

Electronic Supplementary Information

Deprotonation Routes of Anthocyanidins in Aqueous Solution, pKa Values, and Speciation under Physiological Conditions

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Table 1S. Set of phenols used to obtain the k and C_0 parameters, their experimental pKa and calculated ΔG_0 values.

	ΔG_0 (kcal/mol)	pKa exp
phenol	288.79	9.98
<i>m</i> -aminophenol	289.38	9.87
<i>p</i> -aminophenol	291.24	10.30
<i>o</i> -chlorophenol	284.79	8.56
<i>m</i> -chlorophenol	286.17	9.02
<i>p</i> -chlorophenol	287.28	9.38
<i>o</i> -methylphenol	289.50	10.29
<i>m</i> -methylphenol	289.45	10.08
<i>p</i> -methylphenol	289.95	10.14
<i>o</i> -nitrophenol	280.48	7.23
<i>m</i> -nitrophenol	284.60	8.40
<i>p</i> -nitrophenol	279.53	7.15
<i>m</i> -hydroxyphenol	288.03	9.44
<i>p</i> -hydroxyphenol	290.30	9.96
<i>m</i> -methoxyphenol	287.88	9.65
<i>p</i> -methoxyphenol	289.55	10.21

Table 2S. Relative Gibbs energies of each possible first deprotonation reaction (from cationic to neutral form), in aqueous solution at 298.15 K.

	R ₃ '	R ₄ '	R ₅ '	R ₃	R ₅	R ₆	R ₇
Arn	-	5.15	-	5.83	5.58	2.14	0.00
Cpn	-	1.91	-	2.14	-	-	0.00
Cyn	6.78	0.00	-	3.54	1.74	-	1.86
Dlp	8.09	0.00	8.57	3.70	3.23	-	3.19
Erp	-	0.00	7.99	3.31	-	-	1.49
Ltl	6.22	0.00	-	-	0.79	-	0.40
Mlv	-	1.46	-	2.72	0.00	-	1.45
Plg	-	1.83	-	2.26	0.14	-	0.00
Pnd	-	0.83	-	1.97	0.34	-	0.00
Ptn	8.59	1.17	-	2.89	0.00	-	1.82
Rsn	-	0.00	-	0.70	0.38	-	-
6Dlp	8.70	0.61	9.02	4.81	1.87	4.21	0.00

Table 3S. Relative Gibbs energies of each possible second deprotonation reaction (from neutral to mono-anionic form), in aqueous solution at 298.15 K.

	R ₃ '	R ₄ '	R ₅ '	R ₃	R ₅	R ₆	R ₇
Arn	-	0.78	-	0.00	0.30	3.04	-
Cpn	-	0.00	-	0.22	-	-	-
Cyn	11.13	-	-	2.73	0.00	-	1.11
Dlp	10.32	-	11.60	2.16	0.00	-	0.65
Erp	-	-	10.38	0.00	-	-	1.31
Ltl	12.24	-	-	-	0.00	-	0.41
Mlv	-	1.46	-	2.66	-	-	0.00
Plg	-	2.36	-	2.17	0.00	-	-
Pnd	-	1.32	-	0.76	0.00	-	-
Ptn	4.65	0.00	-	2.15	-	-	1.22
Rsn	-	-	-	0.00	0.36	-	-
6Dlp	5.99	0.00	5.49	3.58	5.21	8.25	-

Table 4S. Relative Gibbs energies of each possible third deprotonation reaction (from mono-anionic to di-anionic form), in aqueous solution at 298.15 K.

	R ₃ '	R ₄ '	R ₅ '	R ₃	R ₅	R ₆	R ₇
Arn	-	0.00	-	-	0.73	3.69	-
Cpn	-	-	-	0.00	-	-	-
Cyn	8.15	-	-	0.33	-	-	0.00
Dlp	9.41	-	10.27	0.77	-	-	0.00
Erp	-	-	9.65	-	-	-	0.00
Ltl	9.93	-	-	-	-	-	0.00
Mlv	-	0.00	-	0.02	-	-	-
Plg	-	0.00	-	0.14	-	-	-
Pnd	-	0.88	-	0.00	-	-	-
Ptn	8.55	-	-	0.00	-	-	0.19
Rsn	-	-	-	-	0.00	-	-
6Dlp	9.67	-	10.18	0.00	0.84	4.56	-

Table 5S. pKa values of quercetin and kaempferol.

