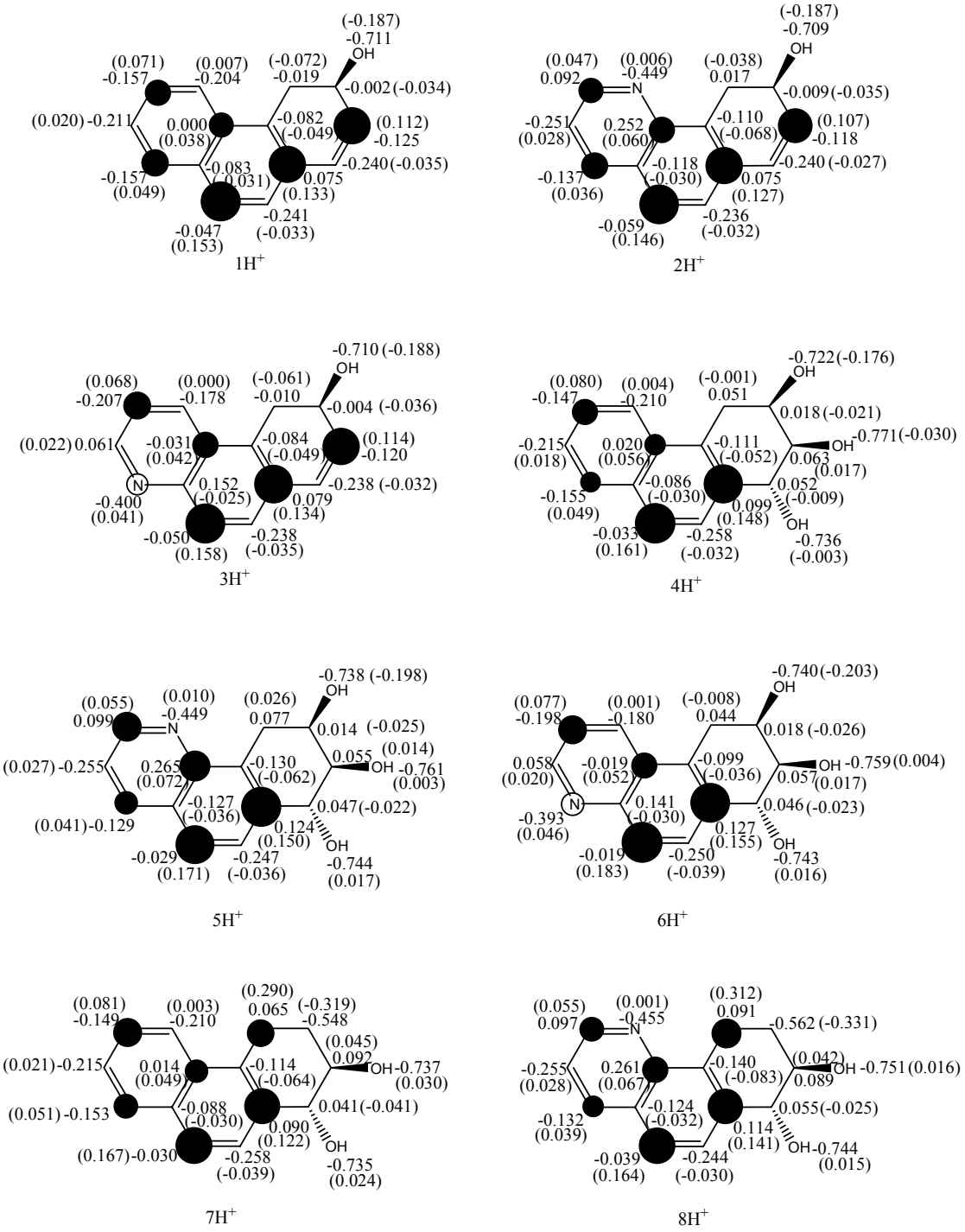
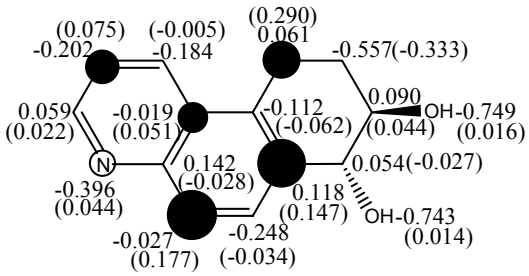
Electronic Supplementary Material for Organic & Biomolecular Chemistry

Theoretical (DFT, GIAO, NICS, AM1) Study of Aza-Polycyclic Aromatic Hydrocarbons (Aza-PAHs), Modeling Carbocations from Oxidized Metabolites and Covalent Adducts with Representative Nucleophiles

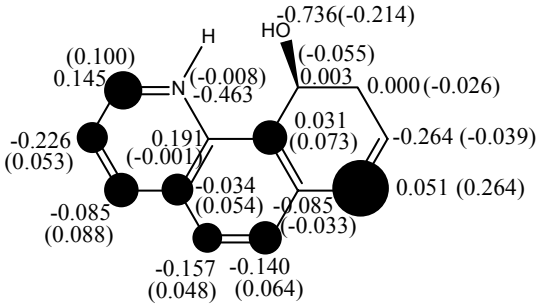
Gabriela L. Borosky and Kenneth K. Laali

Figure S1. Computed NPA-derived heavy atom charges (Δcharges related to the neutral compound in parentheses). *[Dark circles are roughly proportional to the magnitude of C Δcharges, and white circles to N Δcharges; threshold was set to 0.030].*

