681920709,-0.604435986
N,0,2.6917116762,-1.3475718077,0.1538107178	N,0,2.7066172726,-1.3841712754,0.0750762941
N,0,1.9979235601,0.3427195701,-1.165076621	N,0,1.9765687332,0.3519482522,-1.162985854
H,0,1.3612350303,0.8719531925,-1.7416839793	H,0,1.3120215925,0.9059519425,-1.6808286347
N,0,0.4746379115,-1.4306749624,-0.6852813522	N,0,0.4917485455,-1.475991244,-0.7615424269
N,0,-0.4761093392,-0.8436982283,-1.4439899711	N,0,-0.4667108319,-0.8910136249,-1.5054059877
C,0,-1.6147764896,-1.4472402086,-1.5482943756	C,0,-1.6143939015,-1.4800932759,-1.5827388309
H,0,-1.7912495403,-2.4013250811,-1.0439110205	H,0,-1.79556191,-2.4228897103,-1.0567814809
H,0,0.3123777305,-2.3100652385,-0.2026242887	H,0,0.3376937693,-2.350507557,-0.2677399401
H,0,6.118951787,2.4926269609,-0.8417602851	H,0,6.048180813,2.574018543,-0.7210190133
C,0,-2.6942232488,-0.9146501982,-2.3410491338	C,0,-2.7016648939,-0.9452715362,-2.3615500602
C,0,-3.8793158297,-1.6311081258,-2.4741043866	C,0,-3.9088904047,-1.6332335759,-2.4412223507
C,0,-2.5786709964,0.382654754,-2.9829648382	C,0,-2.5740167995,0.3352905773,-3.030812315
C,0,-4.9067649554,-1.1844841331,-3.3120131481	C,0,-4.9503244733,-1.1746179415,-3.2526841596
C,0,-3.5686797428,0.7203483009,-3.9608837867	C,0,-3.5831830528,0.6796073654,-3.9853299544
C,0,-4.7375509909,-0.0204275554,-4.0713109438	C,0,-4.7729234474,-0.0309570263,-4.0398336524

H,0,6.8737184394,0.6416434449,0.6029594013	H,0,6.8417476372,0.6697919449,0.6285694203
H,0,-5.8233101649,-1.7562519651,-3.4040544414	H,0,-5.8875816946,-1.7189240248,-3.2989537559
H,0,-4.0021102952,-2.5692415395,-1.9449181367	H,0,-4.0400739193,-2.5538595765,-1.8837728772
O,0,-3.3479050143,1.8195687247,-4.7269036203	O,0,-3.3577220788,1.7525103846,-4.7865248444
H,0,-4.1027785206,1.9448770755,-5.3207614027	H,0,-4.1254053987,1.8756590781,-5.3626093807
O,0,-2.7507545983,1.6145467441,-1.6487888461	O,0,-2.677332451,1.5817424113,-1.7042842501
H,0,-1.5776992364,0.753073361,-3.174853064	H,0,-1.5716339492,0.6805772602,-3.2564067953
O,0,-5.6563625473,0.4557514716,-4.9704638042	O,0,-5.7141985573,0.4537794462,-4.9188416154
H,0,-6.3802781915,-0.1693930338,-5.0953094397	H,0,-6.4326161082,-0.1771947108,-5.0354171698
O,0,-3.9617876648,1.4929376638,-0.940291527	O,0,-3.8729754096,1.5018701753,-0.9762463152
C,0,-4.8455260117,2.549853585,-1.3245794425	C,0,-4.717385026,2.5951690357,-1.3392638413
H,0,-5.1372239628,2.4583369281,-2.3730401551	H,0,-5.0340708824,2.5196549265,-2.382426988
H,0,-5.7217657978,2.4318574564,-0.6841500276	H,0,-5.5838988022,2.513922556,-0.679709229
H,0,-4.3807944929,3.5225977851,-1.1453059915	H,0,-4.2059970629,3.5461489043,-1.1706714025

TS C16(•OOCH$_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.65050780 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.233501 a.u. 1 imaginary frequency = 494.3557 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2053912 a.u.	**TS C16(•OOCH$_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.67773908 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234660 a.u. 1 imaginary frequency = 435.9571 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2340711 a.u.
0, 2	0, 2
C,0,5.846850166,0.6808871408,0.0832040006	C,0,5.8770366818,0.6680546052,0.0360632887
C,0,5.0410069592,-0.4271408088,0.3346944062	C,0,5.0688787648,-0.4330948477,0.3199812208
C,0,5.3985027914,1.7486458103,-0.7100868998	C,0,5.4196943952,1.7248339586,-0.7681756608
H,0,5.386071459,-1.2519397956,0.9466102543	H,0,5.425900975,-1.2469399595,0.9407740916
C,0,3.7632019645,-0.4522083522,-0.2264236493	C,0,3.7805192693,-0.4609428513,-0.2196157605
C,0,4.1248646878,1.7425082092,-1.2798008724	C,0,4.1348315059,1.7149040659,-1.3161022994
H,0,3.779510237,2.5676301063,-1.892107649	H,0,3.7797655526,2.5287682226,-1.9372343173
C,0,3.3283898583,0.6335747652,-1.0234666729	C,0,3.3371752876,0.6141045098,-1.0273589882
C,0,1.7832003834,-0.9332539157,-0.8508344023	C,0,1.77996927,-0.9379620592,-0.8093570936
N,0,2.7673630849,-1.4194207968,-0.1390151875	N,0,2.7796262771,-1.4208121363,-0.1014531582
N,0,2.037555079,0.2881544732,-1.4152196203	N,0,2.03962829,0.2722785176,-1.3904266486
H,0,1.384192522,0.8106349745,-1.9764747009	H,0,1.3922610179,0.7893468299,-1.9660767621
N,0,0.5846213113,-1.5768069747,-1.0371838004	N,0,0.5776481111,-1.5678866395,-0.9703384166
N,0,-0.3899818281,-1.011195859,-1.7742935482	N,0,-0.3914669315,-0.9919933192,-1.7170152428
C,0,-1.5126666951,-1.6251697563,-1.8785745969	C,0,-1.5092517368,-1.6125165118,-1.8381088934
H,0,-1.6791417292,-2.5794115011,-1.3666093352	H,0,-1.6773635678,-2.5743452893,-1.3463036556
H,0,0.4574867848,-2.4620178142,-0.5561361062	H,0,0.4424037727,-2.4647078586,-0.512968902
H,0,6.0528831031,2.5948440252,-0.8844724129	H,0,6.0748979718,2.5646565521,-0.9686892093
C,0,-2.624165203,-1.0989522223,-2.6711941603	C,0,-2.6126896404,-1.0726513857,-2.6355723174
C,0,-3.8493875503,-1.8140142626,-2.6633331443	C,0,-3.827338054,-1.8103431648,-2.6759249639
C,0,-2.513372817,0.0411960302,-3.4411428207	C,0,-2.5039373136,0.0921291901,-3.3672019292
C,0,-4.9331271598,-1.4028506872,-3.4486256805	C,0,-4.9013082522,-1.3975902664,-3.4698442101
C,0,-3.660056328,0.6015769904,-4.10507622	C,0,-3.6449819932,0.6455363015,-4.0495932625
C,0,-4.8340086334,-0.2586669103,-4.2072546877	C,0,-4.8065168526,-0.2293925748,-4.1950577031
H,0,6.8432310179,0.7217803507,0.5084665501	H,0,6.880674432,0.7101599716,0.444037072
H,0,-5.8393358415,-2.0003889901,-3.4797783686	H,0,-5.7962927296,-2.006248819,-3.5380548132
H,0,-3.9414682126,-2.7116818813,-2.062692419	H,0,-3.9130777336,-2.7278483276,-2.1058389319
O,0,-3.3795943792,1.4196580688,-5.1595931735	O,0,-3.352205969,1.4789217572,-5.0931353285
H,0,-4.210246492,1.748112619,-5.5284886444	H,0,-4.1743009118,1.718508491,-5.5446638437
O,0,-4.2145255899,1.8906065869,-3.0062827938	O,0,-4.2389988597,1.9335250637,-2.9616536848
O,0,-5.7858801282,0.1992799795,-5.0636371744	O,0,-5.7387974954,0.241066962,-5.0538504055
H,0,-6.5414325852,-0.3982210654,-5.0857223468	H,0,-6.4966823125,-0.3552151234,-5.1152010443

H,0,-1.5882815206,0.5975206511,-3.5011459167	H,0,-1.5840285922,0.661400342,-3.3928251309
O,0,-4.489579327,1.4609808423,-1.6919249132	O,0,-4.5783915257,1.5032820187,-1.6544941403
C,0,-5.8891562382,1.5744266632,-1.4610530484	C,0,-5.9991491791,1.5332376236,-1.5094313582
H,0,-6.0310018246,1.2721489717,-0.4210332004	H,0,-6.1840303372,1.2378678365,-0.4746170479
H,0,-6.220781823,2.6076109019,-1.5971851022	H,0,-6.3830249596,2.5422975839,-1.6816791879
H,0,-6.4561407738,0.9113434231,-2.1215162722	H,0,-6.4814778972,0.8253907206,-2.1873956915

TS C16(•$OOCH_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.66169190 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234209 a.u. 1 imaginary frequency = 473.5338 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2171756 a.u.	**TS C17(•$OOCH_3$),** optimization in gas phase UB3LYP/6-311++G**, E= -1100.66499529 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235954 a.u. 1 imaginary frequency = 480.2974 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2162755 a.u.
0, 2	0, 2
C,0,5.8809687251,0.6529757736,0.0216449616	C,0,5.9834393017,0.6089631743,0.0480001889
C,0,5.0717481115,-0.4484507801,0.2951818371	C,0,5.0974375008,-0.4074177904,0.3936153338
C,0,5.4207401745,1.724870912,-0.7597283396	C,0,5.6240615758,1.6186894066,-0.8598224618
H,0,5.4281855851,-1.2753011527,0.8981698774	H,0,5.3728607531,-1.187020722,1.0935358631
C,0,3.7785916791,-0.462079197,-0.231305752	C,0,3.8287085376,-0.3995944327,-0.1900509953
C,0,4.1315744225,1.7296907311,-1.2949455001	C,0,4.3624352834,1.6445767626,-1.4536501858
H,0,3.7757268978,2.5567962837,-1.8982415961	H,0,4.0871313314,2.4244231931,-2.154249769
C,0,3.3323214953,0.6277726051,-1.016743258	C,0,3.4842208883,0.6264454845,-1.1031057959
C,0,1.7750663917,-0.9234104426,-0.8058815703	C,0,1.8287327029,-0.8010071272,-0.8043535777
N,0,2.7759603479,-1.4202050639,-0.1185259803	N,0,2.765752304,-1.2790687304,-0.0253412411
N,0,2.0292227358,0.2955752782,-1.3734513282	N,0,2.1771595309,0.3356084205,-1.4834094011
H,0,1.371508548,0.8242520361,-1.9248695618	H,0,1.5780333748,0.8307501933,-2.1242787977
N,0,0.5653306854,-1.5488538989,-0.9599719927	N,0,0.5899909363,-1.3746918562,-0.9453012978
N,0,-0.4016310316,-0.9834767243,-1.7115894928	N,0,-0.3317184191,-0.8332219087,-1.7564032983
C,0,-1.5220262815,-1.5996359539,-1.8270770118	C,0,-1.4873136124,-1.4214853342,-1.8309189635
H,0,-1.6932850812,-2.5547530269,-1.3204534632	H,0,-1.6863540079,-2.3217576329,-1.2403260322
H,0,0.4419783006,-2.4497055579,-0.5076794168	H,0,0.4106543864,-2.214665158,-0.4016700866
H,0,6.0775844379,2.5653255625,-0.952012978	H,0,6.3407258074,2.3938432144,-1.1048962491
C,0,-2.6233271975,-1.0712841332,-2.6336725187	C,0,-2.5512752728,-0.939072277,-2.66566777
C,0,-3.839543778,-1.8031836683,-2.6661146413	C,0,-3.7913397699,-1.6438999826,-2.664056565
C,0,-2.5090965032,0.0821796295,-3.3825657593	C,0,-2.4046701647,0.1888042525,-3.5045992832
C,0,-4.9081762195,-1.39850526,-3.4740051216	C,0,-4.8437995118,-1.2303934701,-3.4285976354
C,0,-3.6460218592,0.6329679797,-4.0714215147	C,0,-3.4569051178,0.6212961086,-4.27156274
C,0,-4.8043734066,-0.2434366445,-4.2170578358	C,0,-4.7649590377,0.0017633023,-4.1576638993
H,0,6.8887879944,0.6845715865,0.4200612552	H,0,6.9740951105,0.6240833512,0.4877669732
H,0,-5.8047626205,-2.0073657161,-3.5366862698	H,0,-5.7808994459,-1.7733989897,-3.4453692656
H,0,-3.9332696105,-2.710127937,-2.0800765187	H,0,-3.8854499773,-2.539068149,-2.0587712449
O,0,-3.3491777616,1.4651044367,-5.1121250972	O,0,-3.3157409893,1.661957939,-5.1175198513
H,0,-4.1735428831,1.7543593015,-5.5268173016	H,0,-4.1563434402,1.7736450754,-5.5875515595
O,0,-4.2494966848,1.9101978224,-2.9808186432	O,0,-5.7475082385,1.2010048837,-3.1376343998
O,0,-5.7322655876,0.2116065431,-5.0959846942	O,0,-5.5632963448,0.2268437667,-5.2606052897
H,0,-6.4767935631,-0.3979530031,-5.1621257239	H,0,-6.4738198713,0.3346968267,-4.9486978613
H,0,-1.5898743813,0.6510861449,-3.4109572586	H,0,-1.4545310673,0.7020733939,-3.5694205408
O,0,-4.5590804327,1.4726758414,-1.6741111082	O,0,-5.5290526513,1.1426322895,-1.7603368457
C,0,-5.9714834621,1.5300149794,-1.4927915117	C,0,-4.7893518576,2.2972308625,-1.3607887162
H,0,-6.1365777681,1.2281268981,-0.4562645023	H,0,-5.3457452441,3.2081834551,-1.5974909583
H,0,-6.3396343575,2.5479270574,-1.6468874103	H,0,-4.6741532865,2.1987412199,-0.2794331161
H,0,-6.486257331,0.8394307472,-2.1665015886	H,0,-3.8088925474,2.3177407347,-1.8422528441

TS C17(•$OOCH_3$), optimization in solv. water UB3LYP/6-311++G**, E= -1100.68642654 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235117 a.u. 1 imaginary frequency = 444.0297 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2389248 a.u.	**TS C17(•$OOCH_3$),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.67391294 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235250 a.u. 1 imaginary frequency = 471.1687 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2256456 a.u.
0, 2 C,0,5.9464621474,0.6365210735,0.0158002918 C,0,5.0850984073,-0.4039315036,0.3599929903 C,0,5.5510193941,1.6540137357,-0.8695829798 H,0,5.3931611742,-1.1872055341,1.0429934132 C,0,3.8054882897,-0.4112926986,-0.2024157405 C,0,4.277647835,1.6640933198,-1.4413829577 H,0,3.9709416045,2.4473258719,-2.1244251227 C,0,3.4251040472,0.6228589017,-1.0923090326 C,0,1.7967918207,-0.8370023113,-0.7965314326 N,0,2.7604226949,-1.3133657491,-0.0367523202 N,0,2.120243833,0.3152164563,-1.4562346294 H,0,1.5077733772,0.8188549764,-2.0802178924 N,0,0.5683054944,-1.4241289879,-0.9328631966 N,0,-0.3587564598,-0.8719950285,-1.7335317733 C,0,-1.5090623012,-1.4701912225,-1.8210541044 H,0,-1.7054164927,-2.3846080739,-1.2560524425 H,0,0.3920864103,-2.2797552241,-0.412385415 H,0,6.2478935413,2.4471997965,-1.1143752028 C,0,-2.5661442533,-0.9644346333,-2.6512875896 C,0,-3.8067040611,-1.6685043394,-2.6815386711 C,0,-2.4102957164,0.1888626688,-3.4576920109 C,0,-4.8508489888,-1.2320450534,-3.4453334542 C,0,-3.4499898719,0.6413985593,-4.2263493397 C,0,-4.7579619796,0.0158547789,-4.1493848603 H,0,6.9441216424,0.6632680244,0.4391948495 H,0,-5.7872548946,-1.7761200382,-3.4877190038 H,0,-3.9071780729,-2.5799799529,-2.1029590175 O,0,-3.2932001552,1.7093049498,-5.0429916684 H,0,-4.1234988362,1.8614078505,-5.5190964299 O,0,-5.7227093738,1.2042364258,-3.0667197283 O,0,-5.528862311,0.274687147,-5.2493588455 H,0,-6.4421648502,0.0005186064,-5.090944882 H,0,-1.4603435291,0.7065619073,-3.4902988134 O,0,-5.3865899293,1.1897800534,-1.701304673 C,0,-4.651570841,2.3753694738,-1.3855947401 H,0,-5.2515442618,3.2651207193,-1.5948207839 H,0,-4.4472114172,2.3080222448,-0.3152313415 H,0,-3.7129336663,2.4123165593,-1.9421216294	0, 2 C,0,5.972639516,0.6172571413,0.0415513909 C,0,5.0951438168,-0.4086823749,0.383663777 C,0,5.6013849859,1.6315606867,-0.8569342131 H,0,5.3817259222,-1.1908172298,1.0766079077 C,0,3.8231937232,-0.4054000712,-0.1940874046 C,0,4.3362771441,1.6525311321,-1.4446832171 H,0,4.050288146,2.4348667079,-2.1380203169 C,0,3.4670552088,0.6250111807,-1.0977988641 C,0,1.8203373845,-0.8142221359,-0.8049119292 N,0,2.7661684064,-1.293128016,-0.031878607 N,0,2.1614121064,0.3288443023,-1.4746986304 H,0,1.5594893657,0.8285430992,-2.1103977949 N,0,0.5853955542,-1.3919716813,-0.9462768229 N,0,-0.3377317502,-0.8451183963,-1.7537943067 C,0,-1.4917929901,-1.4364202726,-1.8313451893 H,0,-1.6896878929,-2.3407941971,-1.2485335894 H,0,0.4048740868,-2.2374596418,-0.411325468 H,0,6.3111534123,2.41391645,-1.0993691322 C,0,-2.5548433763,-0.946793606,-2.663520601 C,0,-3.7956586642,-1.6505264933,-2.6665953783 C,0,-2.407127151,0.1875067825,-3.4947719802 C,0,-4.8469701964,-1.2305485184,-3.4293053045 C,0,-3.4573689587,0.6256063347,-4.2604083569 C,0,-4.7646434554,0.004072424,-4.1546167503 H,0,6.9652371561,0.6358245167,0.4769376147 H,0,-5.7844344346,-1.7729653489,-3.4501751757 H,0,-3.8911394384,-2.5489900167,-2.0667479238 O,0,-3.3127621267,1.674655872,-5.0986455479 H,0,-4.1534543433,1.8048394477,-5.5636755564 O,0,-5.7438049727,1.2024434058,-3.1164748794 O,0,-5.5550281662,0.2357043143,-5.2572951859 H,0,-6.4827285946,0.2245052532,-4.9820101811 H,0,-1.4572669816,0.7025010559,-3.5521659786 O,0,-5.4860411058,1.1614383558,-1.7419258177 C,0,-4.742722766,2.3251290495,-1.3726890645 H,0,-5.3103341984,3.2304559687,-1.6037599946 H,0,-4.5987001184,2.239072485,-0.2938419081 H,0,-3.7752148036,2.3457857839,-1.8789597994

TS C19(•$OOCH_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.65997825 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235279 a.u. 1 imaginary frequency = 507.3378 i cm^{-1} SP at UM06-2X/6-311++G** (gas phase), E = -1100.2113307 a.u.	**TS C19(•$OOCH_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.68354642 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235087 a.u. 1 imaginary frequency = 458.9979 i cm^{-1} SP at UM06-2X/6-311++G** (water), E = -1100.2359119 a.u.
0, 2	0, 2

C,0,6.1941060361,0.7135678729,0.1558038497	C,0,6.1777205117,0.7278623873,0.1182778949
C,0,5.3348052364,-0.3317144162,0.4841543301	C,0,5.3357241116,-0.3343018033,0.4457341547
C,0,5.7735443661,1.7831483294,-0.650879707	C,0,5.7288473817,1.8051709592,-0.6641756476
H,0,5.6579121627,-1.1576769731,1.1062770345	H,0,5.685623709,-1.1640139017,1.0492098516
C,0,4.0305053765,-0.2914753092,-0.0125573682	C,0,4.0211555724,-0.3017970231,-0.0273407465
C,0,4.4748134733,1.8422741727,-1.1566705152	C,0,4.4191318323,1.8556902843,-1.1456628175
H,0,4.1518141929,2.6685576631,-1.7794993462	H,0,4.0709883213,2.6852099618,-1.7496649133
C,0,3.6241487162,0.795447348,-0.823893668	C,0,3.5868581358,0.7929357503,-0.8139444792
C,0,1.995048864,-0.6633437533,-0.522408951	C,0,1.9742152296,-0.6852624643,-0.5136877359
N,0,2.9831248965,-1.1891480176,0.1566240524	N,0,2.9852943025,-1.2139332276,0.1438768287
N,0,2.295344755,0.5231905198,-1.1372534277	N,0,2.2585578815,0.5117442534,-1.1096032729
H,0,1.6544682535,1.056520661,-1.7024096471	H,0,1.6078626958,1.0577543008,-1.6540760991
N,0,0.7517478138,-1.232831132,-0.626869338	N,0,0.7374731856,-1.2599125254,-0.6094382467
N,0,-0.2190910348,-0.6396097366,-1.3449806187	N,0,-0.2368698758,-0.6544763565,-1.3171739461
C,0,-1.360549153,-1.2466202834,-1.4283946166	C,0,-1.3791692362,-1.2603799127,-1.4022945699
H,0,-1.516144567,-2.2053356682,-0.9240957479	H,0,-1.5364488107,-2.2243914108,-0.9124290892
H,0,0.6101340321,-2.1187419063,-0.1499814132	H,0,0.5950227347,-2.1583254874,-0.1558715799
H,0,6.4704985569,2.5790496645,-0.8862651512	H,0,6.4114821731,2.6134096585,-0.8997568025
C,0,-2.4740157547,-0.7104446453,-2.1668559647	C,0,-2.4849265741,-0.7077633709,-2.1416996429
C,0,-3.7115225614,-1.4630629526,-2.1674101664	C,0,-3.7300951364,-1.4510867683,-2.1561820819
C,0,-2.4206184562,0.5218260208,-2.8318163522	C,0,-2.4140214035,0.5221422757,-2.8090332493
C,0,-4.7372036976,-1.0712383475,-3.0931587241	C,0,-4.7427346584,-1.0557607165,-3.0957024591
C,0,-3.4937821,0.9575145016,-3.5842955747	C,0,-3.4735964843,0.9591945431,-3.5809813465
C,0,-4.6548488214,0.1329061155,-3.7236274394	C,0,-4.6405262233,0.1403847092,-3.7408189821
H,0,7.2115362194,0.7037407732,0.5298285644	H,0,7.2018180736,0.7238892698,0.4740971417
H,0,-5.6163818276,-1.6963220746,-3.2017122242	H,0,-5.6178038151,-1.6810163007,-3.2279222418
H,0,-3.6364724353,-2.5226072363,-1.945028767	H,0,-3.6625679185,-2.5112582211,-1.9347220645
O,0,-3.4427234941,2.1536730535,-4.217499476	O,0,-3.400978129,2.1497167932,-4.2223197982
H,0,-4.2764878965,2.2893497536,-4.6890081349	H,0,-4.2164088874,2.2871722718,-4.7272798806
O,0,-4.4572310098,-1.2249358906,-0.510451402	O,0,-4.4807659224,-1.2088080864,-0.4943604865
O,0,-5.6114231762,0.6629473168,-4.5513999605	O,0,-5.5643517652,0.6659019804,-4.5963134662
H,0,-6.4244082671,0.1491998697,-4.5027226691	H,0,-6.3532301179,0.1117249146,-4.6442902589
H,0,-1.5310829446,1.135894995,-2.7808448513	H,0,-1.519170531,1.1286209429,-2.7506986695
O,0,-4.9770732773,0.0704159406,-0.3585983074	O,0,-4.9601509725,0.1073947007,-0.3112885093
C,0,-4.1467053731,0.800927155,0.5421715894	C,0,-4.0874178595,0.8063300807,0.578889837
H,0,-4.094624061,0.295428291,1.5103974722	H,0,-4.0281916707,0.2921760033,1.5419978732
H,0,-3.1423613526,0.9330201729,0.1321221101	H,0,-3.0904266257,0.9136442962,0.1467723864
H,0,-4.6344129701,1.7718628725,0.6540115168	H,0,-4.5435345149,1.7897719596,0.7106781051

TS C19(•OOCH$_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.67009541 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235394 a.u. 1 imaginary frequency = 489.6971 i cm^{-1} SP at UM06-2X/6-311++G** (benzene), E = -1100.2218687 a.u.	
0, 2 C,0,6.191381692,0.7176024649,0.1345724467 C,0,5.3388720126,-0.3332431438,0.4662424404 C,0,5.7588170013,1.7893164808,-0.6635293295 H,0,5.6734005988,-1.1598151184,1.081900131 C,0,4.0294729751,-0.2959801946,-0.0184934347 C,0,4.4546458299,1.8451926136,-1.1569551661 H,0,4.1208325315,2.6720916484,-1.7729978299 C,0,3.6113056082,0.7930519653,-0.8210832912	

C,0,1.9877983256,-0.6714544762,-0.5144255534 N,0,2.9860825241,-1.1982181327,0.1551023969 N,0,2.2818743933,0.5180583537,-1.1241989303 H,0,1.6373044089,1.0556208466,-1.6822662028 N,0,0.7461096849,-1.2412749081,-0.6122747828 N,0,-0.2256832974,-0.64288786,-1.3272487688 C,0,-1.3672184445,-1.2498788933,-1.4128142822 H,0,-1.523324206,-2.2112205895,-0.9153380768 H,0,0.6039827606,-2.1332172444,-0.1465374783 H,0,6.4502693956,2.5892038613,-0.9018086616 C,0,-2.4769819325,-0.7073848905,-2.1528683986 C,0,-3.7163105658,-1.4584979364,-2.1644955664 C,0,-2.4169193044,0.5256414972,-2.8157256289 C,0,-4.734593581,-1.0649049454,-3.0981637877 C,0,-3.4832197164,0.9618791369,-3.5778501813 C,0,-4.6447694736,0.1378927164,-3.7312219749 H,0,7.2122476049,0.7098915491,0.4993444269 H,0,-5.6109522173,-1.6910304579,-3.220011669 H,0,-3.6427985452,-2.5188044494,-1.9453111801 O,0,-3.4240911551,2.1579570057,-4.2106097462 H,0,-4.2511768775,2.2960641501,-4.6944051379 O,0,-4.469997311,-1.2249476489,-0.5073758694 O,0,-5.5860853958,0.6665605566,-4.5719958339 H,0,-6.3934967882,0.1401152723,-4.559803403 H,0,-1.5267980134,1.1384218173,-2.7573550042 O,0,-4.9814673072,0.0756192014,-0.3423283634 C,0,-4.138018769,0.7987994716,0.5541634577 H,0,-4.0799206294,0.2904748747,1.5204811113 H,0,-3.1374001537,0.9265135021,0.1348139493 H,0,-4.618784943,1.7721466235,0.673674163	

P C1(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.50440294 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234086 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1025.0949963 a.u.	**P C1(•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.52489927 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.233598 a.u. SP at UM06-2X/6-311++G** (water), E = -1025.1165388 a.u.
0, 2 C,0,5.897036758,0.9807238657,0.1637617672 C,0,5.0664105649,-0.1252820754,0.4728001179 C,0,5.5054238885,2.001084445,-0.6645707774 H,0,5.396447662,-0.917556827,1.1316345761 C,0,3.7817299116,-0.1579017637,-0.1147133992 C,0,4.1539370732,2.0674053171,-1.332086237 H,0,4.2864490274,2.1139717744,-2.4232161055 C,0,3.3635632844,0.8665157355,-0.9530755217 C,0,1.8060831227,-0.6730681975,-0.7344872277 N,0,2.7832023822,-1.1217133493,0.0117743266 N,0,2.0873161568,0.5174596762,-1.3544584459 H,0,1.4432522194,1.0464303203,-1.92225789 N,0,0.6048715103,-1.3184928011,-0.9114073186 N,0,-0.387617744,-0.7323830806,-1.6148250665 C,0,-1.5294447251,-1.3190815439,-1.6577548568 H,0,-1.6927088674,-2.2625709162,-1.1245531694 H,0,0.448178591,-2.1530767201,-0.354691287 H,0,6.1777623407,2.8250395238,-0.8766068648 C,0,-2.6668768185,-0.7844362085,-2.4005630375 C,0,-3.8860788117,-1.4730699753,-2.3595727312 C,0,-2.5770132471,0.3990408906,-3.152897733 C,0,-4.9961154061,-0.9916466349,-3.0518264341 C,0,-3.6768091926,0.880045229,-3.8410639537 C,0,-4.8952201306,0.1790588874,-3.7889870906 H,0,6.8902251271,1.0181755838,0.6000069534 H,0,-5.9389138804,-1.5288960448,-3.016232035 H,0,-3.9722479003,-2.3884846955,-1.7851818209 O,0,-3.5729007147,2.0286846297,-4.5652286096 H,0,-4.4274563129,2.2134585885,-4.9760401558 O,0,3.4497266578,3.3146995321,-1.0833437994 C,0,3.1510275679,3.5777960851,0.2838934522 H,0,2.6248069029,4.532590471,0.2996349595 H,0,2.5050634256,2.8040589662,0.7163255926 H,0,4.0597204467,3.655923815,0.8909716487 H,0,-1.6464269209,0.9488350373,-3.2033472556 O,0,-5.9230380864,0.7424996645,-4.5076559029 H,0,-6.7251654625,0.2172463854,-4.4251041572	0, 2 C,0,5.9069139677,0.9888528375,0.0919208005 C,0,5.0808909966,-0.1131419742,0.4351563785 C,0,5.4915795725,2.0037077408,-0.7307655469 H,0,5.434258405,-0.8987853655,1.0907425289 C,0,3.7808510246,-0.1477966492,-0.1153741443 C,0,4.1163857275,2.0739401441,-1.3471871435 H,0,4.2034146465,2.1318442645,-2.4411293279 C,0,3.3370868752,0.8713599115,-0.9490520821 C,0,1.78451484,-0.6715557273,-0.688644439 N,0,2.7866994627,-1.1153486055,0.0390518947 N,0,2.0534727799,0.5176853212,-1.3145312411 H,0,1.4033756062,1.0278970677,-1.8944953684 N,0,0.5825930444,-1.3088743876,-0.8391992091 N,0,-0.4001145298,-0.7275182782,-1.5708854342 C,0,-1.541418167,-1.3161566233,-1.619098998 H,0,-1.7147830463,-2.2511363272,-1.0783099589 H,0,0.4179634827,-2.1517108636,-0.2972732587 H,0,6.1603138504,2.823328072,-0.9695024137 C,0,-2.6649070106,-0.782267121,-2.3847238121 C,0,-3.8855364519,-1.4703664519,-2.3629079513 C,0,-2.5618763639,0.4000683249,-3.1401609279 C,0,-4.984514582,-0.9931452092,-3.076240663 C,0,-3.6509846927,0.8754769848,-3.8484855656 C,0,-4.8725266165,0.1758704549,-3.8175080535 H,0,6.9134379922,1.0247184935,0.4963761654 H,0,-5.927481725,-1.5287854914,-3.0554740514 H,0,-3.9813050862,-2.3830957424,-1.7861386225 O,0,-3.5359957004,2.0255817437,-4.5775255003 H,0,-4.3852455254,2.2106399729,-5.0022759723 O,0,3.4295621992,3.3269955814,-1.0510530464 C,0,3.1590842593,3.5572623059,0.3323247728 H,0,2.6551704895,4.5222669159,0.38772922 H,0,2.5018261172,2.7859251225,0.7490565225 H,0,4.0802134497,3.5972969597,0.9230561735 H,0,-1.6300976849,0.9505464006,-3.1747149469 O,0,-5.8821050851,0.7350520932,-4.5537001376 H,0,-6.6925161214,0.2164516947,-4.4840021302

P C1(•OCH_3), optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.51324918 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234115 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1025.1042701 a.u.	**P C2(•OCH_3),** optimization in gas phase UB3LYP/6-311++G**, E= -1025.50346335 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.233887 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1025.0923788 a.u.
0, 2 C,0,5.9021828299,0.9812648287,0.1353183862 C,0,5.071438855,-0.1209060113,0.4610127845 C,0,5.5024497387,1.9982870715,-0.6928568118	0, 2 C,0,5.7681881308,0.3478093792,0.4832883594 C,0,4.9245149709,-0.7141096005,0.5627333554 C,0,5.4015254473,1.6742123155,-0.1413116404