	pKa1	pKa2	pKa3	Ref.
quercetin	7.30	8.40		1
	6.62	9.70		2
	7.19	9.36	11.56	3
	6.74	9.02	11.55	4
	7.71	9.44	11.46	5
	7.59	9.33	11.56	5
	7.04	8.55	11.26	3
	6.18	7.44	9.68	6
	6.41	7.81	10.19	6
	6.98	8.78	11.04	average
	7.66	7.94	10.26	Calc., this work
kaempferol	8.20	9.50		1
	7.05	9.04	11.04	3
	7.11	9.09	11.33	3
	7.22	8.71	10.40	6
	7.49	9.12	10.90	6
	7.41	9.09	10.92	average
	7.68	8.99	10.34	Calc., this work

Cartesian coordinates of the optimized geometries of the studied anthocyanidins

Flavillium ions

Arn

\\C,4.28809312,-0.3996360164,0.0227564333\C,3.5664111757,
0.7649594957,-0.0562737926\C,2.1523532283,0.7149256101,-0.0364890794\C
,1.5391906431,-0.5431943951,0.0685795505\C,2.2455985579,-1.730627784,0
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8276062992,-0.2314506277\C,1.3296937078,1.8430106791,-0.1264813494\H,1
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\H,-6.1484296267,-1.8862315425,-0.2462449029\O,4.1623467522,1.97504610
6,-0.1531086582\H,5.1231796643,1.8703038824,-0.1334149555\O,4.44057581
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5742,-1.2036286967,0.0636714208\\

Cpn

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Dlp

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Ltl

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MIv

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4.3920567543,-2.5404532796,0.6590448245\H,3.884959073,-3.360079088,0.7
17020333\H,5.2778385453,-0.1672539677,0.4376080168\O,-4.0750627437,-3.
0903578756,-0.7860024402\C,-3.0501281674,-4.0834953803,-0.9265364222\H
, -2.4204951279,-3.8533142792,-1.7850834687\H,-2.4526260601,-4.13654788
3,-0.0171574498\H,-3.5705696944,-5.0215266352,-1.0854668752\O,-5.50402
046,1.3336026529,-0.0862825372\C,-5.9961407161,1.4200480407,1.26673441
21\H,-6.3409954165,0.4431997617,1.6038200715\H,-5.2056685613,1.7880131
286,1.9205521942\H,-6.8240927479,2.1221559657,1.2486858879\

Plg

\C,4.2954744083,-0.390094233,0.0246816122\C,3.570686269
6,0.7693716554,-0.0495645017\C,2.1482208617,0.724226363,-0.0335142753\
C,1.5417350301,-0.537425859,0.0710397141\C,2.2469555292,-1.7241193871,
0.1518164337\C,3.6286082539,-1.6268697627,0.1230594081\H,1.7636094344,
2.8337296319,-0.2282483049\C,1.3263904529,1.8487016869,-0.1238420675\H
,1.7385322798,-2.6740554646,0.2293059921\C,-0.6162364884,0.4513686149,
0.0147155466\C,-0.0481506174,1.7266117565,-0.1002473902\C,-2.020391347
1,0.1013282504,0.0176651709\C,-3.0234662539,1.0199332621,0.3711764265\
C,-2.3909776385,-1.2109297784,-0.3256130085\C,-4.3493878295,0.63847957
56,0.3764865695\H,-2.7669626474,2.0235462622,0.6651438009\C,-3.7160133
321,-1.59013718,-0.3333199557\H,-1.6351513446,-1.9296557651,-0.6052366
19\C,-4.6985639272,-0.6617861817,0.0156843832\H,-5.1255125638,1.335444
1744,0.6586663824\H,-4.0026782943,-2.5956985038,-0.6118927081\O,-0.874

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4509651\O,0.1936858388,-0.6025945022,0.0969481463\O,-6.0155564946,-0.9
815760189,0.0216159049\H,-6.1391150878,-1.9011097259,-0.2433607828\O,4
.1258082306,1.9952506356,-0.139641733\H,5.0894890137,1.9344020943,-0.1
238828052\O,4.4190127542,-2.7178857084,0.1852890387\H,3.886732502,-3.5
216289009,0.242618861\H,5.3767178268,-0.3683903424,0.0106567475\