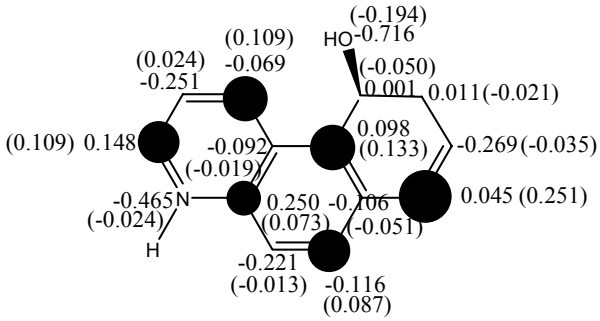




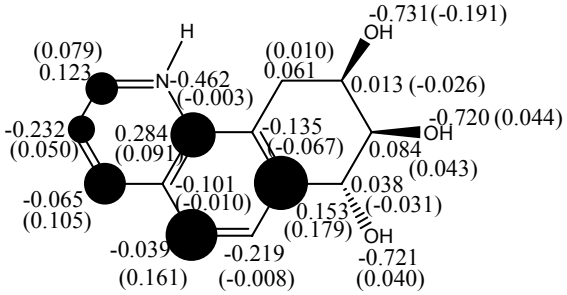
$9H^{+}$



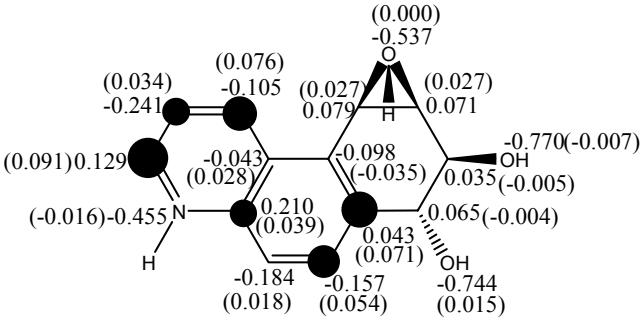
$2H_2^{2+}$



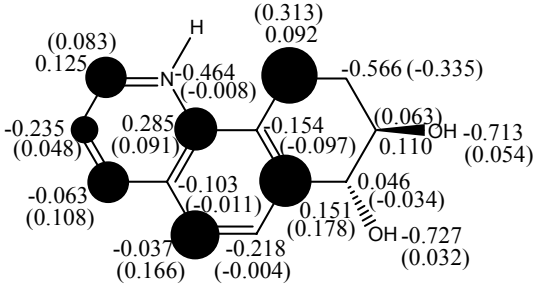
$3H_2^{2+}$



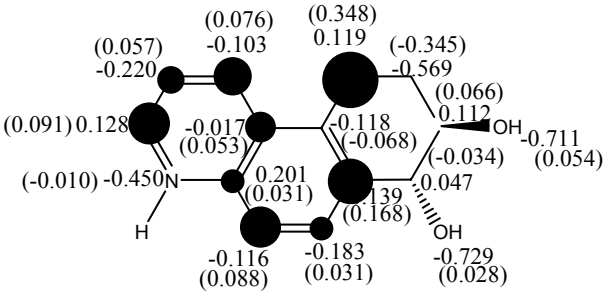
$5H_2^{2+}$



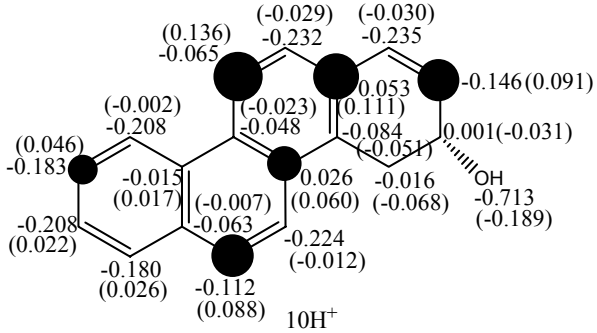
$6H_2^{2+}$



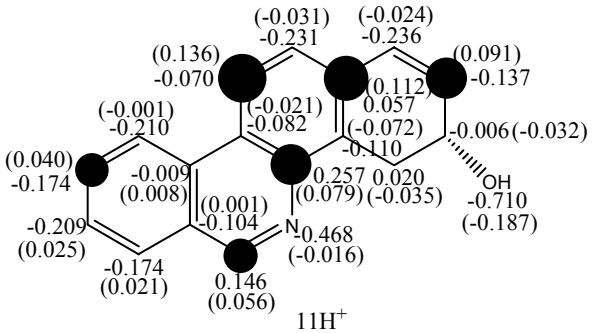
$8H_2^{2+}$



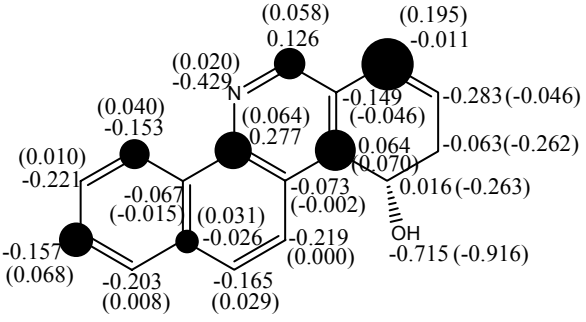
$9H_2^{2+}$



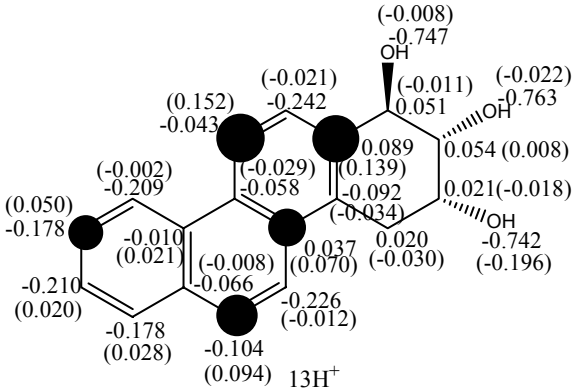
$10H^{+}$



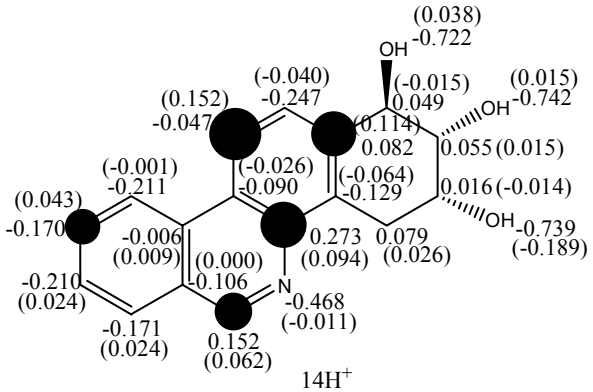
11H+



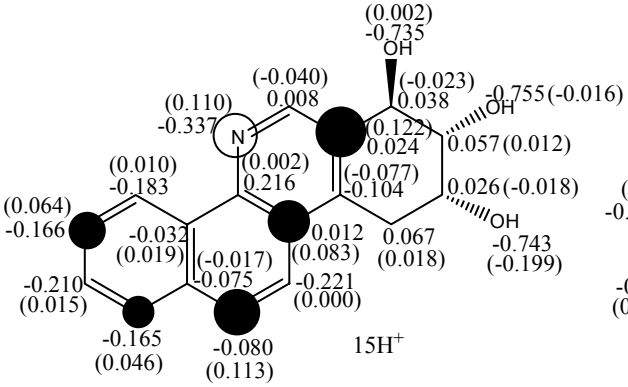
12H+



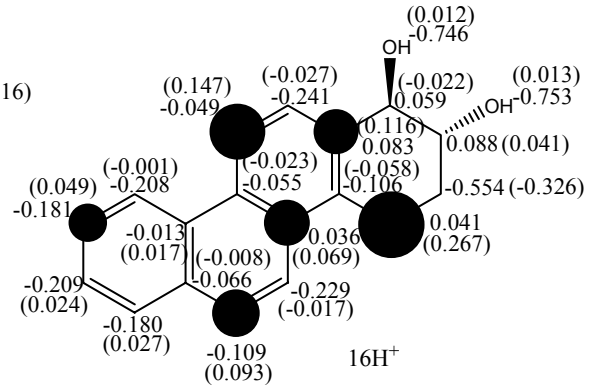
13H+



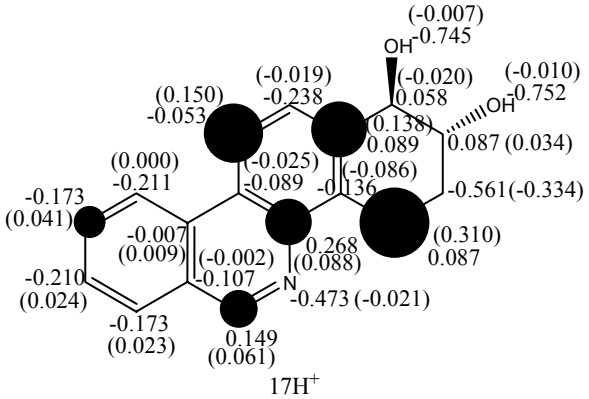
14H+



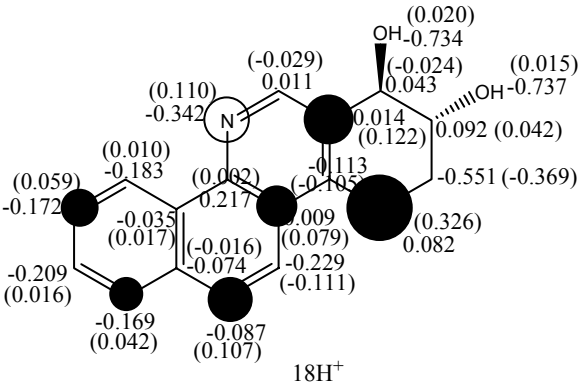
15H+



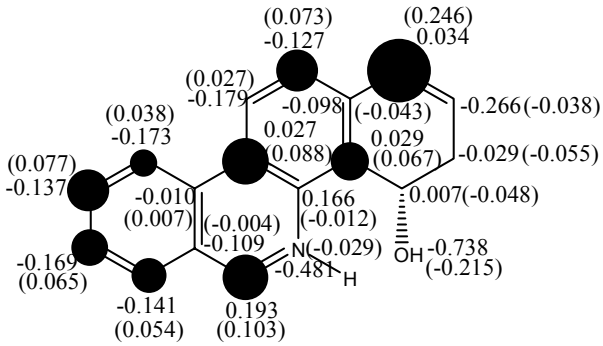
16H+



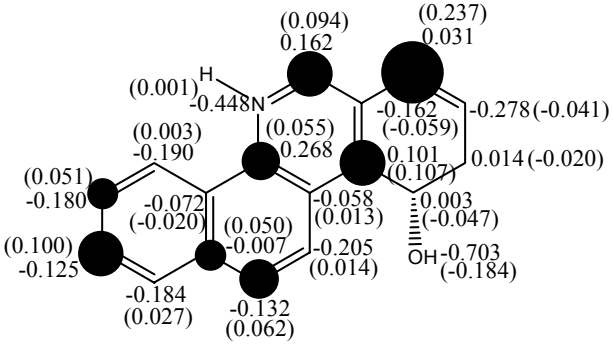
17H+



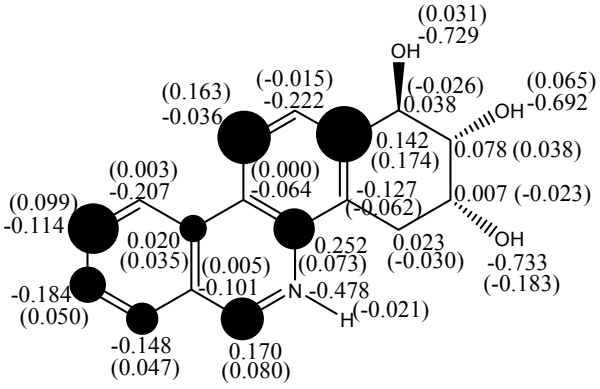
18H+



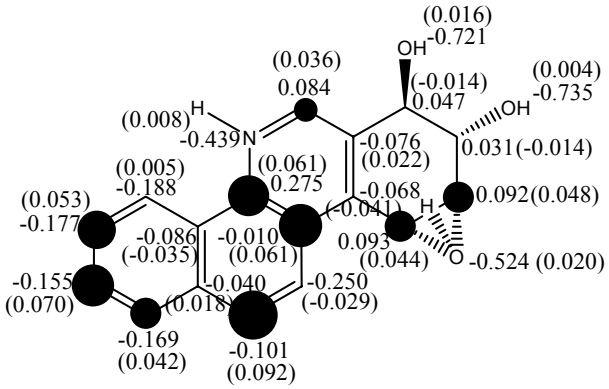
$11H_2^{2+}$



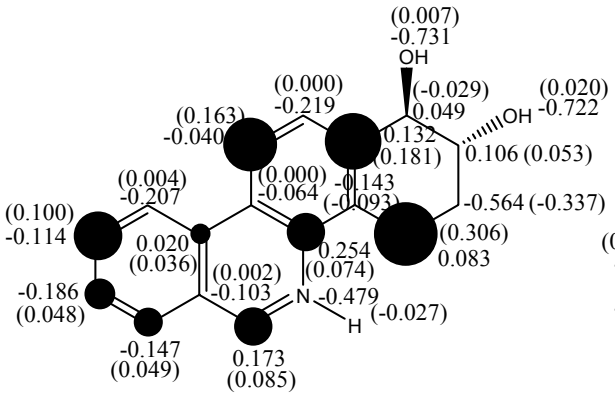
$12H_2^{2+}$



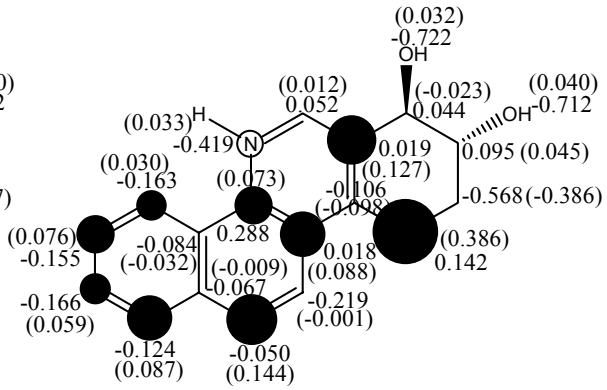
$14H_2^{2+}$



$15H_2^{2+}$

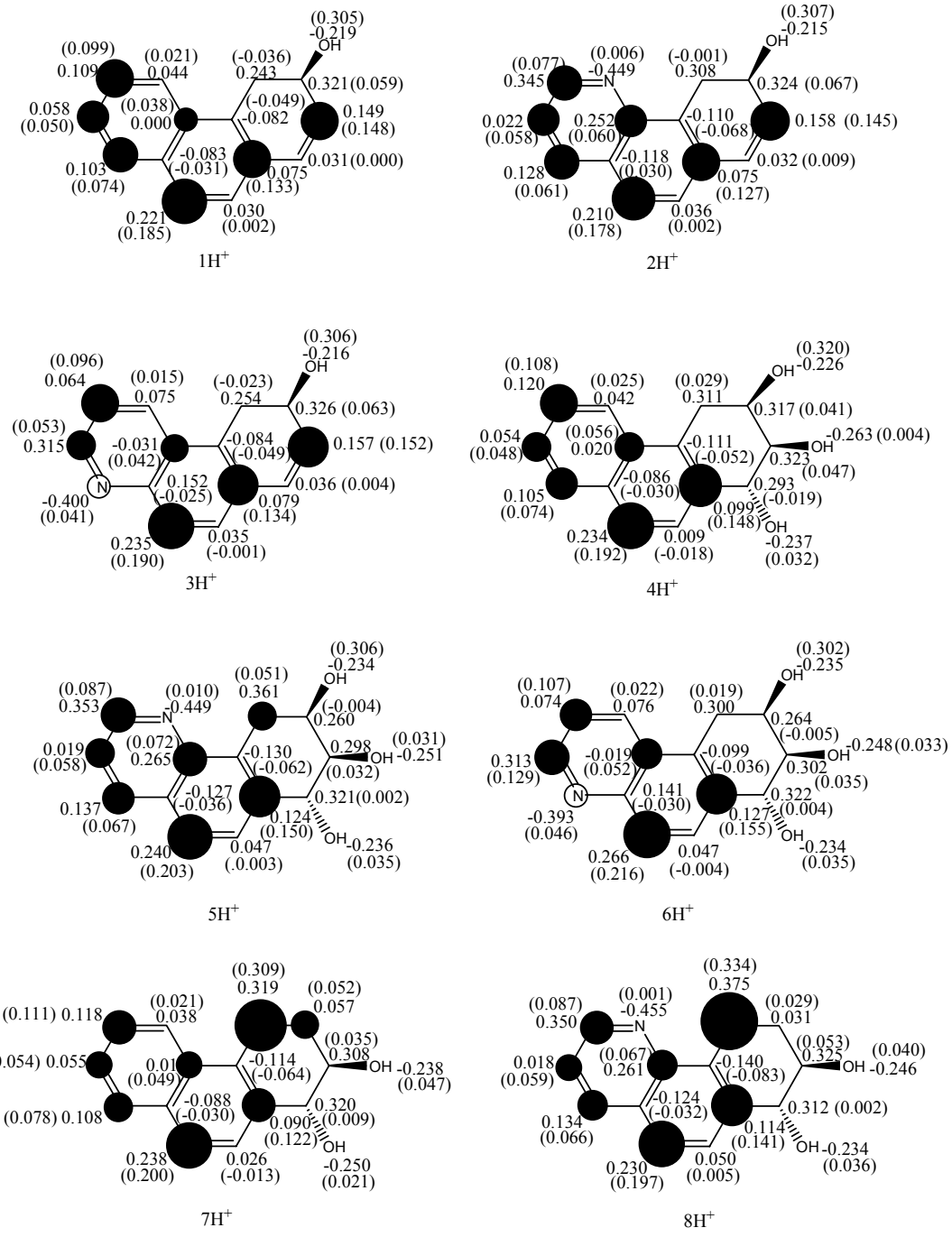


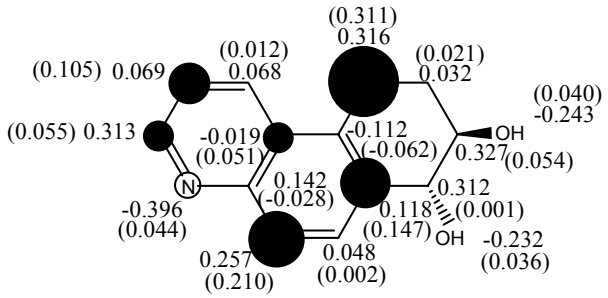
$17H_2^{2+}$



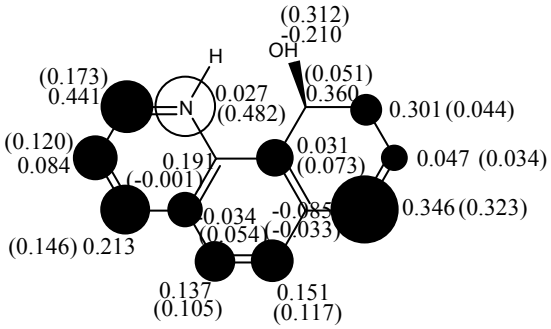
$18H_2^{2+}$

Figure S2. Computed NPA-derived overall charges over CH, NH and OH units (Δcharges related to the neutral compound in parentheses). *[Dark circles are roughly proportional to the magnitude of CH Δcharges, and white circles to NH Δcharges; threshold was set to 0.030]*.

