Electronic Supplementary Information (ESI)

A Theoretical (DFT, GIAO-NMR, NICS) Study of the Carbocations and Oxidation Dications from Azulenes, Homoazulene, Benzazulenes, Benzohomoazulenes, and the Isomeric Azulenoazulenes

Takao Okazaki and Kenneth K. Laali*

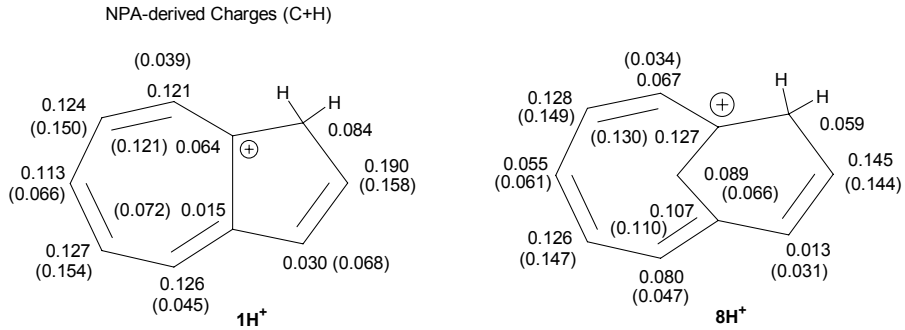


Fig S1. NPA-derived sum of carbon and hydrogen charges

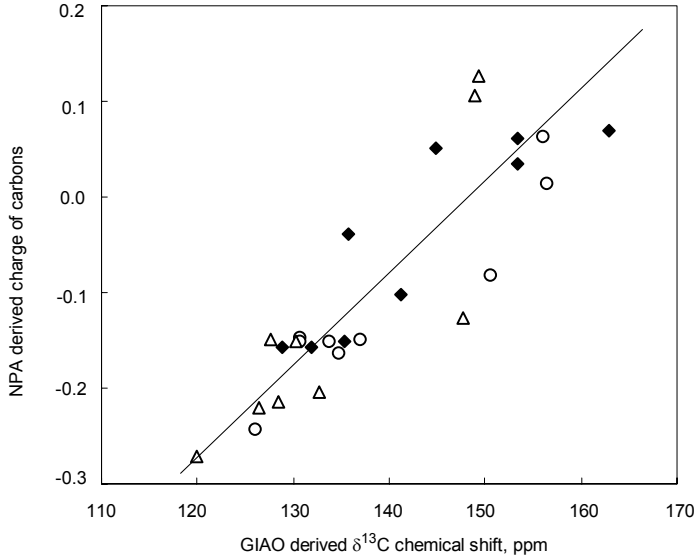


Fig S2: Correlation between NPA-derived charges and $\delta^{13}C$ for $\mathbf{1H}^+$ (o), $\mathbf{2H}^+$ (♦), and $\mathbf{8H}^+$ (Δ).

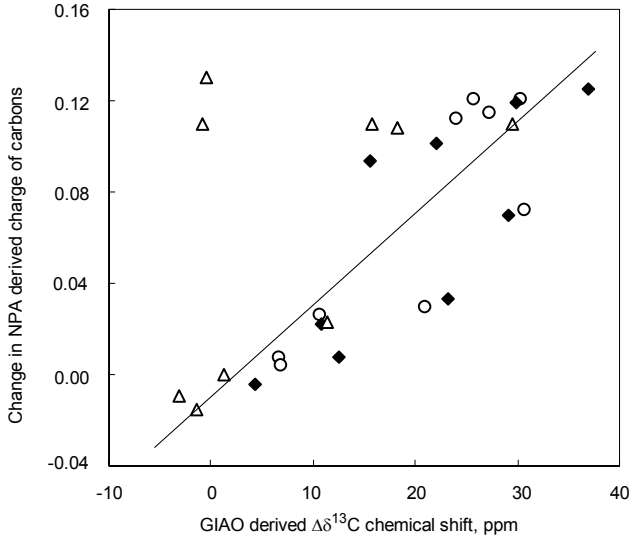
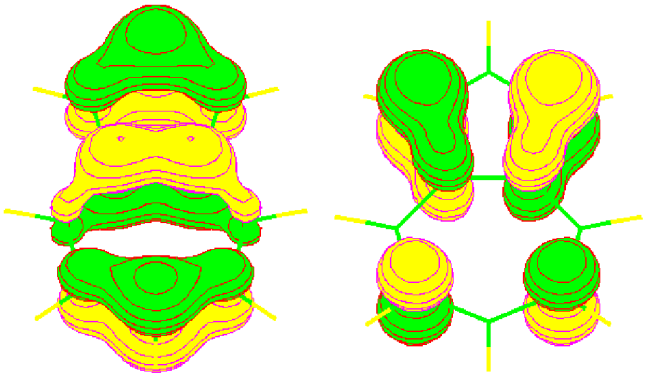
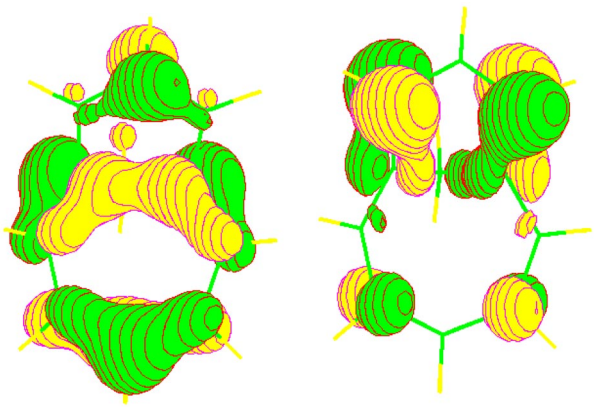


Fig S2a: Correlation between change in NPA-derived charges and $\Delta\delta^{13}C$ for $\mathbf{1H}^+$ (o), $\mathbf{2H}^+$ (♦), and $\mathbf{8H}^+$ (Δ).



HOMO LUMO

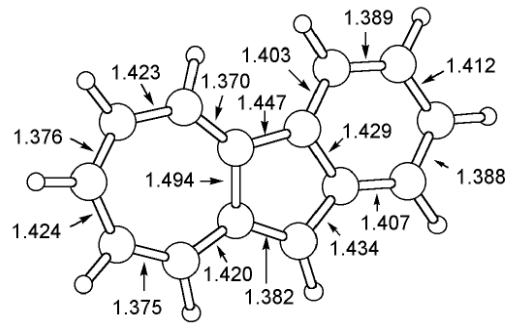
1^{2+}



HOMO LUMO

8^{2+}

Fig. S3: Forms of the HOMO-LUMO for **1^{2+}** and **8^{2+}**.



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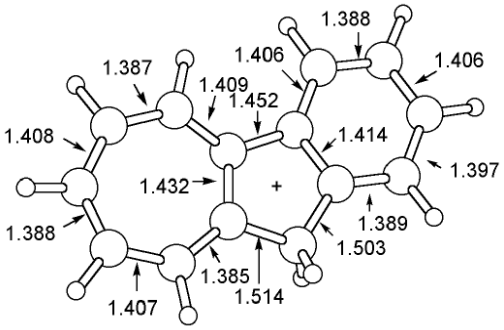
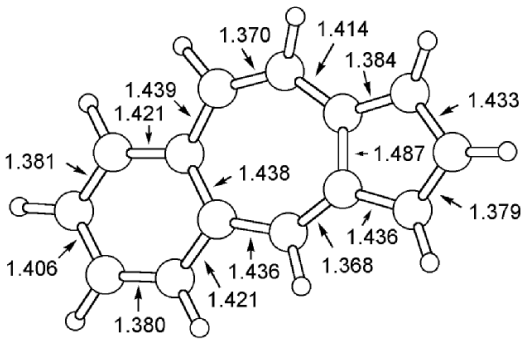
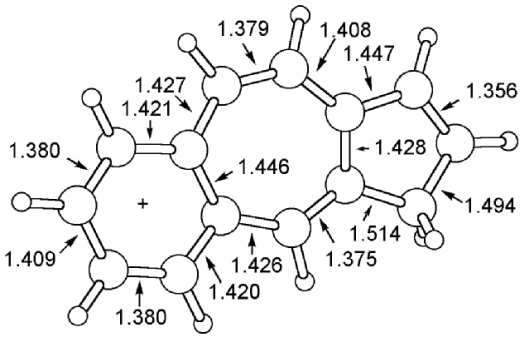


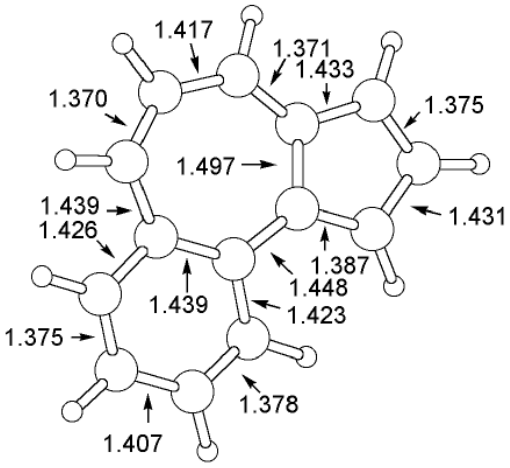
9H$^+$



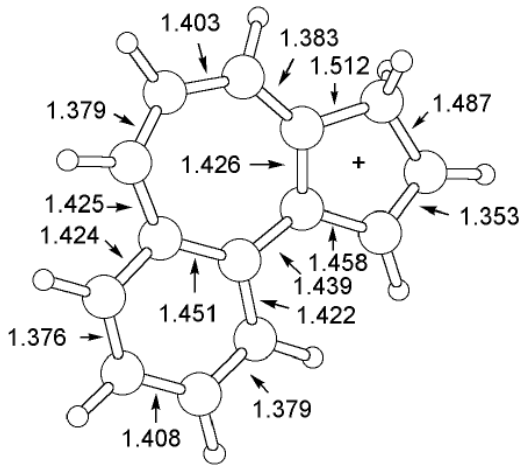
9A



9AH$^+$

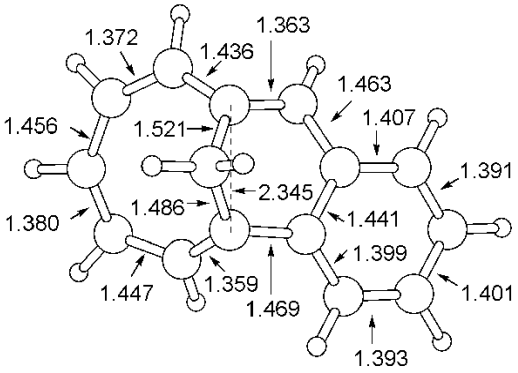


9B



9BH$^+$

Figure S4: B3LYP/6-31G(d) optimized structures for **9**, **9H**$^+$, **9A**, **9AH**$^+$, **9B**, **9BH**$^+$, **10**, **10H**$^+$, **10A**, **10AH**$^+$, **10B**, and **10BH**$^+$; bond lengths (Å).



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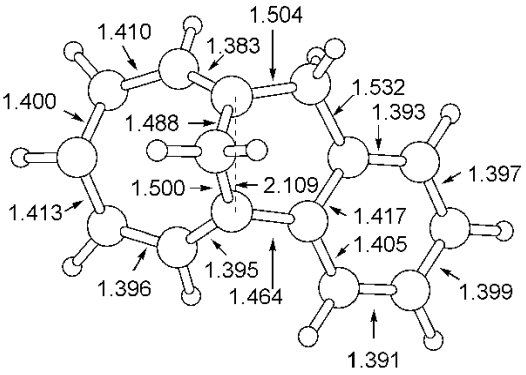
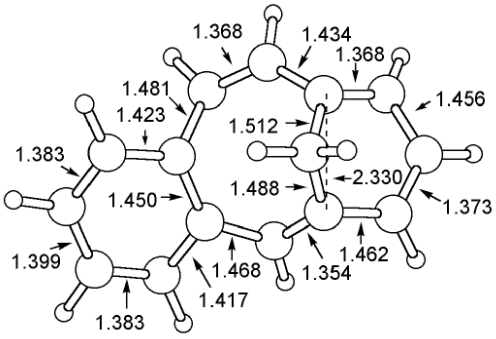
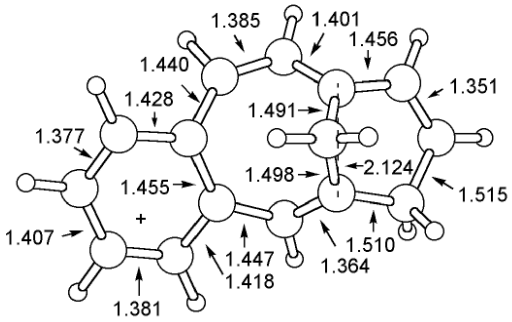


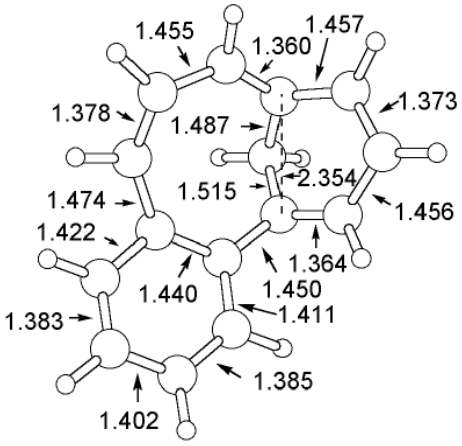
10H$^+$



10A



10AH$^+$



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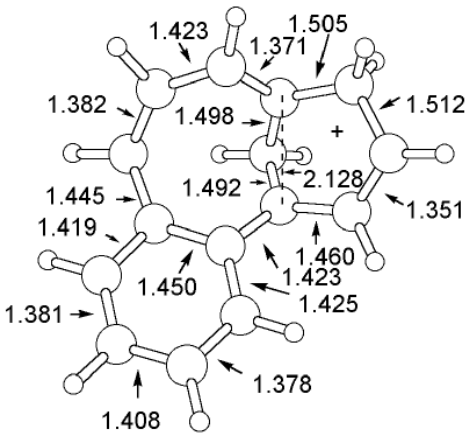


10BH$^+$

Figure S4 (continued):

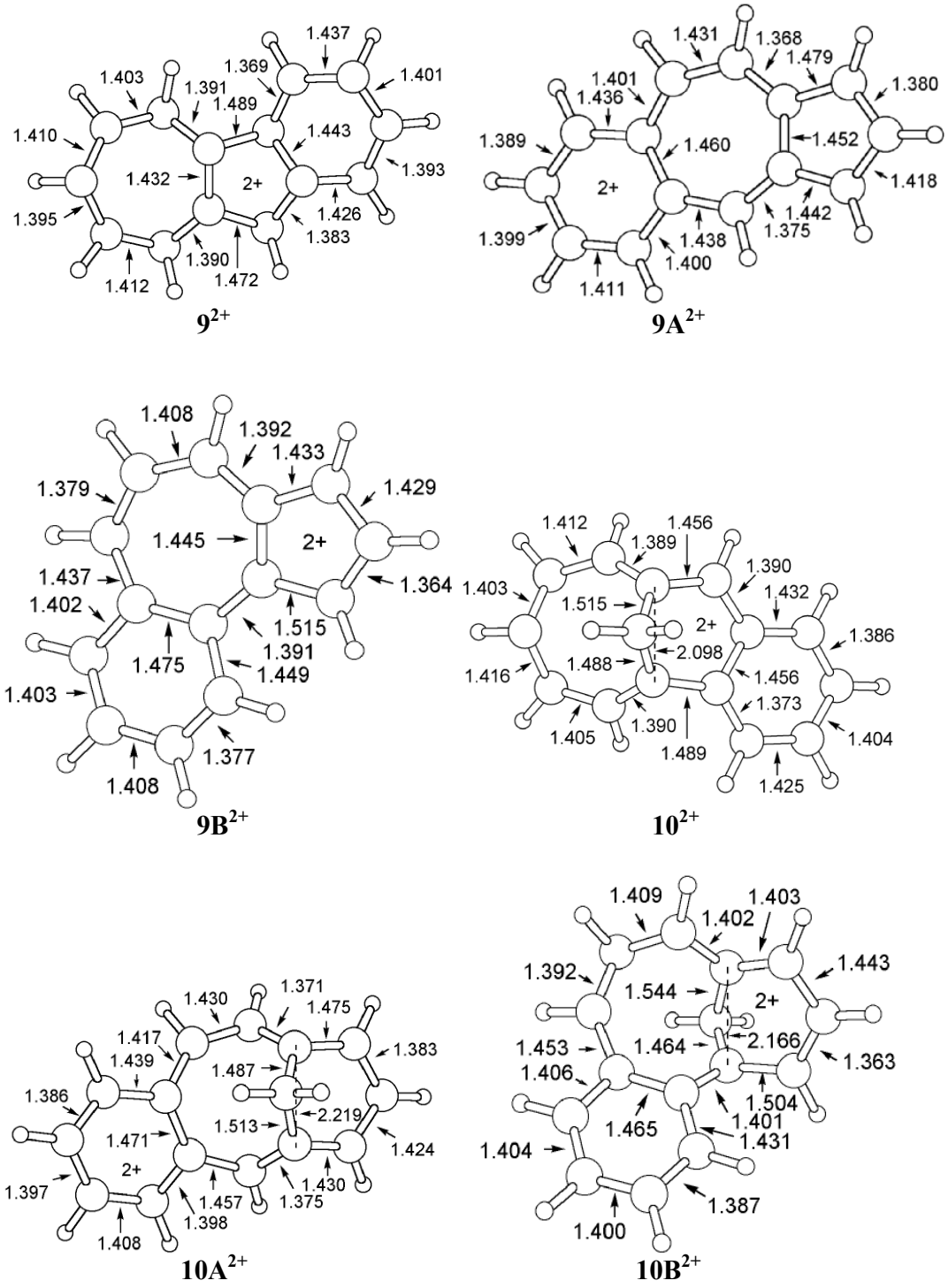


Figure S5: B3LYP/6-31G(d) optimized structures for $\mathbf{9}^{2+}$, $\mathbf{9A}^{2+}$, $\mathbf{9B}^{2+}$, $\mathbf{10}^{2+}$, $\mathbf{10A}^{2+}$, and $\mathbf{10B}^{2+}$; bond lengths (Å).