Pnd

\\C,4.3385750783,-0.328076018,0.0746080968\C,3.604794502
4,0.8217995346,-0.0436850662\C,2.1827233519,0.7665090553,-0.0345264635
\C,1.5863712084,-0.4974480352,0.0909960914\C,2.3003442367,-1.675619150
9,0.2086301729\C,3.6813311023,-1.5674868928,0.2021561851\H,1.781688597
8,2.8669357384,-0.280518517\C,1.3510547513,1.8806922113,-0.158261833\H
,1.7983013965,-2.6270865449,0.3069934747\C,-0.5811609176,0.4710886646,
0.0002963106\C,-0.0230025618,1.7482748317,-0.1453869563\C,-1.982061631
9,0.1076364221,0.0269306597\C,-2.9813293176,1.0293434405,0.3583517775\
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.1171576847,1.9846776514,-0.1820398203\O,4.4799706584,-2.6480792719,0.
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-3.1460903731,-3.87766161,-0.7994161375\H,-2.6155432223,-3.6036635098,
-1.7106623267\H,-2.4459247248,-4.0112424383,0.0243962875\H,-3.71317648
04,-4.7882865143,-0.9586467312\

Ptn

\\C,-5.003643484,0.2216939578,0.1275546125\C,-4.2377
905945,-0.9079670597,0.0169509493\C,-2.8177150701,-0.8061223837,-0.013
426789\C,-2.2582423868,0.4784915192,0.0814671109\C,-3.0059469039,1.635
6232272,0.199083969\C,-4.3827732578,1.4837769037,0.2152570016\H,-2.349
2316519,-2.8973481718,-0.2134861058\C,-1.9526012647,-1.8930288764,-0.1
311931094\H,-2.5321630723,2.6039254748,0.2692341119\C,-0.0612345726,-0.
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8888906721,1.8391099339,-0.284251073\H,0.7931589222,2.1079969038,-0.27
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.1532691327,-0.0679072571\H,-5.7116952907,-2.1305161215,-0.0207524964\
O,-5.2143072525,2.5398635599,0.315423326\H,-4.716543928,3.3663105701,0
.3595283828\H,-6.0830725286,0.159199004,0.1490298481\O,3.1292044414,3.
1775705067,-0.4069035865\H,4.0799080532,3.3352671845,-0.4695246217\O,4
.7795515532,-1.2648551525,-0.1029138415\C,5.0152016792,-1.895171771,1.
1736958241\H,5.1626405362,-1.1327865075,1.9380839101\H,4.1757492307,-2
.5373590216,1.4351532178\H,5.915962862,-2.4892651074,1.0566545462\\

Rsn

\\C,4.3121635615,-0.3473996416,0.0052451274\C,3.58557832
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6\C,1.5655384993,-0.5077419904,0.0464763121\C,2.2723105305,-1.69529991
,0.1467102793\C,3.6558536779,-1.5936297715,0.1273595902\H,1.7667484994
,2.8597618378,-0.2961053435\C,1.3346310745,1.8738062981,-0.1761503788\
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0.4842379294\H,-2.7289422351,2.0420446706,0.6749672306\C,-3.6827935013
, -1.6008015763,-0.2041315588\H,-1.6042753702,-1.9280133291,-0.55619002
58\C,-4.6678075617,-0.6669519215,0.1709859566\H,-5.0859470635,1.328874
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99631239,-0.0312493435\O,4.1358825541,2.0319401085,-0.2170064249\H,5.0
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542228\H,5.3934751789,-0.3219625593,-0.0059825722\O,-4.1633611646,-2.8
410796441,-0.4852310011\C,-3.2202515472,-3.830566024,-0.9162640317\H,-
2.72820147,-3.5043294648,-1.8317417292\H,-2.4853783144,-4.0162381947,-
0.1338273504\H,-3.8003894092,-4.7274535096,-1.1033701113\C,3.887114268
2,-3.9524038786,0.3711641474\H,3.3026731234,-3.9944844085,1.2887200769
\H,3.2654909369,-4.1844990425,-0.491900791\H,4.7213575957,-4.642595008
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6Dlp

\\C,3.9802597303,-0.3155928094,0.0308156904\C,3.2423
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329\C,1.2331268198,-0.5043215622,0.0370805702\C,1.9570871996,-1.682835
9097,0.0991587659\C,3.3337164496,-1.5713151722,0.0926755046\H,1.416970
5658,2.8765212626,-0.1730145636\C,0.9919764873,1.8832288147,-0.0978591
306\H,1.4662894659,-2.6438259441,0.1494425685\C,-0.9328142296,0.456078
487,-0.0089149422\C,-0.3803844061,1.7418585375,-0.0906768591\C,-2.3370
699264,0.0887093631,-0.0101687414\C,-3.3294229388,0.9952716753,0.38138
6347\C,-2.6801641429,-1.2208006631,-0.3840510209\C,-4.6510476252,0.590
118459,0.3963139711\H,-3.0947527978,1.997299512,0.6981962865\C,-4.0056
599466,-1.6006601046,-0.3760220403\H,-1.9291854557,-1.9323745896,-0.69
54220325\C,-4.9999886465,-0.7013594518,0.0126171201\O,-1.2204554875,2.