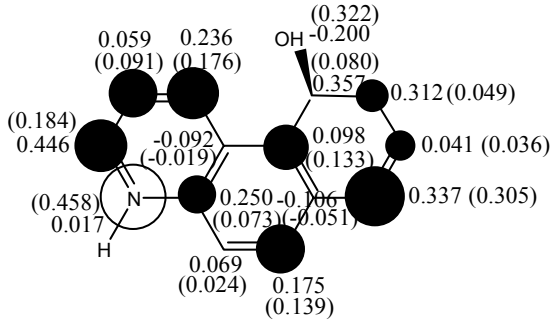




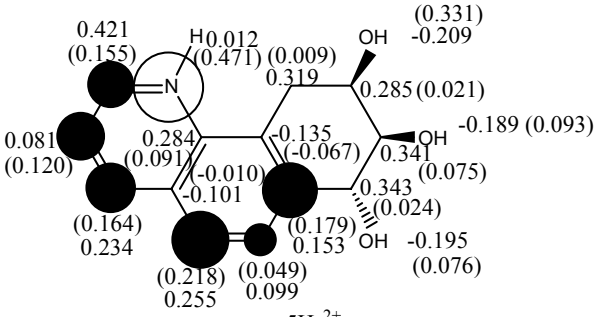
$9H^{+}$



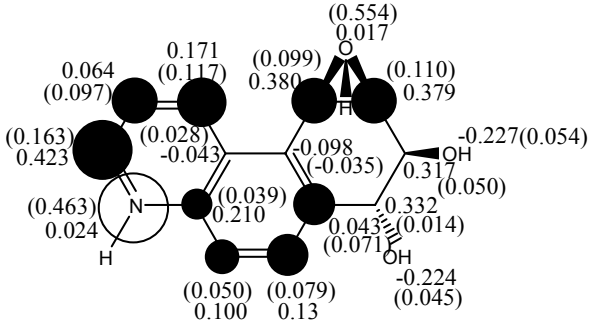
$2H_2^{2+}$



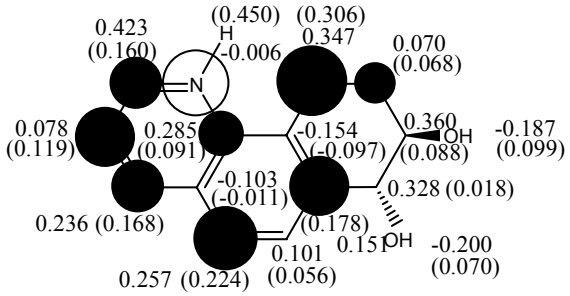
$3H_2^{2+}$



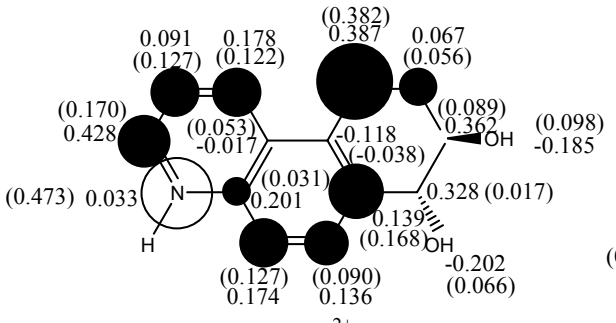
$5H_2^{2+}$



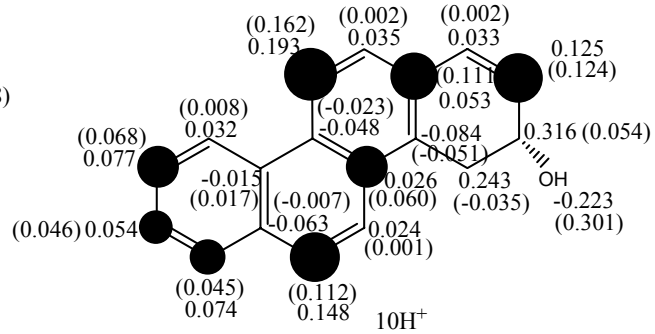
$6H_2^{2+}$



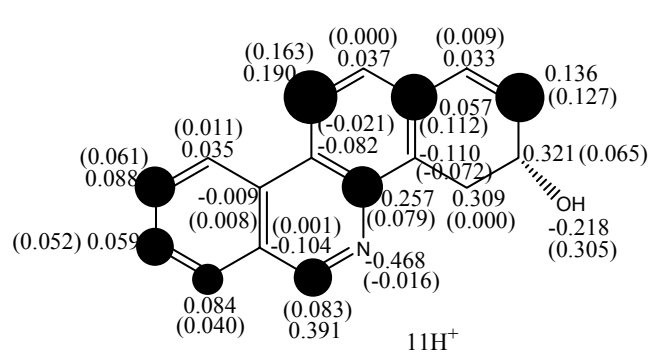
$8H_2^{2+}$

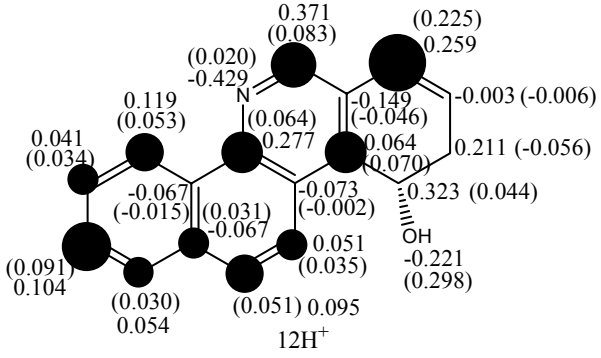


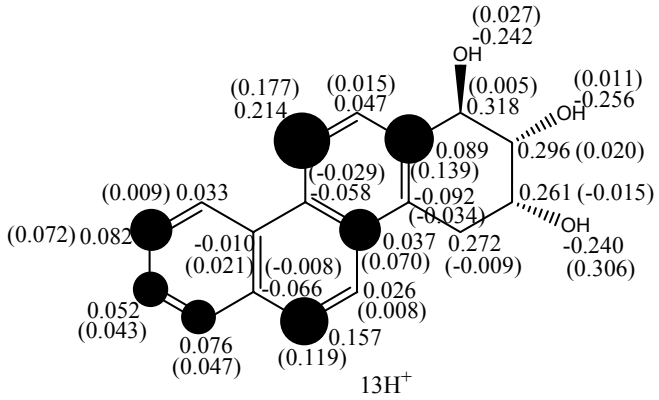
$9H_2^{2+}$

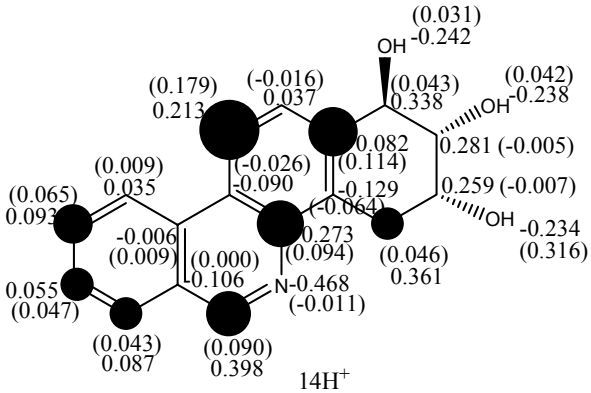


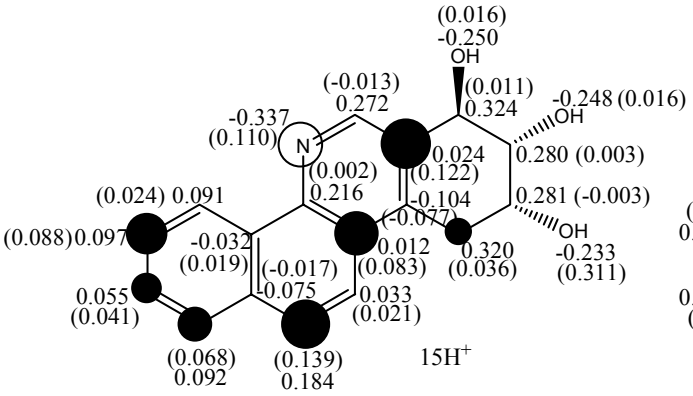
$10H^{+}$

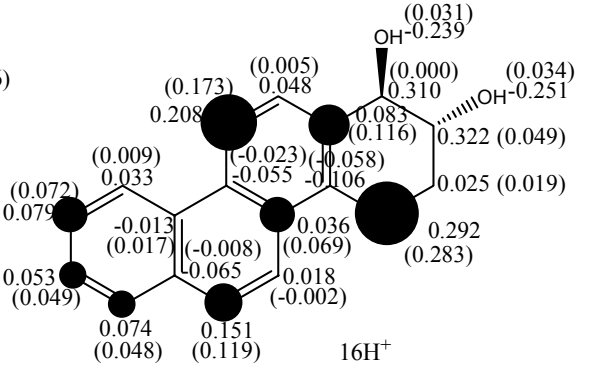

(0.163) 0.190
(0.000) 0.037
(0.009) 0.033
0.136 (0.127)
0.057
(-0.021) -0.082
(0.112) -0.110
(-0.072)
0.321 (0.065)
(0.011) 0.035
(0.061) 0.088
-0.009 (0.008)
(0.001) -0.104
N -0.468 (-0.016)
0.257 (0.079)
0.309 (0.000)
OH -0.218 (0.305)
(0.052) 0.059
0.084 (0.040)
(0.083) 0.391
11H+

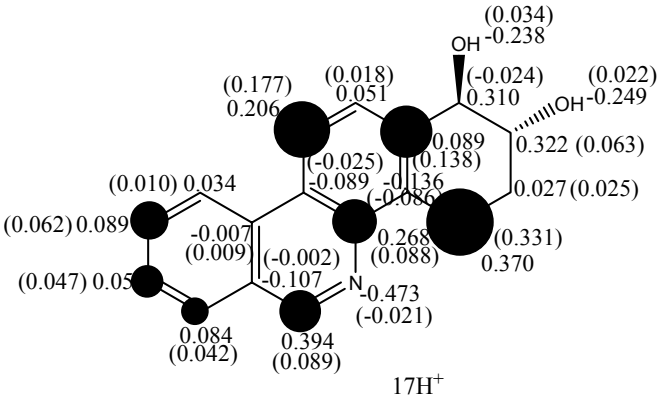

0.371 (0.083)
(0.225) 0.259
(0.020) -0.429
N
-0.149 (-0.046)
-0.003 (-0.006)
0.119 (0.053)
(0.064) 0.277
0.064 (0.070)
0.211 (-0.056)
0.041 (0.034)
-0.067 (-0.015)
(0.031) -0.067
-0.073 (-0.002)
-0.323 (0.044)
OH -0.221 (0.298)
0.051 (0.035)
(0.091) 0.104
(0.030) 0.054
(0.051) 0.095
12H+

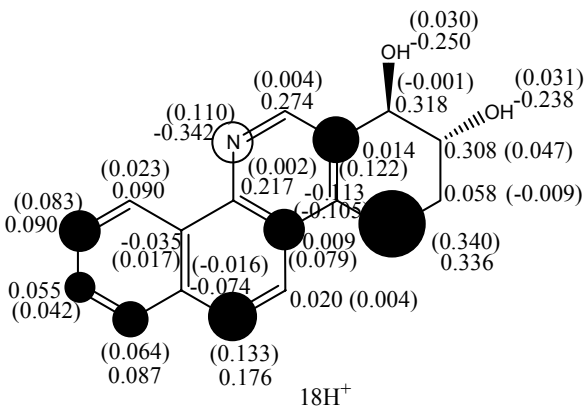

(0.027) -0.242
OH
(0.177) 0.214
(0.015) 0.047
(0.005) 0.318
(0.011) -0.256
OH
0.089 (0.139)
0.296 (0.020)
(-0.029) -0.058
-0.092 (-0.034)
0.261 (-0.015)
(0.009) 0.033
OH -0.240 (0.306)
(0.072) 0.082
-0.010 (0.021)
(-0.008) -0.066
0.037 (0.070)
0.272 (-0.009)
0.026 (0.008)
0.052 (0.043)
0.076 (0.047)
0.157 (0.119)
13H+

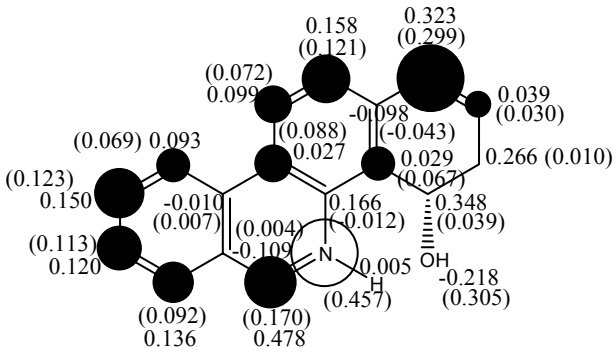

(0.031) -0.242
OH
(0.179) 0.213
(-0.016) 0.037
(0.043) 0.338
(0.042) -0.238
OH
0.082 (0.114)
0.281 (-0.005)
(0.009) 0.035
(-0.026) -0.090
-0.129 (-0.064)
0.259 (-0.007)
(0.065) 0.093
OH -0.234 (0.316)
-0.006 (0.009)
(0.000) -0.106
0.273 (0.094)
0.046 0.361
N -0.468 (-0.011)
0.055 (0.047)
(0.043) 0.087
(0.090) 0.398
14H+


(0.016) -0.250
OH
(-0.013) 0.272
(0.011) 0.324
-0.248 (0.016)
OH
-0.337 (0.110)
N
0.024 (0.122)
0.280 (0.003)
(0.002) 0.216
-0.104 (-0.077)
0.281 (-0.003)
(0.024) 0.091
OH
(0.088) 0.097
-0.032 (0.019)
(-0.017) -0.075
0.012 (0.083)
0.320 (0.036)
-0.233 (0.311)
0.055 (0.041)
0.033 (0.021)
(0.068) 0.092
(0.139) 0.184
15H+

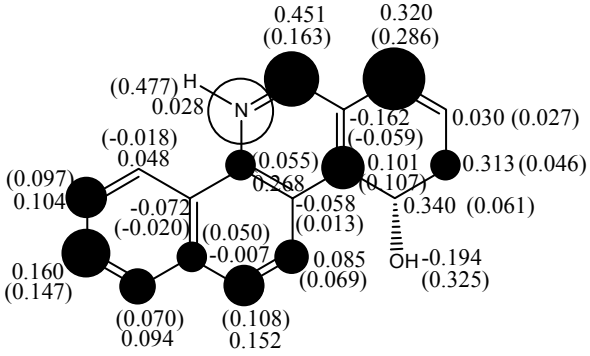

(0.031) -0.239
OH
(0.005) 0.048
(0.000) 0.310
(0.034) -0.251
OH
(0.173) 0.208
0.083 (0.116)
0.322 (0.049)
(0.009) 0.033
(-0.023) -0.055
(-0.058) -0.106
0.025 (0.019)
(0.072) 0.079
-0.013 (0.017)
(-0.008) -0.065
0.036 (0.069)
0.292 (0.283)
0.053 (0.049)
0.018 (-0.002)
0.074 (0.048)
0.151 (0.119)
16H+