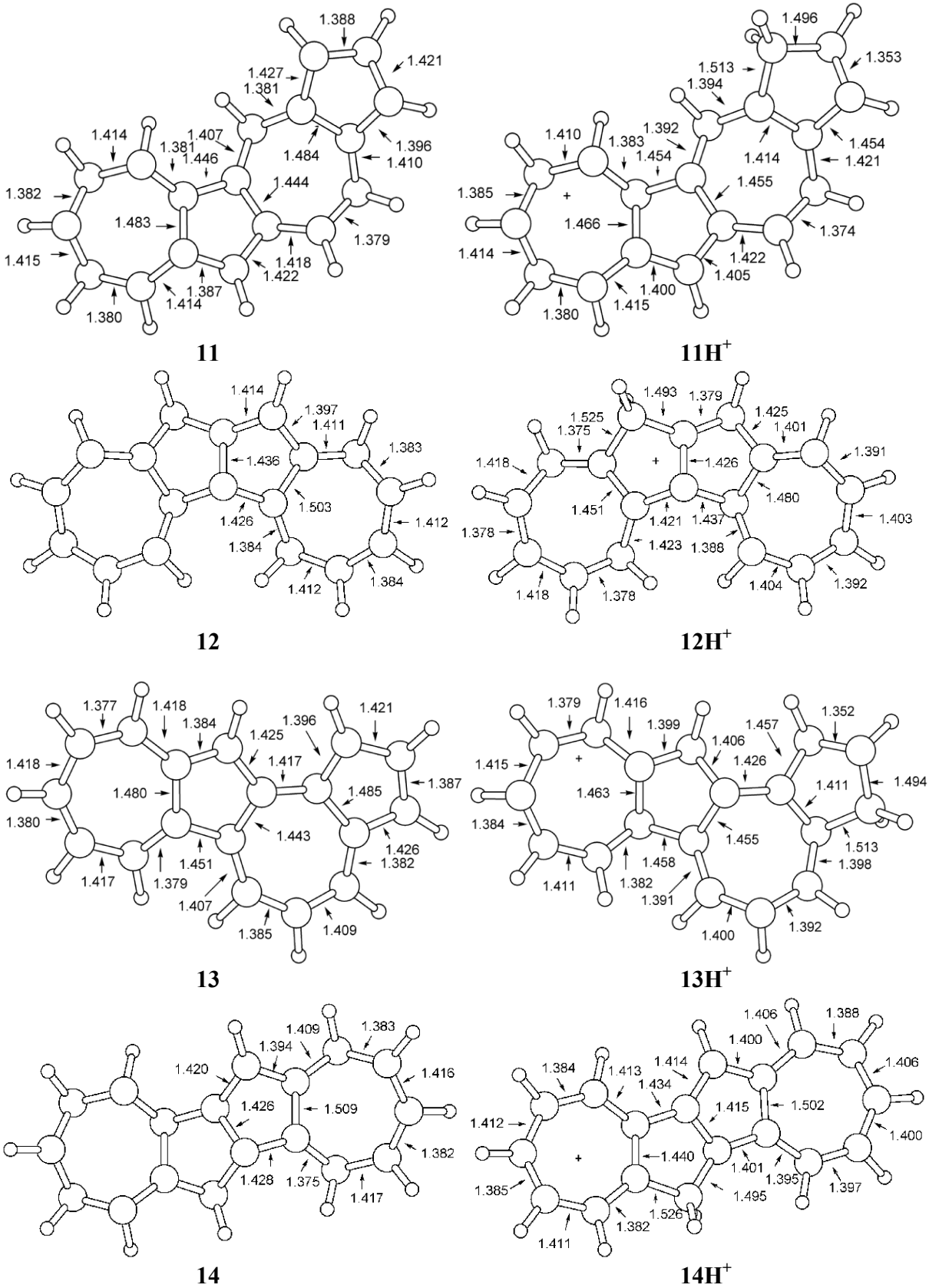
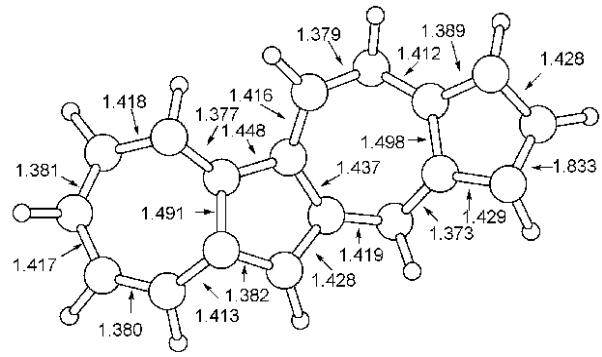


Figure S6: B3LYP/6-31G(d) optimized structures for **11**, **11H**$^+$, **12**, **12H**$^+$, **13**, **13H**$^+$, **14**, **14H**$^+$, **15**, **15H**$^+$, **16**, and **16H**$^+$; bond lengths (Å).



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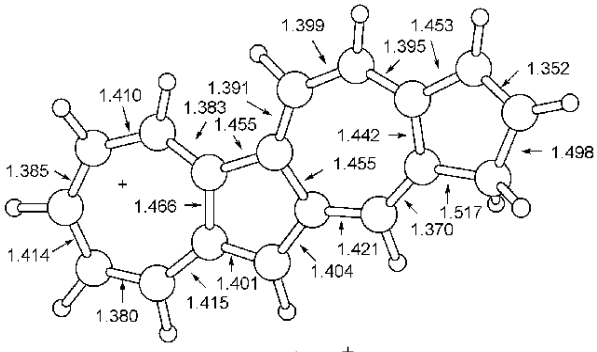
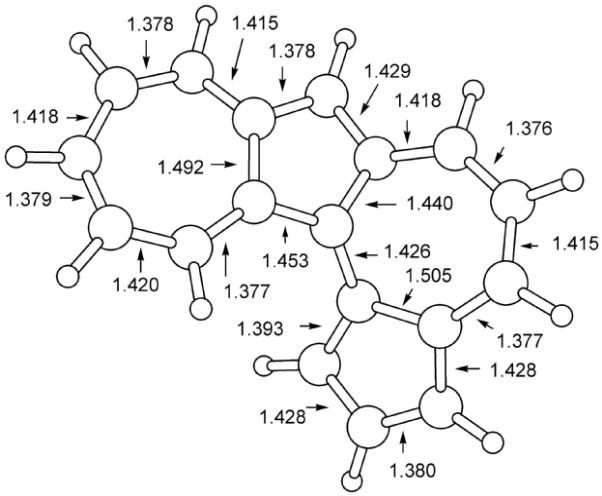


15H$^+$



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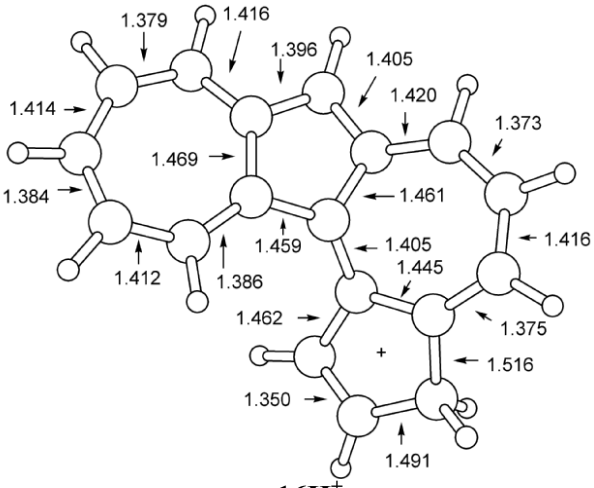
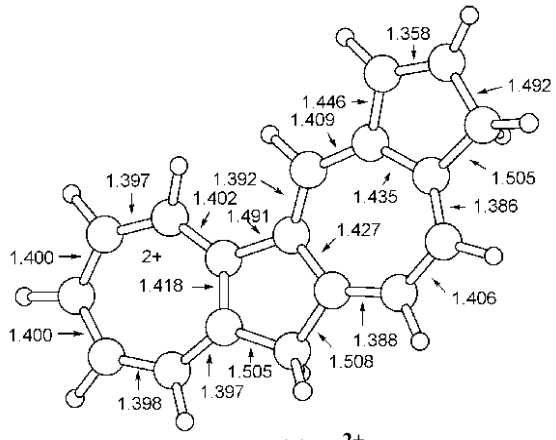
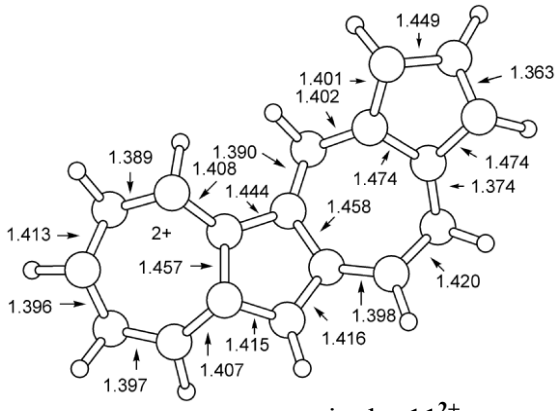


16H$^+$

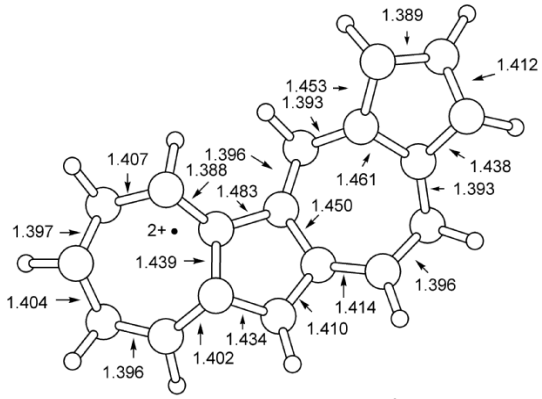
Figure S6 (continued):



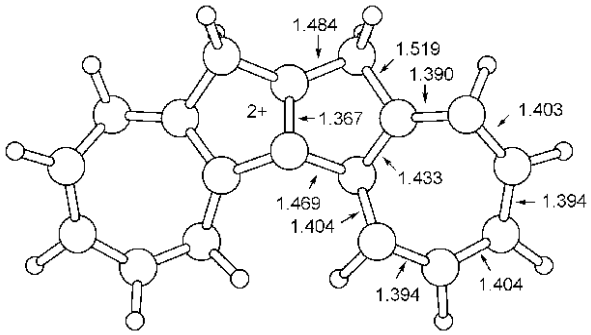
$11H_2^{2+}$



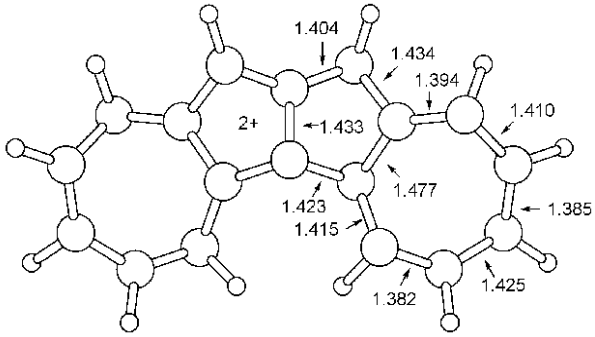
singlet **11^{2+}**



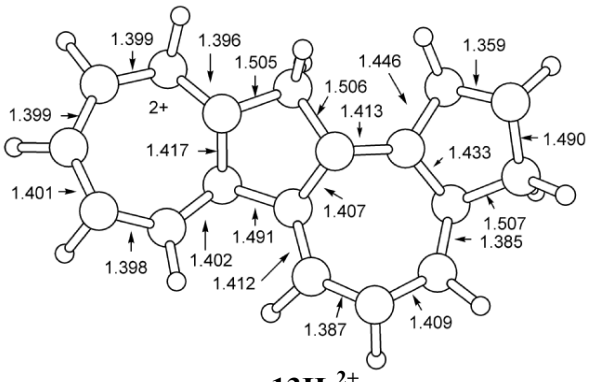
triplet **$11^{2+\cdot}$**



$12H_2^{2+}$

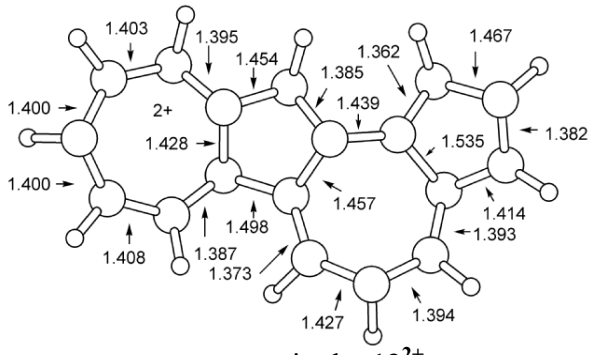


singlet **12^{2+}**

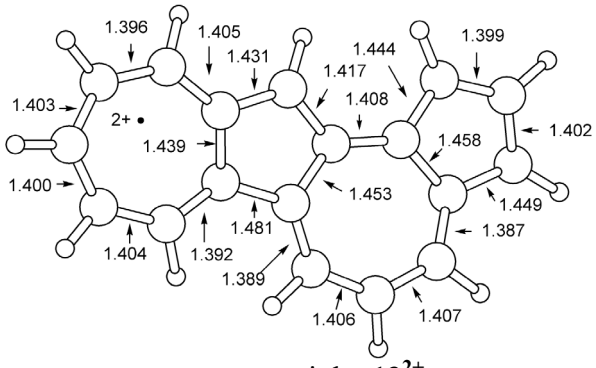


$13H_2^{2+}$

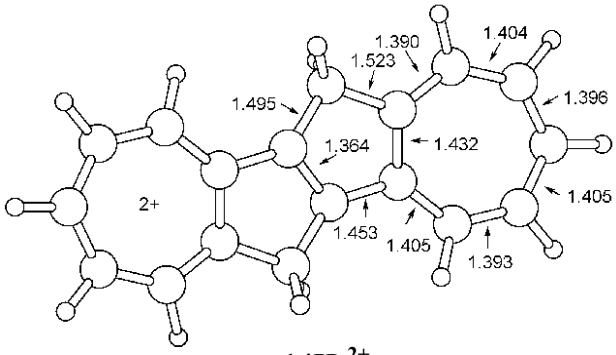
Figure S7: B3LYP/6-31G(d) optimized structures for **$11H_2^{2+}$**, **11^{2+}**, **$12H_2^{2+}$**, **12^{2+}**, **$13H_2^{2+}$**, **13^{2+}**, **$14H_2^{2+}$**, **14^{2+}**, **$15H_2^{2+}$**, **15^{2+}**, **$16H_2^{2+}$**, and **16^{2+}**; bond lengths (Å).