7982501451,-0.1885929627\H,-0.7172229807,3.6201668538,-0.2481835898\O,
-0.1127395777,-0.5865633659,0.0482269349\O,-6.3123518486,-1.040036857,
0.0331060818\H,-6.4215747085,-1.9553189536,-0.2586204773\O,3.820197202
9,2.0600421306,-0.0853126372\H,4.7824535985,1.9698305949,-0.0561659763
\O,4.1703666942,-2.6252143097,0.1419696488\H,3.6840868621,-3.459231522
8,0.1709941353\O,5.3377125381,-0.2128434103,0.0227079534\H,5.737189708
8,-1.0920782597,0.0621661207\O,-4.4531852494,-2.8393406326,-0.73607407
22\H,-3.715758375,-3.4033858333,-0.9969223474\O,-5.61555877,1.47338013
57,0.7913869108\H,-6.4788131699,1.0415543853,0.7682167771\\

Neutral species

Arn

\\C,3.9946917104,-0.2850752228,0.025928476\C,3.263592025
7,0.8523682657,-0.0567627225\C,1.8368720421,0.7756255482,-0.0327599344
\C,1.24860419,-0.5185679922,0.0815317696\C,1.9716667762,-1.6782615184,
0.1684056153\C,3.3869096687,-1.6017181196,0.1430581457\H,1.4237637528,
2.8633378425,-0.217684586\C,1.0081209317,1.868409348,-0.1169246084\H,1
.4793922274,-2.6353230235,0.256721846\C,-0.9282125373,0.4634835347,0.0
282941283\C,-0.385067525,1.7224576562,-0.08875173\C,-2.3373200284,0.08
93846698,0.0368286917\C,-3.3387982956,0.9717126019,0.4657464071\C,-2.7
044649822,-1.1976483864,-0.3800563464\C,-4.6654280286,0.5814299066,0.4
686799578\H,-3.0822768975,1.957888634,0.8166888233\C,-4.0304895441,-1.
5892605737,-0.3849770849\H,-1.948503131,-1.89233826,-0.7160408243\C,-5
.0123447912,-0.6957227071,0.0373759935\O,-1.2120621908,2.8012804162,-0
.202918285\O,-0.1001860561,-0.5977695803,0.1124330419\O,-6.3342945128,
-1.0294403849,0.0505047435\O,3.8212643798,2.0908508921,-0.1626316987\O
,4.1656492536,-2.5942225529,0.2149247726\H,-4.3128622427,-2.5797250188
, -0.717643183\H,-5.4397217361,1.2553390143,0.8076294256\O,5.3572225544
, -0.231732492,0.0012213124\H,-6.4500562519,-1.9354070428,-0.2588861201
\H,-0.6880575061,3.6036557828,-0.3131871606\H,4.7836528202,2.013773484
1,-0.1410665464\H,5.6566670445,-1.153465832,0.0772201105\\

Cpn

\\C,-4.853037,0.719606,0.306394\C,-4.238223,-0.439517,-0
.042247\C,-2.797575,-0.513518,-0.092841\C,-2.073787,0.67152,0.238803\C
, -2.666744,1.845723,0.592979\C,-4.094105,1.913321,0.637851\H,-2.626606
, -2.545076,-0.71225\C,-2.100791,-1.637475,-0.442619\H,-2.07532,2.71587
7,0.837823\C,-0.018458,-0.491752,-0.144397\C,-0.693191,-1.637452,-0.47
7658\C,1.424099,-0.268737,-0.140246\C,2.321228,-1.314404,0.075913\C,1.
900328,1.038222,-0.337309\C,3.683546,-1.057763,0.089113\H,1.986997,-2.
323838,0.253257\C,3.261086,1.277134,-0.332252\H,1.204823,1.844282,-0.5
08875\C,4.166165,0.227804,-0.116383\O,0.006544,-2.745335,-0.860497\H,-
0.600379,-3.437169,-1.150389\O,-0.719991,0.612287,0.202811\O,5.504056,
0.451696,-0.115019\H,5.659746,1.390157,-0.290319\O,-4.862327,-1.589616
, -0.362994\O,-4.69954,2.973234,0.955265\H,-5.928638,0.802454,0.350479\
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,3.423166,-1.708339\H,2.329275,3.781497,0.042532\H,3.654661,4.452873,-
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H,-6.592524,-2.602763,-0.582551\H,-6.633448,-1.363875,0.698974\H,-6.70
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5875\\