H,0,5.4099141952,-0.9097888443,1.1199674148	H,0,5.2267778447,-1.6435465805,1.0327285926
C,0,3.7799381052,-0.1532312577,-0.1104679452	C,0,3.6209272629,-0.6051397845,0.0069146495
C,0,4.1408898383,2.0670153614,-1.339154923	C,0,4.0251383155,1.7097081547,-0.7508547537
H,0,4.2547075113,2.1145718115,-2.431886887	H,0,3.712715772,2.6177996162,-1.2531926315
C,0,3.3525247051,0.8682772967,-0.9485474636	C,0,3.2253437978,0.6133150994,-0.6343743138
C,0,1.7946328073,-0.670093721,-0.709970847	C,0,1.6322511451,-0.9304447085,-0.6794864336
N,0,2.7816871996,-1.116830778,0.0295245916	N,0,2.613473836,-1.5354482417,-0.0394630533
N,0,2.0725089381,0.5184579387,-1.3343974322	N,0,1.9195778853,0.3505518924,-1.0665443937
H,0,1.426910768,1.0388478096,-1.9092089122	H,0,1.2872108381,0.9565700679,-1.5633545266
N,0,0.5918443143,-1.3099763814,-0.8744313397	N,0,0.4284386047,-1.5163606378,-0.9435289379
N,0,-0.3949204225,-0.7266983316,-1.5929835984	N,0,-0.538845493,-0.8435381064,-1.6029910002
C,0,-1.5352904981,-1.3162597863,-1.6422757443	C,0,-1.6506432297,-1.4516605188,-1.8257160042
H,0,-1.7020542759,-2.2573343073,-1.1075792993	H,0,-1.7995460772,-2.4835700892,-1.4884105501
H,0,0.4322528863,-2.1508839788,-0.3281864494	H,0,0.3008462485,-2.4716742589,-0.6223899147
H,0,6.1745936201,2.8189775778,-0.9179007612	H,0,6.1468400877,1.9176349034,-0.9108830641
C,0,-2.6667869677,-0.7835539532,-2.3959185048	C,0,-2.7664780412,-0.8265782977,-2.5254652777
C,0,-3.8830695121,-1.4784797592,-2.3709049447	C,0,-3.9412760834,-1.5645306884,-2.7234483097
C,0,-2.5752748569,0.4042781599,-3.1422431117	C,0,-2.7001404994,0.4926058109,-3.0067435831
C,0,-4.9889564585,-1.0003437588,-3.0723674882	C,0,-5.0290500597,-1.0002833582,-3.3870480743
C,0,-3.6710117123,0.8815492333,-3.8391059888	C,0,-3.7781952256,1.0557602728,-3.6658065273
C,0,-4.8874610101,0.1749259412,-3.8034576805	C,0,-4.9511614922,0.3028443103,-3.8569975893
H,0,6.9012426812,1.0170337686,0.5580579264	H,0,6.7684657719,0.2873430024,0.8985099322
H,0,-5.9289174485,-1.5423286367,-3.0491449505	H,0,-5.9370671021,-1.5760453542,-3.5377483745
H,0,-3.9701267183,-2.3968849441,-1.8015453985	H,0,-4.0092513138,-2.5833247347,-2.3591666507
O,0,-3.5663103141,2.0358941104,-4.5577980145	O,0,-3.6977695575,2.3349487662,-4.1253860229
H,0,-4.4186594144,2.2197073261,-4.9750267017	H,0,-4.532923563,2.5624933141,-4.5543260072
O,0,3.4465481762,3.3193952783,-1.0747152546	O,0,5.6137313213,2.7739269795,0.7929895215
C,0,3.1607346635,3.5741041822,0.2989126543	C,0,4.7880335234,2.7564228801,1.9498847304
H,0,2.6439299726,4.5335930167,0.3279903223	H,0,5.0637954944,3.6362221139,2.5325333928
H,0,2.5104892676,2.8027899525,0.7279924328	H,0,3.7236310358,2.8162860078,1.6929328302
H,0,4.0753060054,3.6381258713,0.8982358119	H,0,4.9530639654,1.8582376384,2.5569038633
H,0,-1.6471258786,0.9596443546,-3.1797342371	O,0,-5.9607027949,0.9561684226,-4.5224355328
O,0,-5.9085429948,0.7364261672,-4.5282470208	H,0,-6.7320546761,0.3882903006,-4.6157959871
H,0,-6.7140181963,0.2135109817,-4.4519001041	H,0,-1.8048426011,1.0839263116,-2.8672051431

P C2(•OCH_3), optimization in solv. water UB3LYP/6-311++G**, E= -1025.52489203 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.233621 a.u. SP at UM06-2X/6-311++G** (water), E = -1025.1149363 a.u.	**P C2(•OCH_3),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.51271484 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.233968 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1025.1021436 a.u.
0, 2	0, 2
C,0,5.7786768582,0.3640756295,0.4491011831	C,0,5.7730184123,0.3561119567,0.4665893129
C,0,4.9410368894,-0.7041909215,0.547761979	C,0,4.9324989362,-0.7089822796,0.5545148517
C,0,5.3865321922,1.6853773813,-0.1666204432	C,0,5.3941395692,1.68080626,-0.1526341855
H,0,5.2636680192,-1.628017311,1.0165299186	H,0,5.2443813341,-1.6362642665,1.0229383549
C,0,3.6292283102,-0.6070505799,0.0115933535	C,0,3.6246937897,-0.6054024281,0.0086946311
C,0,4.0128987573,1.7006853296,-0.7772547845	C,0,4.0184293653,1.7071076413,-0.7616902916
H,0,3.6873847571,2.5947667011,-1.2956816626	H,0,3.6995131306,2.609086807,-1.2707838582
C,0,3.2194757781,0.6015641755,-0.6390320805	C,0,3.2220004384,0.6089392934,-0.6355316355
C,0,1.6306340631,-0.9490864897,-0.662572095	C,0,1.6314286029,-0.9385307693,-0.6712792474
N,0,2.6255774456,-1.545312136,-0.0198263174	N,0,2.6191210267,-1.5396511302,-0.0310755961
N,0,1.9153040479,0.3272801606,-1.0607635316	N,0,1.9166467306,0.3409855022,-1.0621531538
H,0,1.2791656412,0.9332615011,-1.5558522173	H,0,1.2825415461,0.9465743338,-1.5585513968
N,0,0.4312459108,-1.5349024466,-0.9139858115	N,0,0.4293152331,-1.5245010462,-0.9296592797

N,0,-0.5328758196,-0.8522043768,-1.5819716258	N,0,-0.5365623132,-0.8472063414,-1.5929482296
C,0,-1.6460825358,-1.4581450514,-1.8027583873	C,0,-1.6488872688,-1.4540878082,-1.815318541
H,0,-1.8035236663,-2.4862225189,-1.4642219646	H,0,-1.8017556509,-2.4844989116,-1.4778632609
H,0,0.2909203103,-2.4896189257,-0.5953998511	H,0,0.297162271,-2.4804429162,-0.6119667148
H,0,6.1312752348,1.9615462356,-0.9244391724	H,0,6.1386816807,1.9396552024,-0.917374306
C,0,-2.7539808682,-0.8234056326,-2.5083608092	C,0,-2.761312086,-0.8249437211,-2.5178217245
C,0,-3.9328497785,-1.5541897041,-2.7113035297	C,0,-3.9386678728,-1.558961576,-2.7156942281
C,0,-2.6766336751,0.4962140749,-2.990882998	C,0,-2.6892740262,0.493321857,-3.0021272908
C,0,-5.0151384176,-0.9858828205,-3.381135319	C,0,-5.0239969657,-0.9931921879,-3.3823791855
C,0,-3.7494946513,1.0621658268,-3.6555460725	C,0,-3.7648293621,1.0575757971,-3.6639494657
C,0,-4.9284674849,0.317495411,-3.8537989494	C,0,-4.9413031484,0.309067779,-3.8560282448
H,0,6.7868916863,0.3065333138,0.8452588791	H,0,6.7771711925,0.2971556893,0.8725590707
H,0,-5.9252055752,-1.5552565649,-3.5364238934	H,0,-5.9335667475,-1.5657143664,-3.5331803768
H,0,-4.0082102021,-2.5717544915,-2.3457454177	H,0,-4.010572372,-2.5764252182,-2.3487366869
O,0,-3.6604683023,2.344420274,-4.1183157877	O,0,-3.6795079087,2.3370453035,-4.127398413
H,0,-4.4926429447,2.5771602816,-4.5532973463	H,0,-4.5132277645,2.5670046126,-4.5591899261
O,0,5.5702823256,2.7850329339,0.793795178	O,0,5.5939422074,2.7797312737,0.794081785
C,0,4.7254949301,2.7368697413,1.9417523303	C,0,4.7619899398,2.7455830609,1.9484288303
H,0,4.9739900212,3.6120750198,2.5431457534	H,0,5.0249817552,3.6231697446,2.5401840987
H,0,3.6658936651,2.7807934232,1.6670533583	H,0,3.699013512,2.7964838894,1.6856161809
H,0,4.9003606404,1.8333152878,2.5365118895	H,0,4.9340397166,1.8444423607,2.5484404489
O,0,-5.9248498008,0.9745251398,-4.5225976544	O,0,-5.944767841,0.9637237362,-4.5236215526
H,0,-6.703433423,0.4147420824,-4.628284927	H,0,-6.7202445151,0.4004349564,-4.6210806386
H,0,-1.7775368489,1.0821626468,-2.8470862435	H,0,-1.7916910572,1.0816205096,-2.8626652049

P C4(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.50514847 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.233733 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1025.0954065 a.u.	**P C4(•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.52775509 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234171 a.u. SP at UM06-2X/6-311++G** (water), E = -1025.1191434 a.u.
0, 2	0, 2
C,0,5.8844433875,0.8402769427,0.3715926747	C,0,5.8736913968,0.8454315898,0.3748262977
C,0,4.9967400324,-0.2776308026,0.8693336437	C,0,4.9938987586,-0.2751088519,0.8738404158
C,0,5.4744119421,1.822470581,-0.4847694283	C,0,5.4514252893,1.822848039,-0.4832439203
H,0,5.447450905,-1.2468659624,0.6177862582	H,0,5.4599638681,-1.2433987571,0.6481137653
C,0,3.639075696,-0.1842786764,0.2442868117	C,0,3.6409669285,-0.2029806306,0.2410470837
C,0,4.1565141544,1.8738428265,-1.0217956105	C,0,4.1323764344,1.8617644066,-1.0203093749
H,0,3.8551230087,2.6631250603,-1.6984780141	H,0,3.8206582092,2.6462578764,-1.6973681442
C,0,3.2892183328,0.848406461,-0.6296281157	C,0,3.276818822,0.8260123378,-0.6305500232
C,0,1.6239195837,-0.5671584081,-0.3231417394	C,0,1.6248313257,-0.6108543287,-0.3334100425
N,0,2.5979836848,-1.0571029348,0.421653313	N,0,2.6112951199,-1.0918140757,0.4154658105
N,0,1.9644275693,0.5761694798,-0.9811471773	N,0,1.9580656284,0.5366294658,-0.9841433945
H,0,1.3581553639,1.0883524512,-1.6017758036	H,0,1.3504007977,1.0507819897,-1.6041735157
N,0,0.3850980982,-1.1406024252,-0.4289346876	N,0,0.3983285308,-1.1943624301,-0.4488005595
N,0,-0.5563600418,-0.6033869471,-1.2318632789	N,0,-0.5456674033,-0.6363013381,-1.2456864869
C,0,-1.699616695,-1.1883141511,-1.3000910977	C,0,-1.6899043151,-1.2196650062,-1.3143896887
H,0,-1.8972471691,-2.0963688871,-0.7194703167	H,0,-1.8892165052,-2.1329441948,-0.7463503773
H,0,0.2253447267,-1.992552947,0.1002872416	H,0,0.2224473963,-2.0452255524,0.0773899442
H,0,6.1776901734,2.5960645908,-0.7758584524	H,0,6.1478000341,2.6012910457,-0.7779619889
C,0,-2.790226053,-0.6969085822,-2.1347627531	C,0,-2.7793682325,-0.7094830804,-2.1405761131
C,0,-4.0075360942,-1.3908186261,-2.1368609729	C,0,-4.0011930011,-1.3964404511,-2.1469352739
C,0,-2.6581188021,0.4504507698,-2.9358973278	C,0,-2.6431430743,0.4484258872,-2.928417513
C,0,-5.0729708955,-0.951130353,-2.9204158831	C,0,-5.0684644317,-0.9424167247,-2.9204297606
C,0,-3.7136363808,0.8897131039,-3.714837185	C,0,-3.7009556442,0.9006547594,-3.6964945712

C,0,-4.930023892,0.1831697924,-3.7062701466	C,0,-4.9237030282,0.2021118265,-3.6937576472
H,0,6.8981617978,0.8416003347,0.7570257177	H,0,6.8906611724,0.8551493387,0.7520350276
H,0,-6.0140045195,-1.492575834,-2.9184091328	H,0,-6.012108778,-1.4772490364,-2.9229780822
H,0,-4.1266340175,-2.2778348015,-1.5250814373	H,0,-4.1223244683,-2.2898554661,-1.5452741102
O,0,-3.5689975381,2.0035639141,-4.4852035332	O,0,-3.55462308,2.0265806401,-4.4566105115
H,0,-4.3969780221,2.1627343909,-4.956752812	H,0,-4.3854515412,2.1981904441,-4.9215425523
O,0,4.9705741762,-0.3373897058,2.3155803636	O,0,4.942360116,-0.3183835126,2.3327926512
C,0,4.3430192253,0.7643627688,2.9562891718	C,0,4.3384467352,0.8169965432,2.9500315652
H,0,4.8223678894,1.7166076203,2.698154532	H,0,4.8732056467,1.742074039,2.7085596863
H,0,3.2765048787,0.8237866181,2.7083672185	H,0,3.2884984507,0.9257152507,2.6559938228
H,0,4.4479304137,0.5910499554,4.027921467	H,0,4.3901625335,0.6450744884,4.025530138
H,0,-1.7286732916,1.0040950941,-2.9530411552	H,0,-1.7100011501,0.9974597256,-2.9413741522
O,0,-5.912043156,0.7038955638,-4.5150090299	O,0,-5.9007924485,0.736770401,-4.4888389273
H,0,-6.7168354419,0.1794919047,-4.4559949623	H,0,-6.7151330626,0.222573522,-4.4332211171

P C4(•OCH_3), optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.51471022 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234258 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1025.1054938 a.u.	**P C6(•OCH_3),** optimization in gas phase UB3LYP/6-311++G**, E= -1025.51029220 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234501 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1025.1004993 a.u.
0, 2	0, 2
C,0,5.8786925072,0.8447272634,0.3870932875	C,0,6.1442633422,0.217355704,-0.1993709676
C,0,4.9926211818,-0.271372672,0.8891110854	C,0,5.1835386437,-0.655646765,0.2683208709
C,0,5.4682780751,1.815772012,-0.4825880461	C,0,5.786948481,1.4149005648,-0.864365719
H,0,5.4565499853,-1.2415925794,0.6683155171	H,0,5.4428955637,-1.572504147,0.7832868695
C,0,3.6444438654,-0.2008226322,0.243121302	C,0,3.816915125,-0.3275244021,0.0709008994
C,0,4.1547413431,1.8524441675,-1.032180615	C,0,4.455931274,1.7666425195,-1.0871662
H,0,3.8525877013,2.6328353138,-1.7185930495	H,0,4.1995680948,2.6827117541,-1.6059024591
C,0,3.2930160439,0.8219580948,-0.6415209013	C,0,3.4756723137,0.8948727881,-0.6237427307
C,0,1.6369955204,-0.6082152353,-0.3456242284	C,0,1.5927264905,-0.2054268372,0.0611553172
N,0,2.6105914127,-1.0840332541,0.4149190124	N,0,2.7405160198,-1.0086247132,0.4493368046
N,0,1.9759790652,0.533489438,-1.0057553884	N,0,2.1187982439,0.921256688,-0.7089628401
H,0,1.3729529717,1.0394507543,-1.6355712453	H,0,1.5629517717,1.7543175317,-0.8250522026
N,0,0.4080800679,-1.193747035,-0.4670142714	N,0,0.7434308649,-1.0508570517,-0.740022101
N,0,-0.5373565322,-0.6405329273,-1.25926774	N,0,-0.3827208109,-0.4999351785,-1.25145846
C,0,-1.6827895578,-1.2213997708,-1.3255063516	C,0,-1.2879001967,-1.2777440229,-1.7176666609
H,0,-1.8805633937,-2.1344899962,-0.7544839852	H,0,-1.1685628164,-2.367796593,-1.6796953376
H,0,0.2352473775,-2.0363794897,0.0730325609	H,0,0.7530342224,-2.0350816315,-0.4868960456
H,0,6.1688420119,2.5910493005,-0.7758453264	H,0,6.5721818542,2.0754832843,-1.2138385602
C,0,-2.7767252984,-0.7127750495,-2.1460603896	C,0,-2.5194129422,-0.7771161833,-2.3292237725
C,0,-3.9979135066,-1.4001647841,-2.1482129379	C,0,-3.4538157949,-1.6923251463,-2.8290713026
C,0,-2.6452474785,0.4466020485,-2.9307453849	C,0,-2.7923967715,0.5975178002,-2.4271140515
C,0,-5.0687994949,-0.9429649333,-2.9145778172	C,0,-4.6377852934,-1.2485480669,-3.4174256742
C,0,-3.7063657274,0.903268243,-3.6914821068	C,0,-3.9658955978,1.041574857,-3.010905154
C,0,-4.9279726275,0.204551837,-3.6826623858	C,0,-4.8946566371,0.1112117926,-3.509278379
H,0,6.8900608141,0.856698609,0.778722157	H,0,7.194342195,-0.0100938821,-0.0574426129
H,0,-6.0119297356,-1.4799426144,-2.9141507402	H,0,-5.3587015757,-1.9625681652,-3.8042222353
H,0,-4.1159996136,-2.2959150493,-1.5491863075	H,0,-3.258119654,-2.756662542,-2.7621182494
O,0,-3.5636361266,2.0304085779,-4.4460251318	O,0,-4.2162827262,2.3790815919,-3.0993199272
H,0,-4.3972213787,2.2047815154,-4.9033651325	H,0,-5.0718431156,2.5028875041,-3.5301686858
O,0,4.937339494,-0.3028694551,2.3411256375	O,0,0.9390160842,0.3828138512,1.1758611278
C,0,4.3055220879,0.8191082148,2.9465164435	C,0,0.3449387645,-0.5284724317,2.100461921
H,0,4.8074976186,1.7589725402,2.6883607192	H,0,-0.481813647,-1.0802572723,1.6409770895
H,0,3.2490138765,0.8902588006,2.662962408	H,0,1.0847122291,-1.2284558698,2.4971638345

H,0,4.3734520702,0.6621572733,4.0235530232	H,0,-0.0481398882,0.0858824468,2.9097456911
H,0,-1.712942025,0.9958846231,-2.947047166	H,0,-2.0854148399,1.3221310977,-2.0445926043
O,0,-5.9126914557,0.7446775676,-4.4706093849	O,0,-6.0281049262,0.657720516,-4.0687517858
H,0,-6.7300981095,0.2404314628,-4.39596876	H,0,-6.6141101546,-0.0341526903,-4.3907766368

P C6(•OCH_3), optimization in solv. water UB3LYP/6-311++G**, E= -1025.52991152 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235149 a.u. SP at UM06-2X/6-311++G** (water), E = -1025.1219256 a.u.	**P C6(•OCH_3),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.51834402 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234979 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1025.1093228 a.u.
0, 2	0, 2
C,0,6.1512783434,0.2776501819,-0.1809949217	C,0,6.1484225377,0.2406927921,-0.1912569406
C,0,5.2071852217,-0.6184925817,0.2770570525	C,0,5.1938934518,-0.6402670125,0.2744482855
C,0,5.7718473155,1.4740892949,-0.8403654648	C,0,5.782852363,1.4366265885,-0.8565690688
H,0,5.4882500888,-1.5326497189,0.7860850418	H,0,5.4616483965,-1.5551948381,0.7888098119
C,0,3.8343060715,-0.3166948711,0.0742135808	C,0,3.8247921347,-0.3227713153,0.0740551638
C,0,4.4357049766,1.801373238,-1.0658741962	C,0,4.4499537208,1.7788024646,-1.080952512
H,0,4.1603649555,2.7165728552,-1.5755512843	H,0,4.186192446,2.6936623545,-1.5978286231
C,0,3.471813332,0.9040847218,-0.6125924737	C,0,3.4756742617,0.8982030511,-0.6195209237
C,0,1.6039043632,-0.2421635136,0.0441807124	C,0,1.5979873303,-0.2191142398,0.0541351435
N,0,2.7670797877,-1.0220587439,0.4403551161	N,0,2.7516340452,-1.0125510097,0.4482788565
N,0,2.1161483217,0.905727204,-0.6991028933	N,0,2.1198525581,0.9158187859,-0.7035578162
H,0,1.5459233887,1.7209428906,-0.8664263194	H,0,1.5561302109,1.7383919737,-0.85323781
N,0,0.7837568428,-1.0895480521,-0.7907486057	N,0,0.7627472048,-1.0650982653,-0.7641134368
N,0,-0.3443852906,-0.5051192007,-1.3004062062	N,0,-0.3645212044,-0.4991407061,-1.2733214325
C,0,-1.2879596114,-1.2735523839,-1.70319938	C,0,-1.2866688409,-1.2734600374,-1.7113844232
H,0,-1.2106105728,-2.3615336839,-1.6034488706	H,0,-1.1847768575,-2.3633431159,-1.6469708715
H,0,0.7041959458,-2.0460622884,-0.4517859568	H,0,0.7288132603,-2.0373201367,-0.4677116947
H,0,6.5454266235,2.1523872564,-1.1810887658	H,0,6.5637993995,2.1031914077,-1.2040793059
C,0,-2.5151120621,-0.7630153502,-2.3170952309	C,0,-2.5169410313,-0.7695870166,-2.3235670581
C,0,-3.5027681008,-1.6735641591,-2.7143388171	C,0,-3.4700234003,-1.6849771772,-2.7871074483
C,0,-2.7360182599,0.6112764977,-2.5178472904	C,0,-2.7721117567,0.6059215491,-2.4577137171
C,0,-4.6883860077,-1.2291166523,-3.2994192679	C,0,-4.6548648965,-1.2420777965,-3.3746330071
C,0,-3.9112415565,1.0551316737,-3.0984173493	C,0,-3.9465351906,1.0487070371,-3.0406092442
C,0,-4.8964904387,0.1302108246,-3.4922201159	C,0,-4.8952468903,0.1185155833,-3.502233313
H,0,7.2051593421,0.0710987183,-0.0364330645	H,0,7.1999884686,0.0213658516,-0.0478101444
H,0,-5.4495499872,-1.9385786589,-3.6059717686	H,0,-5.3897524435,-1.9558515719,-3.7332255203
H,0,-3.3480043165,-2.7364196468,-2.5676036176	H,0,-3.2880256692,-2.7495912697,-2.6924936568
O,0,-4.1102286558,2.3944118701,-3.2877058655	O,0,-4.179630184,2.3881872568,-3.1643291929
H,0,-4.9738302083,2.5243838241,-3.7037385675	H,0,-5.0390200034,2.5136417093,-3.5884349449
O,0,0.9195819201,0.3079665267,1.1667611192	O,0,0.9285201026,0.352416865,1.1709990714
C,0,0.3221980124,-0.6382372102,2.0627921981	C,0,0.3326642641,-0.5740994744,2.08238538
H,0,-0.4795624269,-1.1995631084,1.5745609612	H,0,-0.4779539856,-1.1356379466,1.6072531194
H,0,1.0673838011,-1.3294061822,2.4626209571	H,0,1.0760372493,-1.2651745572,2.4869939233
H,0,-0.1014780011,-0.0500334082,2.8755650254	H,0,-0.0819660773,0.0291415036,2.8890535421
H,0,-1.9880948112,1.3356118452,-2.2204718148	H,0,-2.0509921344,1.3318877705,-2.1047271103
O,0,-6.0188009484,0.6777009589,-4.0554195517	O,0,-6.0247938642,0.6643003556,-4.0630684365
H,0,-6.6522832084,-0.0062422676,-4.3032650345	H,0,-6.631074786,-0.025648713,-4.3532955745

P C9(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.49580665 a.u.	**P C9(•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.51620046 a.u.

Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235370 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1025.0863389 a.u.	Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235187 a.u. SP at UM06-2X/6-311++G** (water), E = -1025.1080594 a.u.
0, 2 C,0,5.7170428238,0.1620114972,-0.3303027924 C,0,4.6514212049,-0.7207176693,-0.1426852031 C,0,5.4978287664,1.4871948015,-0.8297081108 H,0,4.8217232952,-1.7720086362,0.0601204864 C,0,3.362283114,-0.2611715,-0.3601458105 C,0,4.2484879054,1.9943538476,-1.0180410516 H,0,4.0841008452,2.99130663,-1.4109207849 C,0,3.0744268863,1.2225148594,-0.5193314055 C,0,1.3912103129,-0.1241367169,-1.1480000086 N,0,2.2277102343,-0.9888519311,-0.6110419585 N,0,1.8766163335,1.1450750665,-1.3492757725 H,0,1.2277972646,1.9208802971,-1.3481126564 N,0,0.1423568373,-0.4851605581,-1.540990712 N,0,-0.722018695,0.419398341,-2.0559603981 C,0,-1.8845862004,-0.0018581706,-2.4049358254 H,0,-2.1570800006,-1.056866359,-2.2855837887 H,0,-0.1174429025,-1.4579123072,-1.4008489611 H,0,6.3627980202,2.0883745881,-1.0909484871 C,0,-2.9019328016,0.874026825,-2.9751751564 C,0,-4.1468383075,0.3317269555,-3.3198008358 C,0,-2.6668012177,2.2425099981,-3.1931605996 C,0,-5.1414377896,1.1373623639,-3.8709195346 C,0,-3.6521285305,3.045094339,-3.739789767 C,0,-4.8979595887,2.487090788,-4.0809865314 H,0,6.7340500664,-0.1841145286,-0.1890689266 H,0,-6.1050768962,0.7138236322,-4.1367389969 H,0,-4.3424960597,-0.7223392796,-3.1587281394 O,0,-3.4105866492,4.368875694,-3.945760336 H,0,-4.1989808778,4.7709520967,-4.3329973946 O,0,2.5675610017,1.8286423529,0.7269255375 C,0,3.4269046515,1.8150941553,1.8621150954 H,0,3.6311813384,0.7935931743,2.1992590378 H,0,4.3748779668,2.3253442836,1.6639851414 H,0,2.8897372173,2.3506365531,2.6457864402 O,0,-5.8038942324,3.3702984697,-4.6168105686 H,0,-6.6282237087,2.9243674652,-4.8355822497 H,0,-1.7117330482,2.6825814819,-2.9380482649	0, 2 C,0,5.7127013239,0.1766771306,-0.3533556218 C,0,4.6555770609,-0.7160476779,-0.1510234191 C,0,5.4755211717,1.4981009199,-0.8537571507 H,0,4.8433779926,-1.7637836486,0.057572351 C,0,3.3594625332,-0.2689613245,-0.3555406618 C,0,4.2179111266,1.9934556824,-1.0286365079 H,0,4.0388724896,2.9879921835,-1.4215496614 C,0,3.058524408,1.2102558702,-0.5156073228 C,0,1.367996346,-0.1472111441,-1.1196229793 N,0,2.2240121909,-1.0056840409,-0.5848780655 N,0,1.8535511883,1.1207443058,-1.3276691701 H,0,1.2098708501,1.9002282263,-1.3678205521 N,0,0.1213197559,-0.5030732279,-1.4977512696 N,0,-0.7292043415,0.4162190851,-2.030457473 C,0,-1.8910756725,-0.0035164483,-2.3871720598 H,0,-2.169505615,-1.0543914641,-2.2668205726 H,0,-0.1574217757,-1.4720897741,-1.3661354871 H,0,6.3317973305,2.107265872,-1.1245467973 C,0,-2.8974625189,0.8772559071,-2.9684146316 C,0,-4.1327944803,0.3318956379,-3.3437171902 C,0,-2.6662277784,2.2510066793,-3.1667765445 C,0,-5.121906549,1.1357728514,-3.9071646495 C,0,-3.6466295895,3.0507280454,-3.7253569822 C,0,-4.8842336963,2.4909047289,-4.0994250285 H,0,6.7339925518,-0.159454919,-0.219694082 H,0,-6.0762657178,0.7105388443,-4.1976286841 H,0,-4.324510924,-0.7247425355,-3.1973244345 O,0,-3.4103580068,4.3826280982,-3.9124003902 H,0,-4.1957695729,4.786316851,-4.3075032781 O,0,2.5648905066,1.8070677221,0.7493788157 C,0,3.4553729462,1.8158259329,1.8651838548 H,0,3.696538353,0.8001880401,2.1942342328 H,0,4.3820817881,2.3531145099,1.6432353312 H,0,2.9261213439,2.3341632128,2.6653232026 O,0,-5.7790093249,3.371155212,-4.6411384454 H,0,-6.6058862235,2.9316124483,-4.8738261598 H,0,-1.7203328914,2.6958351073,-2.8844218059

P C9(•OCH$_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.50445197 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235529 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1025.0955407 a.u.	**P C13(•OCH$_3$),** optimization in gas phase UB3LYP/6-311++G**, E= -1025.53406681 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.237084 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1025.1280253 a.u.
0, 2 C,0,5.7160668047,0.1718440847,-0.336605237 C,0,4.6548757402,-0.716789428,-0.1457291791 C,0,5.4883597506,1.4956530534,-0.8353959452 H,0,4.8335418526,-1.7666841444,0.0581371437 C,0,3.3625267835,-0.2641612849,-0.359601665 C,0,4.2350910574,1.9962381814,-1.0196226105 H,0,4.0637189468,2.992080656,-1.4124724722	0, 2 C,0,5.8998500043,0.8490943434,0.3724966043 C,0,4.8740070983,0.2525003426,1.0987482747 C,0,5.7255513208,1.2251223967,-0.970286046 H,0,5.0053555534,-0.037369226,2.134311111 C,0,3.652819693,0.0339782172,0.4553214808 C,0,4.5163808473,1.0152575564,-1.6317391624 H,0,4.3845102289,1.3066099214,-2.6673850574

C,0,3.0673950405,1.2174182551,-0.5178233108	C,0,3.4957192199,0.4185521117,-0.9001372248
C,0,1.38423796,-0.1352222298,-1.1410857706	C,0,1.6584365969,-0.4853903877,-0.0818204794
N,0,2.2292161183,-0.9970059789,-0.6048069499	N,0,2.481173407,-0.5292935288,0.939123318
N,0,1.8682363394,1.134311356,-1.3421701916	N,0,2.191715589,0.0624697744,-1.2182399486
H,0,1.2202953346,1.9108143633,-1.3596251116	H,0,1.6799790133,0.1956005073,-2.0768000929
N,0,0.1372408725,-0.4946373853,-1.5303826894	N,0,0.3697100826,-0.9525184082,-0.059185685
N,0,-0.7217809797,0.4173582731,-2.0504530346	N,0,-0.4256155493,-0.7776997533,-1.1182039256
C,0,-1.8850146857,-0.0018717871,-2.4004835272	C,0,-1.7087770757,-1.4251265414,-0.9363344214
H,0,-2.1611162956,-1.0548179719,-2.2801449659	H,0,-1.5943502581,-2.5025891212,-1.1592092858
H,0,-0.1303447389,-1.4661076035,-1.3954654336	H,0,-0.0167490676,-1.2416749769,0.8370532611
H,0,6.3492702614,2.1015713045,-1.0990457302	H,0,6.5474872041,1.6883462398,-1.5037921145
C,0,-2.8985875156,0.8763368,-2.9736539542	C,0,-2.7187683684,-0.8324090789,-1.8977499557
C,0,-4.1433564875,0.3344465636,-3.3201679751	C,0,-3.2759682602,-1.610183103,-2.9088560541
C,0,-2.6623884901,2.2451079412,-3.1921924631	C,0,-3.0915302247,0.50941318,-1.7705970936
C,0,-5.1371322656,1.1393079109,-3.8738799453	C,0,-4.1987865916,-1.054043328,-3.798577329
C,0,-3.6470267529,3.0464555755,-3.7413943646	C,0,-4.0098227859,1.0678884362,-2.6470005224
C,0,-4.8934645445,2.4895155584,-4.0852149746	C,0,-4.5631389648,0.277386079,-3.6678631696
H,0,6.7351385843,-0.1690178693,-0.1974983571	H,0,6.8559352872,1.0298362881,0.8503754648
H,0,-6.1001406365,0.7164831909,-4.1409142415	H,0,-4.6323565035,-1.6585476154,-4.5895821955
H,0,-4.3394251337,-0.7193124895,-3.158211197	H,0,-2.9911741244,-2.6509414221,-3.0157754228
O,0,-3.4048757901,4.3718600419,-3.9480891928	O,0,-4.3665119231,2.3762732453,-2.5147549042
H,0,-4.1929711875,4.7750091508,-4.3363235826	H,0,-5.0019275954,2.5932701931,-3.2092612114
O,0,2.5634691132,1.8181240476,0.7364618534	O,0,-2.1029340791,-1.3022783558,0.4363647683
C,0,3.4335309677,1.8101052954,1.8653596448	C,0,-3.2070318872,-2.1169368573,0.8096529697
H,0,3.6506607377,0.7899022067,2.1977227801	H,0,-4.1166203713,-1.8268214167,0.2736543225
H,0,4.3742344015,2.3303354773,1.6599871434	H,0,-2.9993075507,-3.177726282,0.6170180428
H,0,2.8990168149,2.337982958,2.6559160541	H,0,-3.3557495944,-1.9683504387,1.8788948287
O,0,-5.7958780327,3.3709097737,-4.6224009182	O,0,-5.4621670309,0.9256713832,-4.4844749341
H,0,-6.623799668,2.9287541943,-4.840111092	H,0,-5.7823146576,0.3352491294,-5.1735103423
H,0,-1.7079216973,2.6856948593,-2.9348278271	H,0,-2.6680172423,1.1301275061,-0.9903923682

P C13(•OCH_3), optimization in solv. water UB3LYP/6-311++G**, E= -1025.55337702 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.236588 a.u. SP at UM06-2X/6-311++G** (water), E = -1025.148308 a.u.	**P C13(•OCH_3),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.54221526 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.237002 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1025.1366004 a.u.
0, 2	0, 2
C,0,5.9148137164,0.8181448574,0.3992895966	C,0,5.9072295545,0.8347055201,0.3802045449
C,0,4.8819624983,0.2177181947,1.1154177697	C,0,4.8795928423,0.2353612169,1.1029344094
C,0,5.7442267404,1.2193506534,-0.9378389731	C,0,5.7323852396,1.2234192625,-0.9593186118
H,0,5.0156348334,-0.0901825345,2.1460300508	H,0,5.0133704581,-0.0634185823,2.1358925179
C,0,3.658737343,0.0221080729,0.4660704823	C,0,3.6565529979,0.0273059776,0.4586543626
C,0,4.5325450002,1.0325083799,-1.6035837695	C,0,4.521067576,1.0240312017,-1.6209568764
H,0,4.4000368629,1.3413977266,-2.6335152918	H,0,4.3872569998,1.3249296524,-2.6534408075
C,0,3.5060001356,0.4322421272,-0.8818449129	C,0,3.4992066644,0.4244073963,-0.8929181138
C,0,1.6551533719,-0.469776289,-0.0908885253	C,0,1.6573144601,-0.4797853843,-0.0845380495
N,0,2.4787729639,-0.5398128576,0.9356313307	N,0,2.4821702515,-0.5362209459,0.9373902082
N,0,2.1999237884,0.097378541,-1.2087050187	N,0,2.1940661754,0.0771385145,-1.2134715895
H,0,1.7134430153,0.2372686222,-2.0818268154	H,0,1.69041203,0.2173805683,-2.0761909846
N,0,0.3647723407,-0.9260137031,-0.0750104049	N,0,0.3679531426,-0.9425296355,-0.0640830528
N,0,-0.4381997949,-0.7310500251,-1.1246570145	N,0,-0.4286963851,-0.7642495339,-1.1216228546
C,0,-1.7219224495,-1.3877904155,-0.9400330124	C,0,-1.7136672036,-1.4126676981,-0.9372064617
H,0,-1.5958830118,-2.4635045593,-1.1517952172	H,0,-1.5962107234,-2.4895287589,-1.1567954727
H,0,-0.0153287158,-1.2681303647,0.8059312262	H,0,-0.0183747491,-1.2471723303,0.8274392001