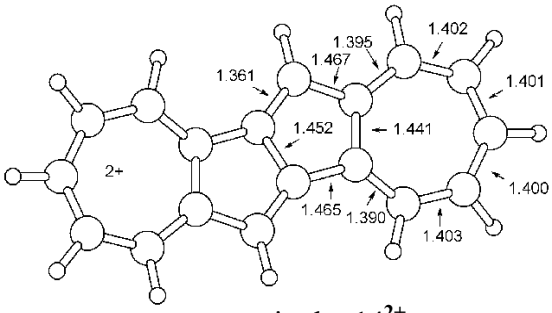
singlet $\mathbf{13}^{2+}$



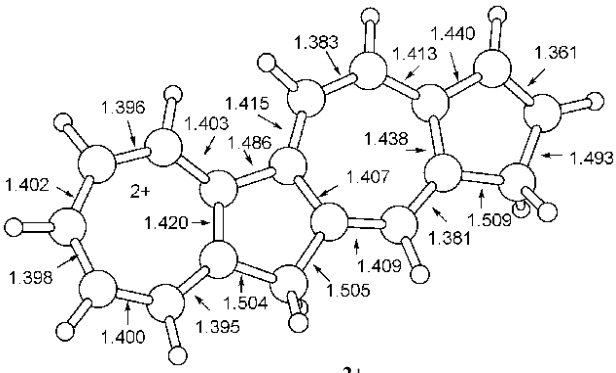
triplet $\mathbf{13}^{2+\cdot}$



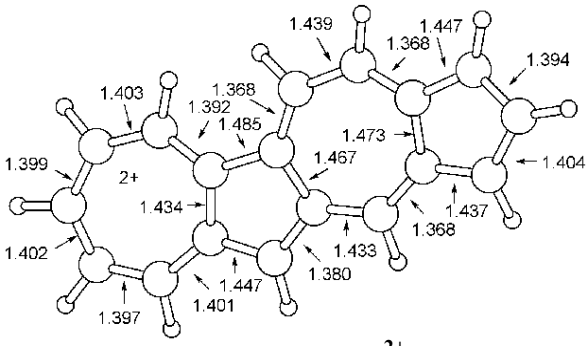
$\mathbf{14H_2}^{2+}$



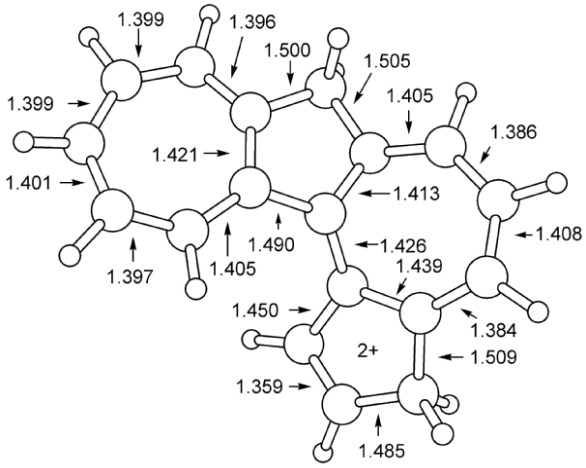
singlet $\mathbf{14}^{2+}$



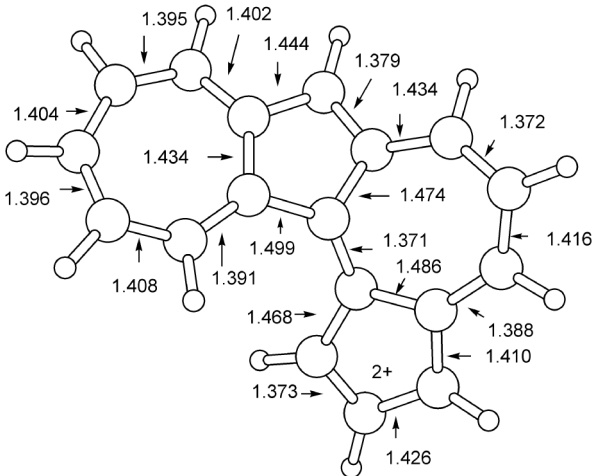
$\mathbf{15H_2}^{2+}$



singlet $\mathbf{15}^{2+}$



$\mathbf{16H_2}^{2+}$



singlet $\mathbf{16}^{2+}$

Figure S7 (continued):

Table S1. Electronic Energies (E), Zero Point Energies (ZPE), and Gibbs Free Energies (G) for Azulene **1**, Guaiazulene **2**, Homoazulene **8**, their Azulenium Ions and Oxidation Dications from DFT Calculations at the B3LYP/6-31G(d) Level

Compd	Protonation site	Point groups	E, hartree	ZPE, hartree	G, hartree	ΔG, kcal[a]
1	Neutral	C_s	-385.8381731	0.146544	-385.723136	(0)
		C_{2v}	-385.8381598	0.146557	-385.722457	
	1	C_s	-386.2159681	0.159402	-386.088473	-229.3
	2	C_s	-386.1788329	0.157514	-386.053354	-207.2
		C_{2v}	-386.1787965	0.157512	-386.052670	
	3a	C_1	-386.1681808	0.158112	-386.042098	-200.2
	4	C_s	-386.1499715	0.156656	-386.028058	-191.3
	5	C_s	-386.1810027	0.158335	-386.054847	-208.2
	6	C_s	-386.1542782	0.156773	-386.029815	-192.4
		C_{2v}	-386.1542759	0.156779	-386.029162	
$\mathbf{1}^{2+}$	Dication	C_{2v}	-385.1178377	0.146553	-385.002680	
		C_s	-385.1178471	0.146551	-385.003346	451.7
2	Neutral	C_1	-582.4142865	0.286917	-582.169032	(0)
	1	C_1	-582.5513830	0.300612	-582.542774	-234.5
	3	C_1	-582.8090643	0.299765	-582.551383	-239.9
8	Neutral	C_s	-425.0993468	0.175213	-424.956477	
		C_1	-425.0993828	0.175202	-424.956514	(0)
	1	C_1	-425.4837386	0.187637	-425.328672	-233.5
	2	C_1	-425.4482126	0.186802	-425.294169	-211.9
		C_s	-425.4481843	0.186775	-425.294182	
	3a	C_1	-425.4566872	0.187860	-425.301645	-216.6
	4	C_1	-425.4434879	0.187003	-425.289309	-208.8
	5	C_1	-425.4536763	0.187312	-425.299164	-215.0
	6	C_1	-425.4406339	0.186778	-425.286685	-207.2
		C_s	-425.4405624	0.186702	-425.286717	-207.2
$\mathbf{8}^{2+}$	Dication	C_s	-424.4050252	0.173772	-424.264576	434.2
		C_1	-424.4050182	0.173762	-424.264569	

[a] Relative to neutral compound.

Table S2. Electronic Energies (E), Zero Point Energies (ZPE), and Gibbs Free Energies (G) for the Isomeric Benzazulenes (**9**, **9A**, **9B**), Isomeric Benzohomoazulenes (**10**, **10A**, **10B**), their Arenium Ions, and Oxidation Dications from DFT Calculations at the B3LYP/6-31G(d) Level

Compd	Protonation site	Point groups	E, hartree	ZPE, hartree	G, hartree	ΔG, kcal[a]
9	Neutral	C_s	-539.4860754	0.193830	-539.327365	(0)
	10	C_1 (almost C_s)	-539.8775494	0.206955	-539.706171	-237.7
		C_s	-539.8775429	0.206918	-539.706203	-237.7
	4a	C_1	-539.8293346	0.205726	-539.659227	-208.2
	9	C_1	-539.8252427	0.205232	-539.656089	-206.3
		C_s[b]	-539.8235743	0.204890	-539.653723	
	8	C_s	-539.8360771	0.205497	-539.666462	-212.8
	7	C_s	-539.8208047	0.204432	-539.652437	-204.0
	6	C_s	-539.8407882	0.205779	-539.670863	-215.5
	5	C_1	-539.8030988	0.202936	-539.636859	-194.2
		C_s[b]	-539.8029988	0.202718	-539.635585	
	4	C_s	-539.8277000	0.204874	-539.658614	-207.9
	3	C_s	-539.8514297	0.205946	-539.681123	-222.0
	2	C_s	-539.8280981	0.204688	-539.659082	-208.2
	1	C_s	-539.8498401	0.205964	-539.679640	-221.1
9^{2+}	Dication	C_s	-538.8339781	0.194814	-538.674728	409.5
9A	Neutral	C_s	-539.4821121	0.193713	-539.323486	(0)
	3	C_s	-539.8715548	0.206564	-539.700447	-236.5
	1	C_s	-539.8665510	0.206331	-539.695690	-233.6
	2	C_s	-539.8349489	0.204991	-539.665575	-214.7
	4	C_1	-539.8136348	0.205189	-539.644382	-201.4
		C_s[b]	-539.809505	0.204496	-539.640233	
	5	C_s	-539.8117488	0.204184	-539.643520	-200.7
	6	C_s	-539.8266468	0.205291	-539.657027	-209.3
	7	C_s	-539.8084029	0.204025	-539.640210	-198.7
	8	C_s	-539.8264441	0.205188	-539.657300	-209.5
	9	C_s	-539.8419457	0.205654	-539.675025	-220.6
	10	C_s	-539.8078480	0.204072	-539.640774	-199.1
9A^{2+}	Dication	C_s	-538.8175392	0.194283	-538.658747	417.1
9B	Neutral	C_s	-539.4751399	0.193582	-539.317090	(0)
	3	C_s	-539.8653997	0.206555	-539.694724	-237.0
	1	C_s	-539.8616153	0.206565	-539.690509	-234.3
9B^{2+}	Dication	C_s	-538.8005889	0.193850	-538.642478	423.3
10	Neutral	C_1	-578.7516966	0.222510	-578.565055	(0)
	10	C_1	-579.1459318	0.235111	-578.946993	-239.7
	4a	C_1	-579.0947448	0.234088	-578.896863	-208.2
10^{2+}	Dication	C_1	-578.1126155	0.222578	-577.926218	400.9
10A	Neutral	C_1	-578.7388639	0.222224	-578.552602	(0)
	1	C_1	-579.1305768	0.234494	-578.932244	-238.2
	3	C_1	-579.1326656	0.234629	-578.934199	-239.5
10A^{2+}	Dication	C_1	-578.0913155	0.222489	-577.905003	406.4
10B	Neutral	C_1	-578.743566	0.222496	-578.556932	(0)
	1	C_1	-579.1288715	0.234804	-578.930161	-234.2
	3	C_1	-579.1321045	0.234881	-578.933402	-236.2
10B^{2+}	Dication	C_1	-578.0857666	0.222182	-577.899691	412.4

[a] Relative to neutral compound. [b] Number of imaginary frequencies = 1.

Table S3. Electronic Energies (E), Zero Point Energies (ZPE), and Gibbs Free Energies (G) for the Azulenoazulenes **11**-**16**, their Monoprotonated, Diprotonated Cations and Singlet and Triplet Oxidation Dications from DFT Calculations at the B3LYP/6-31G(d) Level

Compd	Protonation site	Point groups	E, hartree[a]	ZPE, hartree	G, hartree	ΔG, kcal[b]
11	Neutral	C_s	-693.0866197	0.239533	-692.885968	(0)
	1	C_s	-693.4862628	0.252460	-693.273056	-242.9
	3	C_s	-693.4888348	0.252582	-693.275490	-244.4
	10	C_s	-693.4763042	0.252476	-693.263406	-236.8
	1, 10	C_s	-693.7367884	0.264460	-693.512170	-392.9
	3, 10	C_s	-693.7351397	0.264367	-693.510601	-392.0
$\mathbf{11}^{2+}$	Dication (s)[c]	C_s	-692.4725513	0.240475	-692.271318	385.7
	Dication (t)[d]	C_s	-692.4741681	0.239915	-692.274607	383.6
12	Neutral	C_s	-693.0751377	0.239754	-692.874506	(0)
	11	C_s	-693.4790021	0.253204	-693.265515	-245.4
	11, 12	C_s	-693.7321420	0.264986	-693.507236	-397.0
$\mathbf{12}^{2+}$	Dication (s)[c]	C_s	-692.4689089	0.240471	-692.268043	380.6
		C_{2v}	-692.4689092	0.240472	-692.267395	
	Dication (t)[d]	C_s	-692.4645856	0.240347	-692.264829	382.6
		C_{2v}	-692.4645856	0.240345	-692.264175	
13	Neutral	C_s	-693.0834379	0.239530	-692.882849	(0)
	1	C_s	-693.4847045	0.252633	-693.271311	-243.8
	3	C_s	-693.4870640	0.252688	-693.273640	-245.2
	12	C_s	-693.4752077	0.252592	-693.262226	-238.1
	1, 12	C_s	-693.7324800	0.264552	-693.507768	-392.1
	3, 12	C_s	-693.7342663	0.264542	-693.509503	-393.2
$\mathbf{13}^{2+}$	Dication (s)[c]	C_s	-692.4503592	0.239436	-692.250868	396.6
	Dication (t)[d]	C_s	-692.4701385	0.239985	-692.270509	384.2
14	Neutral	C_s	-693.0703617	0.239250	-692.870125	(0)
	6	C_s	-693.4698845	0.252775	-693.256561	-242.5
	6, 12	C_s	-693.7386309	0.265316	-693.513116	-403.5
$\mathbf{14}^{2+}$	Dication (s)[c]	C_s	-692.5027513	0.242440	-692.299619	358.0
		C_{2h}	-692.5027513	0.242439	-692.298965	
	Dication (t)[d]	C_s	-692.4498968	0.238415	-692.252046	387.9
		C_{2h}	-692.4498977	0.238337	-692.251490	
15	Neutral	C_s	-693.0808070	0.239142	-692.880596	(0)
	1	C_s	-693.4867465	0.252639	-693.273399	-246.5
	3	C_s	-693.4894983	0.252741	-693.276012	-248.1
	5	C_s	-693.4680781	0.252068	-693.255566	-235.3
	1, 5	C_s	-693.7366564	0.264457	-693.512070	-396.3
	3, 5	C_s	-693.7377022	0.264489	-693.513067	-396.3
$\mathbf{15}^{2+}$	Dication (s)[c]	C_s	-692.491588	0.241622	-692.289132	371.1
	Dication (t)[d]	C_s	-692.4632268	0.239055	-692.264522	386.6
16	Neutral	C_1	-693.0834379	0.239530	-692.882849	(0)
	1	C_1	-693.4774481	0.253094	-693.263669	-239.0
	3	C_1	-693.4786596	0.252935	-693.264885	-239.7
	7	C_1	-693.4600356	0.252513	-693.246794	-228.4
	1, 7	C_1	-693.722055	0.264934	-693.497274	-385.6
	3, 7	C_1	-693.7253957	0.264660	-693.500259	-387.4
$\mathbf{16}^{2+}$	Dication (s)[c]	C_1	-692.4739723	0.241617	-692.271566	383.6
$\mathbf{16}^{2+}$	Dication (t)[d]	C_1	-692.4540735	0.239673	-692.254621	394.2

[a] 1 hartree = 627.5096 kcal/mol. [b] Relative to neutral compound. [c] Singlet oxidation dication. [d] Triplet oxidation dication.