Cyn

\\C,4.4795352875,0.5822419571,0.0263360633\C,3.8375221667,-0
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.7259112868,0.4999792259,0.0055256783\C,2.3351555157,1.744175804,0.020
0942785\C,3.7216206529,1.7610329419,0.0303891789\H,2.2020908103,-2.861
4518919,-0.0176470299\C,1.6848564759,-1.9103943358,-0.0139624966\H,1.7
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891\C,-4.5686805604,0.1579205499,-0.0465095789\H,-4.8053432565,-1.9829
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8161803529,0.0070411962\H,5.4545077101,-1.6590430328,0.015320483\O,4.4
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Dlp

\\C,-4.7664784348,0.4328415796,-0.008279357\C,-4.0646014655,
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1\C,-2.0135065383,0.4916301182,-0.0010286795\C,-2.6849669118,1.7028127
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578583\H,-2.1471436852,2.6400237137,0.014697382\C,0.1501333293,-0.5452
203535,-0.0036147865\C,-0.4857612398,-1.8251418755,-0.0148094661\C,1.5
265536999,-0.2349411935,0.0019749033\C,2.5489170529,-1.2269098309,-0.0
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32521\O,-4.6661829952,-1.9658713919,-0.026097715\H,-5.6259768119,-1.86
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54,-0.0013984589\H,5.6976677261,-1.3063586003,0.0042375018\H,4.5841337
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Erp

\\C,4.5284986992,0.8756312969,-0.0286910058\C,3.9694853096,-
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,-2.1948789744,0.7981331483,0.1262179151\C,-3.8833679557,-1.3989919883
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\C,-4.4688645353,-0.0939561731,-0.0280904817\O,-0.1293806785,-3.041794
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Ltl

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,-4.5941174599,-0.1004187174,-0.0214151341\H,-4.7276355297,-2.25141736
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MIv

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Plg

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Pnd

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Ptn

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Rsn

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6Dlp

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Mono-anionic species

Arn

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Cpn

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\O,-0.719083111,0.6265141415,-0.0133522763\O,5.4818720674,0.5095501119
, -0.1531974844\O,-4.8722568694,-1.6103669834,-0.1532840828\O,-4.681911
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58\O,3.7805126939,2.566352997,-0.2870136567\C,2.8678317553,3.661149955
, -0.3573003308\H,2.2483315969,3.5892470391,-1.2519813554\H,2.237856244
9,3.6952201618,0.5322604007\H,3.4799975317,4.5563234961,-0.4065975235\

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8,-0.1392888873\H,-6.6171696072,-2.6197887308,-0.2287712325\H,-6.66623
21606,-1.1653715449,0.7986673643\H,-6.6797124518,-1.0066462113,-0.9828
160143\C,5.076719532,-2.3315614218,1.3334694583\H,5.5124193895,-1.4191
049822,1.7397918314\H,4.2490378028,-2.6605629063,1.9631574663\H,5.8334
369831,-3.1098564518,1.2801532851\\

Cyn

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,0.1207181768\C,3.7125804813,1.7106429303,0.1007217633\H,2.1623719152,
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\H,1.7513851445,2.6396537844,0.1915018785\C,-0.4075598947,-0.657614744
4,-0.0122289238\C,0.2714915544,-1.8841190825,-0.0930431807\C,-1.813503
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51470282\C,-4.6055855793,0.1933848308,0.0792361575\H,-4.8539785864,-1.
8705997117,-0.4652052472\O,-0.4599201299,-3.038195635,-0.136026916\O,0
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Dlp

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,1.5658400994,-0.2018551579,0.000021977\C,2.5940110398,-1.1744881113,0
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Erp

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823\C,-2.2141694439,0.8296120602,0.0792174586\C,-3.9321512312,-1.34019
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Ltl