H,0,6.5707830811,1.6835924306,-1.4631937582	H,0,6.5552932126,1.6882957142,-1.4898951179
C,0,-2.7327998764,-0.8105727979,-1.9092199339	C,0,-2.7237735992,-0.8247254984,-1.9012034982
C,0,-3.3022070619,-1.6087823465,-2.8984085791	C,0,-3.2855316895,-1.6102079823,-2.9041685497
C,0,-3.1017981676,0.5362885647,-1.8119079306	C,0,-3.0949374243,0.5191448987,-1.7852808655
C,0,-4.2315708238,-1.072052527,-3.7941332627	C,0,-4.2108445529,-1.0614644726,-3.796134837
C,0,-4.0255984905,1.0745557726,-2.6948124597	C,0,-4.0152502504,1.0698528498,-2.6643616136
C,0,-4.5931735171,0.264285276,-3.6936468425	C,0,-4.5742033095,0.2718787529,-3.6769095056
H,0,6.8721508199,0.9810116155,0.8811314954	H,0,6.8645501147,1.0074213743,0.8586549033
H,0,-4.6744603804,-1.6931185097,-4.5654857902	H,0,-4.6481715631,-1.6718359485,-4.5798435959
H,0,-3.0257883926,-2.6538591033,-2.9810967727	H,0,-3.0037955522,-2.652648333,-3.002199912
O,0,-4.3783779771,2.3914306884,-2.5900226092	O,0,-4.3705751055,2.3817533518,-2.542647464
H,0,-5.0262866157,2.5942590347,-3.2791711531	H,0,-5.0093743288,2.5938900227,-3.2363659576
O,0,-2.1172526318,-1.2502137388,0.4304483786	O,0,-2.1059421871,-1.2844213758,0.4346642024
C,0,-3.1663384074,-2.132373016,0.8303927439	C,0,-3.1943974291,-2.1196416711,0.8175901309
H,0,-4.0939328516,-1.9162932404,0.2912423103	H,0,-4.1103082291,-1.8503925903,0.282025785
H,0,-2.8850352344,-3.1779608359,0.6604778123	H,0,-2.9649583239,-3.1762928391,0.6309719701
H,0,-3.3213073486,-1.967639815,1.8959389986	H,0,-3.342966643,-1.9662149552,1.885921938
O,0,-5.4936885567,0.8952939679,-4.5129525271	O,0,-5.4742197342,0.9125270007,-4.4945936461
H,0,-5.8462898397,0.2880965715,-5.1741684718	H,0,-5.8037178138,0.31612728,-5.1754735939
H,0,-2.6727049262,1.1749425919,-1.0485976488	H,0,-2.6694934825,1.1465949903,-1.0112376407

P C14(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.49174647 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234178 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1025.0853568 a.u.	**P C14(•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.51368150 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.233403 a.u. SP at UM06-2X/6-311++G** (water), E = -1025.1083608 a.u.
0, 2	0, 2
C,0,5.8345671161,0.8143355152,-0.4649799059	C,0,5.8797226387,0.7772221677,-0.4632496039
C,0,5.131924896,-0.3053850578,-0.0247590815	C,0,5.1727072274,-0.3561894091,-0.0600526954
C,0,5.1957638518,1.8553144185,-1.1564406021	C,0,5.2364424349,1.858163757,-1.0875893566
H,0,5.6240388125,-1.109139829,0.5097563823	H,0,5.6731703903,-1.1884001225,0.4218691274
C,0,3.7631718061,-0.3698496154,-0.2895269286	C,0,3.7959699165,-0.3917458786,-0.2938460499
C,0,3.8284167331,1.8094666581,-1.4313420341	C,0,3.8606332248,1.8406786894,-1.3298072746
H,0,3.3355972932,2.614178486,-1.9649534255	H,0,3.3622452202,2.673495734,-1.8117663244
C,0,3.1362750049,0.6891274678,-0.9890397262	C,0,3.1653787103,0.707634785,-0.9248771941
C,0,1.7066397516,-0.9047542578,-0.4511041252	C,0,1.7199863456,-0.8913163169,-0.4367364988
N,0,2.8348440038,-1.3546723683,0.0338906948	N,0,2.861210312,-1.3804270636,0.0011078044
N,0,1.8001730896,0.3086283882,-1.0798517182	N,0,1.8242131122,0.3498242772,-1.0017533578
H,0,1.0233011174,0.8029474717,-1.489523006	H,0,1.0539134326,0.8793097417,-1.3812879385
N,0,0.5100936193,-1.57591127,-0.3705161875	N,0,0.521276465,-1.5433035573,-0.3574093614
N,0,-0.621259097,-0.9759503979,-0.8057430683	N,0,-0.6069000398,-0.926649846,-0.7945317451
C,0,-1.7383513354,-1.5619783449,-0.6227498821	C,0,-1.7190207654,-1.5351383132,-0.6523356109
H,0,-1.825835058,-2.5283720086,-0.1163957839	H,0,-1.7928121261,-2.524303311,-0.1926900757
H,0,0.4914142782,-2.4229024261,0.1887255708	H,0,0.4938006037,-2.4436427948,0.1111532569
H,0,5.7737273006,2.7119087804,-1.4835541272	H,0,5.8164521108,2.7231261585,-1.3880817952
C,0,-3.0417367878,-0.9662148402,-1.1269681054	C,0,-3.0239984792,-0.9398238395,-1.1501357378
C,0,-3.5506928874,-1.8485599249,-2.2415778586	C,0,-3.556226051,-1.8501713776,-2.2286067244
C,0,-2.8929514187,0.4676094466,-1.5430067588	C,0,-2.8851894657,0.4819381185,-1.6042354013
C,0,-3.8368080936,-1.3670984555,-3.4878689229	C,0,-3.8927182527,-1.400198104,-3.4741925806
C,0,-3.2015537393,0.9072064461,-2.7892725797	C,0,-3.2486714862,0.8905312941,-2.8461863471
C,0,-3.6727345324,-0.002979757,-3.7846170044	C,0,-3.7545724714,-0.0402367631,-3.8072064859
H,0,6.8985823095,0.8855992562,-0.2696221931	H,0,6.949122555,0.8257907956,-0.2913288644
H,0,-4.1970053773,-2.0385424244,-4.2632130333	H,0,-4.2731573046,-2.0912141411,-4.2202845021
H,0,-3.6850255926,-2.8987264644,-2.0094111041	H,0,-3.669150392,-2.8972654104,-1.9725000197

O,0,-3.057968772,2.2265262548,-3.1138600687	O,0,-3.1286445645,2.2065036407,-3.2043311842
H,0,-3.3196433164,2.3505484703,-4.0348861719	H,0,-3.4249475602,2.3098918508,-4.1191024267
O,0,-3.9019698349,-1.0957553561,0.0499430105	O,0,-3.8689458717,-1.0278202913,0.0537188964
C,0,-5.2452934686,-0.6517928163,-0.1112629175	C,0,-5.2269206543,-0.6174532892,-0.1140755016
H,0,-5.2928456622,0.4159166351,-0.3507233021	H,0,-5.2960261645,0.4350712219,-0.4071313427
H,0,-5.7709095672,-1.2155715984,-0.8907932243	H,0,-5.7466093693,-1.2307824994,-0.8574417499
H,0,-5.7346758962,-0.826609953,0.8470347359	H,0,-5.704571479,-0.751159873,0.8566482107
H,0,-2.5196853202,1.1662772209,-0.805308686	H,0,-2.4870177752,1.1992429706,-0.8975475105
O,0,-3.9447398099,0.5548331914,-5.0043717054	O,0,-4.0744642479,0.4933584338,-5.0182359895
H,0,-4.2390881469,-0.1147185811,-5.6309401058	H,0,-4.4079229091,-0.179603075,-5.6247729949

P C14(•OCH_3), optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.50114756 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234095 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1025.0952551 a.u.	**P C15(•OCH_3),** optimization in gas phase UB3LYP/6-311++G**, E= -1025.50886246 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235645 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1025.0989324 a.u.
0, 2	0, 2
C,0,5.8465694438,0.8026615875,-0.4730787744	C,0,5.7257699732,0.8603425028,0.4521793094
C,0,5.1440761291,-0.32093109,-0.039791792	C,0,4.9592773359,-0.289612995,0.6219055475
C,0,5.2041163101,1.8546337737,-1.1448439814	C,0,5.2161439205,1.990659187,-0.2072864372
H,0,5.6410871963,-1.1321723799,0.4791688116	H,0,5.3508887231,-1.1624149884,1.1304667356
C,0,3.7720037055,-0.3774538216,-0.2914624805	C,0,3.6579085841,-0.2936951902,0.1154072311
C,0,3.8331621093,1.8164705629,-1.4060367795	C,0,3.9195855411,2.0066858871,-0.7214665119
H,0,3.3361760355,2.6284670542,-1.9242608259	H,0,3.5277219803,2.8794579469,-1.2309300197
C,0,3.1416807301,0.6927623803,-0.9707166466	C,0,3.1612238319,0.855362177,-0.5478303305
C,0,1.708059907,-0.9019661387,-0.4420917479	C,0,1.6651398502,-0.7626383866,-0.4719546959
N,0,2.8426408976,-1.3632049073,0.0272146528	N,0,2.6921089012,-1.2924380684,0.1446655034
N,0,1.8041163132,0.3191949065,-1.0532635068	N,0,1.864773609,0.515556844,-0.9197055247
H,0,1.0286892254,0.8242830107,-1.4536405247	H,0,1.1623299048,1.0761188312,-1.3778617246
N,0,0.5114492467,-1.5663715521,-0.3600992243	N,0,0.4691774915,-1.405048303,-0.6687257074
N,0,-0.6187956298,-0.9601256815,-0.797584819	N,0,-0.5167387583,-0.7925826415,-1.3449376203
C,0,-1.7344515655,-1.5528070742,-0.6259659394	C,0,-1.6603075113,-1.406202381,-1.4413057892
H,0,-1.8173198325,-2.5258670572,-0.1328251866	H,0,-1.8031746486,-2.3884575562,-0.9757998292
H,0,0.4873043017,-2.4289336242,0.1746945997	H,0,0.3618366393,-2.3259534051,-0.2524628636
H,0,5.7814941813,2.7134592681,-1.4672121101	H,0,5.8415859821,2.8686165443,-0.3201368074
C,0,-3.0380490015,-0.9579090693,-1.1303296882	C,0,-2.7609310308,-0.8542623482,-2.1571142509
C,0,-3.5495596034,-1.8479241903,-2.236952709	C,0,-3.9492168685,-1.5703364869,-2.2771684845
C,0,-2.8933966925,0.4732494866,-1.5552927685	C,0,-2.6241045284,0.528155543,-2.7738006417
C,0,-3.8456173048,-1.3755128395,-3.4844543595	C,0,-5.0133732157,-1.1108550715,-3.0520187992
C,0,-3.2135712232,0.9036685601,-2.8016911398	C,0,-3.7506574482,0.8473046634,-3.7137880524
C,0,-3.6889691801,-0.0121817808,-3.7909281476	C,0,-4.8824104811,0.086596961,-3.794896164
H,0,6.9128207515,0.8674599373,-0.2876073435	H,0,6.7389425324,0.8864974724,0.8369554282
H,0,-4.2080632321,-2.0529620415,-4.2526637958	H,0,-5.9353399044,-1.679026482,-3.111053445
H,0,-3.6779973057,-2.8975392806,-1.9991668105	H,0,-4.0437671147,-2.5252592881,-1.7697096389
O,0,-3.0780561656,2.2231838524,-3.1348041697	O,0,-3.5831191936,1.9706665294,-4.4512252658
H,0,-3.3441965729,2.340971326,-4.056106803	H,0,-4.3682575832,2.0883599878,-5.0052786689
O,0,-3.8968277811,-1.0782658144,0.0528063509	O,0,-2.4560478456,1.5665650324,-1.7821960517
C,0,-5.2442890426,-0.6431003359,-0.1142123702	C,0,-3.5413750133,1.7487164636,-0.8823378283
H,0,-5.2965261852,0.4213420117,-0.3657104906	H,0,-4.4646299603,2.0286609192,-1.4032096865
H,0,-5.7648057244,-1.2187518677,-0.8877887998	H,0,-3.7287558316,0.8510286124,-0.2812733843
H,0,-5.7343370619,-0.8093791672,0.8452257645	H,0,-3.2479159867,2.5640965696,-0.2210465034
H,0,-2.5177161336,1.1775064652,-0.823933075	H,0,-1.6824564356,0.5881281666,-3.3283695902
O,0,-3.9692209934,0.5393727313,-5.0083042303	O,0,-5.8759063778,0.5575545071,-4.6387351152
H,0,-4.2659229824,-0.1303888405,-5.6351220894	H,0,-6.4348729732,-0.1678116961,-4.9341627326

P C15(•OCH_3), optimization in solv. water UB3LYP/6-311++G**, E= -1025.53064038 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235185 a.u. SP at UM06-2X/6-311++G** (water), E = -1025.1217923 a.u.	**P C15(•OCH_3),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.51797016 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235399 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1025.1084892 a.u.
0, 2 C,0,5.805834808,0.79538868,0.4039913012 C,0,4.9845727782,-0.3004746785,0.6685970013 C,0,5.3463521207,1.892214551,-0.3438843132 H,0,5.3432221057,-1.1453064535,1.2454677813 C,0,3.6801447446,-0.2823031819,0.1675123528 C,0,4.0459921685,1.929179386,-0.8522960504 H,0,3.689662853,2.7739462069,-1.4298694117 C,0,3.2346194167,0.8332716653,-0.5832348315 C,0,1.6545738918,-0.6976463261,-0.3821102184 N,0,2.6657985656,-1.227419009,0.2766172064 N,0,1.9211903676,0.5308739232,-0.9207511212 H,0,1.2664518167,1.0811940457,-1.4559951039 N,0,0.436411001,-1.2948184022,-0.533233042 N,0,-0.5337333188,-0.6791643771,-1.246116365 C,0,-1.6574975794,-1.3202562341,-1.3876191118 H,0,-1.7864971798,-2.3138812785,-0.9479734066 H,0,0.3027968057,-2.2148900018,-0.122829216 H,0,6.0124401138,2.7265183968,-0.5311064208 C,0,-2.7522892505,-0.7918538151,-2.1343142803 C,0,-3.8863736207,-1.5692410145,-2.3465308188 C,0,-2.6741705318,0.6172292472,-2.6885673478 C,0,-4.9299704633,-1.1478815933,-3.1727253596 C,0,-3.7522692847,0.9007003835,-3.6902366739 C,0,-4.8321199142,0.0799827998,-3.8691746739 H,0,6.8217923548,0.8021578841,0.7824957873 H,0,-5.8027548858,-1.7746358336,-3.3153152581 H,0,-3.9503852304,-2.5478184274,-1.8821753672 O,0,-3.6069833213,2.0649210806,-4.3751611573 H,0,-4.3571947628,2.1644365968,-4.9803273204 O,0,-2.6658246608,1.6270581705,-1.6388935906 C,0,-3.823208692,1.6637583662,-0.8047612875 H,0,-4.7335035201,1.8678207261,-1.3789248717 H,0,-3.9520282354,0.7282677795,-0.2501197698 H,0,-3.660081224,2.4772883947,-0.0978801624 H,0,-1.7004902116,0.7742802474,-3.1622501976 O,0,-5.7907353287,0.519263285,-4.757581342 H,0,-6.3726886061,-0.2036251298,-5.0189317491	0, 2 C,0,5.7589938514,0.8337693067,0.4403489511 C,0,4.9724421422,-0.299208351,0.6381489102 C,0,5.2680672558,1.9566498927,-0.2458046707 H,0,5.3519903425,-1.1651845448,1.1676078123 C,0,3.6702713148,-0.2931453683,0.1326849131 C,0,3.9704076564,1.9822887252,-0.7587310838 H,0,3.5915721446,2.8482950993,-1.2888698591 C,0,3.1927126422,0.8484836051,-0.5566694309 C,0,1.6651560741,-0.7399902062,-0.4449285297 N,0,2.6864566985,-1.2738674465,0.1848756835 N,0,1.8905964601,0.5235505478,-0.9191665699 H,0,1.2048334508,1.0877221319,-1.3978163398 N,0,0.4615235663,-1.3657233419,-0.6293807343 N,0,-0.5187276183,-0.7495828869,-1.3175845074 C,0,-1.6567470276,-1.3714445064,-1.4264185891 H,0,-1.7949497698,-2.3568211526,-0.9681551667 H,0,0.3430989965,-2.2870672569,-0.2171513821 H,0,5.9082848532,2.8207764007,-0.3807093093 C,0,-2.7574874215,-0.8290726488,-2.151458497 C,0,-3.9278552003,-1.5682479457,-2.2985947752 C,0,-2.644128346,0.5620975634,-2.7493514753 C,0,-4.9881052373,-1.1256161926,-3.0900576525 C,0,-3.7554138439,0.8628802486,-3.7116156321 C,0,-4.8709906833,0.0804170433,-3.8208771365 H,0,6.7729074294,0.8511855849,0.8238509173 H,0,-5.8931340469,-1.716903346,-3.1752612765 H,0,-4.0103208567,-2.5304968566,-1.8033595129 O,0,-3.5961150967,1.9973186333,-4.4366482863 H,0,-4.3705950559,2.1066569927,-5.0078192641 O,0,-2.5356375184,1.5956499148,-1.7384741579 C,0,-3.6464532057,1.722373102,-0.8571434975 H,0,-4.5702063962,1.9660255133,-1.3943261563 H,0,-3.8048465219,0.8116434544,-0.2684142037 H,0,-3.4024664849,2.5434015664,-0.1829968461 H,0,-1.6898924363,0.6578085395,-3.2762520429 O,0,-5.8549171169,0.5375958761,-4.6785413006 H,0,-6.4292689044,-0.185681631,-4.9511477113

P C16(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.50162668 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.232676 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1025.0940509 a.u.	**P C16(•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.52533418 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.233062 a.u. SP at UM06-2X/6-311++G** (water), E = -1025.1190412 a.u.
0, 2 C,0,5.8103769571,0.8101995427,0.2476578284	0, 2 C,0,5.8550907845,0.7856960063,0.142692012

C,0,5.0627286529,-0.3587405858,0.3706588163	C,0,5.085819767,-0.3592051757,0.3525166509
C,0,5.290630527,1.9494665996,-0.3864728987	C,0,5.3379534469,1.9018675965,-0.5348414994
H,0,5.4628383468,-1.2387255042,0.8598953902	H,0,5.4890239758,-1.2188205708,0.8757012454
C,0,3.7707938998,-0.3721832197,-0.1573942152	C,0,3.7756135595,-0.3704043342,-0.1321357319
C,0,4.0014704689,1.9561851633,-0.9203631321	C,0,4.0301898186,1.9095389854,-1.0259873032
H,0,3.6013283362,2.8365579679,-1.4101691649	H,0,3.6292480643,2.7692930353,-1.5497205945
C,0,3.2636500735,0.7860674127,-0.7933885194	C,0,3.2718946215,0.7647651317,-0.8121680299
C,0,1.7959934833,-0.8632632744,-0.7912800243	C,0,1.7631030102,-0.8445951893,-0.6836868914
N,0,2.8221609976,-1.3894565862,-0.173412561	N,0,2.8040839174,-1.3650058067,-0.067433232
N,0,1.9771077265,0.4334004246,-1.193242228	N,0,1.9680481442,0.4235035381,-1.1527351175
H,0,1.2928677778,0.9844698183,-1.6860425485	H,0,1.286226499,0.9722796454,-1.6544577363
N,0,0.6228389332,-1.5342286849,-1.03212236	N,0,0.5685618372,-1.4868672404,-0.8510099961
N,0,-0.4021079768,-0.9231912129,-1.6584108954	N,0,-0.4297782299,-0.8856400378,-1.5406800297
C,0,-1.4884119668,-1.582860014,-1.8369950206	C,0,-1.5147183189,-1.545476761,-1.7269621957
H,0,-1.5812380663,-2.6141980088,-1.4785706466	H,0,-1.6274258771,-2.5636740243,-1.3444284602
H,0,0.5621114028,-2.491322071,-0.6984508582	H,0,0.4906908705,-2.4439015929,-0.5197607014
H,0,5.9009056677,2.8417761804,-0.4640804989	H,0,5.963870684,2.7746824023,-0.680524739
C,0,-2.6572772653,-1.0149252301,-2.5171468444	C,0,-2.6556986579,-0.9845912202,-2.4608275216
C,0,-3.8369923496,-1.810727888,-2.5719480402	C,0,-3.8017288738,-1.8154834055,-2.6213894828
C,0,-2.6432062332,0.2257270732,-3.1035208251	C,0,-2.6456703579,0.2803430469,-2.9948114319
C,0,-4.9930910097,-1.3475427997,-3.226569379	C,0,-4.9267922157,-1.3676445836,-3.3357673464
C,0,-3.8354714963,0.8406171269,-3.7682201088	C,0,-3.8111458472,0.8729282832,-3.7215239143
C,0,-5.0187393472,-0.107586748,-3.8041119126	C,0,-4.9539432217,-0.1089336064,-3.873731403
H,0,6.8165797849,0.8431196794,0.6498403313	H,0,6.8748267178,0.8155836832,0.5098008786
H,0,-5.8708024498,-1.9861371417,-3.2812576857	H,0,-5.7778126206,-2.0279041856,-3.4691765433
H,0,-3.8430837059,-2.7939479867,-2.1163297733	H,0,-3.8037284434,-2.8128864827,-2.1987736355
O,0,-3.4598219671,1.2148132608,-5.07335575	O,0,-3.3583853252,1.308238465,-4.992142529
H,0,-4.172298339,1.7630709921,-5.4293088355	H,0,-4.1131720358,1.7017246566,-5.4529777364
O,0,-4.2032840291,2.0840152324,-3.1350097356	O,0,-4.2653725427,2.0870421672,-3.0793164129
C,0,-4.7025367129,2.0055628893,-1.8032115898	C,0,-4.8552818137,1.9399250765,-1.7843792076
H,0,-5.6557955659,1.4667394717,-1.7566590271	H,0,-5.7900447732,1.371592481,-1.8291572908
H,0,-3.9845692332,1.5258627116,-1.1295288128	H,0,-4.1694033516,1.4542488281,-1.0835857387
H,0,-4.8608303132,3.0349962832,-1.4830682894	H,0,-5.0683670823,2.9495934717,-1.4353562236
O,0,-6.0796559142,0.4080593533,-4.4737264986	O,0,-5.976168471,0.4025165397,-4.598669333
H,0,-6.7864800221,-0.2450652519,-4.5370964911	H,0,-6.6721153939,-0.2558073439,-4.7276419935
H,0,-1.7512005024,0.8384093744,-3.1068527656	H,0,-1.7828304448,0.9271466711,-2.8949844142

P C16(•OCH_3), optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.51156017 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.233333 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1025.1045528 a.u.	**P C17(•OCH_3),** optimization in gas phase UB3LYP/6-311++G**, E= -1025.52064761 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235961 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1025.1118827 a.u.
0, 2	0, 2
C,0,5.7964853512,0.8238070518,0.2625693128	C,0,5.9165214079,0.7473033227,0.1838970135
C,0,5.0582845355,-0.3532069478,0.374611931	C,0,5.0607583328,-0.3146294088,0.4622366985
C,0,5.2688106051,1.9628309319,-0.3660517035	C,0,5.5099273471,1.8265760725,-0.6177950296
H,0,5.4665478256,-1.2319020876,0.8599627184	H,0,5.3726630385,-1.1481500014,1.0799513699
C,0,3.7681075348,-0.3746149083,-0.1587181019	C,0,3.7740485649,-0.2816508511,-0.0800656207
C,0,3.981009865,1.9612186032,-0.904951165	C,0,4.229674408,1.8789708436,-1.1686033726
H,0,3.5735245307,2.8404382632,-1.3903922118	H,0,3.9179807156,2.712566371,-1.7873102055
C,0,3.2531075043,0.7835403534,-0.7889321037	C,0,3.3815765344,0.8152150017,-0.8857702823
C,0,1.796364501,-0.8764119925,-0.8058851933	C,0,1.7636267354,-0.6689338602,-0.6693481571
N,0,2.8274971195,-1.3994749265,-0.1858006056	N,0,2.734425498,-1.1952393047,0.0355364931
N,0,1.9721291274,0.423588702,-1.1963699368	N,0,2.0692973116,0.5319702596,-1.2516298404

H,0,1.2874941529,0.9767260156,-1.6875866468	H,0,1.4397205694,1.0675294972,-1.827766106
N,0,0.6309618609,-1.5513746751,-1.0576438204	N,0,0.532972465,-1.2516255394,-0.8274325069
N,0,-0.3963924022,-0.9326367528,-1.678641268	N,0,-0.4217505791,-0.6576461255,-1.5618665037
C,0,-1.4824440568,-1.5930280047,-1.8562888949	C,0,-1.5681829413,-1.2889713712,-1.6598055213
H,0,-1.5751370318,-2.6246097128,-1.501473865	H,0,-1.7033893696,-2.2504124502,-1.1535268
H,0,0.5645580698,-2.509922746,-0.7289680851	H,0,0.3885482374,-2.1459371197,-0.3661783504
H,0,5.8711168281,2.8612766401,-0.4352713387	H,0,6.2041079001,2.6355287721,-0.8135074479
C,0,-2.6531429812,-1.0204339871,-2.530172327	C,0,-2.6637983397,-0.7852696226,-2.4002756572
C,0,-3.8388082203,-1.808708465,-2.5671802235	C,0,-3.8801783316,-1.5519292618,-2.4499428975
C,0,-2.6358906054,0.217006506,-3.1236194884	C,0,-2.6001230565,0.442204114,-3.1320592237
C,0,-5.0000589536,-1.3403581315,-3.2078458528	C,0,-4.9723229546,-1.1224497729,-3.119392541
C,0,-3.8328247814,0.8356323396,-3.7753236318	C,0,-3.6694638049,0.8927479383,-3.8302549563
C,0,-5.0238806177,-0.1023113257,-3.7906516227	C,0,-5.0157247546,0.2005721572,-3.8202906192
H,0,6.800796206,0.8624847432,0.6691230397	H,0,6.9202344842,0.7437558119,0.5933221095
H,0,-5.8832835977,-1.971304736,-3.247300714	H,0,-5.8832755738,-1.7103330933,-3.1582739312
H,0,-3.8455877984,-2.7895304331,-2.106753121	H,0,-3.9063609241,-2.5094870588,-1.9385436753
O,0,-3.4725219665,1.2009250477,-5.0909274031	O,0,-3.606584576,2.035616784,-4.5488910802
H,0,-4.2106409307,1.7034375187,-5.4629890612	H,0,-4.3962861476,2.0780339302,-5.108202405
O,0,-4.1813360067,2.0877024449,-3.145170958	O,0,-6.0329404386,1.059555426,-3.2572397904
C,0,-4.6611515043,2.0179496564,-1.8031958338	C,0,-5.8795069557,1.4385072497,-1.8890990114
H,0,-5.6138801294,1.4808590637,-1.7404796985	H,0,-6.7509941426,2.0473396589,-1.6510912933
H,0,-3.9334293169,1.5405782645,-1.139001538	H,0,-5.8540219961,0.565896207,-1.2293531236
H,0,-4.8128706965,3.0491089707,-1.485977388	H,0,-4.9717781767,2.0320481187,-1.7401241536
O,0,-6.0874345504,0.4208788429,-4.4476895946	O,0,-5.4178580534,0.0933034798,-5.1794427947
H,0,-6.8089080645,-0.2190663547,-4.4920600444	H,0,-6.3820887451,0.0303847905,-5.1832383441
H,0,-1.7396828355,0.823920578,-3.1362191305	H,0,-1.6762007485,1.005289965,-3.1562293024

P C17(•OCH$_3$), optimization in solv. water UB3LYP/6-311++G**, E= -1025.53960953 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235237 a.u. SP at UM06-2X/6-311++G** (water), E = -1025.1321871 a.u.	**P C17(•OCH$_3$),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.52866820 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235851 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1025.1204693 a.u.
0, 2	0, 2
C,0,5.9167667126,0.7658060876,0.1572041732	C,0,5.9172547731,0.7541913177,0.1745457878
C,0,5.0785087568,-0.3127241378,0.4354843205	C,0,5.0686112452,-0.3147274715,0.4520863277
C,0,5.4858743005,1.8445945589,-0.6338191257	C,0,5.5010678247,1.8338223416,-0.6223014538
H,0,5.4139665763,-1.1433815569,1.0457815997	H,0,5.3900390463,-1.147504226,1.0663361723
C,0,3.7858465707,-0.2955178508,-0.0961086911	C,0,3.7795657228,-0.2878896077,-0.0860749909
C,0,4.1988572606,1.8800500308,-1.1736806556	C,0,4.2181715277,1.8796024061,-1.1688664618
H,0,3.8652039386,2.7108749044,-1.7839636185	H,0,3.8975034209,2.7123495121,-1.7839007575
C,0,3.3695132068,0.8007660916,-0.8908304144	C,0,3.3777145639,0.8092387546,-0.8867584467
C,0,1.7688058528,-0.7041104675,-0.6759881384	C,0,1.7663293997,-0.6830815481,-0.6723794515
N,0,2.7584429641,-1.224596892,0.0205101739	N,0,2.7445825264,-1.2076755297,0.0291364218
N,0,2.060753341,0.5024242992,-1.2483652294	N,0,2.0668410793,0.5205166819,-1.2494906411
H,0,1.4245302392,1.0450100041,-1.8130886665	H,0,1.4357973638,1.0588865589,-1.8224212881
N,0,0.5464065456,-1.2955013419,-0.830744793	N,0,0.5387169521,-1.2686567602,-0.8296630548
N,0,-0.4122244347,-0.6923407486,-1.5582099546	N,0,-0.4177543445,-0.6693524415,-1.5600438355
C,0,-1.5617393077,-1.3188410816,-1.6490585954	C,0,-1.5650903575,-1.2992542622,-1.6564497647
H,0,-1.7040368888,-2.2788581235,-1.1466995954	H,0,-1.7022868484,-2.2612435152,-1.1537146882
H,0,0.3927580525,-2.1890873153,-0.3704934883	H,0,0.3914621483,-2.1652999549,-0.373628733
H,0,6.1652233736,2.6660837722,-0.8296809955	H,0,6.1893648139,2.6479656809,-0.817500852
C,0,-2.6542197308,-0.7952519198,-2.3840608874	C,0,-2.6601864571,-0.7876349441,-2.3937044343
C,0,-3.883429613,-1.5410742904,-2.4270650571	C,0,-3.8814189588,-1.5466419396,-2.4396348876
C,0,-2.5787117228,0.4421089722,-3.1008136909	C,0,-2.5928692805,0.4433577292,-3.1202443932

C,0,-4.9720565057,-1.0911373396,-3.0898432199	C,0,-4.9727663102,-1.1096898166,-3.1058337191
C,0,-3.6444358154,0.9133529182,-3.7903058722	C,0,-3.6610751628,0.9010557292,-3.8152061501
C,0,-4.9900161708,0.2195827939,-3.8169245439	C,0,-5.0070721369,0.2079230949,-3.8184590541
H,0,6.9237703015,0.7742887932,0.5587151409	H,0,6.9222646829,0.7552259774,0.5809615804
H,0,-5.8956688093,-1.6598782432,-3.1156097763	H,0,-5.8887328179,-1.690239898,-3.1384247859
H,0,-3.9256732618,-2.4939377936,-1.9091943615	H,0,-3.9132503286,-2.5021902057,-1.9252549525
O,0,-3.5679678343,2.0788345085,-4.4793327625	O,0,-3.5934944707,2.0525000922,-4.5232429852
H,0,-4.3871297042,2.1975877655,-4.9821260954	H,0,-4.392329523,2.121037232,-5.066740673
O,0,-6.0208050375,1.0954425599,-3.3150523281	O,0,-6.029958422,1.0734004836,-3.2793396435
C,0,-5.9380401021,1.4607517522,-1.9322397638	C,0,-5.9029794984,1.4482505913,-1.9052411064
H,0,-6.7987269044,2.100073284,-1.7415871511	H,0,-6.7703598687,2.069503454,-1.6859729708
H,0,-5.9857652078,0.583196331,-1.2819395242	H,0,-5.9059158076,0.5740858067,-1.2476931783
H,0,-5.020123131,2.0188469219,-1.7229328683	H,0,-4.9904710537,2.0279895742,-1.7339635243
O,0,-5.3283111578,0.0736458259,-5.1909896523	O,0,-5.3837385722,0.0840019934,-5.1836375256
H,0,-6.2699266466,-0.1429244955,-5.2401490409	H,0,-6.3420326903,-0.0415294387,-5.2069786207
H,0,-1.6529670666,1.004092353,-3.1044037107	H,0,-1.6682512413,1.0059574779,-3.1379061259