(0.034) -0.238
OH
(0.177) 0.206
(0.018) 0.051
(-0.024) 0.310
(0.022) -0.249
OH
0.089 (0.138)
0.322 (0.063)
(-0.025) -0.089
-0.136 (-0.086)
0.027 (0.025)
(0.010) 0.034
(0.062) 0.089
-0.007 (0.009)
(-0.002) -0.107
0.268 (0.088)
(0.331) 0.370
N -0.473 (-0.021)
(0.047) 0.05
0.084 (0.042)
0.394 (0.089)
17H+

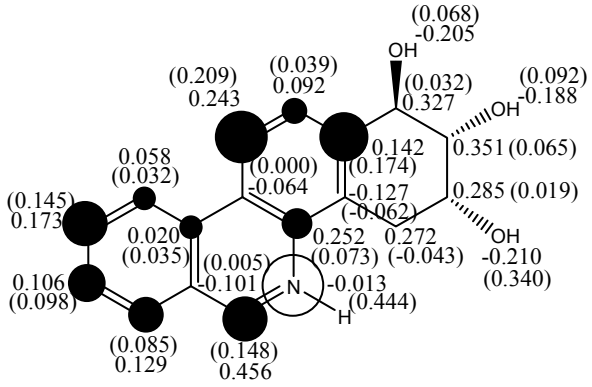

(0.030) -0.250
OH
(0.004) 0.274
(-0.001) 0.318
(0.031) -0.238
OH
(0.110) -0.342
N
0.014 (0.122)
0.308 (0.047)
(0.023) 0.090
(0.002) 0.217
-0.113 (-0.105)
0.058 (-0.009)
(0.083) 0.090
-0.035 (0.017)
(-0.016) -0.074
0.009 (0.079)
(0.340) 0.336
0.055 (0.042)
0.020 (0.004)
(0.064) 0.087
(0.133) 0.176
18H+



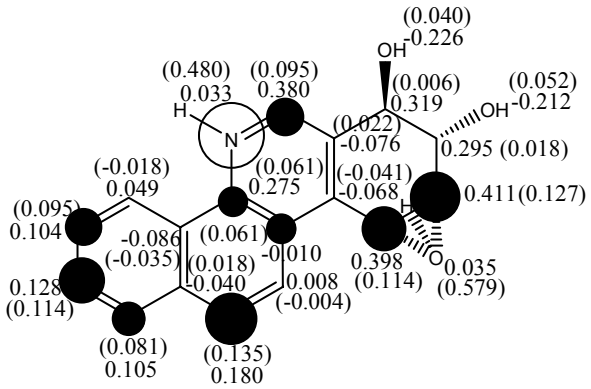
$11H_2^{2+}$



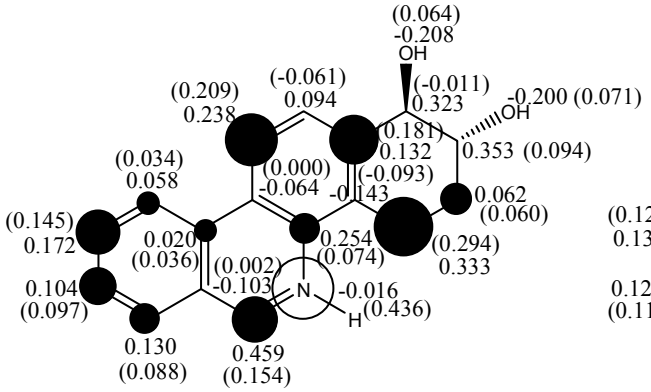
$12H_2^{2+}$



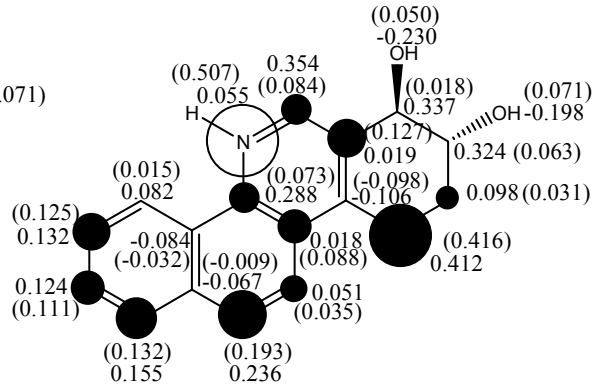
$14H_2^{2+}$



$15H_2^{2+}$

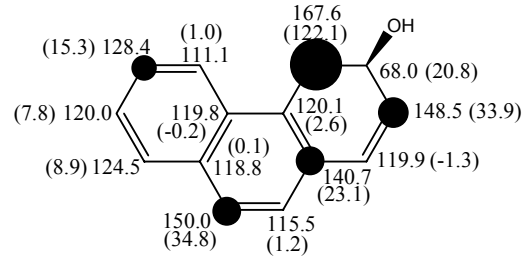


$17H_2^{2+}$

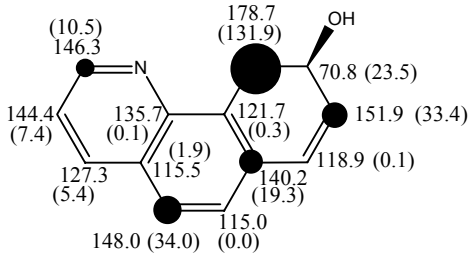


$18H_2^{2+}$

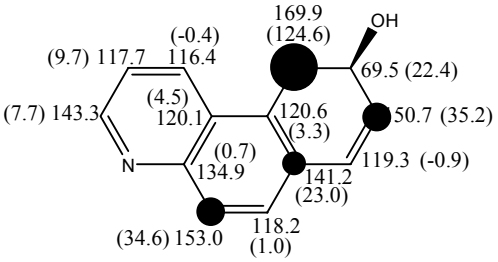
Figure S3. Computed ^{13}C NMR chemical shifts ($\Delta\delta$ ^{13}C's relative to the neutral compound in parentheses). *[Dark circles are roughly proportional to the magnitude of C $\Delta\delta$ ^{13}C; threshold was set to 10 ppm].*