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Mlv

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725909131,-2.7631230963,-0.7977976082\C,-2.2975835042,-1.8328642836,-0
.5093708092\H,-2.5512664212,2.4746985448,0.8702796723\C,-0.2774059374,
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3\C,1.1532310121,-0.2773031921,-0.1650100867\C,2.1069037044,-1.2694479
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8\O,5.189467848,0.6781310374,-0.0730149546\O,-5.1195481851,-1.92297666
45,-0.4395736458\O,-5.1626978024,2.5742758671,0.9929507136\H,-6.276360
1118,0.3310416324,0.3173426339\O,3.422684759,2.6188714024,-0.505747755
9\C,2.4975118041,3.6932013336,-0.7143848782\H,1.9203857335,3.523482604
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\C,4.7789787793,-2.0389954533,1.6736609644\H,5.1672817749,-1.092320194
2,2.0481035953\H,3.9127302477,-2.3478877183,2.2587795973\H,5.550500748
7,-2.8019761315,1.716779353\H,5.294693222,1.6259219444,-0.2330546153\H
,-0.7055974309,-3.5327282369,-1.2335951591\\

Plg

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965141\C,-4.707734565,-0.6136923599,0.056767645\H,-5.0601304118,1.3016
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11308239,-0.2070913537\O,4.3932923335,-2.7847995641,0.2549996367\H,5.4
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Pnd

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587405,-0.0514004222\C,0.6341445476,-1.9338943843,0.1986865207\C,-1.55
49013535,-0.6848594785,-0.1232597279\C,-2.3702817088,-1.7515605337,-0.
5011521535\C,-2.1346047681,0.5594947376,0.1781725063\C,-3.7484776169,-
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\C,-3.5057213251,0.7150262235,0.11590446\H,-1.5064259085,1.386845333,0
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8\O,0.5407869589,0.3747452874,-0.2364998274\O,-5.6731057975,-0.2140461
099,-0.3224958149\O,4.8580704027,-1.574191424,0.3557099809\O,4.3867404
538,3.0513590942,-0.4579533381\H,5.747608762,0.8882889087,-0.016228402
7\O,-4.1824394231,1.8656449225,0.3945644778\C,-3.4043072166,3.02205251
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73\H,-5.8969771309,0.6953349513,-0.0831858867\H,0.6668299442,-3.797923
1093,0.6528036327\

Ptn

\C,-5.08004244,0.15635826,0.0494410649\C,-4.303337
5964,-1.0198199754,-0.0215176369\C,-2.8609186412,-0.8262600277,-0.0192
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, -6.158623944,0.0788587954,0.0501244431\O,3.107099693,3.2392091824,-0.
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Rsn

\C,4.3959799611,0.0512584505,0.0000569893\C,3.72990
68547,-1.1497152067,0.0000613016\C,2.3123311172,-1.1988283561,0.000013

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401,-3.3549455057,0.0000298006\C,1.5207946176,-2.3766319392,-0.0000135
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63014791,-0.7368815313,0.0000370713\C,-2.8736762176,-1.7347804742,-0.0
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,-2.1665444891,-0.000392336\O,-0.5791075515,-3.4375858362,-0.000136587
7\O,0.3021365256,0.047083292,-0.0000635818\O,-5.8725348512,0.280307471
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6Dlp

\C,-4.4616488749,0.3500303634,-0.0047783122\C,-3.7476876
578,-0.8286813559,-0.0144048072\C,-2.3405139747,-0.7979536176,-0.01023
64393\C,-1.714597602,0.4475724142,0.0036138869\C,-2.4057807602,1.64755
5634,0.0136107124\C,-3.7870383383,1.5816380303,0.0091992816\H,-1.96611
68155,-2.9359703248,-0.0296164001\C,-1.517378732,-1.9511641619,-0.0191
244291\H,-1.8863706812,2.5949789977,0.0243044412\C,0.4609163519,-0.557
8155803,-0.000889747\C,-0.1597854102,-1.846852723,-0.0146361943\C,1.83
52548292,-0.2313625806,0.0051846461\C,2.8692255168,-1.2101102598,-0.00
20230586\C,2.201091391,1.1472055609,0.0189797764\C,4.1759783217,-0.820
9750624,0.0043162216\H,2.6476159341,-2.262269535,-0.0124980795\C,3.512
0990914,1.5112873008,0.024973699\H,1.4467722427,1.9189218606,0.0247273
227\C,4.5725452953,0.5500600508,0.0180874306\O,0.6468753413,-2.9389736
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9932,0.5053592856,0.007767044\O,5.7913311981,0.899710726,0.0238772525\
O,-4.3691681082,-2.0353143146,-0.0280015432\H,-5.3269474367,-1.9074093
133,-0.0285062038\O,-4.5888078966,2.6753451971,0.0177584267\H,-4.06197
06812,3.4842124906,0.028018809\O,-5.8266469409,0.2758481228,-0.0095103
402\H,-6.2009078785,1.1661957902,0.0002347599\O,3.8855533874,2.8301587
324,0.0381619224\H,4.8548466214,2.8403694141,0.040020572\O,5.188880099
2,-1.7496815602,-0.0023745221\H,6.0190879657,-1.2498287332,0.0038468877\