Table S4. Cartesian Coordinates of the Optimized Structure for **1** (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.177569	1.610137	0.000000
2	6	0	2.013431	-1.488204	0.000000
3	6	0	-0.892124	-0.273737	0.000000
4	6	0	0.000000	0.932655	0.000000
5	6	0	-2.213135	0.206066	0.000000
6	6	0	-0.845715	2.055361	0.000000
7	6	0	0.783980	-2.154284	0.000000
8	6	0	2.289510	-0.117706	0.000000
9	6	0	-0.504039	-1.610712	0.000000
10	6	0	1.391677	0.954120	0.000000
11	1	0	2.889232	-2.135758	0.000000
12	1	0	-3.050078	2.255322	0.000000
13	1	0	1.841690	1.946980	0.000000
14	1	0	-1.321243	-2.332451	0.000000
15	1	0	-0.513611	3.086934	0.000000
16	1	0	-3.102399	-0.413267	0.000000
17	1	0	3.343634	0.150864	0.000000
18	1	0	0.836671	-3.240798	0.000000

a Number of imaginary frequencies = 0

Table S5. Cartesian Coordinates of the Optimized Structure for **1H$^+$** (C_s) Protonated at C(1) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.276538	1.481963	0.000000
2	6	0	-2.084997	-1.479510	0.000000
3	6	0	0.000000	0.859735	0.000000
4	6	0	0.833573	-0.302812	0.000000
5	6	0	0.902061	2.070511	0.000000
6	6	0	2.218587	0.129479	0.000000
7	6	0	-2.317450	-0.108595	0.000000
8	6	0	-0.856404	-2.165455	0.000000
9	6	0	-1.382461	0.942243	0.000000
10	6	0	0.434120	-1.652333	0.000000
11	1	0	-2.971069	-2.109298	0.000000
12	1	0	3.180930	2.079637	0.000000
13	1	0	1.239226	-2.383747	0.000000
14	1	0	-1.803416	1.945822	0.000000
15	1	0	3.061595	-0.551624	0.000000
16	1	0	-0.929071	-3.250345	0.000000
17	1	0	-3.361218	0.195434	0.000000
18	1	0	0.720812	2.711380	0.876477
19	1	0	0.720812	2.711380	-0.876477

a Number of imaginary frequencies = 0

Table S6. Cartesian Coordinates of the Optimized Structure for $\mathbf{1}^{2+}$ (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.257432	1.609472	0.000000
2	6	0	2.067852	-1.474055	0.000000
3	6	0	-0.827282	-0.285422	0.000000
4	6	0	0.000000	0.874770	0.000000
5	6	0	-2.236594	0.215984	0.000000
6	6	0	-0.933223	2.043900	0.000000
7	6	0	0.840440	-2.151499	0.000000
8	6	0	2.307977	-0.092875	0.000000
9	6	0	-0.482204	-1.620937	0.000000
10	6	0	1.374945	0.984316	0.000000
11	1	0	2.953673	-2.105617	0.000000
12	1	0	-3.140281	2.239001	0.000000
13	1	0	1.804337	1.984408	0.000000
14	1	0	-1.287515	-2.353233	0.000000
15	1	0	-0.604003	3.081781	0.000000
16	1	0	-3.110753	-0.433149	0.000000
17	1	0	3.355753	0.203543	0.000000
18	1	0	0.901920	-3.238653	0.000000

a Number of imaginary frequencies = 0

Table S7. Cartesian Coordinates of the Optimized Structure for **2** (C_1) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.169273	-1.150096	-0.000088
2	6	0	1.374102	1.344590	0.000051
3	6	0	-1.674270	0.573189	-0.000023
4	6	0	-0.935832	-0.733066	-0.000076
5	6	0	-3.038223	0.251884	-0.000052
6	6	0	-1.911016	-1.764487	-0.000117
7	6	0	0.245027	2.170816	0.000064
8	6	0	1.508456	-0.048141	-0.000035
9	6	0	-1.123086	1.864517	0.000023
10	6	0	0.434820	-0.954630	-0.000060
11	1	0	2.313142	1.896549	0.000108
12	1	0	-4.113666	-1.686712	-0.000164
13	1	0	0.722924	-2.006100	-0.000070
14	6	0	-2.087425	3.034480	0.000063
15	6	0	-1.652202	-3.244419	0.000159
16	1	0	-3.858427	0.957815	-0.000101
17	6	0	2.926559	-0.631751	-0.000044
18	1	0	0.473983	3.234817	0.000119
19	1	0	-2.596512	-3.798769	-0.003222
20	1	0	-1.081406	-3.568972	-0.880533
21	1	0	-1.087343	-3.569692	0.884445
22	1	0	-2.739756	3.004998	0.880988
23	1	0	-1.559661	3.991782	0.000125
24	1	0	-2.739719	3.005090	-0.880893
25	6	0	3.712947	-0.254798	-1.270161
26	6	0	3.712861	-0.254916	1.270165
27	1	0	2.821355	-1.724548	-0.000103
28	1	0	3.174705	-0.560078	2.174210
29	1	0	4.694245	-0.744340	1.274935
30	1	0	3.883080	0.826563	1.332252
31	1	0	3.883328	0.826666	-1.332069
32	1	0	4.694267	-0.744350	-1.274973
33	1	0	3.174789	-0.559740	-2.174278

a Number of imaginary frequencies = 0

Table S8. Cartesian Coordinates of the Optimized Structure for **2H$^+$** (C_1) Protonated at C(3) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.142042	-1.229475	-0.000157
2	6	0	1.414976	1.352853	0.000049
3	6	0	-1.604322	0.558854	-0.000028
4	6	0	-0.916012	-0.692478	-0.000070
5	6	0	-3.084391	0.262391	-0.000056
6	6	0	-1.904406	-1.778345	-0.000170
7	6	0	0.293758	2.165150	0.000037
8	6	0	1.540389	-0.057451	0.000056
9	6	0	-1.088825	1.853918	0.000022
10	6	0	0.466003	-0.945929	0.000012
11	1	0	2.356109	1.896301	0.000079
12	1	0	-4.073524	-1.785021	-0.000232
13	1	0	0.736030	-1.999036	0.000040
14	6	0	-2.054885	3.017741	0.000056
15	6	0	-1.562371	-3.238013	-0.000223
16	6	0	2.950966	-0.638349	0.000147
17	1	0	0.513902	3.230101	0.000051
18	1	0	-2.470511	-3.845648	-0.000906
19	1	0	-0.975228	-3.514950	-0.884484
20	1	0	-0.976353	-3.515242	0.884699
21	1	0	-2.706188	2.989801	0.881491
22	1	0	-1.531801	3.975715	0.000107
23	1	0	-2.706157	2.989879	-0.881404
24	6	0	3.725672	-0.246524	-1.275870
25	6	0	3.725603	-0.246281	1.276130
26	1	0	2.848180	-1.729770	0.000245
27	1	0	3.190564	-0.546538	2.182948
28	1	0	4.699715	-0.745214	1.277314
29	1	0	3.909702	0.832704	1.328889
30	1	0	3.909792	0.832447	-1.328820
31	1	0	4.699776	-0.745472	-1.276916
32	1	0	3.190672	-0.546940	-2.182660
33	1	0	-3.587686	0.699318	-0.875779
34	1	0	-3.587676	0.699198	0.875734

a Number of imaginary frequencies = 0

Table S9. Cartesian Coordinates of the Optimized Structure for **8** (C_1) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.886434	1.325791	-0.188482
2	6	0	0.593890	1.883160	-0.150986
3	6	0	-0.534483	1.190887	0.285466
4	6	0	2.388679	0.000198	-0.143786
5	6	0	1.886875	-1.325519	-0.188089
6	6	0	0.594338	-1.883063	-0.151121
7	6	0	-0.534248	-1.190938	0.285074
8	6	0	-1.846404	1.233929	-0.214481
9	6	0	-2.527689	-0.000175	-0.330700
10	6	0	-1.846208	-1.234175	-0.214643
11	6	0	-0.299567	-0.000092	1.163669
12	1	0	2.668954	2.047823	-0.421049
13	1	0	0.483978	2.887103	-0.562815
14	1	0	3.474664	0.000364	-0.239130
15	1	0	2.669697	-2.047456	-0.419954
16	1	0	0.484734	-2.887055	-0.562936
17	1	0	-2.234245	2.101594	-0.743990
18	1	0	-3.508984	-0.000288	-0.799998
19	1	0	-2.234004	-2.101759	-0.744316
20	1	0	0.684685	-0.000047	1.626027
21	1	0	-1.059180	-0.000296	1.956638

a Number of imaginary frequencies = 0

Table S10. Cartesian Coordinates of the Optimized Structure for **8H$^+$** (C_1) Protonated at C(1) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.039630	1.217971	-0.157214
2	6	0	0.730950	1.702142	-0.241741
3	6	0	-0.415968	1.077642	0.245660
4	6	0	2.524676	-0.103066	-0.039367
5	6	0	1.892649	-1.343075	-0.212993
6	6	0	0.528601	-1.681591	-0.314321
7	6	0	-0.540021	-1.031538	0.276915
8	6	0	-1.771468	1.299123	-0.250637
9	6	0	-2.551701	0.208604	-0.392335
10	6	0	-1.974062	-1.175345	-0.157447
11	6	0	-0.318224	0.018037	1.306466
12	1	0	2.817145	1.952974	-0.357360
13	1	0	0.595709	2.658519	-0.745663
14	1	0	3.610051	-0.166069	-0.015725
15	1	0	2.579856	-2.158062	-0.434316
16	1	0	0.298594	-2.578299	-0.889709
17	1	0	-2.091833	2.288331	-0.565284
18	1	0	-3.573173	0.278990	-0.754279
19	1	0	0.650825	-0.032111	1.799418
20	1	0	-1.134109	0.092142	2.027642
21	1	0	-2.067619	-1.780764	-1.067637
22	1	0	-2.555820	-1.689071	0.625005

a Number of imaginary frequencies = 0

Table S11. Cartesian Coordinates of the Optimized Structure for $\mathbf{8}^{2+}$ (C_1) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.941787	-1.276329	-0.194954
2	6	0	-0.585051	-1.660049	-0.314824
3	6	0	0.502444	-1.042145	0.287312
4	6	0	-2.515618	-0.000098	-0.037878
5	6	0	-1.942024	1.276140	-0.194916
6	6	0	-0.585269	1.660099	-0.314645
7	6	0	0.502245	1.042137	0.287377
8	6	0	1.878797	-1.180460	-0.208480
9	6	0	2.597710	0.000136	-0.422563
10	6	0	1.878437	1.180624	-0.208650
11	6	0	0.356718	-0.000055	1.366159
12	1	0	-2.659460	-2.076357	-0.378211
13	1	0	-0.386051	-2.535846	-0.933489
14	1	0	-3.602415	-0.000252	0.007019
15	1	0	-2.659728	2.076151	-0.378120
16	1	0	-0.386378	2.536038	-0.933125
17	1	0	2.312574	-2.160606	-0.415101
18	1	0	3.626509	0.000275	-0.770089
19	1	0	2.312059	2.160803	-0.415447
20	1	0	-0.611565	-0.000198	1.864360
21	1	0	1.174831	-0.000003	2.088576

a Number of imaginary frequencies = 0

Table S12. Cartesian Coordinates of the Optimized Structure for **9** (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.614994	0.000000
2	6	0	-1.318123	-0.088168	0.000000
3	6	0	-2.598210	0.527440	0.000000
4	6	0	-2.059904	2.994797	0.000000
5	6	0	-2.923916	1.863068	0.000000
6	1	0	-2.566641	3.958182	0.000000
7	6	0	-0.685251	3.043232	0.000000
8	6	0	0.242470	1.963578	0.000000
9	1	0	-0.239776	4.035424	0.000000
10	1	0	1.290378	2.260292	0.000000
11	6	0	-1.081486	-1.449361	0.000000
12	6	0	1.005396	-0.425576	0.000000
13	6	0	0.332555	-1.686660	0.000000
14	6	0	1.081439	-2.877839	0.000000
15	6	0	2.407470	-0.369074	0.000000
16	6	0	3.130950	-1.554281	0.000000
17	6	0	2.467229	-2.800144	0.000000
18	1	0	-3.436592	-0.168466	0.000000
19	1	0	-3.986905	2.093393	0.000000
20	1	0	2.928286	0.585436	0.000000
21	1	0	4.216793	-1.525424	0.000000
22	1	0	-1.847215	-2.216944	0.000000
23	1	0	0.582730	-3.843550	0.000000
24	1	0	3.055247	-3.714385	0.000000

a Number of imaginary frequencies = 0

Table S13. Cartesian Coordinates of the Optimized Structure for **9H$^+$** (C_1) Protonated at C(10) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.575278	0.000000
2	6	0	1.290263	-0.136396	0.000000
3	6	0	2.689044	0.433661	0.000000
4	6	0	2.106629	2.971065	0.000000
5	6	0	2.948398	1.899859	0.000000
6	1	0	2.570791	3.953266	0.000000
7	6	0	0.681938	2.980935	0.000000
8	6	0	-0.249050	1.947717	0.000000
9	1	0	0.246811	3.978979	0.000000
10	1	0	-1.291067	2.253610	0.000000
11	6	0	1.020796	-1.471852	0.000000
12	6	0	-1.054039	-0.428901	0.000000
13	6	0	-0.431200	-1.702391	0.000000
14	6	0	-1.184216	-2.855794	0.000000
15	6	0	-2.442043	-0.310219	0.000000
16	6	0	-3.216175	-1.486390	0.000000
17	6	0	-2.599292	-2.731702	0.000000
18	1	0	4.011999	2.134509	0.000000
19	1	0	-2.934032	0.658219	0.000000
20	1	0	-4.298717	-1.416867	0.000000
21	1	0	1.762788	-2.263787	0.000000
22	1	0	-0.723647	-3.839007	0.000000
23	1	0	-3.207122	-3.631344	0.000000
24	1	0	3.247939	0.031604	0.862446
25	1	0	3.247939	0.031604	-0.862446

a Number of imaginary frequencies = 0

Table S14. Cartesian Coordinates of the Optimized Structure for **9^{2+}** (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.651388	0.000000
2	6	0	-1.282211	0.013195	0.000000
3	6	0	-2.556364	0.569179	0.000000
4	6	0	-2.047105	3.044343	0.000000
5	6	0	-2.897727	1.939291	0.000000
6	1	0	-2.533193	4.017321	0.000000
7	6	0	-0.637789	3.074178	0.000000
8	6	0	0.280946	2.013286	0.000000
9	1	0	-0.196384	4.068759	0.000000
10	1	0	1.329059	2.302997	0.000000
11	6	0	-1.048002	-1.440105	0.000000
12	6	0	1.015334	-0.437710	0.000000
13	6	0	0.311074	-1.696675	0.000000
14	6	0	1.009074	-2.940587	0.000000
15	6	0	2.384201	-0.420280	0.000000
16	6	0	3.072455	-1.681419	0.000000
17	6	0	2.402182	-2.911769	0.000000
18	1	0	-3.393228	-0.126540	0.000000
19	1	0	-3.963637	2.155979	0.000000
20	1	0	2.968239	0.495117	0.000000
21	1	0	4.159689	-1.672331	0.000000
22	1	0	-1.843403	-2.181342	0.000000
23	1	0	0.465595	-3.881779	0.000000
24	1	0	2.970854	-3.836075	0.000000

a Number of imaginary frequencies = 0

Table S15. Cartesian Coordinates of the Optimized Structure for **9A** (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.537152	-2.910883	0.000000
2	6	0	-1.339263	0.675549	0.000000
3	6	0	0.427121	-2.015236	0.000000
4	6	0	1.430775	-0.917535	0.000000
5	6	0	1.134718	-3.204918	0.000000
6	6	0	2.722903	-1.544774	0.000000
7	6	0	-1.724429	-0.710593	0.000000
8	6	0	0.000000	1.200190	0.000000
9	6	0	-0.978663	-1.860118	0.000000
10	6	0	1.213263	0.432583	0.000000
11	6	0	-2.406611	1.613577	0.000000
12	1	0	3.325234	-3.656327	0.000000
13	1	0	2.117027	1.042616	0.000000
14	1	0	-1.545318	-2.790968	0.000000
15	1	0	3.667426	-1.013840	0.000000
16	1	0	0.697786	-4.197134	0.000000
17	6	0	0.170395	2.611392	0.000000
18	1	0	-2.802541	-0.859051	0.000000
19	1	0	-3.422395	1.226671	0.000000
20	6	0	-2.202733	2.979049	0.000000
21	6	0	-0.892945	3.490331	0.000000
22	1	0	1.185811	2.999800	0.000000
23	1	0	-3.054182	3.654179	0.000000
24	1	0	-0.718934	4.562369	0.000000

a Number of imaginary frequencies = 0

Table S16. Cartesian Coordinates of the Optimized Structure for **9AH$^+$** (C_s) Protonated at C(3) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.386168	-3.049511	0.000000
2	6	0	-1.358593	0.734501	0.000000
3	6	0	0.368774	-1.958714	0.000000
4	6	0	1.356779	-0.927615	0.000000
5	6	0	1.043848	-3.239064	0.000000
6	6	0	2.717645	-1.592203	0.000000
7	6	0	-1.757098	-0.635202	0.000000
8	6	0	0.000000	1.231014	0.000000
9	6	0	-1.031409	-1.807816	0.000000
10	6	0	1.183706	0.436128	0.000000
11	6	0	-2.416835	1.682501	0.000000
12	1	0	3.136613	-3.832135	0.000000
13	1	0	2.104746	1.017393	0.000000
14	1	0	-1.610511	-2.727827	0.000000
15	1	0	0.528680	-4.192687	0.000000
16	6	0	0.200314	2.636975	0.000000
17	1	0	-2.836046	-0.774659	0.000000
18	1	0	-3.438670	1.315444	0.000000
19	6	0	-2.180022	3.041726	0.000000
20	6	0	-0.856132	3.524461	0.000000
21	1	0	1.218608	3.013896	0.000000
22	1	0	-3.012524	3.738182	0.000000
23	1	0	-0.667478	4.593376	0.000000
24	1	0	3.316853	-1.307031	0.877767
25	1	0	3.316853	-1.307031	-0.877767