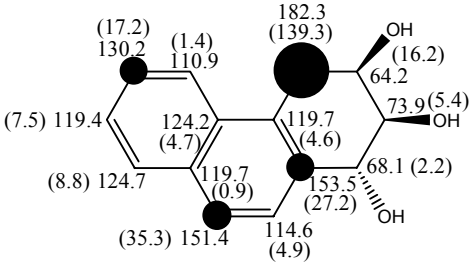
1H$^+$



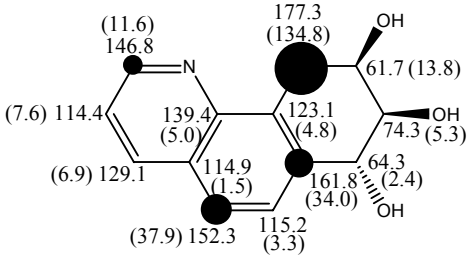
2H$^+$



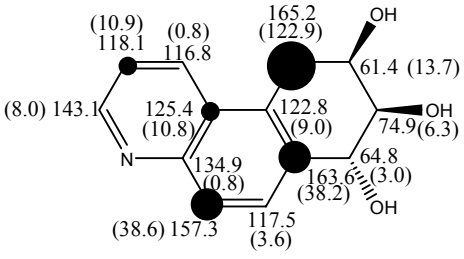
3H$^+$



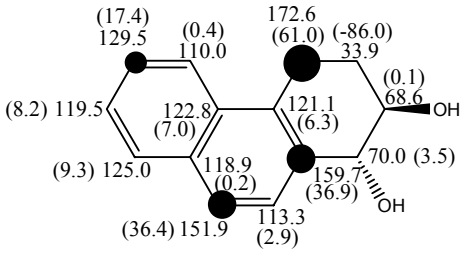
4H$^+$



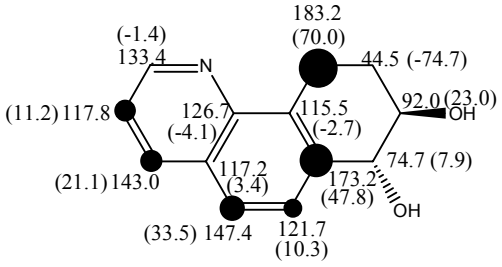
5H$^+$



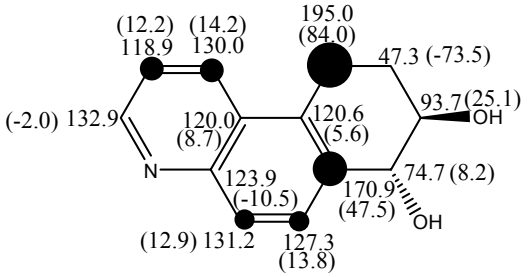
6H$^+$



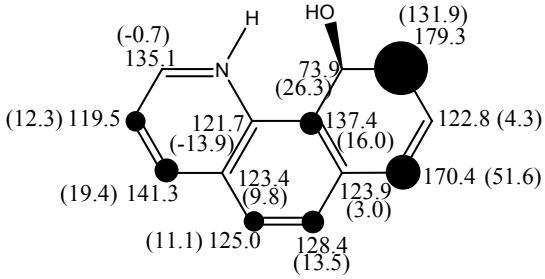
7H$^+$



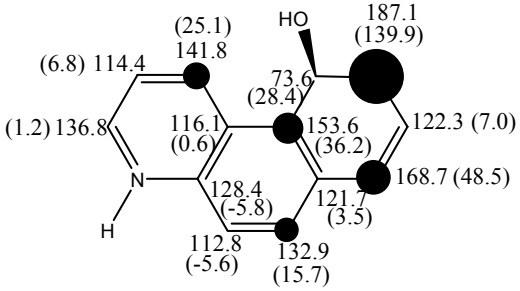
8H$^+$



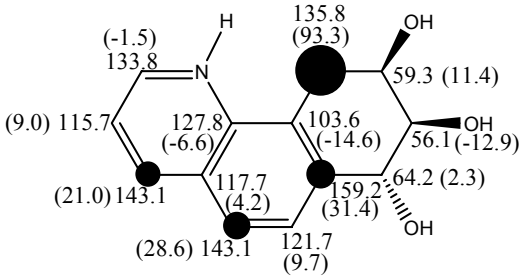
$9H^+$



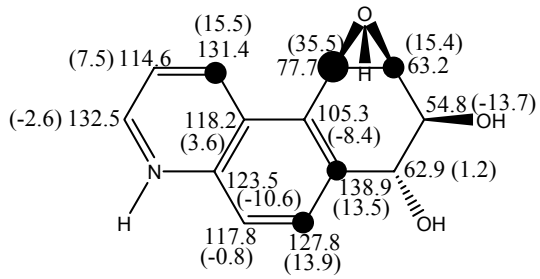
$2H_2^{2+}$



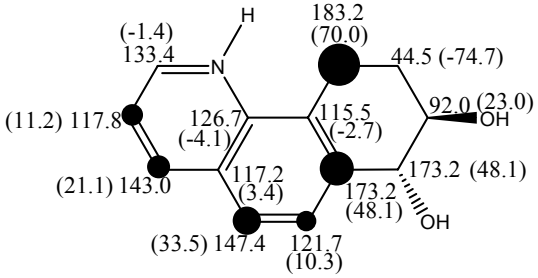
$3H_2^{2+}$



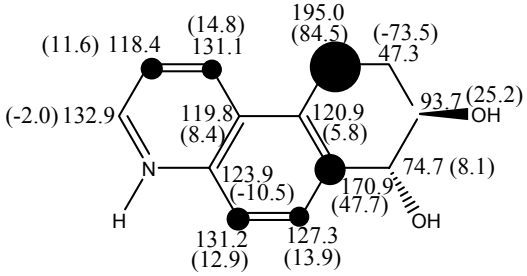
$5H_2^{2+}$



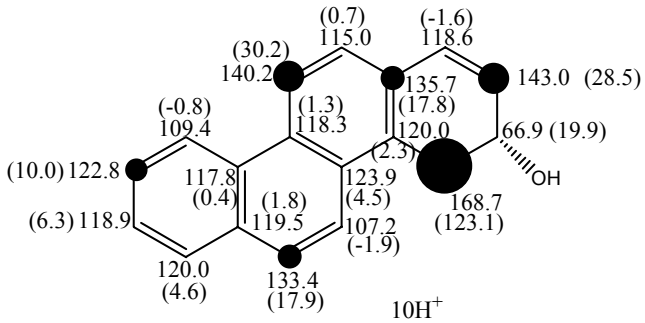
$6H_2^{2+}$



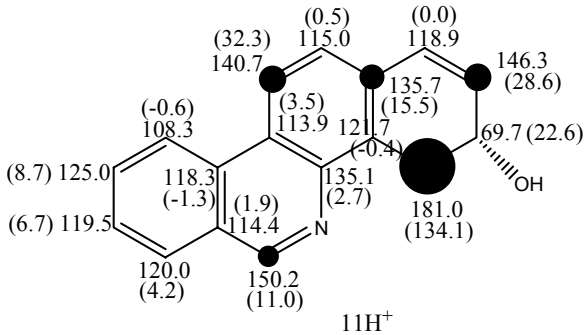
$8H_2^{2+}$



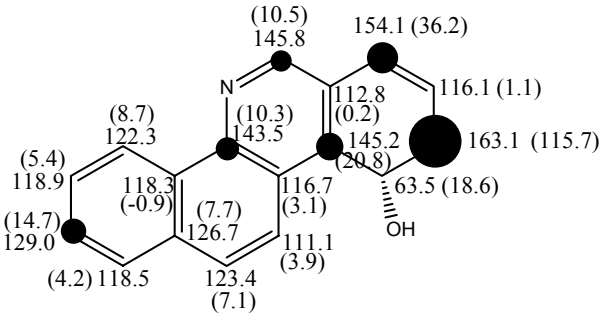
$9H_2^{2+}$



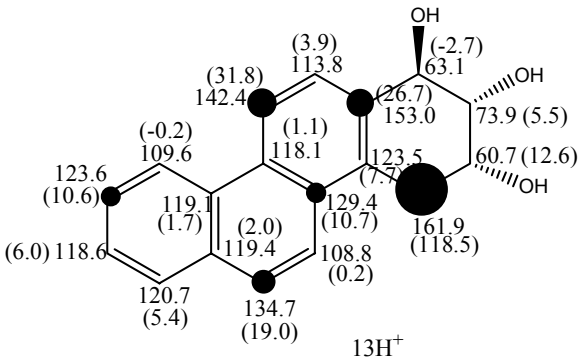
$10H^+$



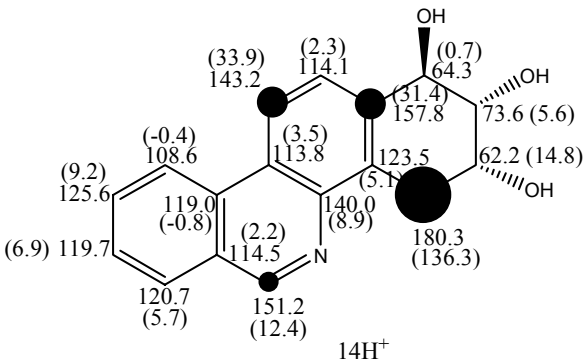
11H$^+$



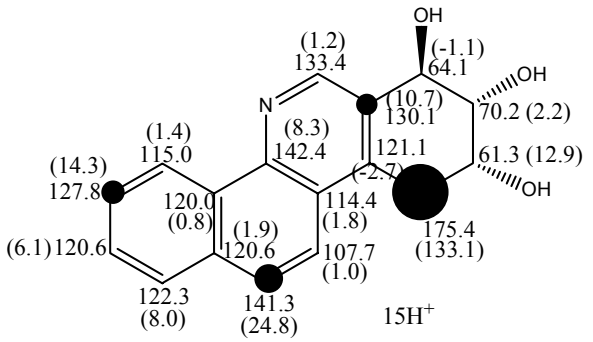
12H$^+$



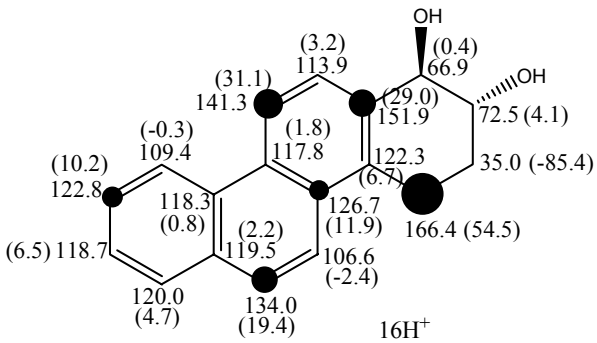
13H$^+$



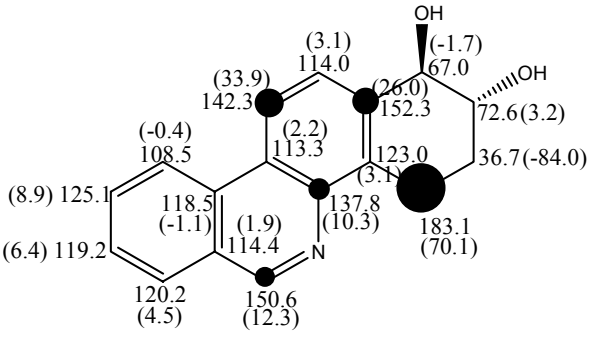
14H$^+$



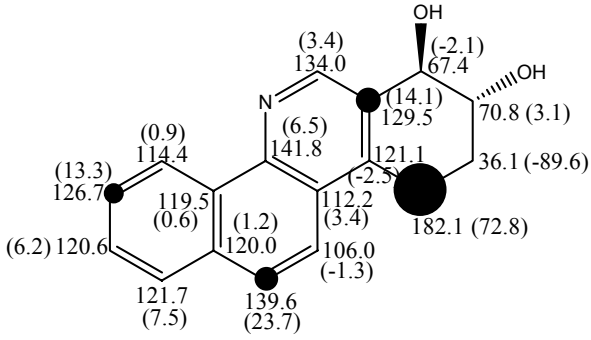
15H$^+$



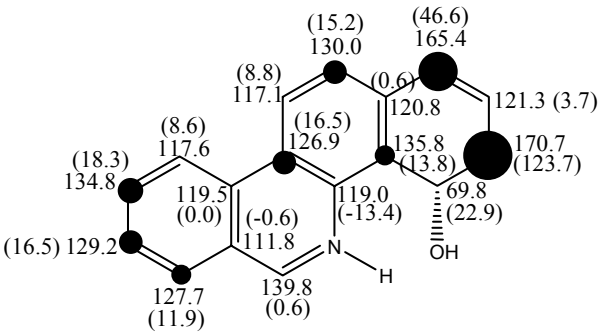
16H$^+$



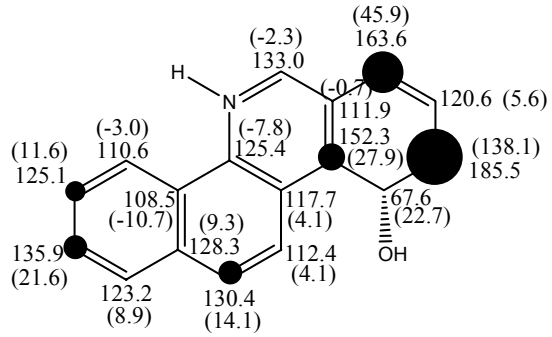
17H$^+$



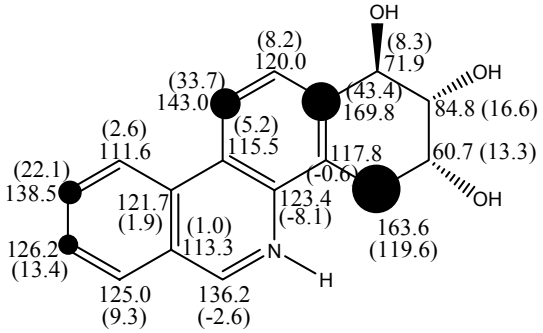
18H$^+$



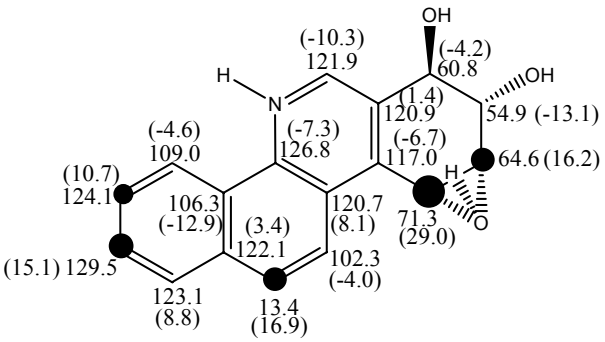
$11H_2^{2+}$



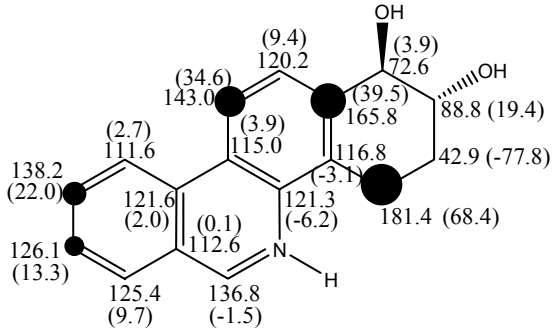
$12H_2^{2+}$



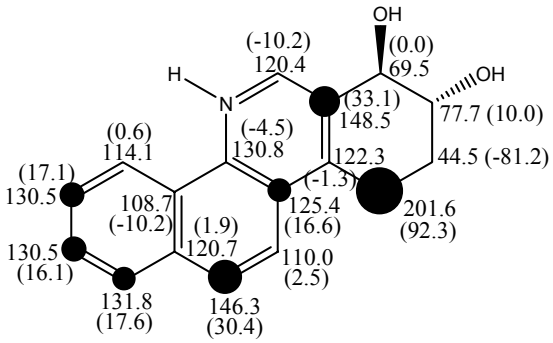
$14H_2^{2+}$



$15H_2^{2+}$

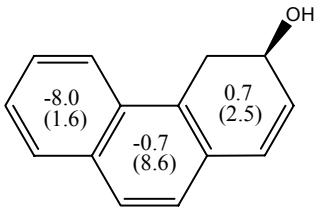


$17H_2^{2+}$

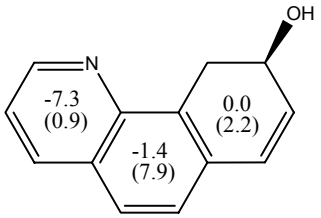


$18H_2^{2+}$

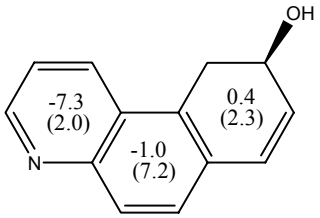
Figure S4. Computed NICS values (ΔNICS related to the neutral compound in parentheses).