P C19(•OCH_3), optimization in gas phase UB3LYP/6-311++G**, E= -1025.51137138 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235413 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1025.1012998 a.u.	**P C19(•OCH_3),** optimization in solv. water UB3LYP/6-311++G**, E= -1025.53168128 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234966 a.u. SP at UM06-2X/6-311++G** (water), E = -1025.1227574 a.u.
0, 2	0, 2
C,0,6.0274900877,0.759506727,0.5070676331	C,0,6.029784053,0.7749798675,0.4764480125
C,0,5.1383904874,-0.2568628114,0.8468936402	C,0,5.164066019,-0.2687380484,0.8026969123
C,0,5.6520980336,1.8063633997,-0.350112452	C,0,5.6192315934,1.8388400302,-0.3440686655
H,0,5.4266950735,-1.0651272817,1.5081773703	H,0,5.4847362801,-1.0879365696,1.4361274537
C,0,3.850153483,-0.2111900419,0.3098542532	C,0,3.8648369549,-0.2317555712,0.2891499822
C,0,4.3703456301,1.8703900459,-0.8972950939	C,0,4.3251763757,1.8935261425,-0.8667904001
H,0,4.0820659068,2.6790399282,-1.5591116409	H,0,4.0062922495,2.7129941361,-1.5000683913
C,0,3.4896095595,0.8525914533,-0.552987869	C,0,3.4693979698,0.8494690501,-0.5362816726
C,0,1.8230071174,-0.5624802393,-0.2468356015	C,0,1.8270545406,-0.6000923571,-0.249089886
N,0,2.7810184395,-1.0815772013,0.480833879	N,0,2.8122845849,-1.1257978518,0.4513358755
N,0,2.1661779435,0.5937054028,-0.8965107735	N,0,2.1470079394,0.5782340219,-0.8653328055
H,0,1.5490857109,1.1198065927,-1.4941339712	H,0,1.5183326074,1.1194084491,-1.4395438735
N,0,0.5724075677,-1.1081162936,-0.3691309044	N,0,0.5866687113,-1.1566670011,-0.3699584961
N,0,-0.3664214151,-0.515061375,-1.1303624796	N,0,-0.3627713665,-0.5449047555,-1.112035693
C,0,-1.5339206006,-1.1019706532,-1.1910583827	C,0,-1.5274129519,-1.1362868504,-1.1786113832
H,0,-1.7131385817,-2.0205385389,-0.6240232174	H,0,-1.6984222347,-2.0696306162,-0.6361568059
H,0,0.3902296726,-1.962031677,0.1507327216	H,0,0.4091386413,-2.0310858286,0.1166308105
H,0,6.3710485933,2.5802858447,-0.5926524552	H,0,6.3189709625,2.633068349,-0.5771844006
C,0,-2.6181267174,-0.596119598,-1.9587454266	C,0,-2.6125371136,-0.6142128979,-1.9371162176
C,0,-3.9260912357,-1.363605305,-1.8614790215	C,0,-3.9279990943,-1.3657286144,-1.8426383807
C,0,-2.525448583,0.5640938827,-2.7364600308	C,0,-2.5131175754,0.5513351188,-2.7070692352
C,0,-4.9835224681,-0.8710304898,-2.8073262995	C,0,-4.9702871342,-0.8877371925,-2.8101355081
C,0,-3.5821997256,0.9986565814,-3.5067640533	C,0,-3.5660429294,0.9868544397,-3.4828890247
C,0,-4.8156947994,0.2447916359,-3.5430887932	C,0,-4.799064954,0.2296552593,-3.5437040188
H,0,7.0330001381,0.7446264789,0.9119896832	H,0,7.0424182506,0.7666339361,0.8637293391
H,0,-5.9098090107,-1.4356074303,-2.8499067006	H,0,-5.8919977966,-1.456462824,-2.8714083752
H,0,-3.7376395603,-2.4252128164,-2.0584761184	H,0,-3.7481758109,-2.4335416499,-2.0050034221
O,0,-3.4716935652,2.124590856,-4.2542456455	O,0,-3.4501783645,2.1177730063,-4.2227634322
H,0,-4.3005502727,2.2592616072,-4.7342112064	H,0,-4.2765395632,2.2589903837,-4.708716835
O,0,-4.4189857664,-1.4183194795,-0.4948705292	O,0,-4.4415520273,-1.3717185401,-0.4737067433
C,0,-4.747583772,-0.1638369561,0.0930527997	C,0,-4.7714308681,-0.0916386374,0.065887128

H,0,-3.8731612724,0.4927813229,0.1668107291	H,0,-3.8893673053,0.5532032243,0.1442022344
H,0,-5.5349913837,0.3540090945,-0.4664320913	H,0,-5.533699671,0.4156666214,-0.5343729147
H,0,-5.1117108338,-0.3870807973,1.0959882307	H,0,-5.1678702634,-0.2750466947,1.0646364242
O,0,-5.7432342544,0.7852180836,-4.4022777347	O,0,-5.7061030108,0.7672713435,-4.4174211174
H,0,-6.559597116,0.2747945254,-4.3834784146	H,0,-6.5353300474,0.2737641636,-4.4055505928
H,0,-1.6034963408,1.1319701229,-2.7520574433	H,0,-1.5896914808,1.1180295577,-2.7158592914

P C19(•OCH_3), optimization in solv. benzene UB3LYP/6-311++G**, E= -1025.52010695 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235081 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1025.110538 a.u.	
0, 2 C,0,6.0249643414,0.7707364215,0.4957313993 C,0,5.1461534712,-0.2565687278,0.8331683011 C,0,5.6352794937,1.8208944851,-0.3514132374 H,0,5.4478084897,-1.0664213954,1.4869253118 C,0,3.8540386584,-0.2180793066,0.303880929 C,0,4.3490773991,1.8775118954,-0.8904665302 H,0,4.0480447217,2.6878126516,-1.5443707635 C,0,3.4793059688,0.8491518553,-0.548670054 C,0,1.8234190618,-0.5803880498,-0.2464681808 N,0,2.7921702402,-1.0985221264,0.4735862507 N,0,2.1570621872,0.5826661463,-0.8869026722 H,0,1.5356989725,1.1118953807,-1.4783471279 N,0,0.5773481166,-1.1314385626,-0.3682379325 N,0,-0.3651708657,-0.5310522212,-1.1230762432 C,0,-1.5317850971,-1.1191284823,-1.1865502828 H,0,-1.7085382575,-2.0434322688,-0.6293062788 H,0,0.3955237329,-1.9917059682,0.1412616829 H,0,6.3459011263,2.6030151779,-0.5923875585 C,0,-2.6157257886,-0.6054148476,-1.950794671 C,0,-3.9279381764,-1.3646267744,-1.8559067719 C,0,-2.5182660885,0.5571685821,-2.7247224908 C,0,-4.9793899715,-0.8738961057,-2.8086956468 C,0,-3.5727087891,0.9950321846,-3.4963897516 C,0,-4.8082206297,0.2431178111,-3.5423828951 H,0,7.0329115269,0.7611725578,0.8948909324 H,0,-5.9047501387,-1.4387588801,-2.8590021278 H,0,-3.7447044426,-2.4286387163,-2.0422967345 O,0,-3.457495752,2.1232160751,-4.2403536231 H,0,-4.2840935266,2.2614129337,-4.7247798298 O,0,-4.428655397,-1.4028853289,-0.4880285595 C,0,-4.7523795976,-0.13851564,0.0852909052 H,0,-3.8720821944,0.5093207286,0.1625584584 H,0,-5.5279079882,0.3805287893,-0.4886259347 H,0,-5.1298924649,-0.34759718,1.0863034586 O,0,-5.7261666353,0.7866198599,-4.4059336735 H,0,-6.5484966674,0.2840208126,-4.394502287 H,0,-1.5945328696,1.1224908333,-2.7376191803	

P C1(•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.34804015 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209185 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1060.9293802 a.u.	**P C1(•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.37213456 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209212 a.u. SP at UM06-2X/6-311++G** (water), E = -1060.9544964 a.u.
0, 2 C,0,5.8889987364,1.0532593016,0.1150712259 C,0,5.0604074412,-0.0460854144,0.4526583224 C,0,5.5018690726,2.0395553734,-0.7554598169 H,0,5.386828924,-0.8098953836,1.1460401569 C,0,3.7843871644,-0.1080254194,-0.1439042333 C,0,4.1571994075,2.0670909635,-1.4237038749 H,0,4.2678661567,2.1374630993,-2.5185505783 C,0,3.366752414,0.8838798238,-1.0229633477 C,0,1.8050450588,-0.6354284941,-0.7366414005 N,0,2.7835878314,-1.0620181327,0.0202866563 N,0,2.0912494845,0.5273682581,-1.4074680551 H,0,1.4328103553,1.057754409,-1.9574579366 N,0,0.5994245191,-1.2773527688,-0.8829926 N,0,-0.3854616119,-0.7194827309,-1.6204325322 C,0,-1.5317833792,-1.2981851264,-1.6365546452 H,0,-1.7046463281,-2.2108438336,-1.0549070234 H,0,0.4336589066,-2.0817955475,-0.2859817891 H,0,6.1769608877,2.8509333471,-1.0046472945 C,0,-2.6617575061,-0.7958409638,-2.4124533297 C,0,-3.8841439861,-1.4766524132,-2.3456227886 C,0,-2.5611536264,0.3479953261,-3.2224589542 C,0,-4.986826709,-1.0268135754,-3.070011804 C,0,-3.653541085,0.7974111921,-3.9429785851 C,0,-4.875213274,0.1044534533,-3.8649582136 H,0,6.8784177041,1.1098169578,0.557354148 H,0,-5.9321505748,-1.5578898373,-3.0145121725 H,0,-3.9784768951,-2.3614720845,-1.7263469231 O,0,-3.5394743043,1.9071858707,-4.7237830385 H,0,-4.3919651364,2.0777309821,-5.1448943299 O,0,3.4394454182,3.3338377352,-1.2129443064 H,0,-1.6284478933,0.8920705225,-3.292012519 O,0,-5.8949594013,0.6341951349,-4.6196811619 H,0,-6.7030950726,0.1238187726,-4.5076685636 O,0,3.0617481479,3.4501996861,0.1823576108 H,0,3.8270961832,3.9113370663,0.5564127278	0, 2 C,0,5.9001334902,1.0369529427,0.0322743607 C,0,5.0637752598,-0.0398482872,0.4265903019 C,0,5.4929781171,2.0160053071,-0.8364352875 H,0,5.4125782056,-0.7981049201,1.1159773792 C,0,3.7647660319,-0.0908887791,-0.1193817983 C,0,4.1138036188,2.0702680103,-1.4248396036 H,0,4.1521295178,2.1663448683,-2.520567674 C,0,3.3262004781,0.8945416892,-0.9971078684 C,0,1.763510207,-0.621674965,-0.6658227694 N,0,2.7638311654,-1.04198072,0.0781666591 N,0,2.0400243689,0.5385593921,-1.3430275183 H,0,1.3916175866,1.0277806364,-1.9428716592 N,0,0.5567283353,-1.252803162,-0.7872220945 N,0,-0.4159961005,-0.7039141758,-1.5568494341 C,0,-1.5530205586,-1.3008342143,-1.6024537798 H,0,-1.7287339819,-2.2186184888,-1.0337978954 H,0,0.3933379465,-2.0860349943,-0.230337955 H,0,6.1696579373,2.8123850026,-1.1249192319 C,0,-2.6675646714,-0.8004156396,-2.4027208486 C,0,-3.8797824805,-1.5033756491,-2.3868133956 C,0,-2.5639684626,0.3635482098,-3.1861109989 C,0,-4.9697698625,-1.0591215733,-3.1342785483 C,0,-3.6443511794,0.806441854,-3.9280466323 C,0,-4.8573165715,0.0917971756,-3.9031769231 H,0,6.9097000846,1.0783137151,0.4275687277 H,0,-5.9060867418,-1.6065071772,-3.1197328043 H,0,-3.9758033254,-2.4020805823,-1.788472906 O,0,-3.5293250881,1.9390757337,-4.6837501892 H,0,-4.3724300248,2.1028993455,-5.1289460989 O,0,3.4342575064,3.353856617,-1.1371643583 H,0,-1.6389046044,0.9255229812,-3.2158236395 O,0,-5.8591163619,0.6180983633,-4.6731734301 H,0,-6.664718494,0.0921510799,-4.6024336205 O,0,3.204237175,3.4840469443,0.2903176195 H,0,4.0042785071,3.9471890102,0.5835729448

P C1(•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.35832268 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209505 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1060.9400784 a.u.	**P C2(•OOH),** optimization in gas phase UB3LYP/6-311++G**, E= -1061.34760984 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209047 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1060.9277445 a.u.
0, 2 C,0,5.8925527467,1.0493409894,0.0875393283 C,0,5.0585158381,-0.0388015303,0.4503617275 C,0,5.5004033487,2.0292323927,-0.7875244502 H,0,5.3916069569,-0.7976420334,1.1462955635 C,0,3.7746196444,-0.0979159495,-0.1288479368	0, 2 C,0,5.8200781313,0.3879559267,0.4222005037 C,0,4.9700642255,-0.6636466157,0.5420197969 C,0,5.4422260812,1.6906313678,-0.2254579803 H,0,5.2699365162,-1.579282896,1.0387556818 C,0,3.6617138966,-0.560271,-0.0015696393

C,0,4.1424549841,2.0660426524,-1.426625647	C,0,4.0811575825,1.7196889022,-0.8497695419
H,0,4.2262029761,2.1419059397,-2.522616145	H,0,3.7837583868,2.6031720118,-1.4027834903
C,0,3.3506682748,0.8888244677,-1.0115534466	C,0,3.2689401716,0.6383549822,-0.6819249841
C,0,1.7886145279,-0.6297641941,-0.7082984262	C,0,1.6696617848,-0.8975718288,-0.6717828885
N,0,2.7739362009,-1.0510618978,0.047931249	N,0,2.6501873888,-1.4856888412,-0.0147236909
N,0,2.0728832761,0.5296933994,-1.3849053322	N,0,1.9628131794,0.3685307194,-1.103000187
H,0,1.4172374489,1.044884051,-1.9532315578	H,0,1.332903325,0.9589751403,-1.6213102831
N,0,0.5839744097,-1.2691682798,-0.8481440933	N,0,0.461812893,-1.4835377159,-0.9107108183
N,0,-0.3947639302,-0.7155015507,-1.6015686286	N,0,-0.5017210365,-0.8271625825,-1.5933489425
C,0,-1.5382497991,-1.3000010167,-1.6275233356	C,0,-1.6191818812,-1.4335750132,-1.7895775528
H,0,-1.7135809429,-2.2118567132,-1.0469412951	H,0,-1.7762746703,-2.4502440394,-1.4122261
H,0,0.4137008668,-2.0780016368,-0.2583537317	H,0,0.3275804541,-2.4253500546,-0.5542081434
H,0,6.1780016281,2.8323668675,-1.0554138245	H,0,6.2102443413,1.9814813204,-0.958620398
C,0,-2.6622093877,-0.8000198121,-2.4140340822	C,0,-2.731146456,-0.8262818818,-2.5107994802
C,0,-3.8796243111,-1.4918491603,-2.3684836126	C,0,-3.9137044553,-1.5598955338,-2.6751311241
C,0,-2.5622385924,0.3532251478,-3.2116749591	C,0,-2.6527346413,0.4713762038,-3.0457183181
C,0,-4.9785116779,-1.0444970808,-3.1004715188	C,0,-4.9977850872,-1.0121441029,-3.358270924
C,0,-3.6511812769,0.8001964129,-3.9385626063	C,0,-3.7269603587,1.0181674556,-3.7243459974
C,0,-4.86910303,0.0975100523,-3.881414752	C,0,-4.9081236111,0.2698996293,-3.88129826
H,0,6.8896101696,1.1002600981,0.5128393784	H,0,6.8194692133,0.3409073084,0.8389764313
H,0,-5.9189276733,-1.584885415,-3.0631733186	H,0,-5.9120343684,-1.5842164165,-3.4827953701
H,0,-3.972972641,-2.3838806127,-1.7595768386	H,0,-3.9907479721,-2.562180715,-2.2692773444
O,0,-3.5388254192,1.9213023141,-4.7068413711	O,0,-3.6347684797,2.2763168909,-4.236266265
H,0,-4.3902220957,2.0928448561,-5.1311748604	H,0,-4.4683480994,2.4946568938,-4.6730483637
O,0,3.4421804656,3.3432093952,-1.1910860233	O,0,5.6397954416,2.8165107199,0.7089403801
H,0,-1.633723963,0.9067691439,-3.263909525	O,0,-5.9126139979,0.9057340615,-4.5699980841
O,0,-5.8834648,0.6274765142,-4.6385588261	H,0,-6.6895360385,0.3420674112,-4.640292199
H,0,-6.6989415893,0.1284553745,-4.5201675733	H,0,-1.7508745822,1.0584667302,-2.9333658663
O,0,3.115632493,3.4700318621,0.2165803288	O,0,4.7925000506,2.636723845,1.8730923818
H,0,3.9044019032,3.9108505021,0.5673191728	H,0,4.0094013723,3.1476625568,1.6221022513

P C2(•OOH), optimization in solv. water UB3LYP/6-311++G**, E= -1061.37361169 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209495 a.u. SP at UM06-2X/6-311++G** (water), E = -1060.9547553 a.u.	**P C2(•OOH),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.35874040 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209440 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1060.9393842 a.u.
0, 2	0, 2
C,0,5.8335094845,0.401210825,0.3826690121	C,0,5.8286343762,0.3965493438,0.3915322033
C,0,4.9933760726,-0.6620215302,0.510135037	C,0,4.9859242988,-0.6625726986,0.5121142723
C,0,5.4206212276,1.7062465136,-0.2313468467	C,0,5.4282306196,1.7050693245,-0.2271558566
H,0,5.3206564824,-1.5814738828,0.9834391216	H,0,5.3025049852,-1.5827861459,0.9901908013
C,0,3.6747670465,-0.5665396262,-0.0077296905	C,0,3.6693550051,-0.5615218154,-0.0108845499
C,0,4.0655043093,1.7178985222,-0.8585666823	C,0,4.0659424103,1.7280359585,-0.8448441612
H,0,3.75099461,2.5961452987,-1.4092796249	H,0,3.7561285921,2.6120158422,-1.3898423536
C,0,3.2641380905,0.6292144647,-0.6836320192	C,0,3.2621417075,0.6398717415,-0.6778761265
C,0,1.6722598946,-0.9155625785,-0.6646507076	C,0,1.6701814215,-0.9042891915,-0.6674072634
N,0,2.6695783479,-1.5004572132,-0.0124990577	N,0,2.6627140819,-1.4931706001,-0.0220647485
N,0,1.9606754283,0.3491132493,-1.0963184751	N,0,1.9555557757,0.3655638898,-1.0901092268
H,0,1.3225986826,0.9477829451,-1.5980727915	H,0,1.3195389486,0.9596698592,-1.5979558459
N,0,0.4700167354,-1.5005811757,-0.8919265335	N,0,0.4642702225,-1.4901418822,-0.8991795672
N,0,-0.4922789435,-0.8325780498,-1.5791278175	N,0,-0.4991048434,-0.8286862899,-1.5836755377
C,0,-1.6136118501,-1.434753938,-1.7654124236	C,0,-1.6188950675,-1.4322581746,-1.7740459456
H,0,-1.780205992,-2.4449432602,-1.3807228668	H,0,-1.7816323886,-2.4448918691,-1.3907039153
H,0,0.3235576461,-2.4427913886,-0.5402468624	H,0,0.3281586451,-2.4352735158,-0.5519642997

H,0,6.1867884962,2.0588973574,-0.9364754294	H,0,6.1905325313,2.032195736,-0.949924062
C,0,-2.718730707,-0.8193246947,-2.4916964453	C,0,-2.7269522324,-0.8223811785,-2.4998656298
C,0,-3.9133364796,-1.537722482,-2.6386298408	C,0,-3.919826761,-1.543482128,-2.6443717476
C,0,-2.6220106542,0.4687240011,-3.0501396833	C,0,-2.6340633761,0.4641108378,-3.0601015039
C,0,-4.9931775217,-0.9873329975,-3.326900083	C,0,-5.0008987296,-0.9953843553,-3.3322911352
C,0,-3.6920870679,1.0164957708,-3.7340130567	C,0,-3.7051052129,1.0106255786,-3.7435575814
C,0,-4.8874836038,0.2847769188,-3.8749596645	C,0,-4.8977956843,0.2755973912,-3.8811418558
H,0,6.84773563,0.3488145893,0.762013119	H,0,6.8367948071,0.3464182709,0.7863710489
H,0,-5.9161608762,-1.5461338102,-3.4378662564	H,0,-5.9230427059,-1.5571229898,-3.4411423768
H,0,-4.003010437,-2.5310384124,-2.214372213	H,0,-4.0073873235,-2.5365270893,-2.2186829863
O,0,-3.5842271761,2.2671714278,-4.2723585506	O,0,-3.5992681921,2.2585673613,-4.2820574189
H,0,-4.4144586459,2.4875522953,-4.7173925645	H,0,-4.4309535354,2.4780876271,-4.7231519806
O,0,5.5696104438,2.8208283152,0.7559428499	O,0,5.6067503939,2.8173615439,0.7400474111
O,0,-5.8793408612,0.9209367036,-4.5692580236	O,0,-5.8945711557,0.9100783246,-4.576714711
H,0,-6.6642840613,0.3652095527,-4.6457554331	H,0,-6.6787207871,0.3541867791,-4.6429175736
H,0,-1.7093931415,1.043112154,-2.9523879561	H,0,-1.7230995141,1.0405003028,-2.9648048856
O,0,4.6728524857,2.6213482945,1.8806732649	O,0,4.7539733476,2.6087732735,1.8956687911
H,0,3.8522456051,3.0280066807,1.5613303856	H,0,3.9416740396,3.0634417774,1.6269755085

P C4(•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.34907466 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209518 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1060.930273 a.u.	**P C4(•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.37566171 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209843 a.u. SP at UM06-2X/6-311++G** (water), E = -1060.9578852 a.u.
0, 2	0, 2
C,0,5.9016792082,0.7768043742,0.4111147852	C,0,5.8959685506,0.7794008284,0.3685356922
C,0,5.0053811339,-0.3421471167,0.8662212077	C,0,5.0132565509,-0.3429643404,0.8318283914
C,0,5.4829112018,1.7947476319,-0.3986612307	C,0,5.4578410568,1.7957573681,-0.4350507403
H,0,5.478375841,-1.3224475563,0.7132372558	H,0,5.4818821986,-1.3217788712,0.6535534986
C,0,3.6791007328,-0.2797504462,0.1932865943	C,0,3.6643187676,-0.268673367,0.2112244071
C,0,4.1689561251,1.8535832701,-0.9455823036	C,0,4.1322090059,1.8544307968,-0.9540050945
H,0,3.8642164146,2.6731656678,-1.5836401383	H,0,3.8121209746,2.6688608411,-1.5905228169
C,0,3.3184492421,0.7936296331,-0.6279331933	C,0,3.2862304547,0.7986562426,-0.6090898817
C,0,1.6898358083,-0.6816880782,-0.43317857	C,0,1.6499635327,-0.6658981267,-0.3672525703
N,0,2.6661906072,-1.1896176752,0.298402778	N,0,2.646929803,-1.1730108582,0.3523300459
N,0,2.009186589,0.5056151148,-1.0196434394	N,0,1.9679755176,0.5137666928,-0.9657365835
H,0,1.3927840292,1.0437283685,-1.6074039352	H,0,1.3511727275,1.049472888,-1.5579866842
N,0,0.4740829755,-1.2858481344,-0.5993530545	N,0,0.4304877468,-1.2555473821,-0.502953587
N,0,-0.4872071963,-0.7019763041,-1.3455996172	N,0,-0.5189931054,-0.6753580811,-1.2787775511
C,0,-1.6352586363,-1.2773707397,-1.40977704	C,0,-1.6573084367,-1.2668496904,-1.3698674947
H,0,-1.8242910817,-2.2081855933,-0.8634319035	H,0,-1.8483836572,-2.2022186449,-0.8360547506
H,0,0.3070512016,-2.1354283583,-0.0682966311	H,0,0.2649422256,-2.1307776537,-0.0145927445
H,0,6.1806992801,2.5853304792,-0.6548938796	H,0,6.1497651614,2.5860561704,-0.7066604567
C,0,-2.7433561521,-0.7442126059,-2.1942545956	C,0,-2.7505455905,-0.7375452909,-2.1785820833
C,0,-3.9724995138,-1.416487573,-2.1744513258	C,0,-3.9674143118,-1.432557828,-2.206858277
C,0,-2.6165631147,0.4232916258,-2.9665236865	C,0,-2.6219535332,0.4457848864,-2.9290400124
C,0,-5.0557902144,-0.9345536366,-2.9069662853	C,0,-5.0378216676,-0.9614250789,-2.9654850182
C,0,-3.68973843,0.904489517,-3.6948500751	C,0,-3.6827169417,0.9148353637,-3.6826641969
C,0,-4.9184640086,0.2201272092,-3.6636557272	C,0,-4.9007820981,0.2080856007,-3.7021051517
H,0,6.9179831945,0.7628472485,0.7898771479	H,0,6.92060547,0.7655513272,0.7233792547
H,0,-6.0063824628,-1.458642255,-2.8876891369	H,0,-5.977872013,-1.5020993977,-2.9845751799
H,0,-4.0872036802,-2.3187092921,-1.5844838136	H,0,-4.0821974342,-2.3454232577,-1.6338666298
O,0,-3.5503452717,2.0372221883,-4.4379609921	O,0,-3.5439023268,2.0647384255,-4.4071933655
H,0,-4.3909029173,2.2253477075,-4.8753711008	H,0,-4.3746389596,2.2435058718,-4.8696135571

O,0,4.8985547901,-0.3797527729,2.3297450313	O,0,4.9589216137,-0.4146166168,2.309222267
H,0,-1.6774954968,0.9596106956,-3.0008510928	H,0,-1.6922597914,1.000735702,-2.9248722723
O,0,-5.9174643273,0.7821407311,-4.4220248115	O,0,-5.8810801701,0.7609759953,-4.4799839205
H,0,-6.7302013479,0.2718945696,-4.3491122388	H,0,-6.6900412841,0.2363596645,-4.446930326
O,0,4.1880703717,0.7979902922,2.7892016274	O,0,4.3162774217,0.7746315649,2.8401738004
H,0,4.9169975851,1.4141612335,2.9534532306	H,0,5.0643850218,1.3840476754,2.9390234296

P C4(•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.36034674 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.210044 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1060.9420219 a.u.	**P C6(•OOH),** optimization in gas phase UB3LYP/6-311++G**, E= -1061.35584913 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.211518 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1060.9381655 a.u.
0, 2	0, 2
C,0,5.8978269575,0.7785246841,0.3932094234	C,0,5.998761589,0.4155053774,-0.3566062418
C,0,5.0079919776,-0.3411894707,0.8555397214	C,0,5.1499083046,-0.4989165243,0.2335385955
C,0,5.4692183366,1.7946518835,-0.4146009919	C,0,5.4971963256,1.5487054807,-1.038784602
H,0,5.4804723124,-1.3209674916,0.6969336043	H,0,5.5197667743,-1.3748294584,0.7520624175
C,0,3.6723478425,-0.2778553929,0.2031302876	C,0,3.7515521696,-0.2815625703,0.135090296
C,0,4.1496466369,1.8515066905,-0.9484784091	C,0,4.1283751226,1.8041956416,-1.1411910488
H,0,3.8369620573,2.6679857368,-1.5864569061	H,0,3.7608148016,2.6830281248,-1.6570744824
C,0,3.3028343862,0.7923623204,-0.6183218487	C,0,3.2640856472,0.8937222206,-0.5484830035
C,0,1.6740270959,-0.6819644381,-0.4052393328	C,0,1.5358853453,-0.3704211045,0.2111692721
N,0,2.6597161934,-1.1878713918,0.3218720015	N,0,2.7602818436,-1.044516984,0.589951301
N,0,1.9908781108,0.5028173704,-0.996386572	N,0,1.9013367707,0.8670390115,-0.4370258736
H,0,1.3729969445,1.0395926185,-1.5849101587	H,0,1.2527388945,1.2984087588,-1.0788889157
N,0,0.4580124447,-1.2819646485,-0.5611982397	N,0,0.7503051613,-1.2244760809,-0.6358671342
N,0,-0.4976558559,-0.6986539604,-1.3203600912	N,0,-0.3155245608,-0.5929230997,-1.2281666784
C,0,-1.642555387,-1.2789198259,-1.3961491049	C,0,-1.3169637589,-1.3079087914,-1.5769008113
H,0,-1.8343853912,-2.2110834181,-0.8547511133	H,0,-1.3408950779,-2.3828375059,-1.3629575909
H,0,0.289198239,-2.1399330088,-0.0443522294	H,0,0.5470544707,-2.1124646644,-0.179288005
H,0,6.1638787945,2.5850452042,-0.6795872614	H,0,6.1973617879,2.2419667458,-1.4904978692
C,0,-2.7437435533,-0.7451843554,-2.1905105276	C,0,-2.4790686824,-0.7593760552,-2.277322821
C,0,-3.9688226057,-1.4254358705,-2.192108299	C,0,-3.5311145704,-1.6168046643,-2.6200804161
C,0,-2.6147571923,0.4304089962,-2.951069328	C,0,-2.5714366181,0.6016021034,-2.6112169369
C,0,-5.0466784096,-0.9446422556,-2.933676998	C,0,-4.6545877277,-1.1296735057,-3.2868458003
C,0,-3.6826254462,0.9101760697,-3.687707786	C,0,-3.6837349739,1.0891035574,-3.2743282697
C,0,-4.9084164758,0.2186031932,-3.6782525308	C,0,-4.7326362373,0.2161146109,-3.6133573352
H,0,6.9185298606,0.7650862441,0.7598013084	H,0,7.0709961398,0.2679536086,-0.3031760497
H,0,-5.9934282599,-1.4750804108,-2.9319632444	H,0,-5.4678957408,-1.7985736909,-3.5513717879
H,0,-4.0845739951,-2.3335092221,-1.6115249925	H,0,-3.4757485894,-2.6694988951,-2.3669231593
O,0,-3.5421944181,2.0520908776,-4.4199295792	O,0,-3.7574177091,2.4118528002,-3.594251147
H,0,-4.3797408145,2.2404837049,-4.8642923497	H,0,-4.599753564,2.5742857578,-4.0382512776
O,0,4.9230372517,-0.384981975,2.3257022584	O,0,0.8278906256,0.0488476126,1.4099917037
H,0,-1.6788487839,0.973481581,-2.9682605188	H,0,-1.7739177416,1.2845426721,-2.3500662928
O,0,-5.8995083909,0.7812888892,-4.4415559846	O,0,-5.7904195145,0.8016036319,-4.2698963671
H,0,-6.7159056733,0.273951829,-4.3765682077	H,0,-6.4780962983,0.1535665656,-4.4519629082
O,0,4.2357581242,0.7974582244,2.8094957497	O,0,0.4092427712,-1.148552137,2.1095080345
H,0,4.9678495664,1.4226304384,2.9214780907	H,0,1.2235151501,-1.3879355799,2.5804165151

P C6(•OOH), optimization in solv. water UB3LYP/6-311++G**, E= -1061.37696367 a.u.	**P C6(•OOH),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.36474604 a.u.

Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.210700 a.u. SP at UM06-2X/6-311++G** (water), E = -1060.9604249 a.u.	Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.211003 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1060.9475176 a.u.
0, 2	0, 2
C,0,6.0382130345,0.3885608452,-0.2818351605	C,0,6.0125534031,0.4021780747,-0.3382301977
C,0,5.1640819943,-0.5165092179,0.2843791572	C,0,5.1553705247,-0.5081882444,0.2457404548
C,0,5.5681208055,1.523940024,-0.9876488916	C,0,5.5212772062,1.5368547521,-1.027540191
H,0,5.5138120788,-1.3908773121,0.8196213793	H,0,5.5189408343,-1.3839172008,0.7691557218
C,0,3.7709088811,-0.2863935818,0.1384573211	C,0,3.7585061768,-0.2848017077,0.1343377852
C,0,4.2065159918,1.7906915658,-1.1373779269	C,0,4.154841707,1.7976565968,-1.1432641518
H,0,3.8607438341,2.6659172412,-1.6730564022	H,0,3.7944514174,2.6756322774,-1.6651514269
C,0,3.3167884053,0.8896599607,-0.5665155325	C,0,3.2821677977,0.891215528,-0.5558619812
C,0,1.5522322556,-0.351652377,0.1478505711	C,0,1.5414153794,-0.3627309742,0.1926702245
N,0,2.7554995661,-1.0395827197,0.5607101785	N,0,2.7587746647,-1.0431190848,0.5805981044
N,0,1.9507193743,0.8726277988,-0.5035320037	N,0,1.9185150302,0.868866205,-0.4585447443
H,0,1.3321567004,1.3321892356,-1.1564370607	H,0,1.2783693767,1.3153001241,-1.0989103903
N,0,0.7614368329,-1.2050888145,-0.6868153005	N,0,0.7506584573,-1.2163893413,-0.6463493594
N,0,-0.3238658539,-0.575462302,-1.2590212985	N,0,-0.3215249579,-0.5849492055,-1.2327228934
C,0,-1.3133722132,-1.3061389571,-1.6153386259	C,0,-1.3178731423,-1.306108616,-1.5854159245
H,0,-1.3144387746,-2.3846443258,-1.4271533543	H,0,-1.3329448892,-2.3825377253,-1.3812088277
H,0,0.5738291447,-2.1025711066,-0.2419378287	H,0,0.552121857,-2.1071347166,-0.1931359116
H,0,6.2892665029,2.2074861634,-1.4201313222	H,0,6.2284830358,2.2260726864,-1.4742267348
C,0,-2.4921934374,-0.7629239695,-2.2920836978	C,0,-2.484905493,-0.7601237415,-2.2798453843
C,0,-3.5397563414,-1.6305215927,-2.6260578023	C,0,-3.527482644,-1.6244021261,-2.6351650614
C,0,-2.606326379,0.6011142296,-2.6139973162	C,0,-2.5911543653,0.6043710997,-2.5975716252
C,0,-4.6815255421,-1.1530446789,-3.2689120635	C,0,-4.6553672097,-1.1418845384,-3.2982325333
C,0,-3.7376318227,1.077617877,-3.2524209759	C,0,-3.7080090096,1.0866864591,-3.2565769044
C,0,-4.7845730125,0.1958977847,-3.5822097661	C,0,-4.7481428425,0.2074193781,-3.6089941126
H,0,7.1067800449,0.2335465383,-0.1923498661	H,0,7.0836665179,0.2508995214,-0.2749182101
H,0,-5.490933463,-1.8277959089,-3.5260863098	H,0,-5.4606153092,-1.8157823914,-3.5727538176
H,0,-3.4665408005,-2.6847234959,-2.3845612948	H,0,-3.4611262912,-2.679527253,-2.3951769461
O,0,-3.8340853709,2.4054170319,-3.5609153978	O,0,-3.7957652529,2.4140080118,-3.5609529553
H,0,-4.6794836596,2.5608245322,-4.0047416608	H,0,-4.638216914,2.5736366692,-4.0070554907
O,0,0.8289634265,0.1177299614,1.336233383	O,0,0.8319944945,0.0779011744,1.3899829407
H,0,-1.8096125903,1.2914453557,-2.3668029779	H,0,-1.8010044173,1.2927539706,-2.3273343775
O,0,-5.8554761456,0.7724880486,-4.2104438551	O,0,-5.8086348436,0.7891762476,-4.2586383468
H,0,-6.532576157,0.1168073458,-4.416260624	H,0,-6.4889231409,0.137214256,-4.4589454073
O,0,0.3386290211,-1.0389547332,2.0575619252	O,0,0.3887812303,-1.1026305322,2.1031529854
H,0,1.1115519986,-1.2863034766,2.5907757108	H,0,1.1886599416,-1.3428426633,2.5980310005

P C9(•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.33841918 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.210390 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1060.9197215 a.u.	**P C9(•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.36364173 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.210158 a.u. SP at UM06-2X/6-311++G** (water), E = -1060.9455948 a.u.
0, 2	0, 2
C,0,5.7311208198,0.1874419525,-0.2816404846	C,0,5.7300356474,0.1926700687,-0.3156002466
C,0,4.674346142,-0.7082656126,-0.1300217957	C,0,4.681166215,-0.7110145135,-0.1406262227
C,0,5.5140811197,1.5088849302,-0.790309748	C,0,5.4942003639,1.510921413,-0.8238488512
H,0,4.8494562903,-1.7519375173,0.1028433028	H,0,4.873530196,-1.7517966273,0.0946354027
C,0,3.3880598812,-0.2674909985,-0.3973683719	C,0,3.3859341209,-0.2808009626,-0.3912534997
C,0,4.2653598972,1.9960518546,-1.0391287377	C,0,4.2368170942,1.9874272134,-1.0550451348
H,0,4.1013679542,2.9828002242,-1.4574135431	H,0,4.0572053009,2.9738494953,-1.466717834
C,0,3.0995794837,1.1977248562,-0.5987483011	C,0,3.089013473,1.1775051821,-0.6023573537
C,0,1.4173442887,-0.1545235364,-1.1928292463	C,0,1.3915953725,-0.1801962366,-1.1544710405

N,0,2.2614197596,-1.0059815963,-0.6507581933	N,0,2.2564797858,-1.0266606935,-0.6144814626
N,0,1.8982390507,1.1194270523,-1.4006204335	N,0,1.8726607264,1.0903152102,-1.3642719875
H,0,1.2548865533,1.897244823,-1.456249874	H,0,1.2485302512,1.8746757761,-1.4957265092
N,0,0.1708949211,-0.517451806,-1.5867133333	N,0,0.1476134516,-0.5376698776,-1.5321314731
N,0,-0.6911582879,0.3896284669,-2.1040443748	N,0,-0.7000606673,0.3845676784,-2.0669304631
C,0,-1.8598230255,-0.0262625275,-2.4387017999	C,0,-1.8642794334,-0.031698735,-2.4199062065
H,0,-2.1393668725,-1.0775102379,-2.3048160259	H,0,-2.1466992369,-1.0808759102,-2.2953843541
H,0,-0.0961655311,-1.4853736749,-1.4281333073	H,0,-0.1339339104,-1.5050921984,-1.3944165801
H,0,6.3803783999,2.1210309399,-1.0198160218	H,0,6.351221311,2.1316640061,-1.0629166514
C,0,-2.8754850383,0.8508719579,-3.0093423221	C,0,-2.8682045917,0.8516722953,-3.0003399824
C,0,-4.1273657076,0.3137747663,-3.3362202418	C,0,-4.1069405685,0.3102805094,-3.3700921176
C,0,-2.6326748197,2.2153146114,-3.2435387356	C,0,-2.6317069903,2.224115404,-3.2018047166
C,0,-5.121566635,1.1208469547,-3.8857225751	C,0,-5.0947240406,1.1171180834,-3.9312640033
C,0,-3.6174328876,3.0193983758,-3.7886964883	C,0,-3.610824948,3.026810554,-3.7579954749
C,0,-4.8706004131,2.4666652125,-4.1118745715	C,0,-4.8521531695,2.47103035,-4.1265530613
H,0,6.7465659531,-0.1410427565,-0.0953464553	H,0,6.7507503675,-0.1282496205,-0.1457773458
H,0,-6.0907750369,0.701622226,-4.1375702368	H,0,-6.051882992,0.6953958732,-4.217471807
H,0,-4.3289728623,-0.7370507068,-3.1620314194	H,0,-4.3022796901,-0.7452815998,-3.2209655847
O,0,-3.3684262127,4.3389585658,-4.0104283015	O,0,-3.3700951397,4.3572564635,-3.947992333
H,0,-4.1582710592,4.7437978962,-4.3918774817	H,0,-4.1556696639,4.7639096434,-4.3397405732
O,0,2.5232853753,1.8098925211,0.6774735363	O,0,2.5252241082,1.7904282082,0.7117072898
O,0,-5.7750230008,3.3507438597,-4.6473694073	O,0,-5.7450248939,3.3536949174,-4.6662338099
H,0,-6.6063093778,2.9101001068,-4.8501594467	H,0,-6.575360673,2.9178207381,-4.8936179248
H,0,-1.6725860925,2.6516738933,-3.0014415168	H,0,-1.6830713454,2.6655810065,-2.9234319713
O,0,3.4791610841,1.7725141212,1.7517297637	O,0,3.5186376594,1.8319771063,1.7547877326
H,0,3.9988215164,2.5751108324,1.5926695094	H,0,4.0046621398,2.6472798087,1.5540194713

P C9(•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.34904483 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.210631 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1060.9306773 a.u.	**P C13(•OOH),** optimization in gas phase UB3LYP/6-311++G**, E= -1061.37528720 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.211547 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1060.9606005 a.u.
0, 2	0, 2
C,0,5.7304342202,0.1927320899,-0.2851717557	C,0,5.9484924608,0.7743917638,0.290952502
C,0,4.6774338707,-0.7075950591,-0.1288071508	C,0,4.9802544041,0.0126877756,0.9359368749
C,0,5.5060491115,1.5123114522,-0.7954759711	C,0,5.680103564,1.4255142325,-0.9259011316
H,0,4.8596366945,-1.7496460294,0.1068647011	H,0,5.1836048257,-0.4897975202,1.8738219578
C,0,3.3879251323,-0.2732583128,-0.3954450724	C,0,3.7204421741,-0.0911545719,0.3391368265
C,0,4.254077852,1.9932436774,-1.0429221365	C,0,4.4317324397,1.3349196072,-1.538649818
H,0,4.0841383877,2.9790885552,-1.4607236866	H,0,4.2279443465,1.8381721997,-2.47664503
C,0,3.0943523015,1.1888565366,-0.6019685085	C,0,3.4681987631,0.5714649401,-0.8887157723
C,0,1.4108833911,-0.168768474,-1.1870246384	C,0,1.7018821539,-0.5332405035,-0.1712977038
N,0,2.2627843991,-1.0167380204,-0.6423792251	N,0,2.5906371439,-0.7745459175,0.7623316972
N,0,1.8909448498,1.1045209768,-1.3942074756	N,0,2.1497452745,0.2602348968,-1.1931278778
H,0,1.2530724888,1.8840381019,-1.481067074	H,0,1.5834943144,0.5565530295,-1.9731340169
N,0,0.1672318508,-0.5303171131,-1.5787129064	N,0,0.4229043092,-1.0293088834,-0.1669033772
N,0,-0.6891396481,0.3847073111,-2.1009285719	N,0,-0.4429505841,-0.6540527299,-1.1134161168
C,0,-1.8582796441,-0.028969469,-2.4375631626	C,0,-1.6886203143,-1.3677120626,-1.0052169116
H,0,-2.1412005081,-1.0783921573,-2.3045605987	H,0,-1.5441292182,-2.4438014182,-1.1766625221
H,0,-0.1078865622,-1.4969794266,-1.4254463357	H,0,0.1200078451,-1.5289645646,0.6669338552
H,0,6.3687827411,2.1289190135,-1.0259084195	H,0,6.4602261534,2.0111164671,-1.3982797438
C,0,-2.8703622651,0.851546264,-3.0089186421	C,0,-2.7141572451,-0.8199447162,-1.9639771383
C,0,-4.1208848825,0.3146562666,-3.3421242569	C,0,-3.4242576738,-1.6809068835,-2.7980369972
C,0,-2.628072111,2.2177890435,-3.2364259505	C,0,-2.9777076616,0.5539727711,-2.0001223333

C,0,-5.1145448559,1.1221977461,-3.8918248269	C,0,-4.3890644862,-1.1768105311,-3.673004054
C,0,-3.612497605,3.0218878764,-3.7816200794	C,0,-3.9356835872,1.0612284902,-2.864898383
C,0,-4.8649675626,2.4699631376,-4.1121876213	C,0,-4.6428153135,0.1864001135,-3.7064359695
H,0,6.7477121616,-0.1309737085,-0.1005598959	H,0,6.93317408,0.8707664591,0.7337624253
H,0,-6.0821419188,0.703553632,-4.1484895822	H,0,-4.9403725129,-1.8459850183,-4.3265867273
H,0,-4.3216382193,-0.7369748074,-3.1724736111	H,0,-3.2286132077,-2.7466227961,-2.773138511
O,0,-3.3646546619,4.3446249025,-3.9968136871	O,0,-4.1817296427,2.4009044134,-2.894898825
H,0,-4.1546656903,4.751459433,-4.3773075763	H,0,-4.8679656299,2.5733404304,-3.5526493837
O,0,2.5161665313,1.8020655518,0.6846322143	O,0,-2.1098458498,-1.2346553265,0.3907313142
O,0,-5.766418956,3.3535103274,-4.645976764	O,0,-5.5681192138,0.7888883252,-4.5270627268
H,0,-6.6006427665,2.9166259815,-4.8500775896	H,0,-6.002149338,0.1375557297,-5.0869107101
H,0,-1.6696662841,2.6548189664,-2.9879815574	H,0,-2.432677629,1.2394276684,-1.3627402512
O,0,3.4811327802,1.7966137155,1.7528000439	O,0,-3.1129769387,-2.2410925,0.6622595038
H,0,3.9972710072,2.5975120485,1.5725806909	H,0,-3.928605326,-1.7233576798,0.5862270655

P C13(•OOH), optimization in solv. water UB3LYP/6-311++G**, E= -1061.39649278 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.211489 a.u. SP at UM06-2X/6-311++G** (water), E = -1060.9826872 a.u.	**P C13(•OOH),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.38442377 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.212257 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1060.9701508 a.u.
0, 2	0, 2
C,0,5.9875503117,0.686295833,0.2346378444	C,0,5.9676977011,0.7312791973,0.2528011132
C,0,5.0315187485,-0.1075725966,0.8617368018	C,0,5.0032199442,-0.0323103682,0.9024316588
C,0,5.6855388008,1.4197230262,-0.9277777984	C,0,5.6847896735,1.4036980237,-0.9496672286
H,0,5.2656490431,-0.6719516333,1.7568608499	H,0,5.2199454607,-0.5504669808,1.8289499743
C,0,3.7503550324,-0.1578638319,0.301776774	C,0,3.7324700284,-0.1154812634,0.324821288
C,0,4.4153796123,1.383090579,-1.5016474326	C,0,4.4252504878,1.3337768299,-1.5425777106
H,0,4.1821969516,1.9473100416,-2.3965368345	H,0,4.2089719619,1.852341841,-2.4691531139
C,0,3.464948241,0.5876521049,-0.869342815	C,0,3.4657908839,0.5688021623,-0.8877323504
C,0,1.7049995856,-0.5406627447,-0.1752140053	C,0,1.6995573827,-0.5304212727,-0.1623961974
N,0,2.6236995921,-0.8560390878,0.7142269813	N,0,2.6023095902,-0.7957963823,0.7544063094
N,0,2.1340682923,0.3151552247,-1.148985276	N,0,2.1402597865,0.2756319759,-1.1755680511
H,0,1.5645207374,0.6683938189,-1.903844627	H,0,1.5704835629,0.5920242369,-1.9457032669
N,0,0.4223224461,-1.0229140308,-0.1559024062	N,0,0.4171613661,-1.0160500301,-0.145059014
N,0,-0.4729160104,-0.6005477671,-1.0530647225	N,0,-0.458501423,-0.6297445265,-1.0779245902
C,0,-1.7272673274,-1.3012104484,-0.9205472579	C,0,-1.7095035569,-1.335190274,-0.9564811869
H,0,-1.5911937862,-2.3851137854,-1.0290824494	H,0,-1.5688675166,-2.4157204054,-1.0974654045
H,0,0.1597894078,-1.611997068,0.63177121	H,0,0.1276607397,-1.5384617898,0.6795031851
H,0,6.4566351283,2.0267786831,-1.3876796136	H,0,6.4622822337,1.9894828985,-1.4261582612
C,0,-2.734007861,-0.7960277723,-1.9204815485	C,0,-2.7239384744,-0.8079791914,-1.9380139404
C,0,-3.3185570578,-1.6723907211,-2.8327933897	C,0,-3.3420010781,-1.6701538827,-2.841049556
C,0,-3.0930947799,0.5576984097,-1.9328293515	C,0,-3.0592766107,0.5511636455,-1.9366063323
C,0,-4.2521431767,-1.2059859913,-3.7614838796	C,0,-4.2861719595,-1.1824781568,-3.7475143398
C,0,-4.0220495157,1.0256438023,-2.8493314486	C,0,-3.9988315876,1.0409675826,-2.8310186703
C,0,-4.6043613401,0.1369652677,-3.7702741987	C,0,-4.6141798218,0.1657380981,-3.7422024673
H,0,6.9877922603,0.7425073422,0.6485921722	H,0,6.9604435031,0.8118652471,0.680569376
H,0,-4.7060365944,-1.8856262305,-4.4748391809	H,0,-4.7659247877,-1.8512590015,-4.4550254855
H,0,-3.048982724,-2.7222252619,-2.8293437205	H,0,-3.090429082,-2.7244105736,-2.8466809976
O,0,-4.3660499159,2.3480730027,-2.8528334654	O,0,-4.3184514531,2.3670990962,-2.82188262
H,0,-5.0229062385,2.4957879765,-3.5475815728	H,0,-4.9813828499,2.5299337358,-3.5063322658
O,0,-2.152838603,-1.0745173777,0.4642257398	O,0,-2.1337630102,-1.1555500413,0.4329224944
O,0,-5.508292312,0.7015762281,-4.6310595629	O,0,-5.5285036157,0.7498737445,-4.5839732671
H,0,-5.8853055201,0.0391922929,-5.2222359033	H,0,-5.9161222297,0.0966326519,-5.1764434827
H,0,-2.6517703578,1.2557095939,-1.2311128011	H,0,-2.5883411197,1.2379709009,-1.2435466602

O,0,-3.2047390984,-2.0160859708,0.7838725783 H,0,-4.0040490923,-1.493235218,0.6118063004	O,0,-3.1638503364,-2.1284122365,0.7267974749 H,0,-3.9698509135,-1.602809801,0.6066555767

P C14(•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.33570114 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208958 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1060.9200269 a.u.	**P C14(•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.36106866 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209082 a.u. SP at UM06-2X/6-311++G** (water), E = -1060.9461339 a.u.
0, 2 C,0,5.9130163838,0.8117683677,-0.4192455442 C,0,5.2068036702,-0.3256627851,-0.0347369158 C,0,5.2745868326,1.8948480083,-1.0435737561 H,0,5.6981985076,-1.1620615281,0.4477115548 C,0,3.8346775259,-0.3644859566,-0.2870652503 C,0,3.9041484867,1.8753684077,-1.3043822832 H,0,3.4122243526,2.7124051491,-1.7865068396 C,0,3.2081483719,0.7368897338,-0.9175192435 C,0,1.7734986068,-0.8756189595,-0.457200873 N,0,2.9026157898,-1.360327015,-0.0114250842 N,0,1.8677618199,0.3719796903,-1.0139043126 H,0,1.0950116908,0.8882258652,-1.4034373765 N,0,0.5732178967,-1.5434385288,-0.3942146246 N,0,-0.5532220327,-0.9486060804,-0.8300357032 C,0,-1.6583884722,-1.582946991,-0.7478225284 H,0,-1.7287049647,-2.5918523635,-0.3310065159 H,0,0.5711592079,-2.4565416528,0.0496520157 H,0,5.8559467634,2.7638789005,-1.329100711 C,0,-2.9527906299,-0.9792032685,-1.252442926 C,0,-3.5573409042,-1.8895396242,-2.2801760143 C,0,-2.8248402554,0.4360642473,-1.7054616501 C,0,-4.0069033632,-1.4284047843,-3.4838285328 C,0,-3.3062435356,0.8592936999,-2.9023482464 C,0,-3.9047680086,-0.0662986557,-3.8117611725 H,0,6.9796730587,0.8642340828,-0.2329077725 H,0,-4.4564684174,-2.1141796709,-4.196803402 H,0,-3.6587796477,-2.934530812,-2.0137593406 O,0,-3.2085490688,2.1720557046,-3.2622634698 H,0,-3.5885156536,2.282859195,-4.1430755556 O,0,-3.7605340698,-1.0495473557,0.0062501286 H,0,-2.3435885015,1.1407353562,-1.0400527069 O,0,-4.3421095489,0.474764717,-4.988596607 H,0,-4.7452897293,-0.197783177,-5.547955798 O,0,-5.1387662282,-0.709063134,-0.2757788675 H,0,-5.1476623037,0.2378508676,-0.0715208346	0, 2 C,0,5.9521544783,0.8072589769,-0.3452629263 C,0,5.2530215483,-0.3615505306,-0.0438196469 C,0,5.3038257327,1.9302737859,-0.8852519161 H,0,5.756742302,-1.2261501747,0.3731688015 C,0,3.8788896969,-0.3894565858,-0.2937923715 C,0,3.9310657831,1.9209785452,-1.1422645092 H,0,3.4291091913,2.7861506838,-1.5589739255 C,0,3.2432146657,0.7520162572,-0.8386588498 C,0,1.8104382029,-0.893428084,-0.497104113 N,0,2.9509160417,-1.4072814624,-0.0904207276 N,0,1.9062474536,0.3900052016,-0.9574935209 H,0,1.135903514,0.9416011277,-1.3042818604 N,0,0.6157532653,-1.5619157868,-0.4741899927 N,0,-0.5086582358,-0.9397160391,-0.8898586284 C,0,-1.6116192928,-1.5827489693,-0.8417690606 H,0,-1.6747798716,-2.6098498287,-0.4753121194 H,0,0.6037024933,-2.5092803041,-0.1080335057 H,0,5.878344966,2.8221289314,-1.107357164 C,0,-2.9054843351,-0.9574387448,-1.315295411 C,0,-3.6023558484,-1.8956838256,-2.2499744049 C,0,-2.7721325925,0.4289642536,-1.8396552805 C,0,-4.1572937148,-1.4739116486,-3.4246622125 C,0,-3.358348722,0.8154734286,-3.0024511104 C,0,-4.0661996264,-0.1259879976,-3.8152888397 H,0,7.0193076943,0.851485242,-0.1590904674 H,0,-4.6720452484,-2.1783330484,-4.0704897524 H,0,-3.6752312482,-2.9334322491,-1.9475670966 O,0,-3.261552209,2.1102635255,-3.4270717861 H,0,-3.7190799428,2.1982506272,-4.27470714 O,0,-3.6467561383,-0.9271782684,0.0117825158 H,0,-2.212298347,1.1460540737,-1.253554161 O,0,-4.5981177655,0.3828864672,-4.9573314213 H,0,-5.062726123,-0.2939121638,-5.4657920951 O,0,-5.0220439232,-0.5204928901,-0.1854094619 H,0,-4.9546902147,0.4470871245,-0.1590625984

P C14(•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.34659799 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208610 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1060.9312731 a.u.	**P C15(•OOH),** optimization in gas phase UB3LYP/6-311++G**, E= -1061.35288704 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.210701 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1060.9336306 a.u.
0, 2 C,0,5.9322297043,0.8064735132,-0.391362325	0, 2 C,0,5.7963876047,0.7949224818,0.3763248856

C,0,5.2250825065,-0.3378651282,-0.0267001937	C,0,5.0128397233,-0.3408931859,0.5616411847
C,0,5.2940102857,1.9004630933,-0.9973885556	C,0,5.2986907469,1.9293601468,-0.2853339996
H,0,5.7181640322,-1.1817193823,0.4413760588	H,0,5.3950029317,-1.2167176415,1.072136501
C,0,3.8525637487,-0.371823427,-0.280245298	C,0,3.7063147516,-0.3264150607,0.0686499685
C,0,3.923003253,1.8855181114,-1.2588380189	C,0,3.9974735399,1.9636739388,-0.7864641839
H,0,3.4301445835,2.7299044789,-1.7267167363	H,0,3.6149084446,2.8397892981,-1.2972551615
C,0,3.2264133761,0.7406436792,-0.8915557376	C,0,3.2220261215,0.8262495825,-0.5973148419
C,0,1.7873245736,-0.8773762188,-0.4619129015	C,0,1.6997973585,-0.7660408478,-0.4945306776
N,0,2.9191134306,-1.3715850475,-0.0230747033	N,0,2.7246108097,-1.3084976099,0.1146183466
N,0,1.8866380209,0.3790322427,-0.9949597324	N,0,1.9166651267,0.5050056776,-0.9546057964
H,0,1.1171755897,0.9071072069,-1.3764323105	H,0,1.2170560087,1.0788935922,-1.3994958865
N,0,0.5881033204,-1.5427586776,-0.4111279259	N,0,0.4922318609,-1.3917849415,-0.671637584
N,0,-0.5362254208,-0.9390342899,-0.8468963124	N,0,-0.489293568,-0.7841652445,-1.3578005387
C,0,-1.6396606969,-1.5785223341,-0.7792084961	C,0,-1.6383855332,-1.3909622462,-1.4342868479
H,0,-1.7064561777,-2.5935873978,-0.3787793381	H,0,-1.7870002069,-2.3602118068,-0.9452908414
H,0,0.5790679722,-2.4664906717,0.0104526197	H,0,0.3738042956,-2.3016974233,-0.234694437
H,0,5.8755676178,2.7741702203,-1.2679655355	H,0,5.9372807911,2.7961805341,-0.4099215931
C,0,-2.9338275381,-0.9719806565,-1.2784711874	C,0,-2.7384424148,-0.8473552506,-2.1546718929
C,0,-3.5614536605,-1.8935105707,-2.2798422639	C,0,-3.9304753587,-1.5582562632,-2.2666424086
C,0,-2.8095651545,0.4356656641,-1.7514440123	C,0,-2.6041850919,0.5177871094,-2.7899375174
C,0,-4.0532312933,-1.4446600562,-3.4718719106	C,0,-4.988780134,-1.1048566371,-3.0495176994
C,0,-3.3338356385,0.8474057759,-2.9344936598	C,0,-3.7220783295,0.844577637,-3.7243857205
C,0,-3.9681730403,-0.0843120565,-3.8142834174	C,0,-4.8543060678,0.0871120486,-3.8014882062
H,0,6.9988779324,0.8550503882,-0.2036039031	H,0,6.8137240786,0.8068554421,0.7506264444
H,0,-4.5194527954,-2.1377673939,-4.1659980902	H,0,-5.913004464,-1.6698172978,-3.1040083513
H,0,-3.6425267134,-2.9385370104,-2.0064859512	H,0,-4.030232604,-2.5043141836,-1.7447997682
O,0,-3.2456102958,2.1570770541,-3.3111230966	O,0,-3.5537881207,1.9767476744,-4.4552679322
H,0,-3.6563848187,2.2613331304,-4.1795868279	H,0,-4.3320360478,2.0891208894,-5.0197784408
O,0,-3.7261203715,-1.01528617,0.0021684265	O,0,-2.4165620146,1.5728936144,-1.7985401943
H,0,-2.3041363562,1.1456967774,-1.110043986	H,0,-1.6452852059,0.6041061104,-3.3157832372
O,0,-4.4483833592,0.4474278399,-4.9744644858	O,0,-5.8451390223,0.5579202864,-4.6460939087
H,0,-4.8850660704,-0.2236264741,-5.5119458555	H,0,-6.4367197257,-0.1571297763,-4.8999542921
O,0,-5.1052074539,-0.6589320917,-0.2538466336	O,0,-3.5945329939,1.6424575123,-0.9524053849
H,0,-5.0909394627,0.2995355293,-0.1096244628	H,0,-3.9828765502,2.4766181204,-1.2531792167

P C15(•OOH), optimization in solv. water UB3LYP/6-311++G**, E= -1061.37761181 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.210751 a.u. SP at UM06-2X/6-311++G** (water), E = -1060.9595412 a.u.	**P C15(•OOH),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.36330858 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.210890 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1060.9445329 a.u.
0, 2	0, 2
C,0,5.8348131546,0.7666939442,0.3430720382	C,0,5.822381677,0.7723989142,0.3504319643
C,0,5.0153954578,-0.3291929151,0.6123107301	C,0,5.0212842763,-0.3459876087,0.5705804907
C,0,5.3709765481,1.8633577618,-0.4026223046	C,0,5.3385442064,1.8971632194,-0.3378772332
H,0,5.3771490743,-1.1737965458,1.187529473	H,0,5.3951286399,-1.2132850568,1.101871132
C,0,3.7082744052,-0.3111743742,0.1181552951	C,0,3.7115195067,-0.3231635544,0.08548394
C,0,4.0681226487,1.9001389096,-0.9041504809	C,0,4.0336937933,1.9393610692,-0.8307678212
H,0,3.7084820928,2.7447717554,-1.4798277733	H,0,3.6604090955,2.8069342747,-1.3622974818
C,0,3.2584230184,0.8040336142,-0.6304644926	C,0,3.2414227336,0.8198533938,-0.606548141
C,0,1.6798542994,-0.7263598264,-0.4193142187	C,0,1.6910184311,-0.7433004943,-0.45723726
N,0,2.694514072,-1.25608061,0.2334909675	N,0,2.7135179595,-1.2875601289,0.1613091675
N,0,1.9431158724,0.5015671062,-0.9603831378	N,0,1.9291765326,0.5119527031,-0.9469853708
H,0,1.2850546635,1.0532569047,-1.4901273304	H,0,1.2441626702,1.0862757709,-1.413856172
N,0,0.4605352197,-1.3246088844,-0.5619058088	N,0,0.4759122257,-1.3537045772,-0.616348304

N,0,-0.5140123966,-0.7117541566,-1.2680354628	N,0,-0.5016043184,-0.7445801987,-1.3128717475
C,0,-1.641386678,-1.3490878614,-1.3962337468	C,0,-1.6417964805,-1.3648706292,-1.4105315317
H,0,-1.773138162,-2.3393621969,-0.9508670999	H,0,-1.7832504411,-2.3423793318,-0.9380097077
H,0,0.3283095876,-2.2411545313,-0.1430942365	H,0,0.3517863679,-2.2676434496,-0.189505126
H,0,6.0358934913,2.6977961893,-0.5933249791	H,0,5.9902085754,2.74977553,-0.4900504231
C,0,-2.7387062138,-0.8148084866,-2.1346184047	C,0,-2.7403992102,-0.8287606171,-2.1413899002
C,0,-3.8848388157,-1.5761413241,-2.3374125498	C,0,-3.9109661998,-1.565593878,-2.2961625091
C,0,-2.6522005436,0.5811621998,-2.6993384758	C,0,-2.6298841464,0.5516979204,-2.7435245904
C,0,-4.9274137608,-1.140484283,-3.1563181277	C,0,-4.9595882365,-1.1246826353,-3.1011179252
C,0,-3.7261939784,0.8911260001,-3.685335232	C,0,-3.7219500172,0.8632936083,-3.711096973
C,0,-4.8197844489,0.0863658871,-3.8530179177	C,0,-4.8352678624,0.0813372877,-3.8317960773
H,0,6.8527427816,0.7739295695,0.7161811848	H,0,6.8423116758,0.7770211407,0.7179603625
H,0,-5.8094142355,-1.7554878283,-3.2928351598	H,0,-5.8645907433,-1.7147224133,-3.1944540448
H,0,-3.9581543392,-2.5535523966,-1.8726947958	H,0,-4.0001042947,-2.5246859363,-1.7969327071
O,0,-3.5672108153,2.0576487069,-4.3640832403	O,0,-3.5555556183,2.0085790914,-4.4229847266
H,0,-4.3208041201,2.1746634739,-4.961787588	H,0,-4.3180307978,2.1169521471,-5.0100281942
O,0,-2.6051053986,1.6044732439,-1.6404474588	O,0,-2.5220612218,1.5928055603,-1.7175483919
H,0,-1.6672514646,0.7605326548,-3.1463722991	H,0,-1.6542968979,0.6866988888,-3.2256513997
O,0,-5.778617078,0.5403678616,-4.7309738031	O,0,-5.8088137779,0.5394715109,-4.6982171268
H,0,-6.380350301,-0.1703712714,-4.980894567	H,0,-6.4064609615,-0.1740012336,-4.9453544516
O,0,-3.8221566558,1.5493329146,-0.8514241141	O,0,-3.7284140912,1.5971705149,-0.9100656702
H,0,-4.3192262413,2.3033550745,-1.2039241126	H,0,-4.16375231,2.4013354774,-1.229515279

P C16(•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.34329023 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208373 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1060.926315 a.u.	**P C16(•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.37039617 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.209188 a.u. SP at UM06-2X/6-311++G** (water), E = -1060.9548347 a.u.
0, 2	0, 2
C,0,5.8496527767,0.7626301889,0.1614562438	C,0,5.8318828539,0.7899055696,0.1538159797
C,0,5.0722407415,-0.3788765481,0.3432194702	C,0,5.0688022427,-0.3632565168,0.3390313829
C,0,5.3526603042,1.8881349201,-0.514248659	C,0,5.3175883869,1.908027157,-0.5227988611
H,0,5.4547364378,-1.2481572051,0.8646107443	H,0,5.4695368832,-1.2241653065,0.8619611325
C,0,3.7734210024,-0.3785525836,-0.1678828654	C,0,3.767868164,-0.3809414012,-0.1698983401
C,0,4.0572121903,1.9082609302,-1.0321148388	C,0,4.0192370595,1.9091988263,-1.0381466366
H,0,3.6744637459,2.7779773893,-1.5537650281	H,0,3.6204245112,2.7707051012,-1.5605865777
C,0,3.2894879264,0.7655223476,-0.8462237919	C,0,3.2671569787,0.7559384725,-0.8491887912
C,0,1.7783719474,-0.8411132509,-0.7576335072	C,0,1.7692352654,-0.8657918051,-0.7603758454
N,0,2.7978484697,-1.3694624393,-0.1307050787	N,0,2.8031254645,-1.3835153091,-0.1305177381
N,0,1.9892669397,0.4317195445,-1.2164100443	N,0,1.9725793595,0.4072186027,-1.2162936493
H,0,1.3109764584,0.9836861124,-1.7164739256	H,0,1.2937518141,0.9569883992,-1.7209852561
N,0,0.5828714512,-1.4878086338,-0.9525936024	N,0,0.5840041286,-1.5175355067,-0.9572447129
N,0,-0.4176885032,-0.8913833152,-1.6281001355	N,0,-0.4185603066,-0.9060141617,-1.6283191771
C,0,-1.5149942302,-1.5361487395,-1.7921656666	C,0,-1.5179615427,-1.5482560771,-1.7901856233
H,0,-1.6356204287,-2.5477974899,-1.3890548322	H,0,-1.6462676914,-2.558414625,-1.392066048
H,0,0.5043259689,-2.431770897,-0.5866832983	H,0,0.4923969035,-2.4629022267,-0.5972515248
H,0,5.9858881998,2.7591329414,-0.6369738772	H,0,5.9383273045,2.7876407954,-0.6483462398
C,0,-2.6597916368,-0.974393282,-2.5161118612	C,0,-2.6573558949,-0.9701796381,-2.5126573154
C,0,-3.8364132204,-1.7705727175,-2.6087673025	C,0,-3.8512008382,-1.7455176795,-2.5840322151
C,0,-2.6255991449,0.2635374154,-3.1053794992	C,0,-2.6010046558,0.2583354346,-3.1215828599
C,0,-4.9722212249,-1.3091854548,-3.2981237025	C,0,-4.9786892891,-1.2797261271,-3.2804622862
C,0,-3.7927677914,0.8589819857,-3.8121361175	C,0,-3.767145385,0.8632713543,-3.8158791459
C,0,-4.9767202545,-0.0705697064,-3.8747317279	C,0,-4.9590731985,-0.0520779225,-3.8861460273
H,0,6.8616418723,0.7846595115,0.5496376088	H,0,6.8443297889,0.8251261792,0.5400975704

H,0,-5.8508883415,-1.9438312492,-3.3730475496	H,0,-5.8664720476,-1.899768072,-3.3480587471
H,0,-3.8584019751,-2.7509918219,-2.1477730249	H,0,-3.8879761337,-2.7162446032,-2.104831857
O,0,-3.389523366,1.2908020546,-5.0855380221	O,0,-3.3753562291,1.3299713801,-5.0826561351
H,0,-4.1610715316,1.6679295578,-5.530752594	H,0,-4.1701776901,1.5957471799,-5.5681253677
O,0,-4.180722195,2.1352683616,-3.1857543888	O,0,-4.1532405105,2.1452073053,-3.1623812476
O,0,-6.0178990072,0.4611916415,-4.5716740956	O,0,-5.9703700738,0.4825537286,-4.6102272255
H,0,-6.7210914091,-0.1906684551,-4.6747332975	H,0,-6.7028428244,-0.1415081772,-4.7018013285
H,0,-1.7415725949,0.8855800319,-3.0658667045	H,0,-1.7011478047,0.8599716964,-3.1000096019
O,0,-4.7066078613,1.8733471577,-1.8585697146	O,0,-4.6158840151,1.8893488785,-1.8136607883
H,0,-5.6313399961,2.1318416072,-1.9816172135	H,0,-5.5753892577,1.989579005,-1.9128707957