a Number of imaginary frequencies = 0

Table S17. Cartesian Coordinates of the Optimized Structure for **9A**$^{2+}$ (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.587883	-2.924590	0.000000
2	6	0	-1.345938	0.655884	0.000000
3	6	0	0.461842	-1.961467	0.000000
4	6	0	1.430409	-0.879830	0.000000
5	6	0	1.240015	-3.218612	0.000000
6	6	0	2.725802	-1.513525	0.000000
7	6	0	-1.696189	-0.700661	0.000000
8	6	0	0.000000	1.221974	0.000000
9	6	0	-0.904135	-1.892000	0.000000
10	6	0	1.231050	0.480528	0.000000
11	6	0	-2.460968	1.560210	0.000000
12	1	0	3.404327	-3.636896	0.000000
13	1	0	2.129907	1.094327	0.000000
14	1	0	-1.463557	-2.824599	0.000000
15	1	0	3.672941	-0.979614	0.000000
16	1	0	0.796414	-4.209707	0.000000
17	6	0	0.123863	2.615995	0.000000
18	1	0	-2.767010	-0.895197	0.000000
19	1	0	-3.464668	1.144580	0.000000
20	6	0	-2.295142	2.938887	0.000000
21	6	0	-1.000483	3.468047	0.000000
22	1	0	1.113736	3.063038	0.000000
23	1	0	-3.160089	3.594820	0.000000
24	1	0	-0.850056	4.544203	0.000000

a Number of imaginary frequencies = 0

Table S18. Cartesian Coordinates of the Optimized Structure for **9B** (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.126981	-1.263629	0.000000
2	6	0	-2.065008	-0.809242	0.000000
3	6	0	0.907525	-1.752942	0.000000
4	6	0	1.048192	-0.262816	0.000000
5	6	0	2.229285	-2.305565	0.000000
6	6	0	2.414166	-0.022557	0.000000
7	6	0	-1.580359	-2.090150	0.000000
8	6	0	-1.415031	0.472194	0.000000
9	6	0	-0.229757	-2.518079	0.000000
10	6	0	0.000000	0.735661	0.000000
11	1	0	4.208115	-1.351501	0.000000
12	6	0	0.391850	2.104077	0.000000
13	1	0	-0.076520	-3.596950	0.000000
14	1	0	2.899886	0.944384	0.000000
15	1	0	2.450464	-3.366096	0.000000
16	6	0	-2.314295	1.579307	0.000000
17	1	0	-2.326220	-2.881875	0.000000
18	6	0	-1.891515	2.888183	0.000000
19	1	0	1.448843	2.340221	0.000000
20	6	0	-0.508600	3.147639	0.000000
21	1	0	-2.610220	3.702329	0.000000
22	1	0	-0.143732	4.171412	0.000000
23	1	0	-3.379655	1.363146	0.000000
24	1	0	-3.151559	-0.737555	0.000000

a Number of imaginary frequencies = 0

Table S19. Cartesian Coordinates of the Optimized Structure for **9BH$^+$** (C_s) Protonated at C(3) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.086524	-1.262268	0.000000
2	6	0	2.145766	-0.689926	0.000000
3	6	0	-0.782242	-1.725263	0.000000
4	6	0	-0.979585	-0.312486	0.000000
5	6	0	-2.133209	-2.403829	0.000000
6	6	0	-2.419424	-0.085060	0.000000
7	6	0	1.711045	-1.998752	0.000000
8	6	0	1.437554	0.546846	0.000000
9	6	0	0.387036	-2.464033	0.000000
10	6	0	0.000000	0.741910	0.000000
11	1	0	-4.164651	-1.375527	0.000000
12	6	0	-0.472715	2.083174	0.000000
13	1	0	0.265901	-3.545853	0.000000
14	1	0	-2.900433	0.882372	0.000000
15	6	0	2.276443	1.697763	0.000000
16	1	0	2.485585	-2.760522	0.000000
17	6	0	1.771358	2.978203	0.000000
18	1	0	-1.536541	2.273873	0.000000
19	6	0	0.376646	3.169661	0.000000
20	1	0	2.442166	3.831441	0.000000
21	1	0	-0.035007	4.174066	0.000000
22	1	0	3.351361	1.546769	0.000000
23	1	0	3.226963	-0.573233	0.000000
24	1	0	-2.264121	-3.054519	0.877761
25	1	0	-2.264121	-3.054519	-0.877761

a Number of imaginary frequencies = 0

Table S20. Cartesian Coordinates of the Optimized Structure for **9B^{2+}** (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.171673	-1.155899	0.000000
2	6	0	-2.091223	-0.856685	0.000000
3	6	0	0.877875	-1.704340	0.000000
4	6	0	0.990884	-0.264239	0.000000
5	6	0	2.215277	-2.218135	0.000000
6	6	0	2.479641	0.019067	0.000000
7	6	0	-1.592556	-2.142859	0.000000
8	6	0	-1.447538	0.428405	0.000000
9	6	0	-0.239860	-2.533648	0.000000
10	6	0	0.000000	0.712097	0.000000
11	1	0	4.248313	-1.277064	0.000000
12	6	0	0.414649	2.100722	0.000000
13	1	0	-0.047653	-3.605092	0.000000
14	1	0	2.934091	1.000904	0.000000
15	1	0	2.462002	-3.277862	0.000000
16	6	0	-2.323738	1.523393	0.000000
17	1	0	-2.324958	-2.945131	0.000000
18	6	0	-1.869328	2.851222	0.000000
19	1	0	1.468268	2.343699	0.000000
20	6	0	-0.490760	3.138134	0.000000
21	1	0	-2.593413	3.661873	0.000000
22	1	0	-0.145385	4.167244	0.000000
23	1	0	-3.394193	1.342076	0.000000
24	1	0	-3.177055	-0.794065	0.000000

a Number of imaginary frequencies = 0

Table S21. Cartesian Coordinates of the Optimized Structure for **10** (C_1) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.451401	1.737165	-0.325838
2	6	0	1.009160	1.781872	-0.220817
3	6	0	0.254205	0.890842	0.474153
4	6	0	3.348788	0.688693	-0.342850
5	6	0	3.285747	-0.765672	-0.364993
6	6	0	2.282325	-1.678298	-0.157153
7	6	0	0.976331	-1.335678	0.333684
8	6	0	-1.149160	0.540144	0.219589
9	6	0	-1.390083	-0.867365	0.024033
10	6	0	-0.238861	-1.759210	-0.116412
11	6	0	0.926157	-0.154301	1.289687
12	1	0	2.910373	2.701589	-0.546594
13	1	0	0.512539	2.558726	-0.804211
14	1	0	4.372537	1.028697	-0.500277
15	1	0	4.229000	-1.200321	-0.694450
16	1	0	2.488626	-2.714349	-0.425554
17	6	0	-2.205653	1.449080	0.096014
18	6	0	-2.705559	-1.279630	-0.257178
19	1	0	-0.332177	-2.612323	-0.785997
20	1	0	1.914339	0.140652	1.636718
21	1	0	0.310253	-0.422145	2.157104
22	6	0	-3.499843	1.004833	-0.164750
23	6	0	-3.748208	-0.362851	-0.335804
24	1	0	-2.011140	2.508999	0.240435
25	1	0	-2.900722	-2.337181	-0.419748
26	1	0	-4.315785	1.719593	-0.228208
27	1	0	-4.758310	-0.709684	-0.537414

a Number of imaginary frequencies = 0

Table S22. Cartesian Coordinates of the Optimized Structure for **10H$^+$** (C_1) Protonated at C(10) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.526313	1.712290	-0.206654
2	6	0	1.133372	1.709625	-0.109400
3	6	0	0.335266	0.716807	0.458336
4	6	0	3.446261	0.641013	-0.254182
5	6	0	3.248927	-0.727032	-0.479399
6	6	0	2.070964	-1.501726	-0.475339
7	6	0	0.939149	-1.296782	0.292236
8	6	0	-1.083291	0.503997	0.166732
9	6	0	-1.479913	-0.849059	0.024676
10	6	0	-0.398574	-1.933805	0.036635
11	6	0	0.932668	-0.294313	1.391889
12	1	0	2.971384	2.680581	-0.429570
13	1	0	0.616959	2.572876	-0.527679
14	1	0	4.482211	0.958485	-0.346738
15	1	0	4.134118	-1.246710	-0.842916
16	1	0	2.076527	-2.385839	-1.112528
17	6	0	-2.024576	1.535836	0.018503
18	6	0	-2.817976	-1.144015	-0.227412
19	1	0	1.919321	-0.026881	1.766016
20	1	0	0.250410	-0.553840	2.203658
21	6	0	-3.358021	1.222440	-0.223324
22	6	0	-3.753779	-0.113779	-0.342697
23	1	0	-1.722795	2.571750	0.143155
24	1	0	-3.130463	-2.176778	-0.356421
25	1	0	-4.091204	2.017582	-0.313165
26	1	0	-4.793898	-0.354342	-0.539987
27	1	0	-0.400641	-2.490269	-0.907218
28	1	0	-0.612681	-2.655592	0.839785

a Number of imaginary frequencies = 0

Table S23. Cartesian Coordinates of the Optimized Structure for $\mathbf{10^{2+}}$ (C_1) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.553580	1.636482	-0.364381
2	6	0	1.150931	1.651889	-0.291781
3	6	0	0.339993	0.781664	0.428327
4	6	0	3.478393	0.569117	-0.260103
5	6	0	3.285508	-0.817830	-0.342377
6	6	0	2.089381	-1.568436	-0.322455
7	6	0	0.924733	-1.231485	0.355496
8	6	0	-1.107972	0.555308	0.166424
9	6	0	-1.443447	-0.846479	-0.040215
10	6	0	-0.386901	-1.749606	-0.006663
11	6	0	0.899858	-0.164280	1.431068
12	1	0	3.003875	2.575773	-0.683382
13	1	0	0.652034	2.451879	-0.839276
14	1	0	4.517427	0.878679	-0.346801
15	1	0	4.179001	-1.384094	-0.602760
16	1	0	2.086501	-2.493123	-0.900012
17	6	0	-2.102209	1.500857	0.118130
18	6	0	-2.796056	-1.227622	-0.314843
19	1	0	-0.522184	-2.799920	-0.264188
20	1	0	1.889379	0.090147	1.806567
21	1	0	0.214898	-0.403851	2.245742
22	6	0	-3.441832	1.084759	-0.130859
23	6	0	-3.786937	-0.259535	-0.339637
24	1	0	-1.894191	2.554082	0.279989
25	1	0	-3.030787	-2.271493	-0.505885
26	1	0	-4.218971	1.844034	-0.171497
27	1	0	-4.819132	-0.530937	-0.535283

a Number of imaginary frequencies = 0

Table S24. Cartesian Coordinates of the Optimized Structure for **10A** (C_1) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.129924	-0.707179	-0.133632
2	6	0	0.117788	-1.472684	-0.246690
3	6	0	1.302496	-1.162045	0.330205
4	6	0	-1.307062	0.730862	-0.076999
5	6	0	-0.363316	1.857671	-0.261760
6	6	0	0.987638	2.055058	-0.183329
7	6	0	1.938137	1.078533	0.262058
8	6	0	2.623062	-1.607603	-0.110525
9	6	0	3.558460	-0.622457	-0.309124
10	6	0	3.145144	0.773116	-0.305729
11	6	0	1.404310	0.031662	1.212937
12	6	0	-2.290918	-1.519971	-0.159755
13	1	0	0.056968	-2.368226	-0.866792
14	6	0	-2.650311	1.189059	0.030964
15	1	0	-0.902133	2.743533	-0.593877
16	1	0	1.359498	3.009509	-0.556448
17	1	0	2.813825	-2.634378	-0.412157
18	1	0	4.535945	-0.882084	-0.708714
19	1	0	3.648548	1.460141	-0.983767
20	1	0	0.458202	0.323924	1.665847
21	1	0	2.135924	-0.151452	2.010116
22	1	0	-2.145131	-2.594058	-0.245860
23	6	0	-3.576308	-1.024646	-0.040094
24	6	0	-3.754737	0.358312	0.072104
25	1	0	-2.811260	2.262869	0.077574
26	1	0	-4.427152	-1.700139	-0.035935
27	1	0	-4.749977	0.784221	0.166232

a Number of imaginary frequencies = 0

Table S25. Cartesian Coordinates of the Optimized Structure for **10AH$^+$** (C_1) Protonated at C(3) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.148382	-0.673326	-0.149103
2	6	0	0.130880	-1.334878	-0.290044
3	6	0	1.315137	-1.034599	0.317068
4	6	0	-1.402753	0.755168	-0.036617
5	6	0	-0.487779	1.844174	-0.264240
6	6	0	0.892807	1.934813	-0.322713
7	6	0	1.810519	1.029146	0.224820
8	6	0	2.659479	-1.593345	-0.082454
9	6	0	3.604894	-0.441681	-0.357719
10	6	0	3.168830	0.833443	-0.262614
11	6	0	1.400427	0.087236	1.305643
12	6	0	-2.269343	-1.538510	-0.221534
13	1	0	0.114859	-2.236374	-0.902691
14	6	0	-2.762892	1.171092	0.091435
15	1	0	-0.998629	2.758909	-0.559351
16	1	0	1.302328	2.786465	-0.863555
17	1	0	4.603924	-0.672173	-0.717185
18	1	0	3.755120	1.674702	-0.621778
19	1	0	0.452461	0.333777	1.780588
20	1	0	2.186406	-0.060728	2.048944
21	1	0	-2.086523	-2.599640	-0.362534
22	6	0	-3.565022	-1.090626	-0.055248
23	6	0	-3.814425	0.283264	0.121334
24	1	0	-2.964259	2.235854	0.162910
25	1	0	-4.388106	-1.798376	-0.067298
26	1	0	-4.830382	0.644675	0.243836
27	1	0	3.071494	-2.223355	0.722130
28	1	0	2.587048	-2.231974	-0.972099

a Number of imaginary frequencies = 0

Table S26. Cartesian Coordinates of the Optimized Structure for **10A**$^{2+}$ (C_1) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.144141	-0.708704	-0.130562
2	6	0	0.111973	-1.441307	-0.224075
3	6	0	1.308301	-1.106193	0.365666
4	6	0	-1.332903	0.749353	-0.079467
5	6	0	-0.395675	1.791364	-0.285546
6	6	0	1.030059	1.831609	-0.390435
7	6	0	1.900121	1.031708	0.304825
8	6	0	2.536502	-1.526937	-0.233915
9	6	0	3.595852	-0.582502	-0.344634
10	6	0	3.270730	0.749543	-0.161040
11	6	0	1.425014	0.058688	1.323744
12	6	0	-2.287493	-1.513075	-0.164912
13	1	0	0.088292	-2.335874	-0.846528
14	6	0	-2.685460	1.231244	0.013034
15	1	0	-0.859082	2.756776	-0.488955
16	1	0	1.429323	2.591148	-1.062576
17	1	0	2.625052	-2.501421	-0.713347
18	1	0	4.561245	-0.875925	-0.744819
19	1	0	3.954328	1.545529	-0.452208
20	1	0	0.479464	0.322428	1.794390
21	1	0	2.174339	-0.138383	2.095918
22	1	0	-2.173060	-2.587384	-0.278668
23	6	0	-3.585502	-0.989593	-0.008726
24	6	0	-3.783460	0.389180	0.096733
25	1	0	-2.847079	2.305369	0.012837
26	1	0	-4.433360	-1.668857	0.003813
27	1	0	-4.782957	0.800318	0.196009

a Number of imaginary frequencies = 0

Table S27. Cartesian Coordinates of the Optimized Structure for **10B** (C_1) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.833978	2.412705	-0.235953
2	6	0	-2.090499	1.702375	-0.312268
3	6	0	-2.330511	0.504395	0.285787
4	6	0	0.476009	2.020940	-0.065173
5	6	0	1.295231	0.798730	0.025644
6	6	0	0.907702	-0.584250	0.128186
7	6	0	-0.482079	-0.953466	0.323430
8	6	0	-3.228353	-0.532183	-0.205012
9	6	0	-2.650945	-1.760092	-0.412221
10	6	0	-1.204591	-1.909522	-0.328369
11	6	0	-1.308968	-0.048842	1.214669
12	1	0	-0.924481	3.478343	-0.449995
13	1	0	-2.851244	2.144775	-0.957117
14	1	0	1.138882	2.884892	-0.100939
15	6	0	2.689274	1.053297	-0.094002
16	6	0	1.894645	-1.588722	0.042884
17	1	0	-4.228796	-0.312575	-0.569333
18	1	0	-3.232753	-2.555682	-0.871595
19	1	0	-0.728343	-2.639545	-0.979592
20	1	0	-0.711944	0.718648	1.704491
21	1	0	-1.796540	-0.661506	1.985059
22	1	0	3.016921	2.088017	-0.157210
23	6	0	3.641109	0.051294	-0.155844
24	6	0	3.238964	-1.290136	-0.100259
25	1	0	1.573681	-2.623199	0.127979
26	1	0	4.692679	0.307697	-0.249871
27	1	0	3.973875	-2.089004	-0.150866