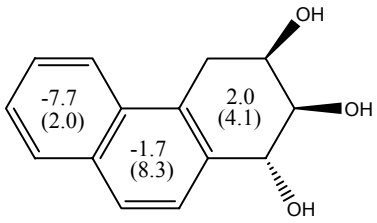
$1H^+$



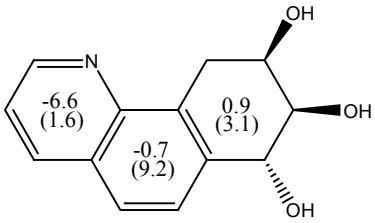
$2H^+$



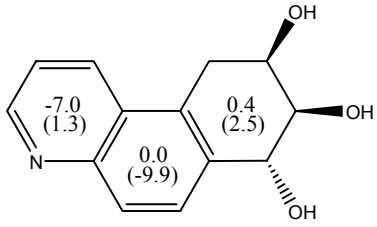
$3H^+$



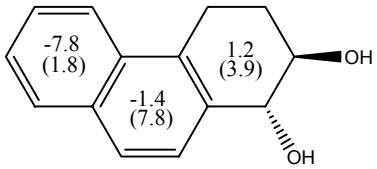
$4H^+$



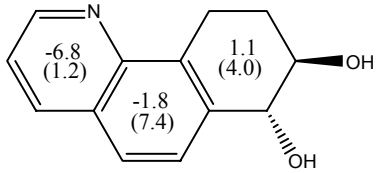
$5H^+$



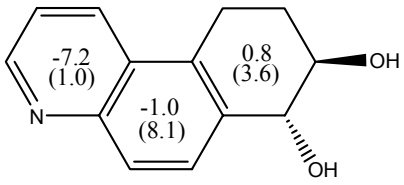
$6H^+$



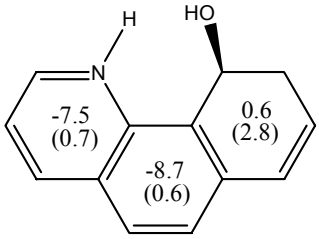
$7H^+$



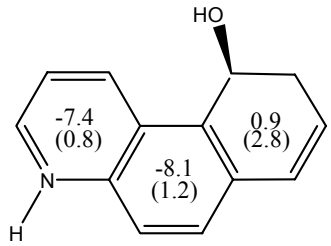
$8H^+$



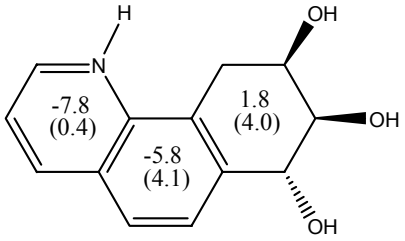
$9H^+$



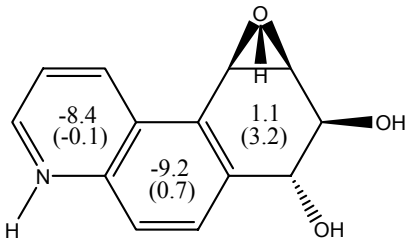
$2H_2^{2+}$



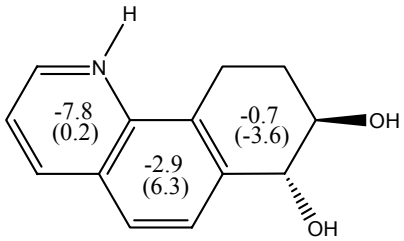
$3H_2^{2+}$



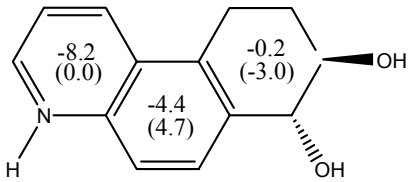
$5H_2^{2+}$



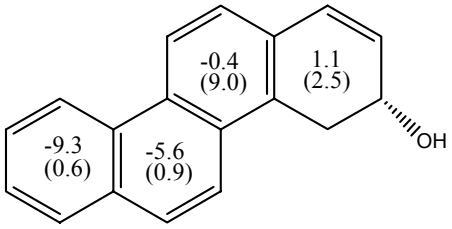
$6H_2^{2+}$



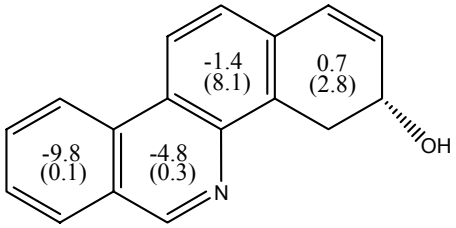
$8H_2^{2+}$



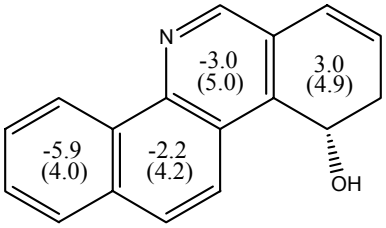
$9H_2^{2+}$



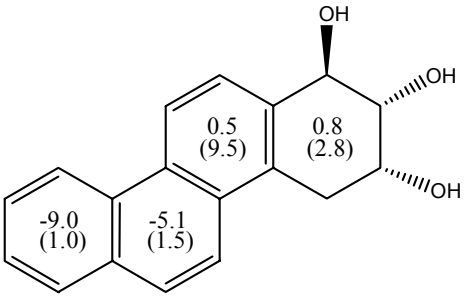
$10H^+$



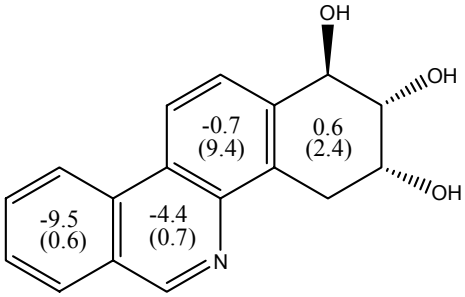
$11H^+$



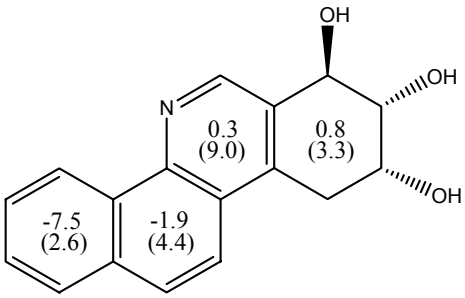
$12H^+$



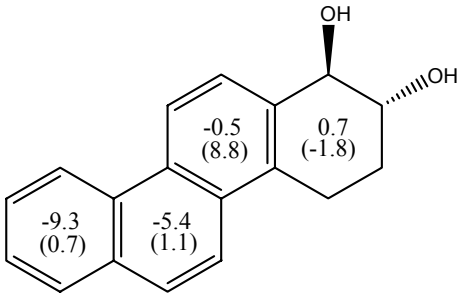
$13H^+$



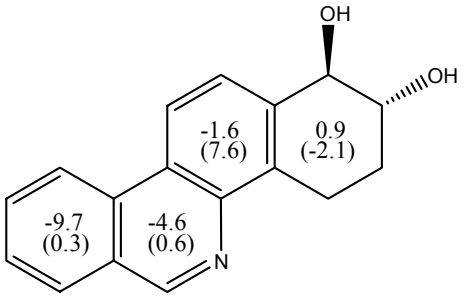
$14H^+$



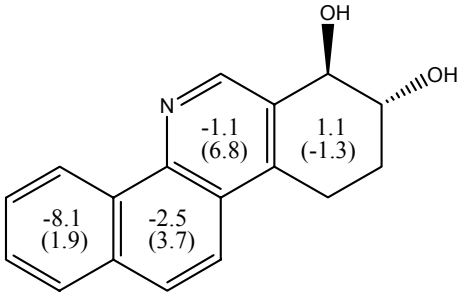
$15H^+$



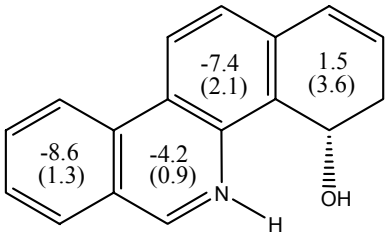
$16H^+$



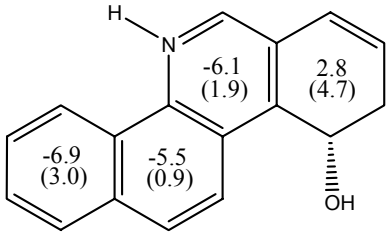
$17H^+$



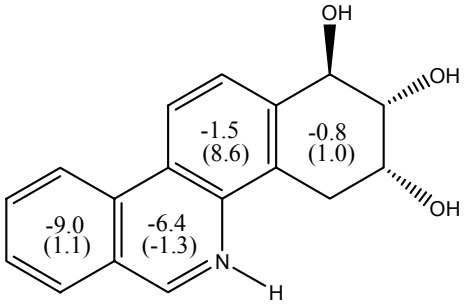
$18H^+$



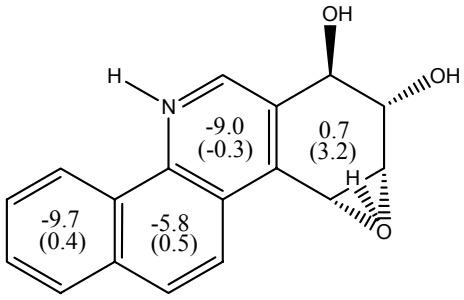
$11H_2^{2+}$



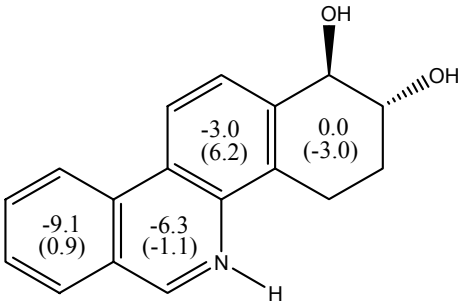
$12H_2^{2+}$



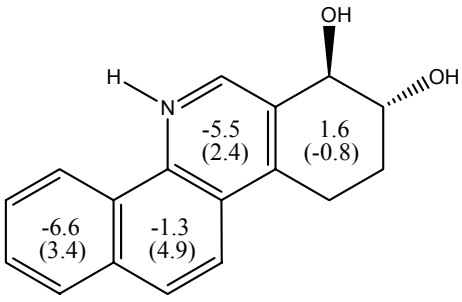
$14H_2^{2+}$



$15H_2^{2+}$

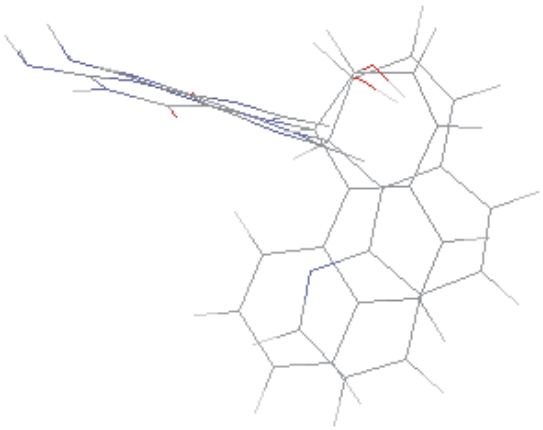


$17H_2^{2+}$

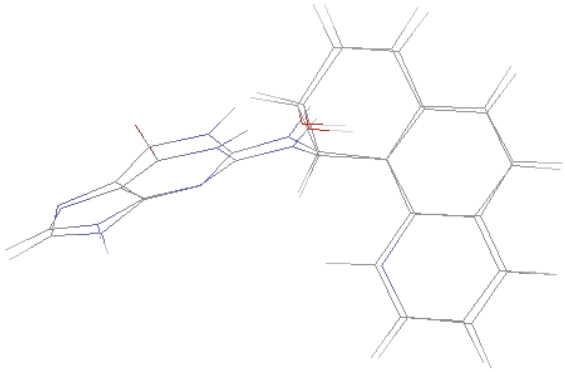


$18H_2^{2+}$

Figure S4. Superimposed structures of the adducts of **1H**$^+$ and **2H**$^+$ with guanine. (a) N-7 adduct. (b) Exocyclic N-adduct.



a



b

Table S1. Cartesian coordinates of the optimized structure for **1H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.911774	1.274140	-0.045865
2	6	0	-0.432625	-0.104167	-0.089540
3	6	0	1.013234	-0.371357	-0.043071
4	6	0	1.904872	0.743234	0.053457
5	6	0	1.372890	2.058116	0.088738
6	6	0	0.013023	2.321572	0.038880
7	6	0	3.305031	0.535711	0.101476
8	6	0	3.822707	-0.744299	0.051786
9	6	0	2.947555	-1.838794	-0.052287
10	6	0	1.568155	-1.656618	-0.103313
11	6	0	-1.372599	-1.098512	-0.123545
12	6	0	-2.836814	-0.850704	-0.273562
13	8	0	-3.640875	-1.790663	0.408800
14	1	0	-3.593608	-1.609483	1.362450
15	6	0	-3.248642	0.575443	-0.110205
16	6	0	-2.326674	1.560002	-0.047148
17	1	0	-0.341873	3.346640	0.073740
18	1	0	2.068717	2.890952	0.158380
19	1	0	3.962789	1.396847	0.177063
20	1	0	4.894930	-0.906119	0.088484
21	1	0	3.350324	-2.846048	-0.097784
22	1	0	0.935207	-2.532383	-0.196066
23	1	0	-1.097374	-2.148507	-0.090465
24	1	0	-3.016555	-1.070029	-1.350378
25	1	0	-4.315122	0.780726	-0.100125
26	1	0	-2.630462	2.600102	0.029502

Table S2. Cartesian coordinates of the optimized structure for **2H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.883294	1.300273	0.029172
2	6	0	-0.058616	2.342437	-0.043422
3	6	0	-1.414964	2.068758	-0.074551
4	6	0	-1.931069	0.742426	-0.041568
5	6	0	-1.023869	-0.350743	0.032799
6	6	0	0.413927	-0.070955	0.077413
7	6	0	1.328621	-1.090060	0.118850
8	6	0	2.788197	-0.843554	0.270095
9	8	0	3.613665	-1.806287	-0.343238
10	6	0	3.209430	0.579587	0.083240
11	6	0	2.298345	1.577642	0.020143
12	7	0	-1.424188	-1.629182	0.072362
13	6	0	-2.733087	-1.871311	0.036572
14	6	0	-3.719282	-0.865788	-0.033797
15	6	0	-3.316072	0.453190	-0.073769
16	1	0	3.562495	-1.697877	-1.307531
17	1	0	0.286062	3.370992	-0.078900
18	1	0	-2.120064	2.895140	-0.129269
19	1	0	-4.038347	1.262881	-0.130218
20	1	0	-4.769196	-1.137209	-0.056031
21	1	0	-3.024420	-2.918670	0.065763
22	1	0	0.989815	-2.122885	0.104073
23	1	0	2.931591	-1.015413	1.364112
24	1	0	4.278069	0.773017	0.065981
25	1	0	2.614858	2.613172	-0.065679

Table S3. Cartesian coordinates of the optimized structure for **3H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.887256	1.271497	-0.041503
2	6	0	0.052520	2.312539	0.038269
3	6	0	1.405691	2.036703	0.084889
4	6	0	1.917446	0.704008	0.050726
5	6	0	1.015436	-0.391659	-0.040070
6	6	0	-0.424134	-0.111233	-0.085100
7	6	0	-1.371530	-1.099699	-0.115321
8	6	0	-2.830930	-0.833756	-0.268064
9	8	0	-3.654913	-1.777333	0.378959
10	6	0	-3.229749	0.594732	-0.099314
11	6	0	-2.297314	1.571695	-0.039411
12	6	0	1.581825	-1.678135	-0.096202
13	6	0	2.958762	-1.808931	-0.045611
14	6	0	3.762554	-0.651483	0.053502
15	7	0	3.265119	0.572326	0.098572
16	1	0	-3.631473	-1.612899	1.336550
17	1	0	-0.293875	3.340676	0.071444
18	1	0	2.137393	2.836875	0.150813
19	1	0	0.964167	-2.566010	-0.182600
20	1	0	4.845676	-0.738285	0.094880
21	1	0	3.423678	-2.788704	-0.084607
22	1	0	-1.104990	-2.152292	-0.083692
23	1	0	-2.991019	-1.028545	-1.354630
24	1	0	-4.294343	0.809547	-0.088388
25	1	0	-2.591673	2.614360	0.037825