P C16(•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.35465700 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.208850 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1060.9382926 a.u.	**P C17(•OOH),** optimization in gas phase UB3LYP/6-311++G**, E= -1061.36097824 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.211540 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1060.9431067 a.u.
0, 2	0, 2
C,0,5.8471051949,0.7696417973,0.1461467322	C,0,5.8911429195,0.7196545364,0.1644647302
C,0,5.0722634495,-0.3726847475,0.340026027	C,0,5.0205147376,-0.3250498833,0.4603998667
C,0,5.3446408249,1.8891385261,-0.5360728122	C,0,5.5055887818,1.782423629,-0.6692986371
H,0,5.4612175673,-1.2362433874,0.8666281426	H,0,5.3158600989,-1.1456167556,1.1030441738
C,0,3.7707327629,-0.378927514,-0.165449624	C,0,3.7402353662,-0.291557822,-0.0971256661
C,0,4.0461984308,1.9022629162,-1.0483468607	C,0,4.232383599,1.8349378297,-1.2358649961
H,0,3.6579998116,2.7660938066,-1.5753660377	H,0,3.9371170414,2.6557935177,-1.8791371502
C,0,3.2815299437,0.7593143519,-0.8501779745	C,0,3.3691550352,0.7882750569,-0.9353176844
C,0,1.7704540838,-0.8474380111,-0.7458196645	C,0,1.7318075792,-0.6707332807,-0.6975899238
N,0,2.7962267993,-1.3709648215,-0.1175283519	N,0,2.6887945812,-1.18965145,0.0309372573
N,0,1.9813571361,0.4216278984,-1.212408193	N,0,2.0577171367,0.5104934689,-1.3082398072
H,0,1.3027510418,0.9725054211,-1.7144768027	H,0,1.4401427587,1.0396342119,-1.9029361233
N,0,0.5758392403,-1.4924270157,-0.9336208967	N,0,0.4959028718,-1.2438800353,-0.8525873844
N,0,-0.4223378927,-0.8916508003,-1.614132504	N,0,-0.4469246262,-0.6566252315,-1.6054650334
C,0,-1.5205880475,-1.5348163998,-1.7780217375	C,0,-1.6024917708,-1.2730193776,-1.6907460854
H,0,-1.6460424989,-2.5443784645,-1.3737833922	H,0,-1.7545919803,-2.2179112052,-1.1591776946
H,0,0.4906884099,-2.4369884141,-0.5704696357	H,0,0.3341904115,-2.1191218426,-0.3611205538
H,0,5.9753971657,2.7605724658,-0.6684534898	H,0,6.2110671537,2.578326821,-0.8776394323
C,0,-2.6604329091,-0.9687043525,-2.507556901	C,0,-2.6878278858,-0.7707878947,-2.4468551238
C,0,-3.8380620888,-1.7633522418,-2.6083664528	C,0,-3.9172877808,-1.5146578783,-2.4767176124
C,0,-2.6195775839,0.270040496,-3.0950953167	C,0,-2.6022502979,0.4404328663,-3.2030716829
C,0,-4.9664440498,-1.3031256745,-3.3095248212	C,0,-5.0008540556,-1.081991902,-3.1564242605
C,0,-3.7834429615,0.8669009611,-3.803771557	C,0,-3.6620659429,0.8916951087,-3.9134660419
C,0,-4.9634445833,-0.0647449766,-3.8892482169	C,0,-5.0048698329,0.2126453501,-3.8917755352
H,0,6.8607586467,0.7962087492,0.5298576415	H,0,6.8901315009,0.7157779894,0.5852094196
H,0,-5.843332732,-1.9379085413,-3.3949249278	H,0,-5.9315357133,-1.6389913953,-3.1591848725
H,0,-3.8646021851,-2.7429798644,-2.1463000981	H,0,-3.9664091996,-2.4518721891,-1.9314177124
O,0,-3.3750690263,1.3251599014,-5.067228794	O,0,-3.5843272031,2.0266839533,-4.6498027728
H,0,-4.1552896466,1.6582327245,-5.5330583383	H,0,-4.3675764789,2.0751959992,-5.2166092534
O,0,-4.184835966,2.1371373932,-3.1600242787	O,0,-6.0273459024,1.1293759807,-3.3410209065
O,0,-5.9883969225,0.4665065411,-4.6051381158	O,0,-5.4483754164,0.1314853255,-5.2318553402
H,0,-6.6954037208,-0.1800120412,-4.7233354602	H,0,-6.3720946239,-0.1526570641,-5.2305013226
H,0,-1.7341630478,0.8900960222,-3.0483416619	H,0,-1.6708712802,0.9906311876,-3.2330463066
O,0,-4.6946663571,1.8620075446,-1.8303490738	O,0,-5.8184343366,1.3075906082,-1.9227002393
H,0,-5.6348965695,2.0628196615,-1.9489484521	H,0,-5.3981774159,2.1805111572,-1.9016031124

P C17(•OOH), optimization in solv. water UB3LYP/6-311++G**, E= -1061.38327209 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.210968 a.u. SP at UM06-2X/6-311++G** (water), E = -1060.9666206 a.u.	**P C17(•OOH),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.37049856 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.211296 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1060.9531451 a.u.
0, 2	0, 2
C,0,5.8860045471,0.7333110175,0.1237722477	C,0,5.8882859416,0.7265783842,0.1533663823
C,0,5.032165245,-0.3255806576,0.4277348045	C,0,5.0229053884,-0.3221165649,0.4542802275
C,0,5.4729425821,1.7961447509,-0.6981341006	C,0,5.4946196687,1.7867878676,-0.6804646197
H,0,5.3536591428,-1.1438536228,1.0617621928	H,0,5.3266505871,-1.1397229926,1.097179479
C,0,3.7419122995,-0.3049907577,-0.1098105412	C,0,3.7399007782,-0.2947802442,-0.0983569121
C,0,4.1889134172,1.8347674038,-1.2442762938	C,0,4.2183941952,1.8327291305,-1.2419896084
H,0,3.8690218442,2.6531605607,-1.8782482323	H,0,3.9152451509,2.6505151525,-1.885321341
C,0,3.3437206747,0.7748618599,-0.935719194	C,0,3.3609075632,0.7823755326,-0.9364362703
C,0,1.7222313861,-0.7013654957,-0.6870969751	C,0,1.7277577441,-0.6809959036,-0.6930907056
N,0,2.7013720044,-1.2163082311,0.0274843311	N,0,2.6915308407,-1.1967037901,0.0341215442
N,0,2.0325098716,0.4849712796,-1.290574502	N,0,2.0501555127,0.4997935875,-1.3041795113
H,0,1.4066074787,1.020528121,-1.8733035512	H,0,1.4319799276,1.0298578234,-1.8984491848
N,0,0.4921727745,-1.2811739029,-0.8309728542	N,0,0.4939381658,-1.2560751059,-0.8447033568
N,0,-0.4539217016,-0.6867258294,-1.5781690899	N,0,-0.4488870997,-0.6661220928,-1.5973658642
C,0,-1.6094617799,-1.3019171089,-1.6648185655	C,0,-1.6039494597,-1.2829531688,-1.684810252
H,0,-1.7674038011,-2.2495560203,-1.1443008983	H,0,-1.7579855149,-2.229129121,-1.1579792831
H,0,0.3268603751,-2.1621496537,-0.3504886609	H,0,0.3292326781,-2.1331853564,-0.3572956022
H,0,6.1644536373,2.6025138672,-0.9132692142	H,0,6.1957389415,2.5855504554,-0.8927570172
C,0,-2.6881775966,-0.7795691524,-2.4213919945	C,0,-2.6869703872,-0.7738329468,-2.4412444425
C,0,-3.924869091,-1.5110514051,-2.4641510185	C,0,-3.9186792402,-1.5139477845,-2.4753726406
C,0,-2.5890604541,0.4429546591,-3.1589955225	C,0,-2.5975138685,0.4414382941,-3.1911142272
C,0,-4.9987009945,-1.0623541686,-3.1514300007	C,0,-4.9999821606,-1.0753597532,-3.1558441522
C,0,-3.6392481987,0.9125140777,-3.8728312043	C,0,-3.6548426405,0.8989491144,-3.9014017192
C,0,-4.9788822955,0.2266862354,-3.8978087017	C,0,-4.9972210267,0.2186797213,-3.8928504179
H,0,6.8914927366,0.739131132,0.5290530112	H,0,6.888943564,0.7272261511,0.5703085854
H,0,-5.9327040862,-1.6136740455,-3.1735958805	H,0,-5.9314677195,-1.6311035953,-3.1643316534
H,0,-3.9873097245,-2.4509949292,-1.9257661101	H,0,-3.9714809242,-2.4526405907,-1.933292867
O,0,-3.5390576926,2.0625677185,-4.5866650883	O,0,-3.5703979541,2.0395594514,-4.6304381175
H,0,-4.3454539225,2.1886746662,-5.1070092925	H,0,-4.3583948349,2.1096128654,-5.1885563463
O,0,-6.0249563451,1.1494677741,-3.3922744594	O,0,-6.0253363154,1.1381895959,-3.3513992673
O,0,-5.3697638065,0.1242768829,-5.2492708995	O,0,-5.4263938163,0.1345500449,-5.2357309241
H,0,-6.2241399844,-0.3268041832,-5.299298952	H,0,-6.3316956559,-0.2045639513,-5.2524458759
H,0,-1.6568165277,0.9937153806,-3.1622989428	H,0,-1.6655681841,0.9914065461,-3.2136432685
O,0,-5.8420157399,1.3775498276,-1.9747054374	O,0,-5.8246027739,1.3260055603,-1.9322502958
H,0,-5.4566564445,2.2677113394,-1.9673732293	H,0,-5.4073772413,2.2008670736,-1.9103832944

P C19(•OOH), optimization in gas phase UB3LYP/6-311++G**, E= -1061.35544721 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.211022 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1060.9363334 a.u.	**P C19(•OOH),** optimization in solv. water UB3LYP/6-311++G**, E= -1061.37913109 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.210664 a.u. SP at UM06-2X/6-311++G** (water), E = -1060.9610518 a.u.
0, 2	0, 2
C,0,6.0445222469,0.7647329595,0.4481032105	C,0,6.0390326941,0.7793562799,0.4107027956
C,0,5.1813483026,-0.2872151633,0.7426392933	C,0,5.1927093559,-0.2883290636,0.7079531412
C,0,5.6375546888,1.8462566842,-0.3498289092	C,0,5.6041395933,1.8650256326,-0.3679831203
H,0,5.4938122614,-1.1222912315,1.3579940975	H,0,5.531834989,-1.1243473481,1.3089052943
C,0,3.8868910002,-0.2416971998,0.2206433184	C,0,3.8879840532,-0.2529935903,0.2082427599

C,0,4.3491938277,1.9108749591,-0.8806815287	C,0,4.3045410158,1.9184045404,-0.8762212519
H,0,4.0367507648,2.7464599921,-1.4964192924	H,0,3.9671752637,2.7546803103,-1.477046328
C,0,3.4942598306,0.8572293569,-0.5817906315	C,0,3.4678664791,0.8501621167,-0.5747410269
C,0,1.862178225,-0.6078372731,-0.3340009672	C,0,1.8511303329,-0.633215952,-0.3227363198
N,0,2.8383962197,-1.1430022899,0.3562156616	N,0,2.8506597322,-1.1681916395,0.3488668844
N,0,2.1727661099,0.5878472143,-0.9254163069	N,0,2.1464905207,0.5704216962,-0.9004141768
H,0,1.5395833568,1.1301025687,-1.4909371742	H,0,1.5041165086,1.1223858672,-1.4486932368
N,0,0.6221941697,-1.1754955847,-0.4713800587	N,0,0.6175220176,-1.2055604263,-0.449971062
N,0,-0.3400336494,-0.564188614,-1.1856047543	N,0,-0.348114082,-0.5846357732,-1.1586209857
C,0,-1.4992641322,-1.1670012396,-1.2552908664	C,0,-1.5074866191,-1.18503433,-1.2280356746
H,0,-1.6517817427,-2.1141768403,-0.7277978569	H,0,-1.6634175256,-2.1359148558,-0.7121320178
H,0,0.467324015,-2.0596963545,0.0051659147	H,0,0.4586198139,-2.0967551502,0.0124347747
H,0,6.3371774344,2.6472973498,-0.5583561097	H,0,6.2894898726,2.6776754851,-0.5792922582
C,0,-2.6021483538,-0.6468323389,-1.9864867003	C,0,-2.6052480955,-0.6478304887,-1.9587130411
C,0,-3.9060083957,-1.402782687,-1.8727244088	C,0,-3.9150474604,-1.3918204757,-1.8627401253
C,0,-2.535104759,0.5315214473,-2.7391601169	C,0,-2.524079207,0.5341537895,-2.7050924606
C,0,-4.9723782394,-0.9424215834,-2.8096496015	C,0,-4.9668716493,-0.9306978243,-2.8136612965
C,0,-3.6124021322,0.9675526511,-3.4787730098	C,0,-3.5902453785,0.9738952375,-3.4599881303
C,0,-4.8343842814,0.1949889987,-3.5164732379	C,0,-4.815027284,0.2039848032,-3.5251557052
H,0,7.0543113003,0.7511000973,0.8421591871	H,0,7.0554890336,0.7732043123,0.7878017452
H,0,-5.8915292555,-1.517453284,-2.8426133884	H,0,-5.8796660622,-1.5120956413,-2.8778177986
H,0,-3.7361689313,-2.4817679732,-1.9865976485	H,0,-3.7537857886,-2.4724994019,-1.9622790112
O,0,-3.5325875017,2.1104784461,-4.2000119354	O,0,-3.4935548404,2.118610681,-4.1785989703
H,0,-4.3792405428,2.2537013691,-4.6459890748	H,0,-4.325438048,2.2610917357,-4.6549007016
O,0,-4.3974394312,-1.4192264774,-0.4857110566	O,0,-4.4235333051,-1.3958693585,-0.471461848
O,0,-5.7817716048,0.7403674261,-4.3475966952	O,0,-5.7339281155,0.7446496764,-4.3816265376
H,0,-6.6196683882,0.2742194877,-4.258165401	H,0,-6.5607957659,0.24713281,-4.3662100244
H,0,-1.6187712571,1.1076258291,-2.7636745048	H,0,-1.6037079687,1.1051912749,-2.7174437035
O,0,-4.7688273974,-0.0724027432,-0.0937288157	O,0,-4.7575046455,-0.0432946143,-0.0617846869
H,0,-4.003958348,0.1869142709,0.4406399186	H,0,-3.9665540251,0.2128419148,0.4371546543

P C19(•OOH), optimization in solv. benzene UB3LYP/6-311++G**, E= -1061.36566227 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.210937 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1060.9470142 a.u.	
0, 2 C,0,6.0416114826,0.7723721437,0.4339200846 C,0,5.1864751789,-0.2871063603,0.7290310399 C,0,5.6223502535,1.8555420695,-0.3559071303 H,0,5.5106490138,-1.1224284628,1.338402603 C,0,3.8878586045,-0.2469994491,0.2158582421 C,0,4.3293897897,1.9144147196,-0.877661405 H,0,4.0057851948,2.7501875555,-1.4871470493 C,0,3.4830877745,0.8536287712,-0.5782308718 C,0,1.8584243044,-0.6204304172,-0.3297029111 N,0,2.844589222,-1.1550081364,0.3529158739 N,0,2.1618919234,0.5791679802,-0.9146755833 H,0,1.5253609709,1.1245801841,-1.4744644046 N,0,0.6211935528,-1.1904569376,-0.4634372065 N,0,-0.3428519678,-0.5740259771,-1.1741188859 C,0,-1.5018574999,-1.1764450493,-1.2453329419 H,0,-1.6551729711,-2.1263367198,-0.7246106285 H,0,0.4659467714,-2.0801381308,0.0028313192	

H,0,6.3154330994,2.6621157219,-0.565172574 C,0,-2.6028889766,-0.6486771561,-1.9755883114 C,0,-3.9099095693,-1.3982662389,-1.867731107 C,0,-2.5298320111,0.5308391488,-2.7261857456 C,0,-4.9701382901,-0.9383508224,-2.8108096147 C,0,-3.6029445338,0.9687943651,-3.4712087903 C,0,-4.8265703805,0.1978118854,-3.5197596789 H,0,7.0540841855,0.7626922375,0.821335538 H,0,-5.8871247547,-1.5154381271,-2.8558638115 H,0,-3.7446554097,-2.4783399496,-1.973411728 O,0,-3.5161767084,2.1123179949,-4.1914993426 H,0,-4.3582222827,2.2572773545,-4.6471089005 O,0,-4.4076986153,-1.4062229076,-0.4782019941 O,0,-5.7619100202,0.7415297745,-4.361177058 H,0,-6.5996629193,0.2692991705,-4.295370224 H,0,-1.611493329,1.1041712356,-2.7470647835 O,0,-4.7651779171,-0.0567319294,-0.0820374269 H,0,-3.9850477553,0.2084426891,0.4278859587	

P C1(•OOCH$_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.66312523 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234833 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1100.2223344 a.u.	**P C1(•OOCH$_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.68577443 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235079 a.u. SP at UM06-2X/6-311++G** (water), E = -1100.2462814 a.u.
0, 2 C,0,6.039470481,0.7187419727,0.043207497 C,0,5.2094713599,-0.4014250799,0.2958104315 C,0,5.6438178855,1.7834908313,-0.7243220938 H,0,5.5425869121,-1.2275525016,0.9100134025 C,0,3.9197958907,-0.3983028028,-0.276744166 C,0,4.2896203814,1.8790344577,-1.3684112291 H,0,4.3929448709,2.0205931996,-2.4580551027 C,0,3.4938114244,0.6717309466,-1.0522470939 C,0,1.924385768,-0.8561546431,-0.874906476 N,0,2.9136221743,-1.3566142528,-0.1797724026 N,0,2.2076235296,0.3593359623,-1.4441789209 H,0,1.5424149552,0.9446313218,-1.9258251733 N,0,0.7096934139,-1.4753339911,-1.0526099759 N,0,-0.2891627092,-0.8431988462,-1.7050728299 C,0,-1.4430565273,-1.406099273,-1.7399178505 H,0,-1.6115982462,-2.3660202496,-1.2385995406 H,0,0.5495129558,-2.3259016442,-0.5215874905 H,0,6.3169080016,2.6142158161,-0.9030704916 C,0,-2.5876078817,-0.8224359336,-2.4333789149 C,0,-3.8193259705,-1.4879933175,-2.3861967671 C,0,-2.4917549478,0.3854224916,-3.1451157761 C,0,-4.9357822371,-0.9601065353,-3.032790136 C,0,-3.5978716515,0.9124321473,-3.7879521584 C,0,-4.8286989343,0.2341214592,-3.7302728789 H,0,7.0364376412,0.7303779982,0.4718076593 H,0,-5.8883151922,-1.4796172083,-2.9928457464 H,0,-3.9101437733,-2.4215959485,-1.8426210947 O,0,-3.4881199372,2.0840476325,-4.4737364667 H,0,-4.3491603424,2.30107549,-4.8540412269 O,0,3.5805707891,3.1238209406,-1.0707573151 H,0,-1.5515463745,0.9182721154,-3.198596963 O,0,-5.862035719,0.8428964571,-4.4030175539 H,0,-6.6734187528,0.3329713644,-4.3151813571 O,0,3.2409930829,3.1342018938,0.3511330401 C,0,3.7657365423,4.3386160689,0.8819573358 H,0,3.4392218606,4.3404897534,1.9250952982 H,0,4.8589988227,4.3551268367,0.8358429385 H,0,3.3529210737,5.2116331302,0.3666389895	0, 2 C,0,6.0278865249,0.7395457747,-0.0454997873 C,0,5.2005020556,-0.3724449233,0.2587137306 C,0,5.6028874313,1.7997426615,-0.8033403502 H,0,5.5630176039,-1.1939126991,0.863406849 C,0,3.8892379959,-0.3707394918,-0.2622543669 C,0,4.213724061,1.9076831192,-1.364466136 H,0,4.2447145773,2.0829678366,-2.4515272754 C,0,3.4337901609,0.6938807479,-1.0307417821 C,0,1.8749151415,-0.8467846629,-0.8128839988 N,0,2.8906309744,-1.3368761902,-0.1353876531 N,0,2.1391456287,0.3722890907,-1.3817638294 H,0,1.4785174737,0.9180044216,-1.9157962452 N,0,0.6638031904,-1.464337935,-0.967156659 N,0,-0.3251499735,-0.8415885263,-1.6553836909 C,0,-1.475389587,-1.4123663278,-1.7042339177 H,0,-1.6532779236,-2.3640862948,-1.1951549149 H,0,0.502163627,-2.3316363245,-0.4642641952 H,0,6.2732232779,2.6227288459,-1.0223394275 C,0,-2.6040138324,-0.8348072676,-2.4296014661 C,0,-3.8370329313,-1.5001264939,-2.4019825413 C,0,-2.4932375167,0.366940969,-3.1525722433 C,0,-4.9411407337,-0.9809709087,-3.0771149322 C,0,-3.5871761966,0.8836272831,-3.8235310764 C,0,-4.8213869611,0.2067725152,-3.7868080712 H,0,7.0451296807,0.744799724,0.3321689138 H,0,-5.8938806112,-1.4988120118,-3.0510960748 H,0,-3.938542576,-2.4275680873,-1.8502413138 O,0,-3.4644815658,2.0516490144,-4.5220280937 H,0,-4.3175286374,2.2631616825,-4.9263554792 O,0,3.5302170354,3.1511458836,-0.9788271503 H,0,-1.5514192377,0.8997371709,-3.191636914 O,0,-5.8342939881,0.8068197498,-4.485288576 H,0,-6.6509937593,0.2971819758,-4.4230586518 O,0,3.3239819258,3.1520715281,0.4692699196 C,0,3.9293293868,4.3388438847,0.9700150235 H,0,3.705682202,4.3281331678,2.0393889419 H,0,5.0114077421,4.3291433367,0.8159729153 H,0,3.4879989545,5.229115821,0.5130819196

P C1(•OOCH$_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.67268398 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235015 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1100.2323925 a.u.	**P C2(•OOCH$_3$),** optimization in gas phase UB3LYP/6-311++G**, E= -1100.66257942 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234281 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1100.2202748 a.u.
0, 2 C,0,6.0390584191,0.7230069315,-0.0098166462 C,0,5.2075707965,-0.3912434461,0.2669986269	0, 2 C,0,5.7065082357,0.2876274966,0.356750817 C,0,4.8683326567,-0.7765309905,0.4447845236

C,0,5.6292665461,1.7900675799,-0.7664851421	C,0,5.324056185,1.5975616227,-0.2794428281
H,0,5.5543032306,-1.2189665577,0.8718070946	H,0,5.1727644919,-1.6964757214,0.930893543
C,0,3.9043401118,-0.3817012742,-0.2735738393	C,0,3.5664738862,-0.6797908704,-0.1150283764
C,0,4.2551692316,1.898861621,-1.363884169	C,0,3.964870253,1.6224134518,-0.9101353911
H,0,4.3197547375,2.0583996199,-2.453201484	H,0,3.6545720014,2.5201511288,-1.4313073532
C,0,3.4636632769,0.6907475151,-1.0384684998	C,0,3.1669825786,0.5271405957,-0.7747853276
C,0,1.8954444334,-0.8387476626,-0.8394838231	C,0,1.5817638415,-1.023426521,-0.8031975227
N,0,2.8994486109,-1.3409030117,-0.1612107397	N,0,2.5639124794,-1.6151056614,-0.1523822697
N,0,2.1704342999,0.3795163084,-1.405900731	N,0,1.8652189008,0.2527667291,-1.2088776141
H,0,1.5035162222,0.95412174,-1.898876486	H,0,1.2292328295,0.8513055408,-1.7099777034
N,0,0.6787506154,-1.4521055208,-0.9990997203	N,0,0.3807950863,-1.6179902261,-1.0604151661
N,0,-0.3137088881,-0.8288341685,-1.6743690974	N,0,-0.5874197994,-0.9606415986,-1.7335365575
C,0,-1.4652660876,-1.3967921364,-1.7151467892	C,0,-1.6965714671,-1.5767551167,-1.9475547911
H,0,-1.6373530642,-2.350287909,-1.204711127	H,0,-1.842485995,-2.6029216061,-1.5919717207
H,0,0.5194911048,-2.3129538716,-0.484747398	H,0,0.2557717009,-2.5677049369,-0.7220472087
H,0,6.3031523903,2.6156726049,-0.9645252476	H,0,6.0925288846,1.8862641326,-1.0145261927
C,0,-2.6024021256,-0.8240183443,-2.4299305276	C,0,-2.8127768051,-0.9687293878,-2.6615810909
C,0,-3.8311342595,-1.4961954692,-2.3946709548	C,0,-3.9843151085,-1.7144827665,-2.849366583
C,0,-2.5033099378,0.3785699902,-3.1511901295	C,0,-2.7496470109,0.3414671503,-3.1672584933
C,0,-4.94189999,-0.9812457776,-3.0614838014	C,0,-5.0719566482,-1.1667220915,-3.5268536165
C,0,-3.603663677,0.891856053,-3.8144167311	C,0,-3.827566179,0.8882238539,-3.8401675105
C,0,-4.8324308512,0.2075744695,-3.7691081302	C,0,-4.9971726972,0.1276272663,-4.020969015
H,0,7.0480957736,0.7265961363,0.389599854	H,0,6.7003836118,0.246089849,0.787322457
H,0,-5.8917867558,-1.5052305943,-3.0296618148	H,0,-5.977432536,-1.7484979328,-3.6695382286
H,0,-3.9240088675,-2.4255493287,-1.8443347395	H,0,-4.0497712962,-2.7265372127,-2.4663262291
O,0,-3.4913023449,2.0593386682,-4.51057627	O,0,-3.7502127758,2.1589185006,-4.3235775167
H,0,-4.3478843796,2.2670543779,-4.907381406	H,0,-4.5844552346,2.3747890274,-4.7602581869
O,0,3.5650524532,3.1458612689,-1.0188433148	O,0,5.5269448348,2.7107710047,0.6532973908
H,0,-1.5653721696,0.9166890779,-3.1958159775	O,0,-6.0069190263,0.7646980467,-4.7018187323
O,0,-5.8570919979,0.8039147894,-4.4606397674	H,0,-6.7749015029,0.1913483014,-4.7892948641
H,0,-6.6665561291,0.2860408703,-4.3924596722	H,0,-1.8567479613,0.9383191156,-3.0361860319
O,0,3.2910570533,3.147994234,0.4173412309	O,0,4.6424139744,2.5124081944,1.8028385195
C,0,3.8687786672,4.3344385866,0.9404226808	C,0,4.0364003007,3.7668563891,2.0453112615
H,0,3.5930695102,4.3272656552,1.9978621013	H,0,3.400061715,4.0759936105,1.2091149203
H,0,4.9580234968,4.3265989649,0.8410531693	H,0,3.4258152632,3.6095284547,2.9383554728
H,0,3.450691164,5.2235160696,0.4586108187	H,0,4.7865210922,4.5388898777,2.2469809763

P C2(•OOCH$_3$), optimization in solv. water UB3LYP/6-311++G**, E= -1100.68674897 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235072 a.u. SP at UM06-2X/6-311++G** (water), E = -1100.2460593 a.u.	**P C2(•OOCH$_3$),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.67278793 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235335 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1100.2314367 a.u.
0, 2	0, 2
C,0,5.7552742123,0.2966563363,0.3131130203	C,0,5.7425729368,0.2987279182,0.3284759885
C,0,4.9219334256,-0.7740417374,0.4198169216	C,0,4.9077707897,-0.7689240221,0.4265487407
C,0,5.3405711263,1.6092117949,-0.2905990477	C,0,5.3408641854,1.6118188997,-0.285514496
H,0,5.2528492127,-1.6971051165,0.8837008572	H,0,5.226434932,-1.6908696192,0.9001028073
C,0,3.6056111154,-0.6806286805,-0.1041549509	C,0,3.5968940792,-0.6736665232,-0.1113727166
C,0,3.9823181671,1.6204188284,-0.9149444232	C,0,3.9822920273,1.6285531259,-0.9138309551
H,0,3.6597586487,2.5068974656,-1.4468694917	H,0,3.6657110506,2.5197806761,-1.4421182903
C,0,3.1899796364,0.5224443402,-0.7618104292	C,0,3.1876099996,0.5314620912,-0.7684440137
C,0,1.606407953,-1.0321330872,-0.7706979036	C,0,1.6041560161,-1.0219581549,-0.7844804635
N,0,2.605393284,-1.6213434123,-0.1264666852	N,0,2.5956782566,-1.6120403672,-0.1397260399
N,0,1.8870801165,0.2416724928,-1.1796665064	N,0,1.8844740605,0.2535899214,-1.1920521151

H,0,1.2473793514,0.843179934,-1.6757534997	H,0,1.2455117894,0.8522020852,-1.6906075685
N,0,0.4078284185,-1.6218026464,-1.0117458005	N,0,0.4027769972,-1.6136488567,-1.0310161407
N,0,-0.5566291284,-0.9498273825,-1.6909394672	N,0,-0.5633713897,-0.9496707866,-1.7074112582
C,0,-1.6708639148,-1.558593892,-1.8977230564	C,0,-1.6782376906,-1.558260582,-1.9112779893
H,0,-1.8296072831,-2.5789280322,-1.537119874	H,0,-1.8343768183,-2.5785347118,-1.5457873664
H,0,0.2689064137,-2.572568497,-0.6808618355	H,0,0.2708827615,-2.5630302121,-0.6940637281
H,0,6.1020878409,1.9495169499,-1.008445521	H,0,6.1053446643,1.9326580013,-1.010137873
C,0,-2.7778311304,-0.9377317235,-2.6168178065	C,0,-2.7889799427,-0.9439819665,-2.6294502442
C,0,-3.9622273913,-1.6664721377,-2.7928097463	C,0,-3.9744455354,-1.6729430892,-2.7945610086
C,0,-2.6931552077,0.3658382357,-3.1400330017	C,0,-2.7063832384,0.3548819862,-3.1621001895
C,0,-5.0433527005,-1.1113903704,-3.4753881606	C,0,-5.0578418572,-1.1207307519,-3.4756210736
C,0,-3.7646020923,0.9184074607,-3.8179958556	C,0,-3.7798098269,0.9054935621,-3.8386037205
C,0,-4.9494472313,0.1760858326,-3.9885665644	C,0,-4.9647638958,0.1624833985,-3.997012607
H,0,6.7671196273,0.2464219151,0.6993778832	H,0,6.7457721473,0.2536383166,0.7366138251
H,0,-5.9581922975,-1.6785868939,-3.6090321588	H,0,-5.974067256,-1.6888929332,-3.6002925693
H,0,-4.0428779414,-2.6718193396,-2.3959407581	H,0,-4.0543714041,-2.6756002054,-2.390409204
O,0,-3.6682045686,2.1845723078,-4.3215041232	O,0,-3.6838287552,2.1658537237,-4.3499329137
H,0,-4.4979564931,2.4070813644,-4.7663432222	H,0,-4.5159506109,2.3865910025,-4.7895475387
O,0,5.5177071434,2.7126045116,0.6883465996	O,0,5.5264251205,2.7152068641,0.6775389187
O,0,-5.943824664,0.8185243242,-4.6738921787	O,0,-5.9651164172,0.802356312,-4.6832359781
H,0,-6.7220325785,0.2563939437,-4.7696097484	H,0,-6.743875883,0.2408178704,-4.7632534696
H,0,-1.7889368744,0.9490218344,-3.0189628707	H,0,-1.8016133117,0.9380084058,-3.050124833
O,0,4.6300892268,2.4984149355,1.8293458844	O,0,4.6554133357,2.4903274179,1.8286936888
C,0,3.7829368922,3.6381536001,1.9139755196	C,0,3.8465202343,3.6482169528,1.9567074968
H,0,3.1320606608,3.7167386577,1.0391604475	H,0,3.1784763376,3.7674203922,1.0981226191
H,0,3.1816679769,3.4681279776,2.8105268502	H,0,3.2591556031,3.4747118595,2.8620709197
H,0,4.3667538074,4.5554346059,2.0345984637	H,0,4.4582692684,4.5467986988,2.0843791194

P C4(•OOCH$_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.66398904 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234124 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1100.2229142 a.u.	**P C4(•OOCH$_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.68905416 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234722 a.u. SP at UM06-2X/6-311++G** (water), E = -1100.249426 a.u.
0, 2	0, 2
C,0,5.9647782891,0.8084164645,0.0750140459	C,0,5.9231782055,0.8303642301,0.0786619165
C,0,5.0395052346,-0.206143807,0.6914826908	C,0,5.0167068243,-0.2013715903,0.6885245865
C,0,5.5701190029,1.716553031,-0.8657121476	C,0,5.5053707165,1.7475905001,-0.8454844888
H,0,5.469498802,-1.2172791081,0.6367559015	H,0,5.4517610361,-1.2085778512,0.6002496617
C,0,3.6974795631,-0.1758338646,0.0422299167	C,0,3.6580814498,-0.1581684726,0.079512282
C,0,4.2489506099,1.7530691033,-1.3949736361	C,0,4.1744354078,1.7839302081,-1.3518830588
H,0,3.9621558601,2.4872421813,-2.1369504416	H,0,3.8688066012,2.5209678144,-2.0828115086
C,0,3.3627812753,0.7857850661,-0.914753525	C,0,3.3009764528,0.8085680036,-0.8637918529
C,0,1.6806695654,-0.5776911289,-0.491142734	C,0,1.6236457166,-0.5600210549,-0.4227728561
N,0,2.6502554162,-1.0194830555,0.2891425768	N,0,2.6143149282,-1.0051593913,0.3435457589
N,0,2.0347390311,0.5021895862,-1.2422549677	N,0,1.9691446418,0.5247964075,-1.1675968549
H,0,1.4291248242,0.9784625476,-1.8913214954	H,0,1.3614267556,1.0011790743,-1.8171109379
N,0,0.4377243328,-1.1479393026,-0.5546258637	N,0,0.3831498196,-1.1212698661,-0.4711029212
N,0,-0.5166689409,-0.6314154068,-1.3556261685	N,0,-0.5591841784,-0.6084598759,-1.3004910708
C,0,-1.6797476065,-1.179873665,-1.3429559571	C,0,-1.7114213287,-1.1793558946,-1.3204511077
H,0,-1.884312273,-2.039241323,-0.6945808518	H,0,-1.918539675,-2.04826412,-0.689200251
H,0,0.2551410784,-1.9229992707,0.0758474745	H,0,0.2028666675,-1.9354178655,0.1089323529
H,0,6.2914734264,2.4370859038,-1.237205662	H,0,6.2169583564,2.4747802386,-1.2225741111
C,0,-2.7848415636,-0.7086453041,-2.1702439223	C,0,-2.7998324064,-0.712484689,-2.1731711985
C,0,-4.0208551376,-1.3633110578,-2.0865137829	C,0,-4.0279484368,-1.3867295366,-2.1311037987