a Number of imaginary frequencies = 0

Table S28. Cartesian Coordinates of the Optimized Structure for **10BH$^+$** (C_1) Protonated at C(3) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.540355	2.473091	-0.348521
2	6	0	-1.731234	1.725734	-0.567744
3	6	0	-2.122795	0.610900	0.127779
4	6	0	0.719220	2.073701	0.056352
5	6	0	1.392118	0.798276	0.149555
6	6	0	0.804090	-0.525359	0.086858
7	6	0	-0.550702	-0.791181	0.432385
8	6	0	-3.207984	-0.339774	-0.299159
9	6	0	-2.631463	-1.736913	-0.320585
10	6	0	-1.328728	-1.938050	-0.026017
11	6	0	-1.328409	0.136393	1.305399
12	1	0	-0.606594	3.523870	-0.625346
13	1	0	-2.421546	2.120992	-1.312873
14	1	0	1.417101	2.903459	0.146021
15	6	0	2.808165	0.880025	0.097424
16	6	0	1.645989	-1.634021	-0.216646
17	1	0	-3.265956	-2.552974	-0.654716
18	1	0	-0.864909	-2.903306	-0.196839
19	1	0	-0.735246	0.915370	1.780750
20	1	0	-1.936337	-0.402053	2.035429
21	1	0	3.271588	1.859119	0.171746
22	6	0	3.603482	-0.230760	-0.105918
23	6	0	3.014998	-1.496342	-0.292562
24	1	0	1.210546	-2.621416	-0.309697
25	1	0	4.682679	-0.121822	-0.149025
26	1	0	3.637544	-2.365870	-0.477506
27	1	0	-4.053248	-0.303136	0.407170
28	1	0	-3.613965	-0.086562	-1.286720

a Number of imaginary frequencies = 0

Table S29. Cartesian Coordinates of the Optimized Structure for **10B**$^{2+}$ (C_1) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.635086	2.542533	-0.261920
2	6	0	-1.791949	1.793437	-0.555753
3	6	0	-2.112300	0.564382	0.037949
4	6	0	0.623207	2.109166	0.146728
5	6	0	1.295253	0.821135	0.187307
6	6	0	0.713934	-0.522407	0.141821
7	6	0	-0.563416	-0.829296	0.628527
8	6	0	-2.837254	-0.412800	-0.660646
9	6	0	-2.530058	-1.799095	-0.402855
10	6	0	-1.360860	-2.047674	0.252903
11	6	0	-1.405980	0.132858	1.341225
12	1	0	-0.686520	3.600270	-0.516521
13	1	0	-2.465033	2.182895	-1.320718
14	1	0	1.324405	2.930554	0.279375
15	6	0	2.693441	0.905398	0.065057
16	6	0	1.544419	-1.627642	-0.228563
17	1	0	-3.557234	-0.136850	-1.430392
18	1	0	-3.173152	-2.595415	-0.765035
19	1	0	-1.039466	-3.053458	0.513961
20	1	0	-0.889450	0.958713	1.826159
21	1	0	-2.124534	-0.332994	2.021951
22	1	0	3.172874	1.878021	0.125612
23	6	0	3.492054	-0.216680	-0.208708
24	6	0	2.912912	-1.477332	-0.399232
25	1	0	1.111164	-2.620412	-0.287434
26	1	0	4.567286	-0.092227	-0.301324
27	1	0	3.529770	-2.334998	-0.648680

a Number of imaginary frequencies = 0

Table S30. Cartesian Coordinates of the Optimized Structure for **11** (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.759575	-0.551994	0.000000
2	6	0	-0.419440	-1.346541	0.000000
3	6	0	2.727238	-1.616299	0.000000
4	6	0	2.510041	-0.148682	0.000000
5	6	0	4.109325	-1.814998	0.000000
6	6	0	3.803541	0.454370	0.000000
7	6	0	0.374103	-2.521392	0.000000
8	6	0	0.000000	0.035619	0.000000
9	6	0	1.749068	-2.631569	0.000000
10	6	0	1.313621	0.540563	0.000000
11	1	0	5.833896	-0.403591	0.000000
12	1	0	1.412643	1.625470	0.000000
13	1	0	2.142564	-3.648093	0.000000
14	1	0	3.987669	1.522691	0.000000
15	1	0	4.600298	-2.781909	0.000000
16	6	0	-1.193235	0.851977	0.000000
17	1	0	-0.185383	-3.454811	0.000000
18	6	0	-1.841041	-1.370252	0.000000
19	1	0	-2.439075	-2.274827	0.000000
20	6	0	-2.347512	-0.078692	0.000000
21	6	0	-1.237203	2.232186	0.000000
22	6	0	-3.721389	0.257335	0.000000
23	1	0	-0.278160	2.745571	0.000000
24	6	0	-2.358474	3.093304	0.000000
25	6	0	-4.317417	1.501891	0.000000
26	1	0	-4.398210	-0.596347	0.000000
27	1	0	-2.121109	4.155051	0.000000
28	6	0	-3.704206	2.776794	0.000000
29	1	0	-5.405311	1.506709	0.000000
30	1	0	-4.389397	3.622370	0.000000

a Number of imaginary frequencies = 0

Table S31. Cartesian Coordinates of the Optimized Structure for **11H$^+$** (C_s) Protonated at C(3) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.918759	-3.837349	0.000000
2	6	0	-1.287748	-0.623365	0.000000
3	6	0	0.774865	-3.005837	0.000000
4	6	0	1.614569	-1.867605	0.000000
5	6	0	1.613927	-4.193631	0.000000
6	6	0	3.049988	-2.347296	0.000000
7	6	0	-1.538829	-2.022705	0.000000
8	6	0	0.000000	0.054600	0.000000
9	6	0	-0.644551	-3.065359	0.000000
10	6	0	1.269220	-0.516867	0.000000
11	1	0	3.765790	-4.513543	0.000000
12	1	0	2.112891	0.170664	0.000000
13	1	0	-1.071381	-4.065425	0.000000
14	1	0	1.222081	-5.204476	0.000000
15	6	0	-0.276824	1.482022	0.000000
16	1	0	-2.591657	-2.297658	0.000000
17	6	0	-2.302817	0.348011	0.000000
18	1	0	-3.365284	0.137212	0.000000
19	6	0	-1.735743	1.628135	0.000000
20	6	0	0.674820	2.485725	0.000000
21	6	0	-2.481559	2.830441	0.000000
22	1	0	1.715719	2.170858	0.000000
23	6	0	0.491920	3.883450	0.000000
24	6	0	-2.025814	4.133371	0.000000
25	1	0	-3.562136	2.701311	0.000000
26	1	0	1.405851	4.471247	0.000000
27	6	0	-0.692026	4.602369	0.000000
28	1	0	-2.791642	4.904490	0.000000
29	1	0	-0.583349	5.684519	0.000000
30	1	0	3.605090	-1.983930	0.878195
31	1	0	3.605090	-1.983930	-0.878195

a Number of imaginary frequencies = 0

Table S32. Cartesian Coordinates of the Optimized Structure for **11H$_2^{2+}$** (C_s) Diprotonated at C(1) and C(10) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.147612	-4.274728	0.000000
2	6	0	1.373383	-0.355062	0.000000
3	6	0	-0.088940	-3.127294	0.000000
4	6	0	-1.180917	-2.195933	0.000000
5	6	0	-0.674400	-4.513852	0.000000
6	6	0	-2.418235	-2.943752	0.000000
7	6	0	1.927283	-1.627889	0.000000
8	6	0	0.000000	0.032326	0.000000
9	6	0	1.273454	-2.873034	0.000000
10	6	0	-1.124117	-0.788134	0.000000
11	1	0	-2.882731	-5.071952	0.000000
12	1	0	-2.096513	-0.303210	0.000000
13	1	0	1.926972	-3.743122	0.000000
14	1	0	-3.403232	-2.491345	0.000000
15	6	0	-0.060382	1.522180	0.000000
16	1	0	3.014350	-1.674666	0.000000
17	6	0	2.237980	0.880067	0.000000
18	6	0	1.264693	2.027824	0.000000
19	6	0	-1.250058	2.264062	0.000000
20	6	0	1.704498	3.354085	0.000000
21	1	0	-2.179779	1.702664	0.000000
22	6	0	-1.418210	3.651059	0.000000
23	6	0	0.945046	4.527825	0.000000
24	1	0	2.783823	3.494354	0.000000
25	1	0	-2.450272	3.993371	0.000000
26	6	0	-0.448450	4.661196	0.000000
27	1	0	1.511911	5.455821	0.000000
28	1	0	-0.828417	5.680127	0.000000
29	1	0	2.899799	0.916419	0.878122
30	1	0	2.899799	0.916419	-0.878122
31	1	0	-0.342906	-5.100279	0.872797
32	1	0	-0.342906	-5.100279	-0.872797

a Number of imaginary frequencies = 0

Table S33. Cartesian Coordinates of the Optimized Structure for **11**$^{2+}$ (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.836424	0.011151	0.000000
2	6	0	-0.219407	-1.355403	0.000000
3	6	0	2.897642	-1.240063	0.000000
4	6	0	2.501626	0.179375	0.000000
5	6	0	4.371630	-1.270465	0.000000
6	6	0	3.698543	0.908189	0.000000
7	6	0	0.695719	-2.412695	0.000000
8	6	0	0.000000	0.086361	0.000000
9	6	0	2.114632	-2.369235	0.000000
10	6	0	1.221499	0.750584	0.000000
11	1	0	5.872236	0.327555	0.000000
12	1	0	1.205598	1.837964	0.000000
13	1	0	2.620167	-3.331625	0.000000
14	1	0	3.769898	1.991669	0.000000
15	1	0	4.959250	-2.181031	0.000000
16	6	0	-1.304917	0.705535	0.000000
17	1	0	0.262607	-3.411620	0.000000
18	6	0	-1.616235	-1.590595	0.000000
19	1	0	-2.086310	-2.568206	0.000000
20	6	0	-2.305073	-0.354518	0.000000
21	6	0	-1.555734	2.091039	0.000000
22	6	0	-3.708752	-0.264795	0.000000
23	1	0	-0.687743	2.744896	0.000000
24	6	0	-2.779569	2.747577	0.000000
25	6	0	-4.507071	0.881490	0.000000
26	1	0	-4.239833	-1.214866	0.000000
27	1	0	-2.727242	3.833385	0.000000
28	6	0	-4.088139	2.213413	0.000000
29	1	0	-5.580997	0.715588	0.000000
30	1	0	-4.884545	2.954624	0.000000

a Number of imaginary frequencies = 0

Table S34. Cartesian Coordinates of the Optimized Structure for **12** (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000369	1.671784	0.000000
2	6	0	4.329799	-1.304602	0.000000
3	6	0	2.184993	1.032284	0.000000
4	6	0	1.351258	-0.218732	0.000000
5	6	0	1.333646	2.139642	0.000000
6	6	0	0.000000	0.236280	0.000000
7	6	0	4.533038	0.092656	0.000000
8	6	0	3.137580	-2.008263	0.000000
9	6	0	3.594310	1.108099	0.000000
10	6	0	1.811931	-1.523447	0.000000
11	1	0	5.235785	-1.907820	0.000000
12	6	0	-1.334781	2.138902	0.000000
13	1	0	1.048167	-2.297481	0.000000
14	1	0	3.992531	2.122331	0.000000
15	6	0	-1.351204	-0.219432	0.000000
16	1	0	1.662628	3.172173	0.000000
17	1	0	3.228588	-3.092720	0.000000
18	1	0	5.573110	0.412660	0.000000
19	6	0	-2.185444	1.031185	0.000000
20	1	0	-1.664271	3.171274	0.000000
21	6	0	-3.594962	1.106271	0.000000
22	6	0	-1.811119	-1.524286	0.000000
23	6	0	-4.533048	0.090441	0.000000
24	6	0	-3.136653	-2.009860	0.000000
25	6	0	-4.329104	-1.306883	0.000000
26	1	0	-5.234853	-1.910452	0.000000
27	1	0	-3.993624	2.120329	0.000000
28	1	0	-5.573318	0.409808	0.000000
29	1	0	-1.046990	-2.297953	0.000000
30	1	0	-3.226987	-3.094375	0.000000

a Number of imaginary frequencies = 0

Table S35. Cartesian Coordinates of the Optimized Structure for **12H$^+$** (C_s) Protonated at C(11) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.009465	1.689452	0.000000
2	6	0	-4.255966	-1.505485	0.000000
3	6	0	-2.231468	0.902718	0.000000
4	6	0	-1.330737	-0.234516	0.000000
5	6	0	-1.416034	2.191350	0.000000
6	6	0	0.000000	0.262997	0.000000
7	6	0	-4.524234	-0.154260	0.000000
8	6	0	-2.990302	-2.145018	0.000000
9	6	0	-3.606607	0.926465	0.000000
10	6	0	-1.724128	-1.601665	0.000000
11	1	0	-5.115916	-2.170041	0.000000
12	6	0	1.277661	2.184360	0.000000
13	1	0	-0.915182	-2.324544	0.000000
14	1	0	-4.060345	1.915842	0.000000
15	6	0	1.368493	-0.175463	0.000000
16	1	0	-3.026986	-3.231971	0.000000
17	1	0	-5.573933	0.128741	0.000000
18	6	0	2.166737	1.070865	0.000000
19	1	0	1.589894	3.221139	0.000000
20	6	0	3.562612	1.192556	0.000000
21	6	0	1.850248	-1.477237	0.000000
22	6	0	4.532017	0.195511	0.000000
23	6	0	3.177721	-1.933064	0.000000
24	6	0	4.358555	-1.196867	0.000000
25	1	0	5.275488	-1.781536	0.000000
26	1	0	3.935564	2.215037	0.000000
27	1	0	5.562643	0.540851	0.000000
28	1	0	1.106701	-2.269029	0.000000
29	1	0	3.295586	-3.013568	0.000000
30	1	0	-1.652068	2.806443	0.879182
31	1	0	-1.652068	2.806443	-0.879182

a Number of imaginary frequencies = 0

Table S36. Cartesian Coordinates of the Optimized Structure for **12H$_2^{2+}$** (C_s) Diprotonated at C(11) and C(12) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000020	1.655469	0.000000
2	6	0	-4.319886	-1.395509	0.000000
3	6	0	-2.231768	0.950050	0.000000
4	6	0	-1.383719	-0.204942	0.000000
5	6	0	-1.377978	2.206147	0.000000
6	6	0	0.000000	0.288823	0.000000
7	6	0	-4.556154	-0.021684	0.000000
8	6	0	-3.087222	-2.066739	0.000000
9	6	0	-3.619487	1.023504	0.000000
10	6	0	-1.793136	-1.547701	0.000000
11	1	0	-5.201984	-2.031095	0.000000
12	6	0	1.377919	2.206174	0.000000
13	1	0	-1.009222	-2.297269	0.000000
14	1	0	-4.040058	2.027383	0.000000
15	6	0	1.383724	-0.204900	0.000000
16	1	0	-3.149841	-3.152333	0.000000
17	1	0	-5.599831	0.283257	0.000000
18	6	0	2.231741	0.950122	0.000000
19	6	0	3.619457	1.023601	0.000000
20	6	0	1.793178	-1.547652	0.000000
21	6	0	4.556155	-0.021567	0.000000
22	6	0	3.087273	-2.066658	0.000000
23	6	0	4.319926	-1.395394	0.000000
24	1	0	5.202038	-2.030960	0.000000
25	1	0	4.040009	2.027488	0.000000
26	1	0	5.599823	0.283408	0.000000
27	1	0	1.009278	-2.297235	0.000000
28	1	0	3.149921	-3.152249	0.000000
29	1	0	-1.585759	2.838159	0.877052
30	1	0	-1.585759	2.838159	-0.877052
31	1	0	1.585681	2.838206	-0.877044
32	1	0	1.585681	2.838206	0.877044