Di-anionic species

Arn

\C,3.9888787343,-0.3676350464,0.00

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464845,-0.0026748874\C,1.2583136096,-0.5062582095,0.0015589086\C,1.957
941577,-1.7040754742,0.0053073539\C,3.3614476521,-1.6675349448,0.00507
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09962,0.5090500901,-0.0003861588\C,-0.3621952366,1.8272958364,-0.02332
04102\C,-2.3041845975,0.1422238014,-0.0053354885\C,-3.345651888,1.0700
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647069514,0.6779926062,0.2507222371\H,-3.0949203412,2.1025306854,0.405
2573681\C,-3.9956438202,-1.5995566464,-0.2097916222\H,-1.916720508,-1.
9476435637,-0.4068998515\C,-5.0583830393,-0.6743234741,0.0307886034\O,
-1.102530809,2.894171699,-0.061363157\O,-0.0922994654,-0.5603937334,0.
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.4410298026\O,5.3615625175,-0.3422955074,0.0001684464\H,4.8519931878,1
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Cpn

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.7861539507,-0.0935275841\H,-2.0871906476,2.7570678573,0.113261737\C,0
.0205521246,-0.5603297175,-0.0700972723\C,-0.6258447541,-1.8279338032,
-0.1072423111\C,1.4335280225,-0.2947040245,-0.0959006017\C,2.393049034
5,-1.3222588079,-0.12875682\C,1.8984922086,1.0468926388,-0.0904782223\
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9,-0.1355474299\C,3.2411707757,1.3292458226,-0.1207374091\H,1.18164851
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3\O,0.0241954311,-2.9535709359,-0.1556459878\O,-0.7207199241,0.5723007
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8121,-1.7301053123,-0.0678870096\O,-4.725036293,3.0382540336,0.1588266
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,-0.1246429967\C,2.8247039556,3.6818519124,-0.0949004226\H,2.176680784
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,3.4202845038,4.5896291758,-0.105389949\O,4.65706298,-2.0662233179,-0.
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-2.7612168787,-0.1340275768\H,-6.6429974383,-1.2698438386,0.8345995825
\H,-6.6250440076,-1.1793779345,-0.9512754491\C,5.1445766906,-2.4247252
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Cyn

\C,4.5149679204,-0.5099909567,0.032252727\C,3.8960698476,0.7355939891,-0.0651
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69233,-1.7390346006,0.1556083281\H,2.1812261591,2.833128198,-0.2505251
891\C,1.6809018712,1.8783086073,-0.1362579599\H,1.8048572042,-2.630223
9619,0.2771784366\C,-0.3777750311,0.6502187782,0.0191826585\C,0.276800
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789\C,-2.7471790622,1.3747476467,0.3613425837\C,-2.2656053131,-0.91907
22734,-0.2408061949\C,-4.1012770158,1.0826914696,0.3976768013\H,-2.423
2812481,2.3730376588,0.6068630676\C,-3.6055272651,-1.1917552362,-0.211
9395402\H,-1.5736288263,-1.7097563501,-0.4943030253\C,-4.5924321085,-0
.2075394084,0.1075903359\H,-4.8146301333,1.854752404,0.6568832484\O,-0
.4476445144,3.012225108,-0.2511783621\O,0.3700349751,-0.4817992974,0.1
214712474\O,-5.838485665,-0.5530040975,0.1115743609\O,4.5204085236,1.8
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,3.7386904122,-0.4396642096\