Table S4. Cartesian coordinates of the optimized structure for **4H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.563006	-1.100155	0.035986
2	6	0	0.015423	0.212578	0.197838
3	6	0	1.471396	0.381968	0.120420
4	6	0	2.266653	-0.769253	-0.198184
5	6	0	1.629894	-2.011668	-0.396961
6	6	0	0.247686	-2.179857	-0.273864
7	6	0	3.679150	-0.658164	-0.304606
8	6	0	4.297993	0.554812	-0.092158
9	6	0	3.517731	1.681314	0.233663
10	6	0	2.133614	1.598490	0.339768
11	6	0	-0.844741	1.278427	0.335024
12	6	0	-2.342375	1.199317	0.375329
13	6	0	-2.862442	-0.102861	-0.259259
14	8	0	-2.686777	0.049739	-1.663181
15	1	0	-3.409223	-0.395129	-2.131851
16	6	0	-2.051079	-1.292783	0.271576
17	8	0	-2.303318	-1.328280	1.673079
18	1	0	-1.990882	-2.170930	2.039552
19	8	0	-2.903672	2.331529	-0.241183
20	1	0	-0.188054	-3.163002	-0.426417
21	1	0	2.245557	-2.872470	-0.648224
22	1	0	4.259118	-1.542789	-0.551412
23	1	0	5.376361	0.645378	-0.169736
24	1	0	4.004663	2.635725	0.410114
25	1	0	1.580839	2.492163	0.607233
26	1	0	-0.462723	2.294540	0.391298
27	1	0	-2.637729	1.212074	1.434885
28	1	0	-3.915213	-0.239294	0.008538
29	1	0	-2.384839	-2.214836	-0.223091
30	1	0	-2.903123	2.141671	-1.198047

Table S5. Cartesian coordinates of the optimized structure for $\mathbf{5}^{+}$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.529541	0.899826	0.116178
2	6	0	0.188641	2.091040	0.154720
3	6	0	1.581792	2.068631	0.122328
4	6	0	2.329136	0.866437	0.039323
5	6	0	1.633849	-0.374758	-0.031823
6	6	0	0.164791	-0.359156	-0.016777
7	6	0	-0.539024	-1.520924	-0.197572
8	8	0	-2.429950	-1.916056	1.100496
9	6	0	-2.043175	-1.580067	-0.224285
10	6	0	-2.647405	-0.216716	-0.620250
11	8	0	-4.035974	-0.216514	-0.320983
12	1	0	-4.546587	-0.442843	-1.114356
13	6	0	-2.023579	0.895516	0.244299
14	8	0	-2.532518	2.164635	-0.074349
15	1	0	-3.490546	2.136370	0.085930
16	7	0	2.261407	-1.553838	-0.122202
17	6	0	3.593790	-1.550241	-0.132228
18	6	0	4.382090	-0.383277	-0.056392
19	6	0	3.745681	0.837409	0.025518
20	1	0	-0.348875	3.028935	0.225164
21	1	0	2.123958	3.010655	0.173537
22	1	0	4.307561	1.765809	0.078587
23	1	0	5.464000	-0.458670	-0.067902
24	1	0	4.070460	-2.525025	-0.205204
25	1	0	0.023192	-2.443625	-0.319250
26	1	0	-2.367407	-2.355827	-0.934823
27	1	0	-2.461568	0.004933	-1.678912
28	1	0	-2.244507	0.624177	1.292919
29	1	0	-3.394268	-1.766882	1.140180

Table S6. Cartesian coordinates of the optimized structure for **6H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.525854	0.871375	0.128010
2	6	0	0.193760	2.060643	0.137965
3	6	0	1.583325	2.032481	0.067938
4	6	0	2.324685	0.819548	0.000978
5	6	0	1.631479	-0.422541	-0.022532
6	6	0	0.160802	-0.400433	-0.018242
7	6	0	-0.581214	-1.527303	-0.252749
8	8	0	-2.475938	-1.945811	1.032279
9	6	0	-2.087512	-1.561244	-0.278272
10	6	0	-2.672920	-0.177395	-0.618687
11	8	0	-4.057238	-0.166960	-0.305000
12	6	0	-2.017024	0.886534	0.281701
13	8	0	-2.511190	2.173716	0.021816
14	6	0	2.417600	-1.587720	-0.044485
15	6	0	3.796948	-1.466072	-0.058467
16	6	0	4.383701	-0.180075	-0.050791
17	7	0	3.676640	0.934936	-0.019537
18	1	0	1.969309	-2.575547	-0.031281
19	1	0	-4.581533	-0.327985	-1.105325
20	1	0	-3.465939	2.156042	0.201714
21	1	0	-0.341578	2.999561	0.210056
22	1	0	2.159191	2.953962	0.083735
23	1	0	5.465476	-0.071300	-0.065909
24	1	0	4.429185	-2.348133	-0.069415
25	1	0	-0.081439	-2.475333	-0.430284
26	1	0	-2.423488	-2.303562	-1.018301
27	1	0	-2.492886	0.081109	-1.669808
28	1	0	-2.226718	0.575780	1.321637
29	1	0	-3.437790	-1.783487	1.082974

Table S7. Cartesian coordinates of the optimized structure for **7H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.770560	0.707860	-0.153877
2	6	0	-0.006804	-0.511540	-0.099196
3	6	0	-1.474477	-0.434172	-0.034759
4	6	0	-2.078413	0.866040	0.005285
5	6	0	-1.253647	2.011136	-0.030841
6	6	0	0.138105	1.940572	-0.108499
7	6	0	-3.490052	1.001126	0.074549
8	6	0	-4.295399	-0.117825	0.102865
9	6	0	-3.703328	-1.393780	0.063036
10	6	0	-2.322371	-1.550625	-0.001736
11	6	0	0.667994	-1.713097	-0.097232
12	6	0	2.143015	-1.856816	-0.105504
13	6	0	2.872297	-0.601040	0.375638
14	8	0	4.229805	-0.758356	0.064097
15	1	0	4.682412	0.082237	0.249959
16	6	0	2.276425	0.635772	-0.314310
17	8	0	2.942816	1.818565	0.086139
18	1	0	2.801702	1.953698	1.039771
19	1	0	2.465690	-2.064819	-1.142662
20	1	0	0.733673	2.845329	-0.156928
21	1	0	-1.729611	2.989004	-0.008395
22	1	0	-3.921382	1.997550	0.104226
23	1	0	-5.374710	-0.020369	0.154251
24	1	0	-4.334300	-2.277295	0.082108
25	1	0	-1.922702	-2.558232	-0.029754
26	1	0	0.098872	-2.638810	-0.090924
27	1	0	2.445787	-2.741137	0.467207
28	1	0	2.716633	-0.493028	1.465757
29	1	0	2.493537	0.542537	-1.389015

Table S8. Cartesian coordinates of the optimized structure for **8H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.756806	0.725637	0.161510
2	6	0	-0.129459	1.965848	0.070385
3	6	0	1.258387	2.040343	-0.020426
4	6	0	2.088640	0.890857	-0.027942
5	6	0	1.484531	-0.397510	0.044919
6	6	0	0.024271	-0.481498	0.121946
7	6	0	-0.603456	-1.708471	0.106039
8	1	0	-2.387939	-2.032950	1.174078
9	6	0	-2.076023	-1.868108	0.126421
10	6	0	-2.806825	-0.609320	-0.388685
11	8	0	-4.187515	-0.632273	-0.095688
12	6	0	-2.247242	0.624908	0.336898
13	8	0	-2.855180	1.811117	-0.098204
14	7	0	2.194948	-1.535075	0.036154
15	6	0	3.520338	-1.438681	-0.035905
16	6	0	4.222694	-0.216479	-0.106313
17	6	0	3.502399	0.958525	-0.105314
18	1	0	-4.671928	-1.069564	-0.812858
19	1	0	-3.814498	1.685311	0.004395
20	1	0	-0.733780	2.865006	0.076264
21	1	0	1.730513	3.018651	-0.081866
22	1	0	3.995956	1.924716	-0.162898
23	1	0	5.305835	-0.217341	-0.162579
24	1	0	4.066018	-2.379511	-0.039464
25	1	0	0.031313	-2.591317	0.062325
26	1	0	-2.371737	-2.776310	-0.411916
27	1	0	-2.628954	-0.489074	-1.467023
28	1	0	-2.432574	0.460839	1.418399

Table S9. Cartesian coordinates of the optimized structure for **9H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.756806	0.725637	0.161510
2	6	0	-0.129459	1.965848	0.070385
3	6	0	1.258387	2.040343	-0.020426
4	6	0	2.088640	0.890857	-0.027942
5	6	0	1.484531	-0.397510	0.044919
6	6	0	0.024271	-0.481498	0.121946
7	6	0	-0.603456	-1.708471	0.106039
8	1	0	-2.387939	-2.032950	1.174078
9	6	0	-2.076023	-1.868108	0.126421
10	6	0	-2.806825	-0.609320	-0.388685
11	8	0	-4.187515	-0.632273	-0.095688
12	6	0	-2.247242	0.624908	0.336898
13	8	0	-2.855180	1.811117	-0.098204
14	7	0	2.194948	-1.535075	0.036154
15	6	0	3.520338	-1.438681	-0.035905
16	6	0	4.222694	-0.216479	-0.106313
17	6	0	3.502399	0.958525	-0.105314
18	1	0	-4.671928	-1.069564	-0.812858
19	1	0	-3.814498	1.685311	0.004395
20	1	0	-0.733780	2.865006	0.076264
21	1	0	1.730513	3.018651	-0.081866
22	1	0	3.995956	1.924716	-0.162898
23	1	0	5.305835	-0.217341	-0.162579
24	1	0	4.066018	-2.379511	-0.039464
25	1	0	0.031313	-2.591317	0.062325
26	1	0	-2.371737	-2.776310	-0.411916
27	1	0	-2.628954	-0.489074	-1.467023
28	1	0	-2.432574	0.460839	1.418399

Table S10. Cartesian coordinates of the optimized structure for **10H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.842743	0.625517	-0.008363
2	6	0	-0.105643	-0.440253	-0.081499
3	6	0	-1.540904	-0.116544	-0.105659
4	6	0	-1.971973	1.277900	-0.072444
5	6	0	-1.002972	2.272755	-0.015579
6	6	0	0.351730	1.948158	0.015960
7	6	0	-3.377739	1.613199	-0.052614
8	6	0	-4.333732	0.662861	-0.089253
9	6	0	-3.975616	-0.781201	-0.232661
10	6	0	-2.516298	-1.076397	-0.108385
11	8	0	-4.783594	-1.672807	0.513414
12	6	0	0.362121	-1.769000	-0.147392
13	6	0	1.711709	-2.045062	-0.119012
14	6	0	2.691721	-1.023907	-0.032098
15	6	0	2.268900	0.342113	0.023392
16	6	0	3.266652	1.338476	0.108218
17	6	0	4.608424	1.000392	0.135029
18	6	0	5.019439	-0.347066	0.078410
19	6	0	4.072230	-1.344344	-0.004047
20	1	0	3.002420	2.388704	0.156635
21	1	0	5.354212	1.786671	0.200925
22	1	0	6.076285	-0.592871	0.100150
23	1	0	4.368959	-2.388399	-0.048563
24	1	0	2.043663	-3.078734	-0.168178
25	1	0	-0.331363	-2.597419	-0.229442
26	1	0	-2.283327	-2.135379	-0.057642
27	1	0	-4.200107	-1.035327	-1.291466
28	1	0	-5.391930	0.905633	-0.066173
29	1	0	-3.642228	2.664680	0.015403
30	1	0	-1.302703	3.315580	0.012742
31	1	0	1.056463	2.770806	0.060756
32	1	0	-4.706340	-1.447066	1.455511

Table S11. Cartesian coordinates of the optimized structure for **11H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.853138	0.688992	0.001570
2	6	0	-0.080430	-0.376721	-0.056075
3	6	0	-1.511346	-0.074138	-0.087116
4	6	0	-1.967116	1.302812	-0.042561
5	6	0	-1.007557	2.317003	0.014577
6	6	0	0.349334	2.012465	0.031864
7	6	0	-3.380854	1.595433	-0.019506
8	6	0	-4.302988	0.609464	-0.070246
9	6	0	-3.899494	-0.820975	-0.249369
10	6	0	-2.439522	-1.081778	-0.112983
11	8	0	-4.718530	-1.765048	0.405830
12	7	0	0.272509	-1.683429	-0.093783
13	6	0	1.556521	-1.973829	-0.073167
14	6	0	2.609107	-1.016577	-0.021349
15	6	0	2.265313	0.368102	0.018845
16	6	0	3.308046	1.316056	0.073076
17	6	0	4.629009	0.900538	0.085396
18	6	0	4.964819	-0.469114	0.044862
19	6	0	3.965432	-1.418459	-0.007925
20	1	0	3.092792	2.378671	0.105402
21	1	0	5.420256	1.643025	0.126748
22	1	0	6.007617	-0.769546	0.055533
23	1	0	4.204488	-2.477791	-0.039565
24	1	0	1.810424	-3.033147	-0.099024
25	1	0	-2.114086	-2.118465	-0.091535
26	1	0	-4.068101	-1.018495	-1.333872
27	1	0	-5.369101	0.814929	-0.045287
28	1	0	-3.683527	2.635414	0.064173
29	1	0	-1.323137	3.354962	0.049459
30	1	0	1.050276	2.840180	0.073755
31	1	0	-4.655698	-1.620983	1.364690