C,0,-2.6491620394,0.3820476418,-3.0464549789	C,0,-2.6558489367,0.3909872321,-3.0343508465
C,0,-5.1009998317,-0.9405997137,-2.8591948747	C,0,-5.093762008,-0.9734574196,-2.9290219791
C,0,-3.7193090195,0.8044075085,-3.8147801575	C,0,-3.7120201866,0.8025059029,-3.8271062597
C,0,-4.9543091204,0.1377483774,-3.7195814137	C,0,-4.9409651656,0.1166974537,-3.7759650533
H,0,6.9835433519,0.8141847566,0.4460432535	H,0,6.9506779922,0.8326802203,0.424332994
H,0,-6.0565558636,-1.4513904251,-2.7902276425	H,0,-6.0426631222,-1.4978468484,-2.893805639
H,0,-4.1430269327,-2.2065873206,-1.4163015948	H,0,-4.1550772692,-2.2384932705,-1.4729607958
O,0,-3.5711910781,1.8635094901,-4.6583535016	O,0,-3.5579284073,1.8756106338,-4.6586125022
H,0,-4.411587045,2.0194994419,-5.1084915589	H,0,-4.3871443752,2.022110121,-5.1348277495
O,0,4.971881881,-0.0770898935,2.1422847807	O,0,4.9866117493,-0.1228073488,2.1566989301
H,0,-1.705730998,0.9051976989,-3.1300234321	H,0,-1.7177213859,0.9292032961,-3.0856501717
O,0,-5.9501272574,0.6375722095,-4.5248879219	O,0,-5.9158327538,0.6076265853,-4.6010895063
H,0,-6.7678553408,0.1452296645,-4.4021493375	H,0,-6.7301066901,0.0966431281,-4.5205868333
O,0,4.3428612746,1.2062361928,2.453500107	O,0,4.3952774953,1.1547522405,2.5546388475
C,0,5.1660956809,1.8179315374,3.4278544534	C,0,5.344471858,1.8017112132,3.3937581096
H,0,5.2612712938,1.1880437111,4.3184808215	H,0,5.5826194497,1.1866542478,4.2664394441
H,0,6.1580869147,2.0522216207,3.027550749	H,0,6.2566538426,2.0504549321,2.845044938
H,0,4.6434532598,2.7420315118,3.6884398786	H,0,4.8441702793,2.7172130116,3.7185026117

P C4(•OOCH$_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.67436197 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234843 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1100.2340205 a.u.	**P C6(•OOCH$_3$),** optimization in gas phase UB3LYP/6-311++G**, E= -1100.67049432 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.236899 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1100.2307981 a.u.
0, 2	0, 2
C,0,5.9489275324,0.79880823,0.1134277014	C,0,6.0743447142,0.4221728417,-0.58405079
C,0,5.0219600788,-0.2133215651,0.7284643779	C,0,5.2528088129,-0.5336483892,-0.0196973768
C,0,5.557892961,1.6971367023,-0.8391339635	C,0,5.540666034,1.5873423868,-1.1809788445
H,0,5.4605162874,-1.2216809257,0.6982760463	H,0,5.6473966299,-1.4348727501,0.4332211664
C,0,3.6892407888,-0.2003944513,0.0616849474	C,0,3.850410195,-0.325195097,-0.0572428951
C,0,4.2420129569,1.7217262499,-1.3830856686	C,0,4.166318351,1.8340341057,-1.2214060231
H,0,3.9581592387,2.4478250487,-2.133854248	H,0,3.7740410437,2.7371145279,-1.6734523405
C,0,3.357594638,0.7511329953,-0.9065302189	C,0,3.3305303215,0.8824569297,-0.6533851393
C,0,1.6792828084,-0.6225960965,-0.4957244619	C,0,1.6389668451,-0.4457871959,0.0869721512
N,0,2.6452400594,-1.0509872549,0.3023157785	N,0,2.882429087,-1.1254279734,0.3847372458
N,0,2.0369309272,0.454130675,-1.2482894203	N,0,1.9727761083,0.834753342,-0.4969341417
H,0,1.4379938132,0.9231533401,-1.9097321078	H,0,1.2994701284,1.2979789424,-1.0889947446
N,0,0.4447717083,-1.2027575399,-0.576530213	N,0,0.8517557436,-1.2630754694,-0.7969074435
N,0,-0.508523547,-0.6700375287,-1.3739799957	N,0,-0.2387750767,-0.6266291244,-1.3311625109
C,0,-1.6695687037,-1.2227041023,-1.3749538168	C,0,-1.2273342971,-1.3442943036,-1.7103170536
H,0,-1.873512234,-2.0965057925,-0.7474052524	H,0,-1.2210277575,-2.4309185015,-1.5650008351
H,0,0.2504711534,-1.9757506016,0.0530833449	H,0,0.6863891612,-2.1859570609,-0.3979132886
H,0,6.2792671673,2.4179419708,-1.2101578913	H,0,6.2186992421,2.312845863,-1.6156030769
C,0,-2.7744858579,-0.7307345975,-2.1910016325	C,0,-2.4127147196,-0.7823353752,-2.3595168256
C,0,-4.0046145855,-1.3999529434,-2.1393826523	C,0,-3.4514238386,-1.6413270268,-2.7374039416
C,0,-2.6458770405,0.3971666554,-3.02070784	C,0,-2.5396808524,0.5934183305,-2.6117945673
C,0,-5.0869290161,-0.9559154715,-2.8973641486	C,0,-4.5955452669,-1.1410525386,-3.357886676
C,0,-3.7185947348,0.8412841185,-3.7726041871	C,0,-3.6724837976,1.094006901,-3.2289270207
C,0,-4.9491200747,0.1613572094,-3.7093058831	C,0,-4.7076850357,0.2194412417,-3.6034838257
H,0,6.9649395256,0.8115959885,0.491696231	H,0,7.1489150421,0.2819125475,-0.5759330934
H,0,-6.0365559566,-1.4797719119,-2.8564681815	H,0,-5.3983867616,-1.8113312005,-3.6496766012
H,0,-4.1204994588,-2.2717159492,-1.5055624568	H,0,-3.369255885,-2.7056981354,-2.5483859304
O,0,-3.5791675937,1.9391245688,-4.5697917674	O,0,-3.7790814952,2.4314370523,-3.4699512914
H,0,-4.4233106884,2.1134385397,-5.0073612728	H,0,-4.6291536921,2.5999662814,-3.8965366644

O,0,4.9304437485,-0.0656391862,2.1828734112	O,0,0.9363408286,-0.0967533647,1.3074764774
H,0,-1.7077468525,0.933827161,-3.0765323257	H,0,-1.7520153892,1.277095363,-2.3239696116
O,0,-5.9457473359,0.6876034743,-4.4918406491	O,0,-5.7884930599,0.8184510154,-4.2091854419
H,0,-6.773812706,0.2129958282,-4.3613092526	H,0,-6.4595230929,0.1647755927,-4.4290618758
O,0,4.3042141976,1.2215329945,2.4797105208	O,0,0.4583188003,-1.3322080958,1.9090328661
C,0,5.1788038651,1.8980792046,3.36745883	C,0,1.1791153299,-1.5133570114,3.1238159148
H,0,5.3478450513,1.3142037983,4.2776402291	H,0,1.0230313156,-0.6653477328,3.796211119
H,0,6.1339283667,2.133000004,2.8878895444	H,0,0.7452803756,-2.4161573383,3.5612118079
H,0,4.6529394321,2.8225427608,3.6194076251	H,0,2.2431309479,-1.6611461801,2.926127022

P C6(•OOCH$_3$), optimization in solv. water UB3LYP/6-311++G**, E= -1100.69053754 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.236400 a.u. SP at UM06-2X/6-311++G** (water), E = -1100.2520832 a.u.	**P C6(•OOCH$_3$),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.67879925 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.236762 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1100.2395991 a.u.
0, 2	0, 2
C,0,6.1269070047,0.3955300046,-0.5110042802	C,0,6.0921504135,0.4099688026,-0.5661695219
C,0,5.2830766391,-0.5589687502,0.0204815315	C,0,5.2634938568,-0.5452878653,-0.0117831222
C,0,5.6190038021,1.568984529,-1.1203026384	C,0,5.566718697,1.5790244418,-1.1652643122
H,0,5.6619343939,-1.4627725983,0.4821270008	H,0,5.6533410915,-1.4479967379,0.442493175
C,0,3.883038828,-0.3403895643,-0.0625996596	C,0,3.8616922221,-0.3322182278,-0.0614144865
C,0,4.2492406888,1.824708851,-1.2056962892	C,0,4.1938630345,1.8299326524,-1.2176932108
H,0,3.8745593297,2.7293207663,-1.6683789311	H,0,3.8071960596,2.7342560845,-1.6716232529
C,0,3.390572483,0.8738774452,-0.6688646169	C,0,3.3507503802,0.8786107603,-0.6590734398
C,0,1.6650124514,-0.4435507299,0.0140568705	C,0,1.6476982846,-0.4447460186,0.0647482178
N,0,2.8930287833,-1.136801695,0.3406706921	N,0,2.8861911823,-1.1306784025,0.3689228233
N,0,2.0281639281,0.8320298307,-0.5612332135	N,0,1.9916497076,0.833557056,-0.5168603159
H,0,1.3822505828,1.328912718,-1.1577313576	H,0,1.3265266116,1.3118994413,-1.1065736024
N,0,0.8802564809,-1.2549512806,-0.872675328	N,0,0.8580720052,-1.2592654063,-0.8174335614
N,0,-0.2321809297,-0.6167172592,-1.3777634733	N,0,-0.2397012632,-0.6209936889,-1.3422088953
C,0,-1.2097159218,-1.3466157202,-1.767281834	C,0,-1.2242540441,-1.3432245198,-1.7249642962
H,0,-1.1787772452,-2.4356276239,-1.6580016577	H,0,-1.2090364139,-2.4307991413,-1.5917898477
H,0,0.7243970503,-2.1865166165,-0.489659196	H,0,0.6946145956,-2.1845508802,-0.4231786678
H,0,6.3159756938,2.2913964216,-1.5286511444	H,0,6.250949977,2.303304185,-1.5919232449
C,0,-2.4165005529,-0.7887784334,-2.3801797594	C,0,-2.4162908795,-0.783334003,-2.3639755658
C,0,-3.4487626233,-1.6584150989,-2.7540737491	C,0,-3.4461335249,-1.6481910211,-2.7535934756
C,0,-2.5728327758,0.5910489846,-2.601633555	C,0,-2.5584496219,0.5950566658,-2.5966187008
C,0,-4.616539343,-1.1677373401,-3.3376481692	C,0,-4.5962747351,-1.1523832562,-3.3667821067
C,0,-3.7299898291,1.0807854074,-3.1811322867	C,0,-3.697475856,1.0905736286,-3.2061933684
C,0,-4.7610681146,0.1967157839,-3.5518305716	C,0,-4.7242150211,0.2106120354,-3.5936911224
H,0,7.1997322235,0.2499437298,-0.4680879213	H,0,7.1661999405,0.2670243706,-0.5488105665
H,0,-5.4133719308,-1.8448914795,-3.6259005512	H,0,-5.3916661415,-1.8263151721,-3.6688407905
H,0,-3.3432239974,-2.7247748452,-2.5904182119	H,0,-3.352032185,-2.7141998817,-2.5800859247
O,0,-3.8667809098,2.4241789127,-3.3918933338	O,0,-3.8193309707,2.4316460107,-3.4284999494
H,0,-4.7258112159,2.5884212157,-3.8053025517	H,0,-4.6718520322,2.5984248892,-3.8522531838
O,0,0.9443242675,-0.0682449899,1.2278701012	O,0,0.9432758554,-0.0851042154,1.2858403739
H,0,-1.7887165122,1.2835841402,-2.3223293946	H,0,-1.7779860428,1.283494224,-2.2996162936
O,0,-5.8600093261,0.7869076508,-4.1160115854	O,0,-5.8093469874,0.8047983304,-4.1897339928
H,0,-6.5254635966,0.1293586778,-4.3514552779	H,0,-6.4766015336,0.1487338946,-4.4183247768
O,0,0.4312861176,-1.2844031614,1.8446576107	O,0,0.4523204719,-1.3126108607,1.8949464676
C,0,1.0958113557,-1.4407346904,3.0982911718	C,0,1.1554228206,-1.4861514915,3.1227613384
H,0,0.909635922,-0.5810262932,3.7469374135	H,0,0.9906074094,-0.6341428143,3.7875499783
H,0,0.6427638644,-2.3348901827,3.532200164	H,0,0.7146212606,-2.3855908282,3.559410544
H,0,2.1673279737,-1.5922133163,2.9544938827	H,0,2.2218464152,-1.6364496404,2.9423465772

P C9(•OOCH$_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.65280261 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.236115 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1100.2122491 a.u.	**P C9(•OOCH$_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.67658619 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235853 a.u. SP at UM06-2X/6-311++G** (water), E = -1100.2371104 a.u.
0, 2 C,0,5.7942255196,0.0705121482,-0.4674031395 C,0,4.7177277848,-0.7849359733,-0.2359913068 C,0,5.5972601794,1.3702659827,-1.0345875978 H,0,4.870748396,-1.8214087022,0.0409264272 C,0,3.4373356391,-0.319602209,-0.4838293668 C,0,4.3566926899,1.8834914179,-1.2623494418 H,0,4.2075337295,2.856721077,-1.7156652599 C,0,3.1818308384,1.1455459352,-0.7456663787 C,0,1.449732276,-0.1900872807,-1.2333906983 N,0,2.2822026562,-1.0366058816,-0.669038075 N,0,1.9605324579,1.057123013,-1.5206079932 H,0,1.3361771415,1.8480474579,-1.6007685775 N,0,0.1825236583,-0.5356157702,-1.5777987616 N,0,-0.6662077585,0.3679930082,-2.1202903003 C,0,-1.8553170212,-0.0279085649,-2.4038923494 H,0,-2.1634643252,-1.0611216855,-2.2070929453 H,0,-0.1072615927,-1.4861491356,-1.3638479356 H,0,6.4723680357,1.9451169965,-1.3199835974 C,0,-2.8578468909,0.8504249423,-2.9959783821 C,0,-4.136547048,0.340786273,-3.2562660266 C,0,-2.5760758747,2.1898565025,-3.3157016884 C,0,-5.1188404112,1.1503670232,-3.8233861182 C,0,-3.5489327111,2.9962750472,-3.8785605367 C,0,-4.8292757155,2.4713819869,-4.1337762932 H,0,6.8056390101,-0.2790928776,-0.2977263378 H,0,-6.1088139454,0.7522520106,-4.0235486189 H,0,-4.3685645861,-0.6905061706,-3.0157326038 O,0,-3.2619964838,4.2915686262,-4.1835893328 H,0,-4.0475010741,4.6999872342,-4.5701138106 O,0,2.6464280957,1.8179136542,0.5070838862 O,0,-5.7191346944,3.3554347767,-4.6942618554 H,0,-6.5690064307,2.9321557478,-4.8517881771 H,0,-1.5945678722,2.6042456752,-3.1267546314 O,0,3.6571939554,1.8205996205,1.5449007361 C,0,3.8828721338,3.1752016121,1.898220787 H,0,4.5972021639,3.1270858233,2.7239757985 H,0,4.314910098,3.7403155147,1.066398565 H,0,2.9588903564,3.6528017437,2.2394447579	0, 2 C,0,5.7893752,0.0701411055,-0.5030307016 C,0,4.7228806276,-0.79662945,-0.2548506628 C,0,5.5696783265,1.3731587453,-1.053946578 H,0,4.8956885666,-1.8337921933,0.0102562162 C,0,3.4326036467,-0.3401903842,-0.4761605528 C,0,4.3188485136,1.8781154651,-1.2516616625 H,0,4.1511743896,2.8550379058,-1.689593205 C,0,3.1633500825,1.1215736726,-0.7257537496 C,0,1.4215085924,-0.2170259716,-1.1906036145 N,0,2.2773874789,-1.0640318152,-0.639725137 N,0,1.9286877405,1.0315276042,-1.4657090851 H,0,1.3161719193,1.8250253947,-1.5980001631 N,0,0.1587198248,-0.5563254117,-1.5231275979 N,0,-0.6762260819,0.3636865667,-2.0803677955 C,0,-1.8590598494,-0.0345996375,-2.3893334569 H,0,-2.1684827287,-1.06809648,-2.2099016002 H,0,-0.1440256959,-1.5095541371,-1.3393195562 H,0,6.433575698,1.9594115012,-1.3492257629 C,0,-2.8497173136,0.8502051093,-2.9905994591 C,0,-4.1126879026,0.3310188232,-3.3060946659 C,0,-2.5757970095,2.2027577025,-3.2657742704 C,0,-5.0880559173,1.1404391537,-3.8852468595 C,0,-3.5424709102,3.0079963207,-3.8397719981 C,0,-4.8086068144,2.4747542269,-4.1525874524 H,0,6.8066660965,-0.2736963472,-0.3586754952 H,0,-6.0639840988,0.7355930848,-4.1297054782 H,0,-4.3368636755,-0.709177294,-3.1002167072 O,0,-3.2651695672,4.3190671702,-4.1016976705 H,0,-4.0465481572,4.7305759903,-4.4967092657 O,0,2.6422093903,1.7764499374,0.5659470669 O,0,-5.6866349804,3.3576740798,-4.7161201322 H,0,-6.5368061859,2.9386273662,-4.8967183097 H,0,-1.6074826485,2.626406606,-3.0309461201 O,0,3.6821409541,1.8409151979,1.5735653397 C,0,3.904733491,3.21728886,1.8666949582 H,0,4.6466360759,3.2110157465,2.6685591902 H,0,4.3003756385,3.7493044437,0.9978677889 H,0,2.9868796637,3.6957879416,2.2198470258

P C9(•OOCH$_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.66269437 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.236135 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1100.2226497 a.u.	**P C13(•OOCH$_3$),** optimization in gas phase UB3LYP/6-311++G**, E= -1100.69080697 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.237151 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1100.254357 a.u.
0, 2	0, 2

C,0,5.79306618,0.0760002086,-0.4706387009	C,0,5.9614455986,0.752846822,0.2632511194
C,0,4.721111298,-0.7859423805,-0.2375133956	C,0,4.9502569489,0.0736079754,0.9343182682
C,0,5.5871236742,1.3758002322,-1.0344165603	C,0,5.7488858053,1.3179579192,-1.0062814534
H,0,4.8826749953,-1.8218235909,0.037674039	H,0,5.1107504045,-0.3623711103,1.9129423437
C,0,3.437018015,-0.3274589952,-0.482252698	C,0,3.7044698936,-0.0350428496,0.3098463915
C,0,4.342311391,1.8825836964,-1.2574907907	C,0,4.5152173202,1.2207748513,-1.6474287374
H,0,4.1857281154,2.85614796,-1.7073937679	H,0,4.354489903,1.6571582665,-2.6264222755
C,0,3.1741106655,1.1355476506,-0.7414009272	C,0,3.5087591752,0.5401127597,-0.9712083901
C,0,1.4428934452,-0.2050656028,-1.2267835007	C,0,1.6865143688,-0.4502465494,-0.2262048387
N,0,2.2842950715,-1.0498059938,-0.6641138667	N,0,2.5407043115,-0.6479969398,0.7492025512
N,0,1.951184339,1.0434690885,-1.5081969901	N,0,2.1893508594,0.2486592975,-1.2907498327
H,0,1.3294499032,1.8340047946,-1.6108290331	H,0,1.6551706394,0.5020542742,-2.1076496628
N,0,0.1790748243,-0.5495782225,-1.5706552843	N,0,0.3915928985,-0.9024102741,-0.2233586667
N,0,-0.6643737516,0.3619556027,-2.1173851674	N,0,-0.4360013579,-0.5683638011,-1.2179562681
C,0,-1.8533046698,-0.0322786439,-2.4047509267	C,0,-1.7101394884,-1.232815184,-1.0938322019
H,0,-2.1643389278,-1.0640162049,-2.2102518029	H,0,-1.5924834842,-2.3199623067,-1.208552554
H,0,-0.117862879,-1.499875766,-1.3649951366	H,0,0.0465975495,-1.3289972933,0.6342925542
H,0,6.4580556012,1.9566245661,-1.3202885819	H,0,6.5611723107,1.8406044624,-1.4979404228
C,0,-2.851907797,0.8495767946,-2.9979727924	C,0,-2.6926053884,-0.7104101649,-2.1115782656
C,0,-4.1293637842,0.3402416981,-3.2658493528	C,0,-3.4568021879,-1.5997479542,-2.8634178653
C,0,-2.5696090506,2.1912753486,-3.3100034648	C,0,-2.8640128854,0.667183369,-2.2842965547
C,0,-5.1107110041,1.1512465561,-3.8326355992	C,0,-4.3880574998,-1.1212192666,-3.7876222697
C,0,-3.5417591235,2.9987376692,-3.871967593	C,0,-3.7865548331,1.1497459567,-3.2002089059
C,0,-4.821964791,2.4751276223,-4.1346258885	C,0,-4.5520850607,0.2459634077,-3.9546731502
H,0,6.8067532496,-0.2686949814,-0.3045012391	H,0,6.9363241014,0.8508845032,0.7269515719
H,0,-6.0990361776,0.7537406503,-4.0395769608	H,0,-4.9830911507,-1.8132858104,-4.3759341659
H,0,-4.3609631667,-0.6924582589,-3.0314059391	H,0,-3.3323711368,-2.668351683,-2.732917186
O,0,-3.2552115902,4.2977385149,-4.1693422998	O,0,-3.9416929961,2.4943331058,-3.3637657269
H,0,-4.0412777497,4.7095403368,-4.5526261871	H,0,-4.6118486968,2.6457795582,-4.0428171405
O,0,2.637895038,1.8013447849,0.5234973633	O,0,-2.1529318172,-1.0177712808,0.2786239275
O,0,-5.7086406244,3.3600555199,-4.691279875	O,0,-5.4375956582,0.8245862484,-4.8356925112
H,0,-6.5659590282,2.945270498,-4.8370722023	H,0,-5.9060667614,0.1504550273,-5.3376882483
H,0,-1.5893879707,2.6060619597,-3.1141775716	H,0,-2.2742683104,1.3743751504,-1.7140659863
O,0,3.655045662,1.8252908659,1.5551199128	O,0,-3.1512592642,-2.0384084936,0.5772695045
C,0,3.8835571902,3.1879839765,1.8853187949	C,0,-4.2913069588,-1.3529537537,1.0774708465
H,0,4.6047225989,3.1540229186,2.7055348567	H,0,-4.9965294302,-2.1502396033,1.3242771656
H,0,4.3080224615,3.7380731377,1.0404241284	H,0,-4.0442311173,-0.7874946859,1.9805855795
H,0,2.9622507469,3.669972589,2.2263878214	H,0,-4.7204514244,-0.69150955,0.3203134367

P C13(•OOCH$_3$), optimization in solv. water UB3LYP/6-311++G**, E= -1100.71033423 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.236694 a.u. SP at UM06-2X/6-311++G** (water), E = -1100.2748018 a.u.	**P C13(•OOCH$_3$),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.69915474 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.236681 a.u. SP at UM06-2X/6-311++G** (benzene), E = 1100.2631214 a.u.
0, 2	0, 2
C,0,5.9964401744,0.6765340775,0.2132346727	C,0,5.9743303678,0.7282597226,0.2394590637
C,0,5.0011948362,-0.0426563836,0.8691620736	C,0,4.9708748272,0.0351902177,0.9092192626
C,0,5.7485306661,1.3250927907,-1.0106392325	C,0,5.7458643493,1.3205285327,-1.0154076252
H,0,5.1938957054,-0.5416023274,1.8117883886	H,0,5.1457928369,-0.420958291,1.8763269703
C,0,3.7361694266,-0.1047891666,0.2750544031	C,0,3.7168405891,-0.0591077372,0.298061095
C,0,4.4950817918,1.2749718946,-1.6195131546	C,0,4.5036313388,1.2379012671,-1.6425107794
H,0,4.3034038435,1.774043117,-2.5617592475	H,0,4.3289562424,1.6945426781,-2.6096116998
C,0,3.5056534389,0.5540319387,-0.9584522844	C,0,3.5053486085,0.5434801124,-0.9675102656
C,0,1.6961877477,-0.4745702385,-0.2357199439	C,0,1.6896391805,-0.4601598143,-0.2247599429

N,0,2.5794331813,-0.7413806853,0.7042232651	N,0,2.5567394885,-0.6806289166,0.7374280351
N,0,2.1769497161,0.2923811729,-1.2584009764	N,0,2.1822861037,0.2614251763,-1.2771070776
H,0,1.6396090938,0.5988636505,-2.0560144162	H,0,1.6451344462,0.5339330257,-2.0864516766
N,0,0.4011254089,-0.9222483284,-0.2208444467	N,0,0.3947428993,-0.9111123363,-0.2152564975
N,0,-0.4562135263,-0.5443383487,-1.1732268285	N,0,-0.4429431733,-0.5642423709,-1.1968547097
C,0,-1.7325994994,-1.2091365918,-1.0331872733	C,0,-1.7190546134,-1.2267231191,-1.0664021956
H,0,-1.6128971359,-2.2981187817,-1.1113777776	H,0,-1.6017474966,-2.314785136,-1.1676192478
H,0,0.0937752497,-1.4351739741,0.603086904	H,0,0.0623216178,-1.3646982736,0.6335104003
H,0,6.5486298946,1.8760630568,-1.4911750351	H,0,6.5522418868,1.8530368637,-1.5062231776
C,0,-2.7043770953,-0.718988811,-2.0763274222	C,0,-2.6958108769,-0.7152781596,-2.0948770175
C,0,-3.3176582378,-1.6223204971,-2.9416746463	C,0,-3.404315355,-1.6111546087,-2.8920706198
C,0,-3.0005265951,0.6456854684,-2.178147554	C,0,-2.9112351674,0.6598711363,-2.2397668389
C,0,-4.2204957261,-1.173346247,-3.9089156785	C,0,-4.3232186455,-1.1430712965,-3.8343443815
C,0,-3.8963609782,1.0975642151,-3.1348126116	C,0,-3.8220578746,1.1315642041,-3.1725455971
C,0,-4.5099565556,0.1808047322,-4.0064104752	C,0,-4.5316659184,0.2216272821,-3.9741601059
H,0,6.9852374736,0.7398908255,0.6529026794	H,0,6.9551140008,0.8156412782,0.6927787391
H,0,-4.6983043406,-1.8754888832,-4.5837513127	H,0,-4.8746153237,-1.8404190869,-4.4571917224
H,0,-3.0955983795,-2.6809245404,-2.8710895323	H,0,-3.2453426845,-2.6779205799,-2.7852198164
O,0,-4.1773915709,2.432380652,-3.2255523181	O,0,-4.0218995075,2.4751478301,-3.3077222897
H,0,-4.8150595556,2.5669476182,-3.9404862774	H,0,-4.6785678561,2.6209605539,-4.001886202
O,0,-2.1724179115,-0.9376298861,0.3305814547	O,0,-2.1605409674,-0.9898461422,0.3029579024
O,0,-5.3772880682,0.7306301394,-4.9142572835	O,0,-5.4081348687,0.7912629217,-4.8661286642
H,0,-5.7580329193,0.0522684908,-5.4845775873	H,0,-5.8461231422,0.1165744646,-5.395975761
H,0,-2.5353054501,1.36563614,-1.5150828192	H,0,-2.3669878698,1.3731602396,-1.6326038037
O,0,-3.2143442062,-1.9078344684,0.6554660156	O,0,-3.1760601817,-1.9907380534,0.6125476885
C,0,-4.3465201799,-1.166076947,1.1024435001	C,0,-4.3180931926,-1.2826384906,1.0814538347
H,0,-5.0805567837,-1.930642398,1.3659442094	H,0,-5.0346541826,-2.0675691313,1.3341642473
H,0,-4.1013535503,-0.5717569471,1.986625362	H,0,-4.0786169974,-0.7010302159,1.9759079687
H,0,-4.7387442032,-0.5272811289,0.3079651866	H,0,-4.7288577084,-0.6345413468,0.3034744876

P C14(•$OOCH_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.65069468 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234203 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1100.2131717 a.u.	**P C14(•$OOCH_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.67423404 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.233719 a.u. SP at UM06-2X/6-311++G** (water), E = -1100.2377475 a.u.
0, 2	0, 2
C,0,6.0212291848,0.7137116696,-0.5223568843	C,0,6.0251134397,0.7340137632,-0.4432982434
C,0,5.2690757147,-0.359804474,-0.0507364546	C,0,5.286978651,-0.3855983725,-0.0590541076
C,0,5.4288017483,1.7646033464,-1.2399340196	C,0,5.4165258613,1.8315292866,-1.0740807139
H,0,5.7250462862,-1.1715805766,0.5032759519	H,0,5.7601422964,-1.2307907648,0.4277245048
C,0,3.8978899318,-0.3670577633,-0.3107015992	C,0,3.9144044125,-0.3899476313,-0.3187090398
C,0,4.0598792142,1.7760721366,-1.5095741704	C,0,4.0458074027,1.8452465511,-1.3420716441
H,0,3.6034188815,2.5884135023,-2.0634922526	H,0,3.5747518247,2.690820148,-1.8291229165
C,0,3.3179651418,0.7013631425,-1.0355842966	C,0,3.3189631344,0.7253441984,-0.9555784296
C,0,1.8194361213,-0.8121488383,-0.4569982572	C,0,1.8325590982,-0.844601362,-0.5033206306
N,0,2.9266650767,-1.300597958,0.0377954712	N,0,2.9535770746,-1.3600894728,-0.0468599821
N,0,1.9650640104,0.3810593186,-1.1131566612	N,0,1.972063084,0.3964417786,-1.0592927488
H,0,1.2151951446,0.8907105656,-1.5530365455	H,0,1.2218008486,0.942894909,-1.4548160604
N,0,0.5944698657,-1.4262928418,-0.3508614363	N,0,0.6182794453,-1.4730347495,-0.4427152843
N,0,-0.5051151792,-0.8307178163,-0.8526695293	N,0,-0.4841358166,-0.8520088383,-0.9196232131
C,0,-1.6319748865,-1.4189480471,-0.7356865133	C,0,-1.6042433421,-1.4598013048,-0.835245969
H,0,-1.7417135242,-2.3875830639,-0.2391524658	H,0,-1.6988686869,-2.4541525921,-0.3928240454
H,0,0.5549595939,-2.3026898293,0.1599496733	H,0,0.5736983963,-2.3884168278,-0.0049225476
H,0,6.0449839553,2.5839033232,-1.5917768858	H,0,6.0206201763,2.6850981466,-1.3592258496

C,0,-2.9003268605,-0.819832531,-1.3136141147	C,0,-2.8790823319,-0.8438243195,-1.3785946601
C,0,-3.4916884838,-1.7918496802,-2.295143292	C,0,-3.53835881,-1.8280394624,-2.2988418632
C,0,-2.7163419497,0.5527505249,-1.8702911832	C,0,-2.7023651365,0.5093369877,-1.9770073362
C,0,-3.8771262773,-1.4136840565,-3.5489849798	C,0,-4.0077176737,-1.4728464148,-3.5312420222
C,0,-3.1370110904,0.8931281345,-3.1147462727	C,0,-3.2052331506,0.8283314846,-3.197114103
C,0,-3.7223241641,-0.0843710843,-3.9756723321	C,0,-3.868780952,-0.1534398221,-3.9977161327
H,0,7.0881610294,0.7404370437,-0.332033504	H,0,7.0918889438,0.7590420111,-0.2514222898
H,0,-4.3163500616,-2.1412369769,-4.2263049981	H,0,-4.4935062033,-2.2089176283,-4.1640203155
H,0,-3.6355934691,-2.8096142523,-1.9534251107	H,0,-3.6512651871,-2.843078611,-1.9373064688
O,0,-2.9912052961,2.1734262554,-3.5680396195	O,0,-3.068266399,2.0973892689,-3.689405098
H,0,-3.3388158036,2.2257920793,-4.4672684047	H,0,-3.4659155972,2.1364329617,-4.5701146779
O,0,-3.7370447545,-0.7869199241,-0.0849491373	O,0,-3.6592862016,-0.7563724413,-0.0960003199
H,0,-2.2495100398,1.2965921965,-1.2386647362	H,0,-2.1783629457,1.2582890206,-1.3980479762
O,0,-4.0969211717,0.3738790955,-5.2091628421	O,0,-4.3170833878,0.2879074829,-5.203780175
H,0,-4.496265994,-0.3307842504,-5.7302208201	H,0,-4.7493609272,-0.4180185936,-5.7011002781
O,0,-5.1059723173,-0.4459315075,-0.4554876535	O,0,-5.0321651446,-0.3561990182,-0.3860074727
C,0,-5.4573154509,0.6939151504,0.3133250223	C,0,-5.2735307874,0.8442647103,0.3410230983
H,0,-5.3690154306,0.4895774796,1.3846539652	H,0,-5.1328793162,0.6892932482,1.4144954592
H,0,-4.8503848488,1.5629617067,0.0426590957	H,0,-4.6355194218,1.6585068833,-0.011727517
H,0,-6.5046835471,0.8786228804,0.0608536328	H,0,-6.3217063707,1.0782694666,0.1397529095