Dlp

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0198348\H,2.3006918759,-2.8778783029,0.0000620968\C,1.8510918552,-1.89
14494805,0.00002719\H,2.2049825184,2.6196709142,-0.0000859697\C,-0.146
0987042,-0.5514990929,-0.0000322964\C,0.448680728,-1.7928241501,0.0000
008652\C,-1.5539157087,-0.2009698844,-0.0000282274\C,-2.5786341102,-1.
1685117281,-0.0000995597\C,-1.9135974599,1.1630140206,0.0000594095\C,-
3.8966797181,-0.7694666837,-0.0000806137\H,-2.3615742228,-2.2226137708
, -0.0001746757\C,-3.2393072826,1.5271515211,0.0000759315\H,-1.16242516
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, -0.3252137502,-2.9268114701,0.0000183285\O,0.6647977145,0.5415050435,
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, -2.0139619656,0.000088535\O,4.8248968366,2.7128767884,-0.0000383564\H
,5.8886539358,0.3411378392,0.0000494232\O,-3.6009350888,2.8576243592,0
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H,0.249129557,-3.7009870945,0.0000615304\

Erp

\C,4.5261547647,0.8841219156,-0.0008689011\C,3.9743273547,-0.3641726485,0.00
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86559285,2.077058282,-0.0015167849\H,2.4774271139,-2.6759306866,0.0016
850107\C,1.8969060226,-1.7623975812,0.001070376\H,1.6532306245,2.77935
91683,-0.0017459658\C,-0.233059216,-0.6772755817,0.0005007262\C,0.4956
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\O,0.4325501256,0.5043646685,-0.0001764364\O,-5.7759692311,0.044590822
1,-0.0017136453\O,4.6815932633,-1.5230600792,0.0006484585\O,4.26743497
8,3.2313151657,-0.0022268376\H,5.5963271589,1.0289592977,-0.0010774217
\O,-4.1698907993,2.2363567492,0.0033812181\C,-3.3104159117,3.374525439
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49,0.0002902065\H,6.4750338211,-2.4434310006,0.0008294418\H,6.45187235
19,-0.9032474566,-0.8943515538\H,6.4522404666,-0.9021837808,0.89417469
87\H,-5.6704069084,-2.0297665577,-0.0036971305\\

Ltl

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9\C,-0.2950718148,-1.9750093804,-0.0000085512\C,1.7695005747,-0.519707
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3812801,-0.0000029654\H,1.6081344473,1.6511902879,-0.0000165348\C,4.58
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018647,-0.000012379\H,5.1080326839,2.1645618996,0.0000241078\\

Mlv

\\C,-5.2249144748,0.3668535769,0.1
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C,-3.1130066043,1.6358872114,0.2715281308\C,-4.5529321354,1.6124556652
,0.3053359954\H,-2.7915818519,-2.8606972802,-0.4608948349\C,-2.3189648
781,-1.8971105813,-0.3072490376\H,-2.5840620855,2.5688840508,0.4022809
909\C,-0.2994527938,-0.6050184511,-0.1499949763\C,-0.9190234895,-1.819
1593655,-0.3471000792\C,1.1127382724,-0.2947110734,-0.1464231479\C,2.1
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99696626,1.824361514,-0.337361865\C,3.8952461413,0.4111649034,-0.10309

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1849,-0.3347600336\C,2.3496479896,3.7118187171,-0.4961446709\H,1.76164
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,-1.172570758,1.8638693724\H,3.9910989821,-2.4445777484,2.0840295549\H
,5.60625304,-2.8644552643,1.4576356027\H,-0.7471768322,-3.6735189218,-
0.810491391\\

Plg

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0775069,0.6525648461,0.3930416982\H,-2.7121959222,2.0133442243,0.71791
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\O,4.2589501313,1.9476247224,-0.0684853398\O,4.4306386328,-2.776136023
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Pnd

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68612142,1.7551585178,-0.1464748105\C,3.8742236579,1.9077743286,-0.109
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74587865,0.0985349645\H,1.8124280852,2.6259248023,-0.2306120508\C,-0.0
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6,-0.5076449802\C,-3.4561597423,0.7414164014,0.0682551501\H,-1.4449741
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31601,0.0301038545\O,-4.1064864596,1.9287212858,0.2569671565\C,-3.3070
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3921\H,-2.6209567808,3.289106799,-0.2561135773\H,-4.0047812815,3.89722
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Ptn

\C,-5.0334953308,0.1344786512,0.
0336195133\C,-4.2548879092,-1.0366875864,-0.0023700719\C,-2.8096819043
, -0.8462928193,-0.0057170235\C,-2.291602843,0.4541115781,0.0286435061\
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,0.0672521188\H,-2.2875643624,-2.920087356,-0.0757073504\C,-1.90266065
68,-1.908522776,-0.0428062002\H,-2.6322893757,2.5865563738,0.094665836
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6Dlp

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