a Number of imaginary frequencies = 0

Table S37. Cartesian Coordinates of the Optimized Structure for **12**$^{2+}$ (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000646	1.648027	0.000000
2	6	0	-4.361802	-1.259146	0.000000
3	6	0	-2.189922	0.989277	0.000000
4	6	0	-1.353109	-0.226921	0.000000
5	6	0	-1.318673	2.129115	0.000000
6	6	0	0.000000	0.214865	0.000000
7	6	0	-4.559815	0.111159	0.000000
8	6	0	-3.143601	-1.997740	0.000000
9	6	0	-3.577007	1.122790	0.000000
10	6	0	-1.832998	-1.557282	0.000000
11	1	0	-5.263051	-1.867852	0.000000
12	6	0	1.317515	2.130371	0.000000
13	1	0	-1.082547	-2.341723	0.000000
14	1	0	-3.952432	2.144331	0.000000
15	6	0	1.352992	-0.225585	0.000000
16	1	0	-1.645976	3.163845	0.000000
17	1	0	-3.270258	-3.077596	0.000000
18	1	0	-5.591195	0.452872	0.000000
19	6	0	2.189078	0.991631	0.000000
20	1	0	1.643779	3.165413	0.000000
21	6	0	3.576314	1.126008	0.000000
22	6	0	1.834168	-1.555752	0.000000
23	6	0	4.559727	0.115219	0.000000
24	6	0	3.144974	-1.995079	0.000000
25	6	0	4.362570	-1.255267	0.000000
26	1	0	5.264325	-1.863245	0.000000
27	1	0	3.950904	2.147864	0.000000
28	1	0	5.590901	0.457527	0.000000
29	1	0	1.084297	-2.340755	0.000000
30	1	0	3.272668	-3.074802	0.000000

a Number of imaginary frequencies = 0

Table S38. Cartesian Coordinates of the Optimized Structure for **13** (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.570001	-0.540396	0.000000
2	6	0	-3.163283	1.280277	0.000000
3	6	0	-2.157506	2.229148	0.000000
4	6	0	-1.927269	-0.912668	0.000000
5	6	0	0.000000	0.784884	0.000000
6	6	0	-3.067288	-0.125315	0.000000
7	6	0	-0.687047	2.024726	0.000000
8	6	0	-0.112512	3.296615	0.000000
9	1	0	-4.013528	-0.660808	0.000000
10	6	0	1.417900	0.647399	0.000000
11	1	0	-2.120334	-1.983186	0.000000
12	6	0	0.528622	-1.488964	0.000000
13	6	0	0.420870	-2.863387	0.000000
14	6	0	1.774915	-0.690229	0.000000
15	6	0	3.107116	-1.176089	0.000000
16	1	0	3.872211	-0.400960	0.000000
17	6	0	3.561970	-2.476068	0.000000
18	1	0	-0.587152	-3.271024	0.000000
19	6	0	1.442604	-3.845011	0.000000
20	1	0	1.088009	-4.873431	0.000000
21	6	0	2.812508	-3.679486	0.000000
22	1	0	4.642553	-2.601096	0.000000
23	1	0	2.119458	1.472169	0.000000
24	1	0	3.402291	-4.593886	0.000000
25	1	0	-4.178501	1.676977	0.000000
26	6	0	-2.376903	3.638330	0.000000
27	1	0	-3.352608	4.110093	0.000000
28	6	0	-1.144407	4.273754	0.000000
29	1	0	0.948681	3.513769	0.000000
30	1	0	-0.982809	5.346270	0.000000

a Number of imaginary frequencies = 0

Table S39. Cartesian Coordinates of the Optimized Structure for **13H$^+$** (C_s) Protonated at C(3) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.561405	-0.598958	0.000000
2	6	0	3.150562	1.193752	0.000000
3	6	0	2.127749	2.146938	0.000000
4	6	0	1.897400	-0.986348	0.000000
5	6	0	0.000000	0.743611	0.000000
6	6	0	3.052773	-0.195159	0.000000
7	6	0	0.727661	1.970192	0.000000
8	6	0	0.102383	3.285870	0.000000
9	1	0	3.993993	-0.737593	0.000000
10	6	0	-1.402072	0.639180	0.000000
11	1	0	2.088168	-2.056365	0.000000
12	6	0	-0.564914	-1.524748	0.000000
13	6	0	-0.470929	-2.903672	0.000000
14	6	0	-1.779418	-0.708458	0.000000
15	6	0	-3.122087	-1.158585	0.000000
16	1	0	-3.871853	-0.369773	0.000000
17	6	0	-3.601648	-2.451651	0.000000
18	1	0	0.531080	-3.325296	0.000000
19	6	0	-1.503677	-3.865095	0.000000
20	1	0	-1.173323	-4.900259	0.000000
21	6	0	-2.872977	-3.664699	0.000000
22	1	0	-4.683287	-2.557438	0.000000
23	1	0	-2.098722	1.466671	0.000000
24	1	0	-3.479648	-4.567355	0.000000
25	1	0	4.163338	1.592962	0.000000
26	6	0	2.413742	3.632217	0.000000
27	6	0	1.052460	4.247910	0.000000
28	1	0	-0.966905	3.454778	0.000000
29	1	0	0.876239	5.317352	0.000000
30	1	0	3.005222	3.934269	0.877545
31	1	0	3.005222	3.934269	-0.877545

a Number of imaginary frequencies = 0

Table S40. Cartesian Coordinates of the Optimized Structure for **13H$_2^{2+}$** (C_s) Diprotonated at C(3) and C(12) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.588337	-0.526245	0.000000
2	6	0	3.103191	1.385411	0.000000
3	6	0	2.043049	2.276943	0.000000
4	6	0	1.958750	-0.864405	0.000000
5	6	0	0.000000	0.751966	0.000000
6	6	0	3.060804	-0.022451	0.000000
7	6	0	0.633957	2.015120	0.000000
8	6	0	-0.063238	3.282176	0.000000
9	1	0	4.028653	-0.517133	0.000000
10	6	0	-1.499514	0.616573	0.000000
11	1	0	2.202971	-1.922028	0.000000
12	6	0	-0.500993	-1.544081	0.000000
13	6	0	-0.288137	-2.930162	0.000000
14	6	0	-1.746437	-0.867609	0.000000
15	6	0	-3.039704	-1.392986	0.000000
16	1	0	-3.848296	-0.664508	0.000000
17	6	0	-3.436491	-2.734165	0.000000
18	1	0	0.742747	-3.271244	0.000000
19	6	0	-1.232867	-3.959421	0.000000
20	1	0	-0.822039	-4.966167	0.000000
21	6	0	-2.631296	-3.878740	0.000000
22	1	0	-4.509905	-2.908104	0.000000
23	1	0	-3.158626	-4.829800	0.000000
24	1	0	4.099389	1.823389	0.000000
25	6	0	2.230710	3.772283	0.000000
26	6	0	0.837556	4.300090	0.000000
27	1	0	-1.139983	3.397567	0.000000
28	1	0	0.597768	5.357797	0.000000
29	1	0	-1.956198	1.095957	0.878900
30	1	0	-1.956198	1.095957	-0.878900
31	1	0	2.806828	4.113265	0.875240
32	1	0	2.806828	4.113265	-0.875240

a Number of imaginary frequencies = 0

Table S41. Cartesian Coordinates of the Optimized Structure for **13**$^{2+}$ (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.780328	0.000000
2	6	0	-3.152521	1.403099	0.000000
3	6	0	-3.154180	0.009773	0.000000
4	6	0	-0.651172	1.989198	0.000000
5	6	0	-0.564215	-0.562703	0.000000
6	6	0	-2.052349	2.259569	0.000000
7	6	0	-1.951277	-0.944266	0.000000
8	6	0	-2.472898	-2.202137	0.000000
9	1	0	-2.297792	3.319288	0.000000
10	6	0	0.497815	-1.451306	0.000000
11	1	0	-0.039386	2.886393	0.000000
12	6	0	1.491489	0.644234	0.000000
13	6	0	2.398448	1.694037	0.000000
14	6	0	1.774627	-0.755030	0.000000
15	6	0	3.003088	-1.416956	0.000000
16	1	0	2.964664	-2.503994	0.000000
17	6	0	4.286085	-0.850262	0.000000
18	1	0	1.998227	2.703758	0.000000
19	6	0	3.804303	1.623965	0.000000
20	1	0	4.311414	2.586044	0.000000
21	6	0	4.643034	0.503547	0.000000
22	1	0	5.111198	-1.558591	0.000000
23	1	0	0.418374	-2.532927	0.000000
24	1	0	5.709746	0.712941	0.000000
25	1	0	-4.127917	1.883811	0.000000
26	6	0	-4.325722	-0.781566	0.000000
27	1	0	-5.340033	-0.404096	0.000000
28	6	0	-3.936564	-2.107661	0.000000
29	1	0	-1.935700	-3.142074	0.000000
30	1	0	-4.600752	-2.965739	0.000000

a Number of imaginary frequencies = 0

Table S42. Cartesian Coordinates of the Optimized Structure for **14** (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.712844	0.000000
2	6	0	4.295490	-2.276705	0.000000
3	6	0	2.191468	0.089260	0.000000
4	6	0	1.353716	-1.165922	0.000000
5	6	0	1.337204	1.190270	0.000000
6	6	0	0.000003	-0.712870	0.000000
7	6	0	4.523360	-0.878926	0.000000
8	6	0	3.105571	-2.979812	0.000000
9	6	0	3.599272	0.150502	0.000000
10	6	0	1.782178	-2.472613	0.000000
11	1	0	5.197835	-2.886481	0.000000
12	6	0	-1.353732	1.165905	0.000000
13	1	0	0.994845	-3.225912	0.000000
14	1	0	4.012877	1.158977	0.000000
15	6	0	-1.337232	-1.190273	0.000000
16	1	0	1.664177	2.223872	0.000000
17	1	0	3.189441	-4.064082	0.000000
18	1	0	5.568518	-0.578200	0.000000
19	6	0	-2.191475	-0.089266	0.000000
20	6	0	-1.782150	2.472594	0.000000
21	6	0	-3.599301	-0.150491	0.000000
22	1	0	-1.664179	-2.223883	0.000000
23	1	0	-0.994814	3.225886	0.000000
24	6	0	-3.105558	2.979817	0.000000
25	6	0	-4.523356	0.878940	0.000000
26	1	0	-4.012904	-1.158966	0.000000
27	6	0	-4.295469	2.276737	0.000000
28	1	0	-3.189397	4.064091	0.000000
29	1	0	-5.568522	0.578240	0.000000
30	1	0	-5.197815	2.886510	0.000000

a Number of imaginary frequencies = 0

Table S43. Cartesian Coordinates of the Optimized Structure for **14H$^+$** (C_s) Protonated at C(6) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.667138	0.000000
2	6	0	-4.332204	-2.210773	0.000000
3	6	0	-2.183982	0.099370	0.000000
4	6	0	-1.371324	-1.163640	0.000000
5	6	0	-1.311443	1.194603	0.000000
6	6	0	-0.033217	-0.747934	0.000000
7	6	0	-4.533519	-0.819450	0.000000
8	6	0	-3.148431	-2.950438	0.000000
9	6	0	-3.586879	0.195949	0.000000
10	6	0	-1.832690	-2.480583	0.000000
11	1	0	-5.244606	-2.803712	0.000000
12	6	0	1.361605	1.117123	0.000000
13	1	0	-1.060614	-3.248939	0.000000
14	1	0	-3.979790	1.211469	0.000000
15	6	0	1.353674	-1.306686	0.000000
16	1	0	-1.610888	2.234755	0.000000
17	1	0	-3.264561	-4.030736	0.000000
18	1	0	-5.571590	-0.498156	0.000000
19	6	0	2.211983	-0.044674	0.000000
20	6	0	1.760500	2.472568	0.000000
21	6	0	3.592261	-0.103083	0.000000
22	1	0	0.948668	3.196061	0.000000
23	6	0	3.041200	2.996563	0.000000
24	6	0	4.522231	0.958658	0.000000
25	1	0	4.025918	-1.101353	0.000000
26	6	0	4.281717	2.322804	0.000000
27	1	0	3.103437	4.082215	0.000000
28	1	0	5.567660	0.659972	0.000000
29	1	0	5.160819	2.962173	0.000000
30	1	0	1.588333	-1.924423	0.879464
31	1	0	1.588333	-1.924423	-0.879464

a Number of imaginary frequencies = 0

Table S44. Cartesian Coordinates of the Optimized Structure for **14H$_2^{2+}$** (C_s) Diprotonated at C(6) and C(12) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.681806	0.000000
2	6	0	-4.233322	-2.468432	0.000000
3	6	0	-2.228366	-0.049419	0.000000
4	6	0	-1.361203	-1.188843	0.000000
5	6	0	-1.392980	1.223963	0.000000
6	6	0	0.000000	-0.681807	0.000000
7	6	0	-4.512613	-1.100330	0.000000
8	6	0	-2.984569	-3.111699	0.000000
9	6	0	-3.617725	-0.018371	0.000000
10	6	0	-1.709650	-2.549550	0.000000
11	1	0	-5.099004	-3.126364	0.000000
12	6	0	1.361203	1.188842	0.000000
13	1	0	-0.882682	-3.256066	0.000000
14	1	0	-4.075863	0.968841	0.000000
15	6	0	1.392981	-1.223962	0.000000
16	1	0	-3.017757	-4.198536	0.000000
17	1	0	-5.566801	-0.833776	0.000000
18	6	0	2.228366	0.049417	0.000000
19	6	0	1.709649	2.549549	0.000000
20	6	0	3.617725	0.018371	0.000000
21	1	0	0.882680	3.256064	0.000000
22	6	0	2.984568	3.111700	0.000000
23	6	0	4.512613	1.100331	0.000000
24	1	0	4.075865	-0.968840	0.000000
25	6	0	4.233322	2.468433	0.000000
26	1	0	3.017756	4.198537	0.000000
27	1	0	5.566801	0.833777	0.000000
28	1	0	5.099003	3.126365	0.000000
29	1	0	1.619862	-1.842993	0.880243
30	1	0	1.619862	-1.842993	-0.880243
31	1	0	-1.619861	1.842991	0.880244
32	1	0	-1.619861	1.842991	-0.880244

a Number of imaginary frequencies = 0

Table S45. Cartesian Coordinates of the Optimized Structure for **14**$^{2+}$ (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.725832	0.000000
2	6	0	4.334614	-2.274171	0.000000
3	6	0	2.186763	0.018741	0.000000
4	6	0	1.392071	-1.183522	0.000000
5	6	0	1.280815	1.184810	0.000000
6	6	0	-0.000003	-0.725836	0.000000
7	6	0	4.530963	-0.887170	0.000000
8	6	0	3.132031	-2.991003	0.000000
9	6	0	3.576371	0.139245	0.000000
10	6	0	1.814791	-2.507905	0.000000
11	1	0	5.239806	-2.876514	0.000000
12	6	0	-1.392072	1.183519	0.000000
13	1	0	1.035471	-3.266488	0.000000
14	1	0	3.971800	1.152659	0.000000
15	6	0	-1.280818	-1.184811	0.000000
16	1	0	1.632922	2.210652	0.000000
17	1	0	3.230625	-4.073901	0.000000
18	1	0	5.567781	-0.559243	0.000000
19	6	0	-2.186765	-0.018743	0.000000
20	6	0	-1.814789	2.507904	0.000000
21	6	0	-3.576374	-0.139244	0.000000
22	1	0	-1.632918	-2.210656	0.000000
23	1	0	-1.035467	3.266485	0.000000
24	6	0	-3.132027	2.991005	0.000000
25	6	0	-4.530963	0.887174	0.000000
26	1	0	-3.971804	-1.152657	0.000000
27	6	0	-4.334612	2.274174	0.000000
28	1	0	-3.230620	4.073903	0.000000
29	1	0	-5.567780	0.559247	0.000000
30	1	0	-5.239803	2.876519	0.000000

a Number of imaginary frequencies = 0

Table S46. Cartesian Coordinates of the Optimized Structure for **15** (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.681401	-1.889981	0.000000
2	6	0	0.000000	0.476270	0.000000
3	6	0	3.088656	-0.241309	0.000000
4	6	0	2.423790	-1.583265	0.000000
5	6	0	4.456680	-0.480223	0.000000
6	6	0	3.469725	-2.557468	0.000000
7	6	0	1.121417	1.341525	0.000000
8	6	0	-0.018236	-0.960205	0.000000
9	6	0	2.463409	1.024842	0.000000
10	6	0	1.078499	-1.859900	0.000000
11	1	0	5.659336	-2.360110	0.000000
12	1	0	0.807938	-2.916352	0.000000
13	1	0	3.148812	1.871894	0.000000
14	1	0	3.316469	-3.629970	0.000000
15	1	0	5.226400	0.283132	0.000000
16	6	0	-1.376342	-1.400256	0.000000
17	1	0	0.900835	2.406253	0.000000
18	6	0	-1.380387	0.914224	0.000000
19	6	0	-1.813366	2.220874	0.000000
20	6	0	-2.228464	-0.312154	0.000000
21	6	0	-3.639601	-0.379453	0.000000
22	1	0	-4.045547	-1.390736	0.000000
23	6	0	-4.565393	0.643628	0.000000
24	1	0	-1.039482	2.985602	0.000000
25	6	0	-3.136139	2.730933	0.000000
26	1	0	-3.211422	3.815907	0.000000
27	6	0	-4.332098	2.040884	0.000000
28	1	0	-5.610542	0.343097	0.000000
29	1	0	-1.684561	-2.439941	0.000000
30	1	0	-5.229548	2.657423	0.000000