P C14(•OOCH$_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.66076509 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234983 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1100.2237108 a.u.	**P C15(•OOCH$_3$),** optimization in gas phase UB3LYP/6-311++G**, E= -1100.66845241 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235855 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1100.2272098 a.u.
0, 2	0, 2
C,0,6.0240912111,0.7208771908,-0.4912306796	C,0,5.6745584862,0.8902492014,0.3974197739
C,0,5.2767082121,-0.3710168608,-0.0530389128	C,0,4.891933258,-0.2386674614,0.6253486951
C,0,5.4262475034,1.7906650758,-1.1763001529	C,0,5.1931039079,1.9779469831,-0.3489563042
H,0,5.7387464391,-1.196477372,0.4755976402	H,0,5.2620343615,-1.0786912259,1.2008011042
C,0,3.9050890218,-0.3767387663,-0.3133880402	C,0,3.6029215581,-0.2651727067,0.0888505711
C,0,4.0566751896,1.803320076,-1.4458176293	C,0,3.9091482032,1.9709073485,-0.8943553875
H,0,3.595131031,2.6291396636,-1.9747363343	H,0,3.5389338709,2.8109272983,-1.4707566837
C,0,3.3199252687,0.7107953724,-1.0050248635	C,0,3.1346406369,0.8410182764,-0.6619589066
C,0,1.8248003588,-0.8249751167,-0.4754031003	C,0,1.6189044144,-0.7546658243,-0.5129850385
N,0,2.9372940262,-1.3246599908,0.005452371	N,0,2.6261100963,-1.250603771,0.1619887459
N,0,1.9692994648,0.38771412,-1.0929880367	N,0,1.843684477,0.4883674789,-1.0415324942
H,0,1.2202859035,0.9122827775,-1.5176965429	H,0,1.1573868288,1.0258436153,-1.5481378852
N,0,0.6038544802,-1.4442594925,-0.3878487913	N,0,0.4224561012,-1.3991813932,-0.6939610908
N,0,-0.4969773594,-0.8366721187,-0.8785751138	N,0,-0.5455430411,-0.8318117421,-1.4346600847
C,0,-1.6206753834,-1.433796481,-0.7745852066	C,0,-1.6854772151,-1.4541624432,-1.5157342753
H,0,-1.7226974451,-2.414243592,-0.3014718802	H,0,-1.8364623918,-2.4039117047,-0.9902641878
H,0,0.5606966295,-2.3372297949,0.0934360002	H,0,0.2962175954,-2.2856214752,-0.2134419698
H,0,6.0382524768,2.6235631832,-1.5026815797	H,0,5.8304851939,2.8404847583,-0.5054515061
C,0,-2.8929592051,-0.8283533288,-1.3366416368	C,0,-2.7730459481,-0.9557281608,-2.2867472682
C,0,-3.5105060762,-1.8052764369,-2.2952563144	C,0,-3.9491576992,-1.6900534692,-2.4044146781
C,0,-2.7131521225,0.5374030886,-1.9087694745	C,0,-2.6434929107,0.390537788,-2.967467721
C,0,-3.9273623729,-1.4363951446,-3.5420046459	C,0,-4.9946203136,-1.2836142479,-3.2308543141
C,0,-3.1640959753,0.8687100266,-3.145223251	C,0,-3.7433661862,0.6618690732,-3.9436771968
C,0,-3.7780695743,-0.1110638385,-3.9846808318	C,0,-4.8596214126,-0.1194482821,-4.023011554
H,0,7.0908928967,0.7465988921,-0.2997411515	H,0,6.6785468624,0.9330136907,0.8041667291
H,0,-4.3853144006,-2.1671900597,-4.2022002545	H,0,-5.907264617,-1.8668499918,-3.2884792624
H,0,-3.6436264878,-2.8216694806,-1.9449702286	H,0,-4.047090209,-2.6187791145,-1.8518048798

O,0,-3.0218684541,2.1452701679,-3.6134827456	O,0,-3.571971204,1.7622439598,-4.7182299866
H,0,-3.38818039,2.1921787818,-4.5063206002	H,0,-4.3408602637,1.8418846293,-5.3008516868
O,0,-3.706907294,-0.7763560538,-0.0860703399	O,0,-2.4962395904,1.4771720784,-2.0170596762
H,0,-2.226419244,1.284071915,-1.29564698	H,0,-1.6750586443,0.4658683527,-3.4778420097
O,0,-4.1798879636,0.339768437,-5.2086493997	O,0,-5.8347163467,0.3010994252,-4.912405245
H,0,-4.5915900433,-0.3653841806,-5.7214741914	H,0,-6.3964249446,-0.4376479239,-5.1662142949
O,0,-5.0799459882,-0.4177068947,-0.4234808136	O,0,-3.7091324923,1.5251668099,-1.1994075836
C,0,-5.3893574158,0.7515973785,0.3228828004	C,0,-4.0406903514,2.8988418856,-1.0882202182
H,0,-5.2774501382,0.5746736703,1.3966232034	H,0,-4.2725522463,3.3339140932,-2.0647883477
H,0,-4.7725054188,1.5993494558,0.0120745715	H,0,-4.9268565975,2.9136535118,-0.4489810796
H,0,-6.4389010604,0.950759811,0.0921189769	H,0,-3.2339081064,3.4619460196,-0.6083313421

P C15(•OOCH$_3$), optimization in solv. water UB3LYP/6-311++G**, E= -1100.69146950 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235676 a.u. SP at UM06-2X/6-311++G** (water), E = -1100.2517941 a.u.	**P C15(•OOCH$_3$),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.67800621 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235447 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1100.2373703 a.u.
0, 2	0, 2
C,0,5.7703211796,0.809321418,0.3471411477	C,0,5.7065707103,0.8653071626,0.3827666985
C,0,4.9438605691,-0.2723821036,0.6505371665	C,0,4.9092253396,-0.2488735887,0.6364283277
C,0,5.3244900555,1.868674724,-0.4607761547	C,0,5.2374084879,1.9433096162,-0.3856030095
H,0,5.2917990199,-1.0881693309,1.2738854635	H,0,5.2720720054,-1.0802163885,1.2292915137
C,0,3.6482256956,-0.2785457104,0.1267707265	C,0,3.618311206,-0.2699244387,0.1032463866
C,0,4.0332709848,1.8807735858,-0.9929246903	C,0,3.9512575599,1.9412590513,-0.9274935645
H,0,3.6873423514,2.6964728468,-1.616772131	H,0,3.5890624605,2.7727036277,-1.5209243655
C,0,3.2166235841,0.7990806011,-0.6849985558	C,0,3.1627590052,0.8265696015,-0.6691882372
C,0,1.6318002674,-0.7194754369,-0.4356473913	C,0,1.6230234835,-0.7442552167,-0.4871443354
N,0,2.6311073274,-1.2168197165,0.264888753	N,0,2.6278098362,-1.2405524675,0.1976520155
N,0,1.9087908638,0.4808475896,-1.0295993385	N,0,1.8669004769,0.4843964166,-1.0383516726
H,0,1.2632181488,1.0060487434,-1.6000492206	H,0,1.1937533129,1.0218162141,-1.5628660995
N,0,0.415421805,-1.3231887784,-0.576898822	N,0,0.4205269664,-1.3754916474,-0.6567163979
N,0,-0.5420734247,-0.7446200189,-1.335156714	N,0,-0.5425540834,-0.8045730043,-1.4063593003
C,0,-1.6674027521,-1.3870388989,-1.4556271226	C,0,-1.6786026173,-1.4323767871,-1.4980144516
H,0,-1.8091681076,-2.3536422974,-0.9635822555	H,0,-1.8279376195,-2.3855016996,-0.9800540633
H,0,0.2713391882,-2.2176426765,-0.1164263274	H,0,0.2842424043,-2.2617594765,-0.1785692632
H,0,5.9943488772,2.693004177,-0.676536741	H,0,5.8855809277,2.7938732943,-0.5622624963
C,0,-2.7488310325,-0.8916207034,-2.2428323283	C,0,-2.7640271714,-0.9362590985,-2.2760021966
C,0,-3.8872976333,-1.6666739539,-2.4347125388	C,0,-3.9275370252,-1.6852027569,-2.4180720329
C,0,-2.6528349308,0.4789614443,-2.8718146843	C,0,-2.64632886,0.4180230559,-2.9400988969
C,0,-4.9133850777,-1.2758681542,-3.2965862934	C,0,-4.9668488882,-1.2860246143,-3.257603792
C,0,-3.7082779898,0.7340685963,-3.8959338305	C,0,-3.7318004151,0.6822017786,-3.9327143239
C,0,-4.7942223266,-0.0838916045,-4.0486234419	C,0,-4.8386289415,-0.1120260307,-4.0359641986
H,0,6.7796238029,0.8345897161,0.7422817259	H,0,6.7120166207,0.9030656254,0.7865621211
H,0,-5.7887462145,-1.9022341744,-3.4247222804	H,0,-5.8657854402,-1.8869886045,-3.3402476911
H,0,-3.9669843952,-2.6214495589,-1.9258705955	H,0,-4.0195530218,-2.6224217994,-1.8791268045
O,0,-3.5362576045,1.8607705044,-4.6352011185	O,0,-3.5606309943,1.791393477,-4.6964398145
H,0,-4.2740274094,1.9385493073,-5.2584862259	H,0,-4.3191130409,1.8706449713,-5.2931962179
O,0,-2.6218921097,1.545104366,-1.8683331063	O,0,-2.5393342525,1.4987742735,-1.9707409012
H,0,-1.6608550164,0.6294340162,-3.3148693916	H,0,-1.668894272,0.5195660389,-3.4278467673
O,0,-5.7341542249,0.3213119359,-4.9708072504	O,0,-5.8016855969,0.3031414509,-4.9359831199
H,0,-6.3335584733,-0.4013850204,-5.1897085492	H,0,-6.3960136347,-0.4220121578,-5.1551523186
O,0,-3.8671090808,1.5049432875,-1.1029199536	O,0,-3.7659430484,1.5178421413,-1.1732401385
C,0,-4.4094952506,2.820849567,-1.1410977808	C,0,-4.1606924006,2.8797809294,-1.0991813758
H,0,-4.6746627179,3.1130498636,-2.1602046946	H,0,-4.3973526629,3.2808705411,-2.0885963483

H,0,-5.3083235428,2.7618694202,-0.5232055111	H,0,-5.0563227259,2.8694900638,-0.4735279825
H,0,-3.7145112857,3.5452677675,-0.7069884831	H,0,-3.3874209708,3.4887757857,-0.6210734257

P C16(•OOCH$_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.65907151 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234083 a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1100.2200707 a.u.	**P C16(•OOCH$_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.68424332 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.234609 a.u. SP at UM06-2X/6-311++G** (water), E = -1100.2470678 a.u.
0, 2	0, 2
C,0,5.8114716761,0.84786873,0.1654026877	C,0,5.8164924377,0.8453428194,0.1485755543
C,0,5.0970788256,-0.3420695641,0.2851264842	C,0,5.0976761757,-0.3413959334,0.2948096694
C,0,5.249939448,1.9821247402,-0.4414762276	C,0,5.2566165137,1.9680866149,-0.4826671021
H,0,5.5295403487,-1.2181755034,0.753384237	H,0,5.5336131157,-1.2057458704,0.7827544726
C,0,3.7957943449,-0.3820388427,-0.2181558524	C,0,3.794730314,-0.3884645264,-0.2071451892
C,0,3.9508119525,1.9625225649,-0.9503625837	C,0,3.9553818979,1.9402689823,-0.9900501016
H,0,3.5180758904,2.839049506,-1.4188951173	H,0,3.5213271481,2.8051737396,-1.4776607687
C,0,3.2463751657,0.7717165514,-0.8268117702	C,0,3.2476795069,0.7537847746,-0.8401364827
C,0,1.8232884096,-0.9160409019,-0.8239184415	C,0,1.8117142301,-0.925198455,-0.8058983782
N,0,2.8745783181,-1.4241845526,-0.2334179646	N,0,2.8681562145,-1.4271175831,-0.2009088239
N,0,1.9625422492,0.390979778,-1.2083338886	N,0,1.9644836126,0.371164699,-1.2133716124
H,0,1.2543213963,0.9308402776,-1.6792646319	H,0,1.2636625102,0.9129546014,-1.6961295264
N,0,0.6613305103,-1.6114129532,-1.0488078825	N,0,0.6500402058,-1.6123371866,-1.02055942
N,0,-0.3673023785,-1.0345993952,-1.7012244397	N,0,-0.3728595545,-1.0194383648,-1.6790468631
C,0,-1.4233343496,-1.7317461449,-1.9139087228	C,0,-1.4375743029,-1.7065336115,-1.883052884
H,0,-1.4856267083,-2.7708368372,-1.5716943232	H,0,-1.5178660541,-2.7393082532,-1.5332057376
H,0,0.6402194875,-2.5825556763,-0.7530289479	H,0,0.6037173616,-2.5803165643,-0.7163308768
H,0,5.835033327,2.8913246657,-0.517140051	H,0,5.8437028077,2.8741059059,-0.5789247059
C,0,-2.5956779736,-1.1987258167,-2.6149737682	C,0,-2.5989161807,-1.154562992,-2.5906589032
C,0,-3.7193467722,-2.0594236229,-2.767273009	C,0,-3.7444090591,-1.99184803,-2.7227569157
C,0,-2.6350855485,0.0726004937,-3.1279690815	C,0,-2.6071395704,0.1078205636,-3.1290102823
C,0,-4.8773266476,-1.6280771024,-3.4381162806	C,0,-4.8898291734,-1.5515245283,-3.4063634706
C,0,-3.8331290277,0.6381990942,-3.8112365775	C,0,-3.7975154669,0.6852722873,-3.8111195596
C,0,-4.9577158952,-0.3587627391,-3.9377283158	C,0,-4.9378359198,-0.2909942468,-3.9384045609
H,0,6.8241170936,0.9014717256,0.548809423	H,0,6.8296786325,0.9035886466,0.5301249728
H,0,-5.7134743509,-2.3107903935,-3.561530068	H,0,-5.7381921146,-2.217766494,-3.5234031551
H,0,-3.6818775628,-3.0660205098,-2.3676705247	H,0,-3.7290740155,-2.9895711953,-2.3012328727
O,0,-3.4443500588,1.1527632628,-5.0613678443	O,0,-3.4103708169,1.2075538323,-5.0620233627
H,0,-4.2350034902,1.5012395885,-5.4962381228	H,0,-4.2109270783,1.462164647,-5.5439658806
O,0,-4.2974909791,1.8463494148,-3.1270193555	O,0,-4.2444225651,1.9124639055,-3.121124987
O,0,-6.0221429761,0.1427036107,-4.6184336064	O,0,-5.9718268028,0.2197872121,-4.6469931627
H,0,-6.6898525076,-0.5411410799,-4.7465270875	H,0,-6.6639053388,-0.4419413692,-4.779539256
H,0,-1.7930250974,0.7457405483,-3.0392301625	H,0,-1.7454496735,0.7593851097,-3.0568797634
O,0,-4.8418940681,1.4493962892,-1.8283926775	O,0,-4.7117830347,1.5557176291,-1.7844546481
C,0,-5.9690822776,2.2849406377,-1.6222647993	C,0,-6.0085929322,2.1306723337,-1.6402361679
H,0,-6.3436222601,1.9975060574,-0.6370658009	H,0,-6.3039995828,1.8764510293,-0.6200862062
H,0,-5.6798133979,3.3403268896,-1.6113270502	H,0,-5.9688250349,3.2177250986,-1.750768226
H,0,-6.7355756958,2.1125358496,-2.3837760548	H,0,-6.7145899927,1.7001794126,-2.3540130157

P C16(•OOCH$_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.66954231 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235009 a.u.	**P C17(•OOCH$_3$),** optimization in gas phase UB3LYP/6-311++G**, E= -1100.67655092 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.236959 a.u.

SP at UM06-2X/6-311++G** (benzene), E = -1100.2312353 a.u.	SP at UM06-2X/6-311++G** (gas phase), E = -1100.237067 a.u.
0, 2	0, 2
C,0,5.8085377981,0.8541560912,0.1690390048	C,0,6.0631600638,0.5879114431,0.0978679052
C,0,5.0984686291,-0.3392482527,0.2895992855	C,0,5.1899116617,-0.4559677051,0.3897048145
C,0,5.2433114082,1.9848701958,-0.4417092834	C,0,5.6765131575,1.660322192,-0.722713902
H,0,5.5358079656,-1.2114495088,0.7611498596	H,0,5.4862719986,-1.2840376737,1.0222168191
C,0,3.7980925309,-0.3858626585,-0.2167742408	C,0,3.905926754,-0.4117032673,-0.1582756476
C,0,3.944798645,1.9582069554,-0.9535470161	C,0,4.3994527614,1.7236012749,-1.2797412947
H,0,3.5080669939,2.8308810155,-1.4251965428	H,0,4.1031819231,2.5519067036,-1.9129614361
C,0,3.2450958269,0.7644780964,-0.8289825271	C,0,3.5337730699,0.6778560333,-0.9833403511
C,0,1.82548989,-0.9271647742,-0.8283766527	C,0,1.8913584821,-0.7761898185,-0.7478161686
N,0,2.8802277662,-1.4314048423,-0.2326558514	N,0,2.8513727578,-1.3063941283,-0.0312293488
N,0,1.9647397021,0.3788082785,-1.2131906993	N,0,2.2184496441,0.4094963802,-1.3493579509
H,0,1.2570717315,0.9202512984,-1.684488118	H,0,1.5984286419,0.9468763658,-1.934060874
N,0,0.6678477624,-1.623223075,-1.0575982589	N,0,0.6516646671,-1.3410779233,-0.8997783888
N,0,-0.3618208025,-1.0378368366,-1.7058882769	N,0,-0.2934760842,-0.7402744472,-1.6406540139
C,0,-1.420817288,-1.7320196534,-1.9137998269	C,0,-1.4540571383,-1.3473885267,-1.7201968975
H,0,-1.4869722102,-2.7697103646,-1.5712076758	H,0,-1.6083927675,-2.2945909034,-1.1932079453
H,0,0.6371021719,-2.5938496519,-0.7606246547	H,0,0.4874363773,-2.2193726353,-0.4148731152
H,0,5.8245286421,2.896535359,-0.5181347792	H,0,6.3839148456,2.4552411934,-0.9283472505
C,0,-2.5925679087,-1.1920284653,-2.611580164	C,0,-2.5428395288,-0.8332598985,-2.4638411328
C,0,-3.72376827,-2.0454352458,-2.7534326828	C,0,-3.7777832791,-1.5684809587,-2.4843944735
C,0,-2.6245356968,0.0773357494,-3.1306149765	C,0,-2.455897414,0.3793126586,-3.2165692102
C,0,-4.8821993601,-1.6087892267,-3.4188187468	C,0,-4.8645560805,-1.1260176122,-3.1520649761
C,0,-3.822665834,0.6471158251,-3.8090265864	C,0,-3.5194717013,0.8425333438,-3.9134871237
C,0,-4.9562542113,-0.340261849,-3.9241509562	C,0,-4.8687739237,0.172607412,-3.8843762373
H,0,6.8200867532,0.9124753212,0.5548188472	H,0,7.0650476697,0.5755082778,0.5115602182
H,0,-5.7236621684,-2.2849807899,-3.53635472	H,0,-5.799510096,-1.6758746403,-3.1467230977
H,0,-3.6909153743,-3.050369594,-2.3497161546	H,0,-3.8280877992,-2.5075409778,-1.9422473676
O,0,-3.4397797874,1.1554791569,-5.0657086217	O,0,-3.4357357524,1.9748811066,-4.6520665154
H,0,-4.2358210534,1.4777041449,-5.5120033294	H,0,-4.2278588161,2.0355549744,-5.2048780782
O,0,-4.2715144797,1.8674614833,-3.128312755	O,0,-5.8871970122,1.0803923869,-3.3367535754
O,0,-6.0179144665,0.1668457175,-4.6004354838	O,0,-5.3074045883,0.0839081667,-5.2288398365
H,0,-6.6978078219,-0.5077987978,-4.7210637983	H,0,-6.2312878648,-0.1993984286,-5.2273652561
H,0,-1.775930235,0.7437146144,-3.0497317018	H,0,-1.5202937825,0.9217388187,-3.2550855316
O,0,-4.7947133946,1.4933977691,-1.8151865703	O,0,-5.6549877758,1.2475091734,-1.9086312369
C,0,-5.979446931,2.2586026364,-1.6403450561	C,0,-5.5715403988,2.6481478359,-1.6774849537
H,0,-6.3333965898,1.9859811037,-0.6436076911	H,0,-6.4992984548,3.1499763381,-1.9679281078
H,0,-5.7628195254,3.3304206853,-1.6722949914	H,0,-5.4311902441,2.7315879438,-0.5973070422
H,0,-6.7311823881,2.0023107292,-2.3919058069	H,0,-4.7193703334,3.0900393017,-2.2008674994

P C17(•OOCH$_3$), optimization in solv. water UB3LYP/6-311++G**, E= -1100.69731970 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.236165 a.u. SP at UM06-2X/6-311++G** (water), E = -1100.2590329 a.u.	**P C17(•OOCH$_3$),** optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.68533331a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.236599 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1100.2463747 a.u.
0, 2	0, 2
C,0,6.0779350389,0.5863793432,0.048983738	C,0,6.0663993837,0.5896650573,0.0817202447
C,0,5.223918955,-0.4755989942,0.3418998804	C,0,5.198953421,-0.4589570592,0.377552979
C,0,5.6593646392,1.6661067441,-0.7475860989	C,0,5.6698632126,1.6619410924,-0.7349399796
H,0,5.5497295264,-1.3069390794,0.9564462508	H,0,5.5050445654,-1.2859153646,1.0072829233
C,0,3.9278878593,-0.4407044105,-0.1806867565	C,0,3.9109910897,-0.4191178257,-0.1624790492
C,0,4.3694230323,1.7191148372,-1.2785866849	C,0,4.3885150369,1.7204217322,-1.2837820299
H,0,4.0452432059,2.5506662559,-1.8929540778	H,0,4.0830109397,2.5475380062,-1.9139677753

C,0,3.5242245114,0.6560756167,-0.9812378338	C,0,3.5291351782,0.6702030318,-0.9833884483
C,0,1.900322078,-0.8194877833,-0.7426365922	C,0,1.8913105419,-0.7887772783,-0.7427613064
N,0,2.8858214582,-1.3512302755,-0.0492216472	N,0,2.8597055338,-1.3179248827,-0.0312172041
N,0,2.2080721576,0.377238051,-1.3267914297	N,0,2.2136479337,0.3981431628,-1.3421034574
H,0,1.5771744034,0.9260700092,-1.8914788219	H,0,1.5917658128,0.938321317,-1.9232716472
N,0,0.6666364568,-1.3917524296,-0.8834965973	N,0,0.6533547009,-1.3552263496,-0.8900261899
N,0,-0.2853906789,-0.7797542994,-1.6099100067	N,0,-0.2929265386,-0.7507450617,-1.6283342183
C,0,-1.445584102,-1.3866668075,-1.6913305105	C,0,-1.4529024802,-1.3586312523,-1.7104139091
H,0,-1.6033707532,-2.3402834051,-1.1817003026	H,0,-1.6085591154,-2.3082407939,-1.1900860853
H,0,0.5025297748,-2.2802304436,-0.4167419351	H,0,0.4877480206,-2.2371987262,-0.4120264895
H,0,6.3510172853,2.4744435401,-0.9547514793	H,0,6.3725447622,2.4602268002,-0.9438921535
C,0,-2.5303883465,-0.847896,-2.4277732243	C,0,-2.5397380573,-0.8366431662,-2.4530209362
C,0,-3.7719703813,-1.5714534451,-2.4645569203	C,0,-3.7761575104,-1.5692867078,-2.4808031733
C,0,-2.4336800306,0.3840315597,-3.1495166196	C,0,-2.449941144,0.382679278,-3.1952670319
C,0,-4.8506029915,-1.1093217918,-3.1348968627	C,0,-4.8602501085,-1.1208108666,-3.1498012227
C,0,-3.4892751429,0.8693128312,-3.8446513607	C,0,-3.5105608293,0.8522697016,-3.8926900125
C,0,-4.8323709678,0.1858997982,-3.8750194689	C,0,-4.8578884904,0.1774959754,-3.8835750593
H,0,7.0878281579,0.5812399734,0.4431932356	H,0,7.0709030233,0.5805265196,0.4892633474
H,0,-5.7884197842,-1.6543951502,-3.150835903	H,0,-5.7953965183,-1.6704865064,-3.1524486128
H,0,-3.834444651,-2.5163700883,-1.9348473255	H,0,-3.8299692573,-2.5107406875,-1.9434988808
O,0,-3.3878256947,2.0274161122,-4.5442453842	O,0,-3.4207291836,1.9933357084,-4.6191255388
H,0,-4.2058955983,2.1759585325,-5.0395873219	H,0,-4.2186212889,2.0795406912,-5.1602816224
O,0,-5.8793992925,1.0946898414,-3.3806270798	O,0,-5.886330033,1.085167157,-3.3513006382
O,0,-5.2057827028,0.0747823222,-5.2345515369	O,0,-5.2747680135,0.0836687112,-5.2332046773
H,0,-6.0610251282,-0.3740942148,-5.2900202249	H,0,-6.1808087798,-0.2531859722,-5.253221134
H,0,-1.4990921948,0.9308451966,-3.1546669147	H,0,-1.5148701912,0.9270886722,-3.2223669761
O,0,-5.6844812781,1.3094110023,-1.9495198977	O,0,-5.6706982735,1.2621246068,-1.9205647004
C,0,-5.6898794585,2.7210924946,-1.7466563725	C,0,-5.599889889,2.6659368132,-1.6929330677
H,0,-6.6370400475,3.1598081255,-2.0713538708	H,0,-6.5264227035,3.160023937,-1.9986959532
H,0,-5.5832030566,2.8358681784,-0.6659940076	H,0,-5.4758174774,2.7543400956,-0.6113803599
H,0,-4.8511526187,3.1990680328,-2.2582081145	H,0,-4.7427936333,3.1105702137,-2.205066034

P C19(•OOCH$_3$), optimization in gas phase UB3LYP/6-311++G**, E= -1100.67059851 a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.236337a.u. SP at UM06-2X/6-311++G** (gas phase), E = -1100.2293683a.u.	**P C19(•OOCH$_3$),** optimization in solv. water UB3LYP/6-311++G**, E= -1100.69253629a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235540 a.u. SP at UM06-2X/6-311++G** (water), E = -1100.2526125 a.u.
0, 2	0, 2
C,0,6.1462125884,0.7351511514,0.3185946051	C,0,6.1337156319,0.7466886659,0.2861219217
C,0,5.2408458028,-0.250324366,0.7035595074	C,0,5.2428715643,-0.2529201064,0.676232737
C,0,5.7860954399,1.7512930374,-0.581033073	C,0,5.7480576097,1.7688828421,-0.5971665413
H,0,5.5175032601,-1.0348079143,1.397640213	H,0,5.5443109836,-1.0399343452,1.3580398143
C,0,3.9517659664,-0.2048682228,0.1685696261	C,0,3.9436579857,-0.2141096764,0.1627020382
C,0,4.5037552929,1.8145367076,-1.1268887967	C,0,4.4545520109,1.8246890069,-1.1208592852
H,0,4.2271273381,2.5994453676,-1.8214304277	H,0,4.1546485704,2.6120071645,-1.802340115
C,0,3.6067976765,0.8276828226,-0.7374188397	C,0,3.5735635631,0.8246779276,-0.7264495154
C,0,1.9167497972,-0.5433849056,-0.367052662	C,0,1.8958898375,-0.5620745941,-0.3497581122
N,0,2.8679351028,-1.0481894532,0.379357286	N,0,2.8689804225,-1.0693486617,0.3802125186
N,0,2.2776003885,0.578245653,-1.0656052291	N,0,2.2437486666,0.568122895,-1.0365687535
H,0,1.6683812909,1.0882730239,-1.6849344787	H,0,1.6281740592,1.0881466318,-1.6436202744
N,0,0.6560050743,-1.0710693492,-0.4620547901	N,0,0.6411517669,-1.0934754531,-0.4351085937
N,0,-0.2735648552,-0.4958265685,-1.2486145599	N,0,-0.2920297416,-0.5068276328,-1.215592
C,0,-1.4513906244,-1.062389063,-1.2832884365	C,0,-1.4683278541,-1.0753831727,-1.2552672142
H,0,-1.6442182683,-1.9521436515,-0.675249834	H,0,-1.6614206206,-1.9739423355,-0.6637873944

H,0,0.4635885439,-1.9038623866,0.0874657388	H,0,0.4455613776,-1.9367019929,0.0975335405
H,0,6.5174713819,2.5016953107,-0.8578629942	H,0,6.4670756244,2.5295110291,-0.8786241253
C,0,-2.5253776089,-0.5749603334,-2.0770756146	C,0,-2.536563011,-0.5727137553,-2.0507894015
C,0,-3.8504187473,-1.2933677139,-1.9392574928	C,0,-3.8649401339,-1.2859627531,-1.937267966
C,0,-2.409050044,0.5350737661,-2.9204992536	C,0,-2.4072468558,0.5426633543,-2.8868785479
C,0,-4.8807862355,-0.880644458,-2.9415643519	C,0,-4.8797589784,-0.873179914,-2.9543147051
C,0,-3.4541199335,0.935371267,-3.7235530518	C,0,-3.4396603152,0.9427706977,-3.707552067
C,0,-4.6931907734,0.1908992536,-3.7344092406	C,0,-4.6793595772,0.1959304643,-3.7496983503
H,0,7.1527150307,0.7198297422,0.7210305707	H,0,7.1468318682,0.7362507118,0.6720806819
H,0,-5.8147122495,-1.4324822691,-2.9527403686	H,0,-5.8054172763,-1.4361828311,-2.9974484168
H,0,-3.6988153751,-2.3806673753,-1.9821075687	H,0,-3.7170443418,-2.3731349616,-1.9736535419
O,0,-3.3260806617,2.0153678336,-4.531589945	O,0,-3.2951436715,2.0244740194,-4.5121628087
H,0,-4.156281115,2.1401755931,-5.0122965977	H,0,-4.1085878961,2.1435812059,-5.0251481761
O,0,-4.3785714173,-1.2080257299,-0.5794435268	O,0,-4.4140418789,-1.1980427147,-0.5779270894
O,0,-5.6052651329,0.6887059986,-4.6336839057	O,0,-5.5604003611,0.6865751136,-4.6747630569
H,0,-6.4534873559,0.243654245,-4.5353484756	H,0,-6.3955476267,0.2034730332,-4.6525082522
H,0,-1.4785551865,1.0869492781,-2.963131866	H,0,-1.474262386,1.0924577972,-2.9156268834
O,0,-4.7236795257,0.191871059,-0.3190713121	O,0,-4.7331825567,0.2039477502,-0.2929426407
C,0,-4.3094400746,0.4507673331,1.010710024	C,0,-4.2509053857,0.4605812477,1.0199785707
H,0,-4.8035683661,-0.2235861745,1.7173919177	H,0,-4.7202434323,-0.2055130042,1.7499240675
H,0,-3.2226959328,0.3756000441,1.1151860951	H,0,-3.1626106932,0.3702853275,1.0704517476
H,0,-4.6308516917,1.4778296874,1.2001997692	H,0,-4.5496681485,1.4915492591,1.2230448504

P C19(•OOCH$_3$), optimization in solv. benzene UB3LYP/6-311++G**, E= -1100.67995935a.u. Thermal correction to Gibbs Free Energy at 25 ^{0}C = 0.235641 a.u. SP at UM06-2X/6-311++G** (benzene), E = -1100.2393429 a.u.	
0, 2 C,0,6.1342731658,0.745725516,0.3101990246 C,0,5.2380190278,-0.2496152635,0.6942459565 C,0,5.7609119648,1.765297143,-0.5805734663 H,0,5.527098423,-1.0357930129,1.3817001871 C,0,3.9450457738,-0.2102017716,0.1671402114 C,0,4.4742027594,1.8222016334,-1.1182684739 H,0,4.1858300883,2.6090160474,-1.8056572241 C,0,3.5870011256,0.8257249594,-0.729959709 C,0,1.9061964678,-0.5581943356,-0.3614324011 N,0,2.8675275049,-1.0624983539,0.3779523267 N,0,2.2587336691,0.5695678953,-1.0525220355 H,0,1.645688436,1.0830494888,-1.6662023439 N,0,0.6492819991,-1.0904299643,-0.454754746 N,0,-0.2824557896,-0.5092324617,-1.2375145331 C,0,-1.4599829975,-1.0759604743,-1.2745644561 H,0,-1.6533446728,-1.9697795357,-0.674116704 H,0,0.4560276343,-1.9282124541,0.0869723245 H,0,6.4848077847,2.523194402,-0.8568069 C,0,-2.5315706157,-0.5802213979,-2.0680400115 C,0,-3.8598805256,-1.2928616974,-1.9388716818 C,0,-2.4077223321,0.5315121613,-2.908707055 C,0,-4.8845977005,-0.8762291445,-2.9450341956 C,0,-3.4473751027,0.9348000051,-3.7175358667 C,0,-4.689716757,0.1940436511,-3.738851066 H,0,7.143244798,0.7349477088,0.7067165775	

H,0,-5.8176682029,-1.4288774491,-2.9663549859 H,0,-3.7128968353,-2.3805769094,-1.9805088706 O,0,-3.3102311832,2.0149458122,-4.5245453176 H,0,-4.1353557983,2.1421750102,-5.0147610236 O,0,-4.3943208167,-1.2066026867,-0.5780787864 O,0,-5.5886614311,0.6933052047,-4.6465267851 H,0,-6.4377223709,0.2434062079,-4.5719686599 H,0,-1.4747469729,1.0798583766,-2.9468462321 O,0,-4.7302765451,0.1934514516,-0.3069292818 C,0,-4.2601065505,0.4628480266,1.0046109053 H,0,-4.7237291863,-0.206423141,1.735865488 H,0,-3.170309809,0.3897091978,1.0630199617 H,0,-4.574789627,1.4907483943,1.2000085093	