Table S12. Cartesian coordinates of the optimized structure for **12H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.654931	-0.664231	-0.005657
2	7	0	-0.267327	-1.976247	0.061938
3	6	0	1.002815	-2.257349	0.043174
4	6	0	2.034062	-1.260152	-0.037485
5	6	0	1.652238	0.114056	-0.096552
6	6	0	0.289066	0.432209	-0.094772
7	6	0	-0.215150	1.780411	-0.186895
8	1	0	0.487698	2.601476	-0.241609
9	6	0	-1.553016	2.019340	-0.182776
10	6	0	-2.514400	0.956627	-0.079941
11	6	0	-2.059295	-0.398051	0.011397
12	6	0	-3.009109	-1.449794	0.109787
13	6	0	-4.359994	-1.166585	0.118852
14	6	0	-4.805111	0.168066	0.028223
15	6	0	-3.896185	1.213109	-0.070715
16	6	0	2.749576	1.164279	-0.218848
17	8	0	2.593640	2.292507	0.630988
18	6	0	4.150613	0.633368	-0.134096
19	6	0	4.443081	-0.691892	-0.081026
20	6	0	3.376592	-1.634768	-0.038510
21	1	0	-2.648957	-2.469249	0.175709
22	1	0	-5.083299	-1.972159	0.194918
23	1	0	-5.870005	0.380873	0.035919
24	1	0	-4.246784	2.238691	-0.140695
25	1	0	-1.920701	3.038871	-0.257854
26	1	0	2.661786	1.579899	-1.239643
27	1	0	4.930743	1.390146	-0.126378
28	1	0	5.469440	-1.041937	-0.043211
29	1	0	3.617031	-2.694617	0.018387
30	1	0	1.284361	-3.309655	0.081951
31	1	0	2.655740	1.999477	1.556058

Table S13. Cartesian coordinates of the optimized structure for **13H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.348479	0.517927	-0.026370
2	6	0	-0.525567	-0.651694	-0.025425
3	6	0	0.939249	-0.488438	-0.002202
4	6	0	1.512324	0.837063	-0.171069
5	6	0	0.680799	1.933439	-0.196907
6	6	0	-0.710517	1.767620	-0.108953
7	6	0	2.999250	0.985045	-0.312849
8	6	0	3.729230	0.021632	0.636114
9	6	0	3.277378	-1.422705	0.351823
10	6	0	1.774919	-1.530357	0.295821
11	8	0	3.740704	-1.836447	-0.925879
12	6	0	-1.136591	-1.919292	-0.059428
13	6	0	-2.511536	-2.039961	-0.048511
14	6	0	-3.371321	-0.914635	-0.000670
15	6	0	-2.799119	0.397412	0.013100
16	6	0	-3.678294	1.499848	0.066199
17	6	0	-5.050065	1.313288	0.097842
18	6	0	-5.609557	0.019343	0.076518
19	6	0	-4.779545	-1.079202	0.027858
20	1	0	-3.297504	2.514584	0.092428
21	1	0	-5.703552	2.179313	0.141006
22	1	0	-6.687307	-0.105808	0.100078
23	1	0	-5.189918	-2.084887	0.012478
24	1	0	-2.956829	-3.030829	-0.082781
25	1	0	-0.537760	-2.820109	-0.127166
26	1	0	1.363914	-2.511207	0.513457
27	1	0	3.659092	-2.093267	1.137652
28	1	0	3.508374	0.305888	1.672883
29	1	0	3.260230	0.667575	-1.337799
30	1	0	1.108432	2.924459	-0.288617
31	1	0	-1.315754	2.667239	-0.138144
32	1	0	4.679164	-1.568916	-0.963691
33	8	0	5.116344	0.146707	0.345118
34	8	0	3.367123	2.323122	-0.085769
35	1	0	5.634999	0.030298	1.156618
36	1	0	4.325686	2.380598	-0.233486

Table S14. Cartesian coordinates of the optimized structure for **14H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.354056	0.582674	0.034465
2	6	0	0.542819	-0.581347	-0.050486
3	6	0	-0.917376	-0.438629	-0.029735
4	6	0	-1.514888	0.870203	0.093396
5	6	0	-0.689290	1.977837	0.153554
6	6	0	0.704061	1.829450	0.132152
7	6	0	-3.020527	1.018325	0.202551
8	6	0	-3.743166	-0.084476	-0.595728
9	6	0	-3.216330	-1.474306	-0.165738
10	6	0	-1.715195	-1.543268	-0.171131
11	8	0	-3.600412	-1.734226	1.175359
12	7	0	1.041001	-1.833166	-0.157373
13	6	0	2.351349	-1.976230	-0.169382
14	6	0	3.290740	-0.911760	-0.079542
15	6	0	2.795682	0.422872	0.021893
16	6	0	3.726457	1.477489	0.102473
17	6	0	5.086187	1.210683	0.085753
18	6	0	5.572113	-0.109785	-0.013060
19	6	0	4.683489	-1.161509	-0.095495
20	1	0	3.395684	2.507564	0.180006
21	1	0	5.790336	2.034720	0.150493
22	1	0	6.641844	-0.291966	-0.023730
23	1	0	5.037360	-2.185755	-0.172515
24	1	0	2.721158	-2.997520	-0.255901
25	1	0	-1.235627	-2.513132	-0.275572
26	1	0	-3.619662	-2.242462	-0.844452
27	1	0	-3.568088	0.067278	-1.672232
28	1	0	-3.284905	0.856463	1.256559
29	1	0	-1.131879	2.963556	0.241496
30	1	0	1.304258	2.731377	0.205949
31	8	0	-5.118784	-0.016203	-0.272942
32	8	0	-3.460488	2.320659	-0.096839
33	1	0	-3.445282	2.453747	-1.059286
34	1	0	-5.653317	-0.284989	-1.036379
35	1	0	-4.542510	-1.477899	1.226917

Table S15. Cartesian coordinates of the optimized structure for **15H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.312834	0.472826	0.034020
2	6	0	0.506081	-0.723582	-0.040077
3	6	0	-0.947730	-0.538385	-0.032662
4	6	0	-1.465210	0.806246	0.109080
5	6	0	-0.564688	1.852105	0.172370
6	7	0	0.771221	1.686091	0.129793
7	6	0	-2.951421	1.030273	0.231351
8	6	0	-3.735072	0.011907	-0.611369
9	6	0	-3.329341	-1.415116	-0.216881
10	6	0	-1.831083	-1.579178	-0.192233
11	8	0	-3.753301	-1.710468	1.106487
12	6	0	1.147506	-1.966429	-0.116686
13	6	0	2.534074	-2.051385	-0.127534
14	6	0	3.369539	-0.911374	-0.065745
15	6	0	2.766625	0.381141	0.017577
16	6	0	3.588668	1.516084	0.082654
17	6	0	4.971646	1.374665	0.065323
18	6	0	5.572629	0.103001	-0.016828
19	6	0	4.783160	-1.028410	-0.081038
20	1	0	3.131491	2.496514	0.147195
21	1	0	5.598262	2.259925	0.117039
22	1	0	6.654322	0.015865	-0.028213
23	1	0	5.231683	-2.015760	-0.143199
24	1	0	2.997736	-3.033059	-0.182153
25	1	0	0.576557	-2.887333	-0.157881
26	1	0	-1.465962	-2.598258	-0.279613
27	1	0	-3.761806	-2.127646	-0.934770
28	1	0	-3.502149	0.175071	-1.678792
29	1	0	-3.230796	0.855780	1.278849
30	1	0	-0.918172	2.872999	0.278771
31	1	0	-4.690120	-1.436711	1.143867
32	8	0	-5.117909	0.103539	-0.365985
33	8	0	-3.365016	2.356048	-0.044825
34	1	0	-5.359475	1.045872	-0.336931
35	1	0	-3.139627	2.574821	-0.966058

Table S16. Cartesian coordinates of the optimized structure for **16H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.106290	-0.466867	-0.042404
2	6	0	0.338842	0.738761	-0.112507
3	6	0	-1.129541	0.641853	-0.135733
4	6	0	-1.760017	-0.661238	-0.216381
5	6	0	-0.981727	-1.796233	-0.161705
6	6	0	0.412783	-1.689627	-0.064206
7	6	0	-3.254339	-0.756190	-0.369884
8	6	0	-3.957885	0.321681	0.463827
9	6	0	-3.423160	1.701151	0.036947
10	6	0	-1.936570	1.746672	0.004092
11	1	0	-3.801449	1.907933	-0.979658
12	6	0	1.015224	1.975300	-0.162264
13	6	0	2.391237	2.030992	-0.114688
14	6	0	3.195545	0.867261	-0.013595
15	6	0	2.560426	-0.413758	0.024538
16	6	0	3.384315	-1.555470	0.125977
17	6	0	4.762325	-1.434485	0.183984
18	6	0	5.383509	-0.169857	0.142170
19	6	0	4.608387	0.965283	0.044409
20	1	0	2.955109	-2.550206	0.166027
21	1	0	5.371977	-2.329397	0.263537
22	1	0	6.465259	-0.095077	0.187689
23	1	0	5.067407	1.949342	0.011343
24	1	0	2.884609	2.998355	-0.160071
25	1	0	0.466756	2.904670	-0.260856
26	1	0	-1.483285	2.726260	0.125353
27	1	0	-3.812750	2.509637	0.666711
28	1	0	-3.732873	0.142872	1.525067
29	1	0	-3.492406	-0.537522	-1.430338
30	1	0	-1.455502	-2.769855	-0.192760
31	1	0	0.975672	-2.615646	-0.022860
32	8	0	-5.339395	0.175141	0.201667
33	8	0	-3.684689	-2.046542	-0.022381
34	1	0	-5.854355	0.496206	0.957719
35	1	0	-4.655364	-2.037738	-0.086637

Table S17. Cartesian coordinates of the optimized structure for **17H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.114162	0.539329	-0.044380
2	6	0	-0.356788	-0.662367	-0.087877
3	6	0	1.103062	-0.582383	-0.138626
4	6	0	1.752320	0.702200	-0.183481
5	6	0	0.984113	1.851597	-0.123212
6	6	0	-0.411077	1.762173	-0.055543
7	6	0	3.249296	0.763815	-0.327615
8	6	0	3.922069	-0.393137	0.425068
9	6	0	3.342275	-1.730198	-0.082403
10	6	0	1.860015	-1.732787	-0.092774
11	1	0	3.692037	-1.877615	-1.120426
12	7	0	-0.911437	-1.897778	-0.073954
13	6	0	-2.224439	-1.982226	-0.025144
14	6	0	-3.114851	-0.872155	0.016554
15	6	0	-2.560412	0.442210	0.009928
16	6	0	-3.442157	1.540609	0.055844
17	6	0	-4.811379	1.334839	0.105277
18	6	0	-5.355957	0.033814	0.111124
19	6	0	-4.516154	-1.059688	0.067187
20	1	0	-3.064861	2.557473	0.052571
21	1	0	-5.477015	2.192057	0.139828
22	1	0	-6.432079	-0.100898	0.150015
23	1	0	-4.915653	-2.069978	0.070796
24	1	0	-2.640798	-2.989223	-0.016610
25	1	0	1.325965	-2.679456	-0.049129
26	1	0	3.722908	-2.592309	0.478270
27	1	0	3.710556	-0.278213	1.497962
28	1	0	3.482007	0.615092	-1.401593
29	1	0	1.471443	2.819166	-0.132153
30	1	0	-0.971075	2.691513	-0.015886
31	8	0	5.304880	-0.272587	0.159831
32	8	0	3.713102	2.014254	0.111063
33	1	0	4.682422	1.991937	0.031416
34	1	0	5.815686	-0.662314	0.885898

Table S18. Cartesian coordinates of the optimized structure for **18H**$^+$ (B3LYP/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.074261	-0.429217	-0.053289
2	6	0	0.317524	0.801112	-0.065081
3	6	0	-1.136974	0.673700	-0.114653
4	6	0	-1.711562	-0.648110	-0.173769
5	6	0	-0.855561	-1.735463	-0.151159
6	7	0	0.482890	-1.624098	-0.092168
7	6	0	-3.207711	-0.824936	-0.306906
8	6	0	-3.974746	0.303697	0.401376
9	6	0	-3.463565	1.664363	-0.082994
10	6	0	-1.987017	1.764390	-0.094447
11	1	0	-3.826610	1.818438	-1.117191
12	6	0	1.011615	2.021050	-0.019999
13	6	0	2.396272	2.048373	0.026851
14	6	0	3.184417	0.870703	0.037734
15	6	0	2.529093	-0.396962	-0.002307
16	6	0	3.302795	-1.568354	0.008788
17	6	0	4.688932	-1.485518	0.057206
18	6	0	5.341184	-0.237547	0.096656
19	6	0	4.599790	0.928164	0.087120
20	1	0	2.804424	-2.530144	-0.021972
21	1	0	5.277857	-2.397702	0.064034
22	1	0	6.425015	-0.194799	0.134123
23	1	0	5.089662	1.897263	0.117104
24	1	0	2.901239	3.010571	0.055058
25	1	0	0.479998	2.966135	-0.025099
26	1	0	-1.568218	2.767469	-0.088521
27	1	0	-3.901998	2.488033	0.492805
28	1	0	-3.781695	0.218113	1.487296
29	1	0	-3.468909	-0.773084	-1.374164
30	1	0	-1.252836	-2.744920	-0.196052
31	8	0	-5.346723	0.249506	0.118810
32	8	0	-3.667861	-2.096691	0.112715
33	1	0	-5.655521	-0.653275	0.308649
34	1	0	-3.438438	-2.222600	1.050139