a Number of imaginary frequencies = 0

Table S47. Cartesian Coordinates of the Optimized Structure for **15H$^+$** (C_s) Protonated at C(3) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.568026	-2.167649	0.000000
2	6	0	0.000000	0.499206	0.000000
3	6	0	-2.986190	-0.494558	0.000000
4	6	0	-2.244954	-1.731824	0.000000
5	6	0	-4.401034	-0.826392	0.000000
6	6	0	-3.245847	-2.871427	0.000000
7	6	0	-1.173483	1.246819	0.000000
8	6	0	0.144427	-0.948760	0.000000
9	6	0	-2.503702	0.814295	0.000000
10	6	0	-0.888442	-1.925015	0.000000
11	1	0	-5.519301	-2.687764	0.000000
12	1	0	-0.545029	-2.958690	0.000000
13	1	0	-3.255814	1.599096	0.000000
14	1	0	-5.188912	-0.081664	0.000000
15	6	0	1.513407	-1.261526	0.000000
16	1	0	-1.056676	2.327753	0.000000
17	6	0	1.345180	1.054160	0.000000
18	6	0	1.658737	2.401254	0.000000
19	6	0	2.269917	-0.082767	0.000000
20	6	0	3.684317	-0.043204	0.000000
21	1	0	4.171789	-1.016205	0.000000
22	6	0	4.520768	1.054662	0.000000
23	1	0	0.822725	3.096490	0.000000
24	6	0	2.926250	3.018443	0.000000
25	1	0	2.913044	4.104988	0.000000
26	6	0	4.178297	2.426523	0.000000
27	1	0	5.586148	0.839819	0.000000
28	1	0	1.922627	-2.264454	0.000000
29	1	0	5.021884	3.112948	0.000000
30	1	0	-3.125113	-3.522877	0.878078
31	1	0	-3.125113	-3.522877	-0.878078

a Number of imaginary frequencies = 0

Table S48. Cartesian Coordinates of the Optimized Structure for **15H$_2^{2+}$** (C_s) Diprotonated at C(3) and C(5) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.635848	-2.074012	0.000000
2	6	0	0.000000	0.457359	0.000000
3	6	0	-3.030411	-0.441760	0.000000
4	6	0	-2.312466	-1.688190	0.000000
5	6	0	-4.441675	-0.726957	0.000000
6	6	0	-3.332004	-2.800528	0.000000
7	6	0	-1.167077	1.256791	0.000000
8	6	0	0.083992	-0.946967	0.000000
9	6	0	-2.493876	0.865264	0.000000
10	6	0	-0.948921	-1.905081	0.000000
11	1	0	-5.597676	-2.575416	0.000000
12	1	0	-0.627496	-2.945545	0.000000
13	1	0	-3.223646	1.671421	0.000000
14	1	0	-5.215254	0.032241	0.000000
15	6	0	1.529736	-1.364868	0.000000
16	1	0	-1.020674	2.332753	0.000000
17	6	0	1.379022	1.010772	0.000000
18	6	0	1.682575	2.380943	0.000000
19	6	0	2.297873	-0.071416	0.000000
20	6	0	3.692646	-0.047825	0.000000
21	1	0	4.183899	-1.019016	0.000000
22	6	0	4.547473	1.060322	0.000000
23	1	0	0.844089	3.071095	0.000000
24	6	0	2.934616	2.998257	0.000000
25	1	0	2.915920	4.085420	0.000000
26	6	0	4.210272	2.417462	0.000000
27	1	0	5.611139	0.834410	0.000000
28	1	0	5.045293	3.114040	0.000000
29	1	0	1.777068	-1.980648	0.878028
30	1	0	1.777068	-1.980648	-0.878028
31	1	0	-3.222645	-3.458753	0.876370
32	1	0	-3.222645	-3.458753	-0.876370

a Number of imaginary frequencies = 0

Table S49. Cartesian Coordinates of the Optimized Structure for **15**$^{2+}$ (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.748135	-1.807237	0.000000
2	6	0	0.000000	0.480959	0.000000
3	6	0	3.055535	-0.215151	0.000000
4	6	0	2.435427	-1.551235	0.000000
5	6	0	4.484771	-0.438110	0.000000
6	6	0	3.522059	-2.492061	0.000000
7	6	0	1.066023	1.338533	0.000000
8	6	0	-0.004614	-0.985829	0.000000
9	6	0	2.469653	1.021577	0.000000
10	6	0	1.109066	-1.887651	0.000000
11	1	0	5.729187	-2.266029	0.000000
12	1	0	0.858929	-2.946874	0.000000
13	1	0	3.136135	1.881218	0.000000
14	1	0	3.402357	-3.570922	0.000000
15	1	0	5.229179	0.351513	0.000000
16	6	0	-1.316245	-1.414989	0.000000
17	1	0	0.857273	2.404472	0.000000
18	6	0	-1.422951	0.907443	0.000000
19	6	0	-1.867639	2.226167	0.000000
20	6	0	-2.219609	-0.285056	0.000000
21	6	0	-3.613470	-0.422063	0.000000
22	1	0	-3.991940	-1.442032	0.000000
23	6	0	-4.579195	0.587708	0.000000
24	1	0	-1.110999	3.006003	0.000000
25	6	0	-3.189295	2.697708	0.000000
26	1	0	-3.294106	3.779929	0.000000
27	6	0	-4.388617	1.976826	0.000000
28	1	0	-5.613111	0.251211	0.000000
29	1	0	-1.641167	-2.449999	0.000000
30	1	0	-5.295936	2.576259	0.000000

a Number of imaginary frequencies = 0

Table S50. Cartesian Coordinates of the Optimized Structure for **16** (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.309749	0.173399	-0.047979
2	6	0	3.414379	0.921096	0.264594
3	6	0	2.799667	2.193377	0.195488
4	6	0	1.421687	-0.716329	-0.118591
5	6	0	0.354572	1.612833	-0.067379
6	6	0	2.857930	-0.329145	0.109151
7	6	0	1.467254	2.487447	0.017753
8	6	0	3.630056	-1.529041	0.044892
9	6	0	-0.980511	2.116365	-0.150859
10	6	0	1.440974	-2.085329	-0.373044
11	6	0	-1.096410	-0.188050	0.000681
12	6	0	-1.609057	-1.435059	0.279683
13	6	0	-1.882331	1.074204	-0.125130
14	6	0	-3.288366	1.212474	-0.201624
15	1	0	-3.633727	2.234767	-0.354448
16	6	0	-4.270312	0.250263	-0.109433
17	1	0	-0.882332	-2.210414	0.494781
18	6	0	-2.961949	-1.860632	0.356023
19	1	0	-3.096482	-2.913233	0.594997
20	6	0	-4.116673	-1.134664	0.154287
21	1	0	-5.295188	0.597933	-0.216610
22	1	0	-1.233922	3.169010	-0.210965
23	1	0	-5.046515	-1.696069	0.230902
24	1	0	4.494317	0.933961	0.410386
25	1	0	3.471885	3.044420	0.281480
26	1	0	1.214407	3.545973	-0.028113
27	1	0	4.706454	-1.574076	0.158240
28	1	0	0.601901	-2.697372	-0.670177
29	6	0	2.780130	-2.569065	-0.270386
30	1	0	3.074463	-3.599755	-0.439240

a Number of imaginary frequencies = 0

Table S51. Cartesian Coordinates of the Optimized Structure for **16H$^+$** (C_s) Protonated at C(3) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.290433	0.192124	-0.006765
2	6	0	3.367018	0.968641	0.235646
3	6	0	2.756174	2.245701	0.191684
4	6	0	1.410377	-0.652971	-0.079982
5	6	0	0.316493	1.652598	-0.046643
6	6	0	2.794602	-0.272068	0.082948
7	6	0	1.424172	2.537926	0.029661
8	6	0	3.645547	-1.525392	0.024558
9	6	0	-1.001642	2.124493	-0.158659
10	6	0	1.404211	-2.090059	-0.349562
11	6	0	-1.118779	-0.186834	0.017273
12	6	0	-1.636261	-1.442375	0.293737
13	6	0	-1.894544	1.052387	-0.127642
14	6	0	-3.300776	1.200761	-0.210215
15	1	0	-3.641167	2.222995	-0.363505
16	6	0	-4.286077	0.240429	-0.123527
17	1	0	-0.922956	-2.221073	0.533698
18	6	0	-2.981031	-1.868210	0.347102
19	1	0	-3.118257	-2.920884	0.579763
20	6	0	-4.139317	-1.141440	0.136337
21	1	0	-5.307953	0.592354	-0.237000
22	1	0	-1.280598	3.168345	-0.234049
23	1	0	-5.067720	-1.704093	0.201024
24	1	0	4.448416	0.976719	0.360402
25	1	0	3.431348	3.093018	0.274769
26	1	0	1.164731	3.593397	-0.016825
27	1	0	0.532165	-2.662731	-0.627304
28	6	0	2.656102	-2.593275	-0.295405
29	1	0	2.926371	-3.626547	-0.482311
30	1	0	4.438454	-1.456717	-0.733694
31	1	0	4.156956	-1.709392	0.981748

a Number of imaginary frequencies = 0

Table S52. Cartesian Coordinates of the Optimized Structure for **16H$_2^{2+}$** (C_s) Diprotonated at C(3) and C(7) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.308769	0.229518	0.022529
2	6	0	-3.395660	0.914222	-0.311061
3	6	0	-2.808882	2.193212	-0.250486
4	6	0	-1.416637	-0.664089	0.109891
5	6	0	-0.377152	1.639963	0.058254
6	6	0	-2.797209	-0.315947	-0.100907
7	6	0	-1.476544	2.510074	-0.037039
8	6	0	-3.615640	-1.581219	-0.014532
9	6	0	1.009120	2.206004	0.212134
10	6	0	-1.371093	-2.076817	0.431277
11	6	0	1.129533	-0.155171	-0.037893
12	6	0	1.613271	-1.431689	-0.371653
13	6	0	1.917221	1.013679	0.142400
14	6	0	3.303238	1.148878	0.235783
15	1	0	3.667406	2.159215	0.412713
16	6	0	4.288643	0.160912	0.140099
17	1	0	0.875182	-2.174671	-0.649806
18	6	0	2.934361	-1.882319	-0.431410
19	1	0	3.052919	-2.924765	-0.717432
20	6	0	4.124438	-1.194768	-0.161631
21	1	0	5.312317	0.498213	0.284189
22	1	0	5.036718	-1.783039	-0.226210
23	1	0	-4.470481	0.898164	-0.480410
24	1	0	-3.489880	3.032940	-0.364172
25	1	0	-1.242739	3.570903	0.020949
26	1	0	-0.491947	-2.620668	0.745778
27	6	0	-2.618817	-2.612073	0.372559
28	1	0	-2.873623	-3.642285	0.596536
29	1	0	1.252397	2.937296	-0.572568
30	1	0	1.108210	2.745656	1.166862
31	1	0	-4.438097	-1.500349	0.712216
32	1	0	-4.098920	-1.810831	-0.978534

a Number of imaginary frequencies = 0

Table S53. Cartesian Coordinates of the Optimized Structure for **16**$^{2+}$ (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.332957	0.137223	0.035096
2	6	0	3.458470	0.892252	0.157227
3	6	0	2.878727	2.183697	0.178747
4	6	0	1.401428	-0.717605	-0.051206
5	6	0	0.413635	1.608769	0.007778
6	6	0	2.837218	-0.342701	0.031510
7	6	0	1.544720	2.487634	0.082630
8	6	0	3.571288	-1.543676	-0.058911
9	6	0	-0.865606	2.104429	-0.129919
10	6	0	1.397872	-2.172099	-0.252195
11	6	0	-1.128164	-0.198476	0.050482
12	6	0	-1.692826	-1.440402	0.319300
13	6	0	-1.837241	1.036162	-0.122455
14	6	0	-3.214772	1.271956	-0.237906
15	1	0	-3.504158	2.308544	-0.396718
16	6	0	-4.259663	0.349613	-0.176714
17	1	0	-1.019846	-2.246370	0.582200
18	6	0	-3.053117	-1.803688	0.331711
19	1	0	-3.244081	-2.849477	0.560160
20	6	0	-4.186656	-1.028039	0.084527
21	1	0	-5.258367	0.754798	-0.320726
22	1	0	-1.123021	3.154736	-0.216527
23	1	0	-5.137194	-1.554804	0.119834
24	1	0	4.545054	0.864183	0.215227
25	1	0	3.569872	3.017815	0.252578
26	1	0	1.289765	3.545103	0.073459
27	1	0	4.653220	-1.611653	-0.002551
28	1	0	0.529330	-2.786368	-0.435870
29	6	0	2.686668	-2.645270	-0.255129
30	1	0	2.989806	-3.675176	-0.398508

a Number of imaginary frequencies = 0

Table S54. Cartesian Coordinates of the Optimized Structure for triplet **11**$^{2+\cdot}$ (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.788903	0.524984	0.000000
2	6	0	-0.093332	-1.405801	0.000000
3	6	0	3.002480	-0.968668	0.000000
4	6	0	2.473792	0.393671	0.000000
5	6	0	4.435298	-0.842867	0.000000
6	6	0	3.624140	1.282664	0.000000
7	6	0	0.934356	-2.377606	0.000000
8	6	0	0.000000	0.041206	0.000000
9	6	0	2.317645	-2.182470	0.000000
10	6	0	1.150767	0.832382	0.000000
11	1	0	5.800568	0.912287	0.000000
12	1	0	1.019941	1.911280	0.000000
13	1	0	2.926935	-3.083141	0.000000
14	1	0	3.565167	2.365304	0.000000
15	1	0	5.128101	-1.677571	0.000000
16	6	0	-1.385773	0.571787	0.000000
17	1	0	0.600488	-3.412364	0.000000
18	6	0	-1.462262	-1.747217	0.000000
19	1	0	-1.852334	-2.759139	0.000000
20	6	0	-2.271898	-0.562509	0.000000
21	6	0	-1.729189	1.917191	0.000000
22	6	0	-3.674241	-0.591663	0.000000
23	1	0	-0.917336	2.639268	0.000000
24	6	0	-3.015225	2.489294	0.000000
25	6	0	-4.559388	0.488603	0.000000
26	1	0	-4.129450	-1.579745	0.000000
27	1	0	-3.037051	3.576240	0.000000
28	6	0	-4.263670	1.861716	0.000000
29	1	0	-5.615942	0.232077	0.000000
30	1	0	-5.123510	2.527312	0.000000

a Number of imaginary frequencies = 0

Table S55. Cartesian Coordinates of the Optimized Structure for triplet **13**$^{2+\cdot}$ (C_s) by B3LYP/6-31G(d)[a]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.598358	-0.536199	0.000000
2	6	0	-3.147198	1.357111	0.000000
3	6	0	-2.101228	2.268652	0.000000
4	6	0	-1.943515	-0.883969	0.000000
5	6	0	0.000000	0.788416	0.000000
6	6	0	-3.074180	-0.048197	0.000000
7	6	0	-0.662599	2.031162	0.000000
8	6	0	-0.035883	3.332005	0.000000
9	1	0	-4.031162	-0.563202	0.000000
10	6	0	1.407650	0.623120	0.000000
11	1	0	-2.177652	-1.944460	0.000000
12	6	0	0.512017	-1.515607	0.000000
13	6	0	0.361718	-2.899314	0.000000
14	6	0	1.741948	-0.768008	0.000000
15	6	0	3.066569	-1.235304	0.000000
16	1	0	3.839921	-0.470123	0.000000
17	6	0	3.516120	-2.556796	0.000000
18	1	0	-0.652016	-3.289471	0.000000
19	6	0	1.362916	-3.883800	0.000000
20	1	0	1.002516	-4.909537	0.000000
21	6	0	2.755233	-3.735527	0.000000
22	1	0	4.595212	-2.688737	0.000000
23	1	0	2.141129	1.420132	0.000000
24	1	0	3.324254	-4.662237	0.000000
25	1	0	-4.151182	1.775816	0.000000
26	6	0	-2.279702	3.706624	0.000000
27	1	0	-3.241153	4.208153	0.000000
28	6	0	-1.021563	4.324575	0.000000
29	1	0	1.031279	3.517342	0.000000
30	1	0	-0.840818	5.392655	0.000000

a Number of imaginary frequencies = 0